Solutions to Dobson & Barnett's An Introduction to Generalized Linear Models

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2026-06-14T13:42:58+11:00

Contents

Solutions to every exercise in the fourth edition of Dobson & Barnett's *An Introduction to Generalized Linear Models* (Chapman & Hall/CRC, 2018) — 78 exercises across 14 chapters, worked in R with the book's own datasets from the `dobson` package, with executed code and committed output throughout. This is the MATH5806 text; the book is filed at An Introduction to Generalized Linear Models (Dobson & Barnett).

1 Introduction

Contents

1.1 Problem 1.1 — Let Y1 and Y2 be independent random variables with

Problem 1.1. Let Y_1 and Y_2 be independent random variables with $Y_1 \sim N(1,3)$ and $Y_2 \sim N(2,5)$. If $W_1 = Y_1 + 2Y_2$ and $W_2 = 4Y_1 - Y_2$, what is the joint distribution of W_1 and W_2? (difficulty: $\star$)

Solution.

$$\begin{pmatrix} W_1 \\ W_2 \end{pmatrix} \sim \text{MVN}\left(\begin{pmatrix} 5 \\ 2 \end{pmatrix}, \begin{pmatrix} 23 & 2 \\ 2 & 53 \end{pmatrix} \right).$$

Indeed $\mathbf{w} = \mathbf{A}\mathbf{y}$ with $\mathbf{y} = [Y_1, Y_2]^T$ and $\mathbf{A} = \begin{pmatrix} 1 & 2 \\ 4 & -1 \end{pmatrix}$, so every linear combination of W_1, W_2 is a linear combination of Y_1, Y_2 and hence Normal (Section 1.4.1 result 4): $\mathbf{w}$ is bivariate Normal. Independence gives $\boldsymbol{\mu}_y = (1,2)^T$ and $\mathbf{V}_y = \text{diag}(3,5)$, so by Equations (1.2) and (1.3),

$$\begin{aligned} E(\mathbf{w}) &= \mathbf{A}\boldsymbol{\mu}_y = (1+4,\ 4-2)^T = (5,2)^T, \\ \text{var}(W_1) &= 1^2(3) + 2^2(5) = 23, \qquad \text{var}(W_2) = 4^2(3) + (-1)^2(5) = 53, \\ \text{cov}(W_1, W_2) &= 4\,\text{var}(Y_1) - 2\,\text{var}(Y_2) = 4(3) - 2(5) = 2, \end{aligned}$$

the cross terms vanishing because $\text{cov}(Y_1, Y_2) = 0$. In particular W_1 and W_2 are **not** independent, the correlation being $2/\sqrt{23 \times 53} = 0.057$.
The matrix arithmetic, checked in R:

```r
A  <- matrix(c(1, 2, 4, -1), nrow = 2, byrow = TRUE)
mu <- c(1, 2)
V  <- diag(c(3, 5))
A %*% mu
A %*% V %*% t(A)
```

```
     [,1]
[1,]    5
[2,]    2
     [,1] [,2]
[1,]   23    2
[2,]    2   53
```

1.2 Problem 1.2 — Let Y1 and Y2 be independent random variables with Y1 ∼ N(0, 1) and Y2 ∼

Problem 1.2. Let Y_1 and Y_2 be independent random variables with $Y_1 \sim N(0,1)$ and $Y_2 \sim N(3,4)$. a. What is the distribution of Y_1^2? b. If $\mathbf{y} = \begin{bmatrix} Y_1 \\ (Y_2 - 3)/2 \end{bmatrix}$, obtain an expression for $\mathbf{y}^T\mathbf{y}$. What is its distribution? c. If $\mathbf{y} = \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix}$ and its distribution is $\mathbf{y} \sim \text{MVN}(\boldsymbol{\mu}, \mathbf{V})$, obtain an expression for $\mathbf{y}^T\mathbf{V}^{-1}\mathbf{y}$. What is its distribution? (difficulty: $\star$)

Solution. (a) $Y_1^2 \sim \chi^2(1)$, since Y_1 is already standard Normal (Section 1.4.2 result 1, $n = 1$).
(b) Since $Y_2 \sim N(3,4)$ gives $(Y_2 - 3)/2 \sim N(0,1)$ independent of Y_1,

$$\mathbf{y}^T\mathbf{y} = Y_1^2 + \frac{(Y_2 - 3)^2}{4} \sim \chi^2(2),$$

a sum of squares of two independent standard Normals, as in Equation (1.4) with $n = 2$.
(c) Independence makes $\mathbf{V} = \text{diag}(1,4)$ and $\mathbf{V}^{-1} = \text{diag}(1, 1/4)$, with $\boldsymbol{\mu} = (0,3)^T$, so

$$\mathbf{y}^T\mathbf{V}^{-1}\mathbf{y} = Y_1^2 + \frac{Y_2^2}{4} \sim \chi^2(2,\ 2.25)$$

by Section 1.4.2 result 6 ($\mathbf{V}$ non-singular), the non-centrality parameter being

$$\lambda = \boldsymbol{\mu}^T \mathbf{V}^{-1} \boldsymbol{\mu} = 0^2 + \frac{3^2}{4} = 2.25.$$

Not centring $\mathbf{y}$ is exactly what leaves $\lambda = (\mu_2/\sigma_2)^2$ behind.
A simulation confirms the moments of (c), using $E = n + \lambda$ and $\text{var} = 2n + 4\lambda$ from Section 1.4.2 result 4:

```r
set.seed(1)
n  <- 2e6
Y1 <- rnorm(n, 0, 1)
Y2 <- rnorm(n, 3, 2)
Q  <- Y1^2 + Y2^2 / 4
c(mean = mean(Q), var = var(Q))
c(theory.mean = 2 + 2.25, theory.var = 2 * 2 + 4 * 2.25)
ks.test(sample(Q, 5000), "pchisq", df = 2, ncp = 2.25)$p.value
```

```
     mean       var
 4.251925 13.007515
theory.mean  theory.var
       4.25       13.00
[1] 0.4517404
```

The simulated mean and variance match the theoretical 4.25 and 13, and a Kolmogorov-Smirnov test against $\chi^2(2, 2.25)$ gives $p = 0.45$, so there is no evidence against the claimed distribution.

1.3 Problem 1.3 — Let the joint distribution of Y1 and Y2 be MVN(μ , V) with

Problem 1.3. Let the joint distribution of Y_1 and Y_2 be $\text{MVN}(\boldsymbol{\mu}, \mathbf{V})$ with

$$\boldsymbol{\mu} = \begin{pmatrix} 2 \\ 3 \end{pmatrix} \quad \text{and} \quad \mathbf{V} = \begin{pmatrix} 4 & 1 \\ 1 & 9 \end{pmatrix}.$$

a. Obtain an expression for $(\mathbf{y} - \boldsymbol{\mu})^T \mathbf{V}^{-1} (\mathbf{y} - \boldsymbol{\mu})$. What is its distribution? b. Obtain an expression for $\mathbf{y}^T \mathbf{V}^{-1} \mathbf{y}$. What is its distribution? (difficulty: ⋆⋆)

Solution. Since $\det \mathbf{V} = 4(9) - 1 = 35 > 0$ with $v_{11} = 4 > 0$, $\mathbf{V}$ is positive definite (Section 1.5 result 3) and

$$\mathbf{V}^{-1} = \frac{1}{35} \begin{pmatrix} 9 & -1 \\ -1 & 4 \end{pmatrix}.$$

(a) Expanding the quadratic form, the cross term doubling because the off-diagonal entries agree,

$$(\mathbf{y} - \boldsymbol{\mu})^T \mathbf{V}^{-1} (\mathbf{y} - \boldsymbol{\mu}) = \frac{9(y_1 - 2)^2 - 2(y_1 - 2)(y_2 - 3) + 4(y_2 - 3)^2}{35},$$

which is $\chi^2(2)$ by Equation (1.5), $\mathbf{V}$ being non-singular.
(b) The same algebra without centring gives

$$\mathbf{y}^T \mathbf{V}^{-1} \mathbf{y} = \frac{1}{35} \left[9y_1^2 - 2y_1 y_2 + 4y_2^2 \right] \sim \chi^2(2,\, 12/7),$$

by Section 1.4.2 result 6, with

$$\lambda = \boldsymbol{\mu}^T \mathbf{V}^{-1} \boldsymbol{\mu} = \frac{9(2)^2 - 2(2)(3) + 4(3)^2}{35} = \frac{60}{35} = \frac{12}{7} \approx 1.714.$$

Confirming the inverse and λ in R:

```r
mu <- c(2, 3)
V  <- matrix(c(4, 1, 1, 9), nrow = 2)
det(V)
Vinv <- solve(V)
35 * Vinv
lambda <- drop(t(mu) %*% Vinv %*% mu)
```

```r
c(lambda = lambda, as.fraction = 60 / 35)
```

```
[1] 35
     [,1] [,2]
[1,]    9   -1
[2,]   -1    4
     lambda as.fraction
   1.714286    1.714286
```

Both forms carry 2 degrees of freedom because $\mathbf{V}^{-1}$ has full rank (Section 1.5 result 4); only the location differs, (a) having expectation 2 and (b) expectation $n + \lambda = 2 + 12/7 \approx 3.71$.

1.4 Problem 1.4 — Let Y1 , . . . ,Yn be independent random variables each with the distribution

Problem 1.4. Let $Y_1, \ldots, Y_n$ be independent random variables each with the distribution $N(\mu, \sigma^2)$. Let

$$\overline{Y} = \frac{1}{n}\sum_{i=1}^{n} Y_i \quad \text{and} \quad S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(Y_i - \overline{Y})^2.$$

a. What is the distribution of $\overline{Y}$? b. Show that $S^2 = \frac{1}{n-1}\left[\sum_{i=1}^{n}(Y_i - \mu)^2 - n(\overline{Y} - \mu)^2\right]$. c. From (b) it follows that $\sum(Y_i - \mu)^2/\sigma^2 = (n-1)S^2/\sigma^2 + \left[(\overline{Y} - \mu)^2 n/\sigma^2\right]$. How does this allow you to deduce that $\overline{Y}$ and S^2 are independent? d. What is the distribution of $(n-1)S^2/\sigma^2$? e. What is the distribution of $\dfrac{\overline{Y} - \mu}{S/\sqrt{n}}$? (difficulty: ⋆⋆)

Solution. (a) $\overline{Y} = \sum a_i Y_i$ with every $a_i = 1/n$, so $\overline{Y} \sim N(\mu, \sigma^2/n)$ by Section 1.4.1 result 4.
(b) Write $Y_i - \overline{Y} = (Y_i - \mu) - (\overline{Y} - \mu)$ and expand; since $\sum(Y_i - \mu) = n(\overline{Y} - \mu)$ the cross term is $-2n(\overline{Y} - \mu)^2$, so

$$\begin{aligned}\sum_{i=1}^{n}(Y_i - \overline{Y})^2 &= \sum(Y_i - \mu)^2 - 2(\overline{Y} - \mu)\sum(Y_i - \mu) + n(\overline{Y} - \mu)^2 \\ &= \sum(Y_i - \mu)^2 - n(\overline{Y} - \mu)^2,\end{aligned}$$

and dividing by $n - 1$ gives the identity (purely algebraic; no distributional assumption).
(c) Dividing by σ^2,

$$\underbrace{\sum \frac{(Y_i - \mu)^2}{\sigma^2}}_{Q} = \underbrace{\frac{(n-1)S^2}{\sigma^2}}_{Q_1} + \underbrace{\frac{n(\overline{Y} - \mu)^2}{\sigma^2}}_{Q_2},$$

where $Q \sim \chi^2(n)$ by Equation (1.4) and Q_1, Q_2 are quadratic forms in the independent $Y_i - \mu \sim N(0, \sigma^2)$ of ranks $m_1 = n - 1$ (matrix $\mathbf{I} - \frac{1}{n}\mathbf{J}$, idempotent with trace $n - 1$) and $m_2 = 1$. As $m_1 + m_2 = n$, Cochran's theorem (Section 1.5 result 5) makes $Q_1 \sim \chi^2(n-1)$ and $Q_2 \sim \chi^2(1)$ independent. That delivers independence of S^2 and $(\overline{Y} - \mu)^2$; for $\overline{Y}$ itself, $\operatorname{cov}(\overline{Y}, Y_i - \overline{Y}) = \sigma^2/n - \sigma^2/n = 0$ for every i and $(\overline{Y}, Y_1 - \overline{Y}, \ldots, Y_n - \overline{Y})$ is multivariate Normal (all entries linear in the Y_i), so $\overline{Y}$ is independent of the residual vector and hence of S^2.
(d) $(n-1)S^2/\sigma^2 \sim \chi^2(n-1)$, by (c); in particular $E(S^2) = \sigma^2$.
(e) With $Z = (\overline{Y} - \mu)/(\sigma/\sqrt{n}) \sim N(0,1)$ from (a) and $X^2 = (n-1)S^2/\sigma^2 \sim \chi^2(n-1)$ independent of Z by (c), so that $S/\sigma = [X^2/(n-1)]^{1/2}$,

$$\frac{\overline{Y} - \mu}{S/\sqrt{n}} = \frac{(\overline{Y} - \mu)/(\sigma/\sqrt{n})}{S/\sigma} = \frac{Z}{[X^2/(n-1)]^{1/2}} \sim t(n-1)$$

by the definition of the t-distribution in Equation (1.6).
A simulation with $n = 8$, $\mu = 10$, $\sigma = 3$ checks (c), (d) and (e) numerically:

```r
set.seed(42)
n <- 8; mu <- 10; sigma <- 3; B <- 2e5
sim  <- matrix(rnorm(n * B, mu, sigma), nrow = B)
ybar <- rowMeans(sim)
s2   <- apply(sim, 1, var)
c(cor.ybar.s2 = cor(ybar, s2))
Q1 <- (n - 1) * s2 / sigma^2
c(mean.Q1 = mean(Q1), df = n - 1, var.Q1 = var(Q1), two.df = 2 * (n - 1))
Tstat <- (ybar - mu) / sqrt(s2 / n)
c(mean.T = mean(Tstat), var.T = var(Tstat), t.var = (n - 1) / (n - 3))
ks.test(sample(Tstat, 5000), "pt", df = n - 1)$p.value
```

```
  cor.ybar.s2
-0.0006370237
  mean.Q1        df    var.Q1    two.df
 7.007965  7.000000 14.053002 14.000000
     mean.T        var.T        t.var
0.0002216423 1.4003904492 1.4000000000
[1] 0.4874567
```

The sample correlation between $\overline{Y}$ and S^2 is essentially zero, consistent with (c); Q_1 has simulated mean 7.01 and variance 14.05 against the $\chi^2(7)$ values 7 and 14, confirming (d); and the t-statistic has simulated variance 1.400 against $(n-1)/(n-3) = 1.4$ with Kolmogorov-Smirnov $p = 0.49$ against $t(7)$, confirming (e).

1.5 Problem 1.5 — This exercise is a continuation of the example in Section 1.6.2 in which

Problem 1.5. This exercise is a continuation of the example in Section 1.6.2 in which $Y_1, \ldots, Y_n$ are independent Poisson random variables with the parameter θ.
a. Show that $E(Y_i) = \theta$ for $i = 1, \ldots, n$. b. Suppose $\theta = e^{\beta}$. Find the maximum likelihood estimator of β. c. Minimize $S = \sum \left(Y_i - e^{\beta}\right)^2$ to obtain a least squares estimator of β. (difficulty: ⋆⋆)

Solution. (a) With $f(y_i;\theta) = \theta^{y_i} e^{-\theta}/y_i!$, the $y = 0$ term dropping and $z = y - 1$,

$$E(Y_i) = \sum_{y=1}^{\infty} \frac{\theta^y e^{-\theta}}{(y-1)!} = \theta e^{-\theta} \sum_{z=0}^{\infty} \frac{\theta^z}{z!} = \theta e^{-\theta} e^{\theta} = \theta.$$

(b) $\widehat{\beta} = \log \overline{y}$ (for $\overline{y} > 0$). Reparameterising the log-likelihood of Section 1.6.2 by $\theta = e^{\beta}$,

$$l(\beta; \mathbf{y}) = \left(\sum y_i\right) \beta - n e^{\beta} - \sum \log y_i!, \qquad \frac{dl}{d\beta} = \sum y_i - n e^{\beta},$$

which vanishes at $e^{\beta} = \overline{y}$; and $d^2 l/d\beta^2 = -n e^{\beta} < 0$ everywhere makes l strictly concave, so the root is the unique maximum. (Equivalently, invariance of maximum likelihood under the one-to-one $\beta = \log \theta$.)
(c) $\widetilde{\beta} = \log \overline{y}$ also. Putting $u = e^{\beta}$, the chain rule gives

$$\frac{dS}{d\beta} = \left[-2 \sum (Y_i - u)\right] e^{\beta} = -2 e^{\beta} \left(\sum Y_i - n e^{\beta}\right),$$

which, since $e^{\beta} > 0$, vanishes only at $\sum Y_i = n e^{\beta}$; there $dS/du = 0$, so $d^2 S/d\beta^2 = e^{2\beta}(2n) > 0$ and the point is a minimum. The two estimators coincide because both estimating equations reduce to $\sum (Y_i - e^{\beta}) = 0$ (comment 2 of Section 1.6.4) – an agreement that depends on the Y_i sharing one θ, so that unweighted least squares is already correctly weighted (Section 1.6.3).
Applying this to the tropical cyclone data of Table 1.2, where Section 1.6.5 reports $\widehat{\theta} = 72/13 = 5.538$:

```r
library(dobson)
data(cyclones)
y <- cyclones$number
c(n = length(y), total = sum(y), ybar = mean(y))
```

```r
betahat <- log(mean(y))
c(betahat = betahat, exp.betahat = exp(betahat))

negll <- function(b) -sum(y * b - exp(b) - lfactorial(y))
opt <- optimize(negll, interval = c(-5, 5), tol = 1e-10)
c(numerical.betahat = opt$minimum, closed.form = betahat)

ss  <- function(b) sum((y - exp(b))^2)
opt2 <- optimize(ss, interval = c(-5, 5), tol = 1e-10)
c(least.squares.betahat = opt2$minimum)

coef(glm(y ~ 1, family = poisson(link = "log")))
```

```
       n     total      ybar
13.000000 72.000000  5.538462
    betahat exp.betahat
   1.711717    5.538462
numerical.betahat       closed.form
         1.711717          1.711717
least.squares.betahat
             1.711717
(Intercept)
   1.711717
```

All four routes agree on $\widehat{\beta} = 1.7117$, and $e^{\widehat{\beta}} = 5.538$ recovers $\widehat{\theta}$, confirming (b) and (c).

1.6 Problem 1.6 — The data in Table 1.4 are the numbers of females and males in the progeny

Problem 1.6. The data in Table 1.4 are the numbers of females and males in the progeny of 16 female light brown apple moths in Muswellbrook, New South Wales, Australia (from Lewis, 1987). Table 1.4 lists, for progeny groups 1 to 16 respectively, the numbers of females $18, 31, 34, 33, 27, 33, 28, 23, 33, 12, 19, 25, 14, 4, 22, 7$ and the corresponding numbers of males $11, 22, 27, 29, 24, 29, 25, 26, 38, 14, 23, 31, 20, 6, 34, 12$.
a. Calculate the proportion of females in each of the 16 groups of progeny. b. Let Y_i denote the number of females and n_i the number of progeny in each group ($i = 1, \ldots, 16$). Suppose the Y_i's are independent random variables each with the Binomial distribution

$$f(y_i; \theta) = \binom{n_i}{y_i} \theta^{y_i} (1-\theta)^{n_i - y_i}.$$

Find the maximum likelihood estimator of θ using calculus and evaluate it for these data. c. Use a numerical method to estimate $\widehat{\theta}$ and compare the answer with the one from (b). (difficulty: ⋆⋆)

Solution. (a) The group size is $n_i = (\text{females})_i + (\text{males})_i$ and the proportion female is $p_i = y_i / n_i$.

```r
library(dobson)
data(moths)
moths$n <- moths$females + moths$males
moths$p <- moths$females / moths$n
print(round(moths[, c("group", "females", "n", "p")], 3), row.names = FALSE)
c(total.females = sum(moths$females), total.progeny = sum(moths$n),
  theta.hat = sum(moths$females) / sum(moths$n))
```

```
 group females  n     p
     1      18 29 0.621
     2      31 53 0.585
     3      34 61 0.557
     4      33 62 0.532
     5      27 51 0.529
     6      33 62 0.532
     7      28 53 0.528
     8      23 49 0.469
     9      33 71 0.465
```

```
      10      12 26 0.462
      11      19 42 0.452
      12      25 56 0.446
      13      14 34 0.412
      14       4 10 0.400
      15      22 56 0.393
      16       7 19 0.368
total.females total.progeny     theta.hat
  363.0000000   734.0000000     0.4945504
```

The proportions range from 0.368 to 0.621, scattered around one half, the smallest groups being the least informative (group 14 has 10 progeny, so its 0.400 is one female from 0.500).

(b) $\widehat{\theta} = T/N = \sum y_i / \sum n_i$, the **pooled** proportion rather than the average of the 16 group proportions. Writing $N = \sum n_i$, $T = \sum y_i$, and dropping the θ-free binomial coefficients from the log-likelihood of the product over the 16 independent groups,

$$l(\theta; \mathbf{y}) = \text{const} + T \log\theta + (N - T)\log(1 - \theta),$$
$$\frac{dl}{d\theta} = \frac{T}{\theta} - \frac{N - T}{1 - \theta} = \frac{T - N\theta}{\theta(1 - \theta)},$$

following Equation (1.9), whose numerator vanishes at T/N; and $d^2l/d\theta^2 = -T/\theta^2 - (N-T)/(1-\theta)^2 < 0$ on $(0, 1)$ whenever $0 < T < N$, so this is the unique interior maximum. Here $T = 363$, $N = 734$ and $\widehat{\theta} = 363/734 = 0.4946$.

(c) Three numerical routes, none using the closed form: direct maximisation of $l^*(\theta) = \sum[y_i \log\theta + (n_i - y_i)\log(1 - \theta)]$ with `optimize`, a bisection search in the spirit of Table 1.3, and the intercept-only binomial generalized linear model.

```r
y <- moths$females; n <- moths$n

lstar <- function(th) sum(y * log(th) + (n - y) * log(1 - th))
opt <- optimize(lstar, interval = c(0.001, 0.999), maximum = TRUE, tol = 1e-12)
c(optimize = opt$maximum, closed.form = sum(y) / sum(n))

lo <- 0.30; hi <- 0.70
for (k in 1:20) {
  mid <- (lo + hi) / 2
  if (lstar(mid + 1e-8) > lstar(mid - 1e-8)) lo <- mid else hi <- mid
}
c(bisection = (lo + hi) / 2)

fit <- glm(cbind(females, males) ~ 1, family = binomial, data = moths)
c(glm.theta = plogis(coef(fit)))
```

```
   optimize closed.form
  0.4945504   0.4945504
bisection
0.4945505
glm.theta.(Intercept)
            0.4945504
```

All three agree with (b) to six decimal places; the bisection differs in the seventh, 20 halvings of an interval of width 0.4 leaving a resolution of about 4×10^{-7}.

A standard error and a check on the single-θ model:

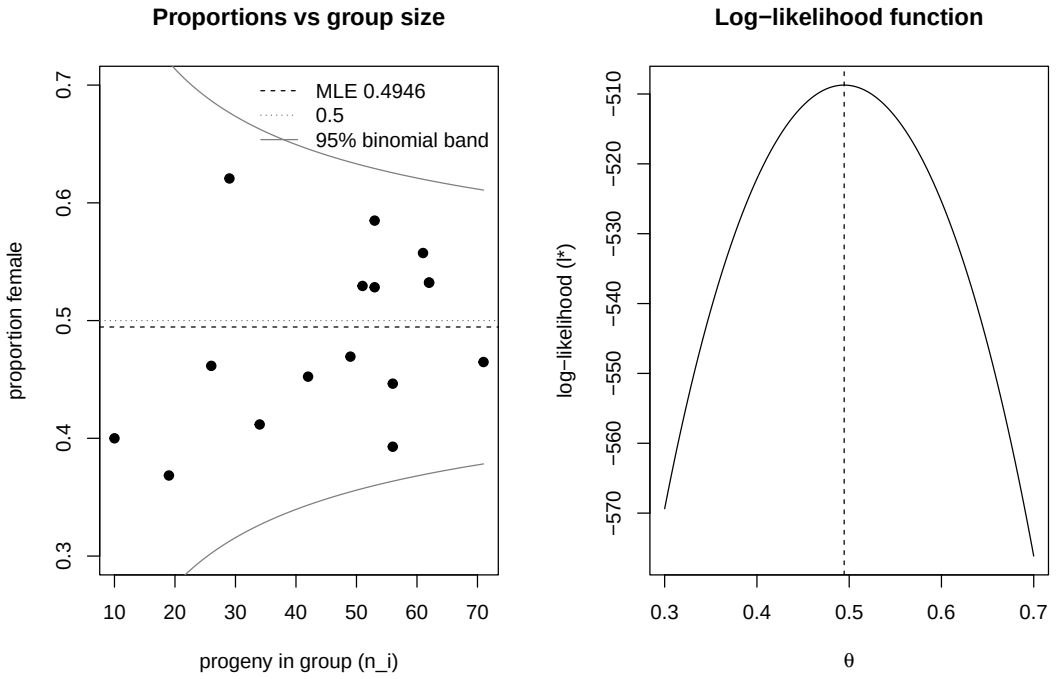
```r
th <- sum(y) / sum(n)
se <- sqrt(th * (1 - th) / sum(n))
c(theta.hat = th, se = se, lower = th - 1.96 * se, upper = th + 1.96 * se)
c(z.vs.half = (th - 0.5) / se, p.value = 2 * pnorm(-abs((th - 0.5) / se)))
c(resid.dev = deviance(fit), df = df.residual(fit),
  p.het = pchisq(deviance(fit), df.residual(fit), lower.tail = FALSE))
```

```
 theta.hat         se      lower      upper
0.49455041 0.01845424 0.45838010 0.53072072
 z.vs.half    p.value
-0.2953029  0.7677625
```

```
  resid.dev         df      p.het
11.9288136 15.0000000  0.6844091
```

The sex ratio is $\widehat{\theta} = 0.495$ with standard error 0.018 and approximate 95% interval $(0.458, 0.531)$, which contains 0.5; the test of $H_0 : \theta = 0.5$ gives $z = -0.30$, $p = 0.77$, so there is no evidence of departure from an even sex ratio. The residual deviance 11.93 on 15 degrees of freedom (16 groups less one fitted parameter) gives $p = 0.68$, so no evidence of heterogeneity between mothers either: the spread of the 16 proportions is no more than binomial sampling variation. The figure shows this, the proportions fanning out for small n_i as the variance $\theta(1-\theta)/n_i$ requires, all 16 inside the pointwise 95% band.

```r
p  <- y / n
th <- sum(y) / sum(n)
par(mfrow = c(1, 2))
plot(n, p, pch = 19, ylim = c(0.3, 0.7), xlab = "progeny in group (n_i)",
     ylab = "proportion female", main = "Proportions vs group size")
abline(h = th, lty = 2); abline(h = 0.5, lty = 3, col = "grey40")
curve(th + 1.96 * sqrt(th * (1 - th) / x), add = TRUE, col = "grey50")
curve(th - 1.96 * sqrt(th * (1 - th) / x), add = TRUE, col = "grey50")
legend("topright", c("MLE 0.4946", "0.5", "95% binomial band"),
       lty = c(2, 3, 1), col = c("black", "grey40", "grey50"), bty = "n")
tt <- seq(0.30, 0.70, length.out = 400)
ls <- sapply(tt, function(t) sum(y * log(t) + (n - y) * log(1 - t)))
plot(tt, ls, type = "l", xlab = expression(theta), ylab = "log-likelihood (l*)",
     main = "Log-likelihood function")
abline(v = th, lty = 2)
```



The right-hand panel shows a single sharply curved peak at $\widehat{\theta} = 0.4946$; the curvature there is $-d^2l/d\theta^2 = N/[\theta(1-\theta)] = 2936.3$, and $1/\sqrt{2936.3} = 0.01845$ reproduces the standard error above.

2 Model Fitting

Contents

2.1 Problem 2.1 — Genetically similar seeds are randomly assigned to be raised in either a

Problem 2.1. Genetically similar seeds are randomly assigned to be raised in either a nutritionally enriched environment (treatment group) or standard conditions (control group) using a completely randomized experimental design. After a predetermined time all plants are harvested, dried and weighed. The results, expressed in grams, for 20 plants in each group are shown in Table 2.7.
Table 2.7 (Dried weight of plants grown under two conditions) has two columns. The treatment group values, read down the two printed sub-columns, are $4.81, 4.17, 4.41, 3.59, 5.87, 3.83, 6.03, 4.98, 4.90, 5.75$ and $5.36, 3.48, 4.69, 4.44, 4.89, 4.71, 5.48, 4.32, 5.15, 6.34$. The control group values are $4.17, 3.05, 5.18, 4.01, 6.11, 4.10, 5.17, 3.57, 5.33, 5.59$ and $4.66, 5.58, 3.66, 4.50, 3.90, 4.61, 5.62, 4.53, 6.05, 5.14$.
We want to test whether there is any difference in yield between the two groups. Let Y_{jk} denote the kth observation in the jth group where $j = 1$ for the treatment group, $j = 2$ for the control group and $k = 1, \ldots, 20$ for both groups. Assume that the Y_{jk}'s are independent random variables with $Y_{jk} \sim \mathrm{N}(\mu_j, \sigma^2)$. The null hypothesis $\mathrm{H}_0 : \mu_1 = \mu_2 = \mu$, that there is no difference, is to be compared with the alternative hypothesis $\mathrm{H}_1 : \mu_1 \neq \mu_2$.

a. Conduct an exploratory analysis of the data looking at the distributions for each group (e.g., using dot plots, stem and leaf plots or Normal probability plots) and calculate summary statistics (e.g., means, medians, standard derivations, maxima and minima). What can you infer from these investigations?

b. Perform an unpaired t-test on these data and calculate a 95% confidence interval for the difference between the group means. Interpret these results.

c. The following models can be used to test the null hypothesis H_0 against the alternative hypothesis H_1, where

$$\mathrm{H}_0 : \mathrm{E}(Y_{jk}) = \mu; \quad Y_{jk} \sim \mathrm{N}(\mu, \sigma^2),$$
$$\mathrm{H}_1 : \mathrm{E}(Y_{jk}) = \mu_j; \quad Y_{jk} \sim \mathrm{N}(\mu_j, \sigma^2),$$

for $j = 1, 2$ and $k = 1, \ldots, 20$. Find the maximum likelihood and least squares estimates of the parameters μ, μ_1 and μ_2, assuming σ^2 is a known constant.

d. Show that the minimum values of the least squares criteria are

$$\text{for } \mathrm{H}_0, \quad \widehat{S}_0 = \sum\sum (Y_{jk} - \overline{Y})^2, \quad \text{where } \overline{Y} = \sum_{j=1}^{2}\sum_{k=1}^{K} Y_{jk}/40;$$

$$\text{for } \mathrm{H}_1, \quad \widehat{S}_1 = \sum\sum (Y_{jk} - \overline{Y}_j)^2, \quad \text{where } \overline{Y}_j = \sum_{k=1}^{K} Y_{jk}/20$$

for $j = 1, 2$.

e. Using the results of Exercise 1.4, show that

$$\frac{1}{\sigma^2}\widehat{S}_1 = \frac{1}{\sigma^2}\sum_{j=1}^{2}\sum_{k=1}^{20}(Y_{jk} - \mu_j)^2 - \frac{20}{\sigma^2}\sum_{k=1}^{20}(\overline{Y}_j - \mu_j)^2,$$

and deduce that if H_1 is true

$$\frac{1}{\sigma^2}\widehat{S}_1 \sim \chi^2(38).$$

Similarly show that

$$\frac{1}{\sigma^2}\widehat{S}_0 = \frac{1}{\sigma^2}\sum_{j=1}^{2}\sum_{k=1}^{20}(Y_{jk} - \mu)^2 - \frac{40}{\sigma^2}\sum_{j=1}^{2}(\overline{Y} - \mu)^2$$

and if H_0 is true, then

$$\frac{1}{\sigma^2}\widehat{S}_0 \sim \chi^2(39).$$

f. Use an argument similar to the one in Example 2.2.2 and the results from (e) to deduce that the statistic

$$F = \frac{\widehat{S}_0 - \widehat{S}_1}{\widehat{S}_1/38}$$

has the central F-distribution $F(1, 38)$ if H_0 is true and a non-central distribution if H_0 is not true.

g. Calculate the F-statistic from (f) and use it to test H_0 against H_1. What do you conclude?

h. Compare the value of F-statistic from (g) with the t-statistic from (b), recalling the relationship between the t-distribution and the F-distribution (see Section 1.4.4). Also compare the conclusions from (b) and (g).

i. Calculate residuals from the model for H_0 and use them to explore the distributional assumptions.

(difficulty: ⋆⋆)

Solution. There is no detectable treatment effect: $F = 0.260$ on $(1, 38)$ degrees of freedom, $p = 0.61$. The data ship in the `dobson` package as `plants`, stacked once and reused throughout.

```
library(dobson)
data(plants)
plant <- data.frame(
  weight = c(plants$treatment, plants$control),
  group  = factor(rep(c("treatment", "control"), each = 20),
                  levels = c("treatment", "control")))
stats <- function(v) c(n = length(v), mean = mean(v), median = median(v),
                       sd = sd(v), min = min(v), max = max(v))
round(t(sapply(split(plant$weight, plant$group), stats)), 3)
```

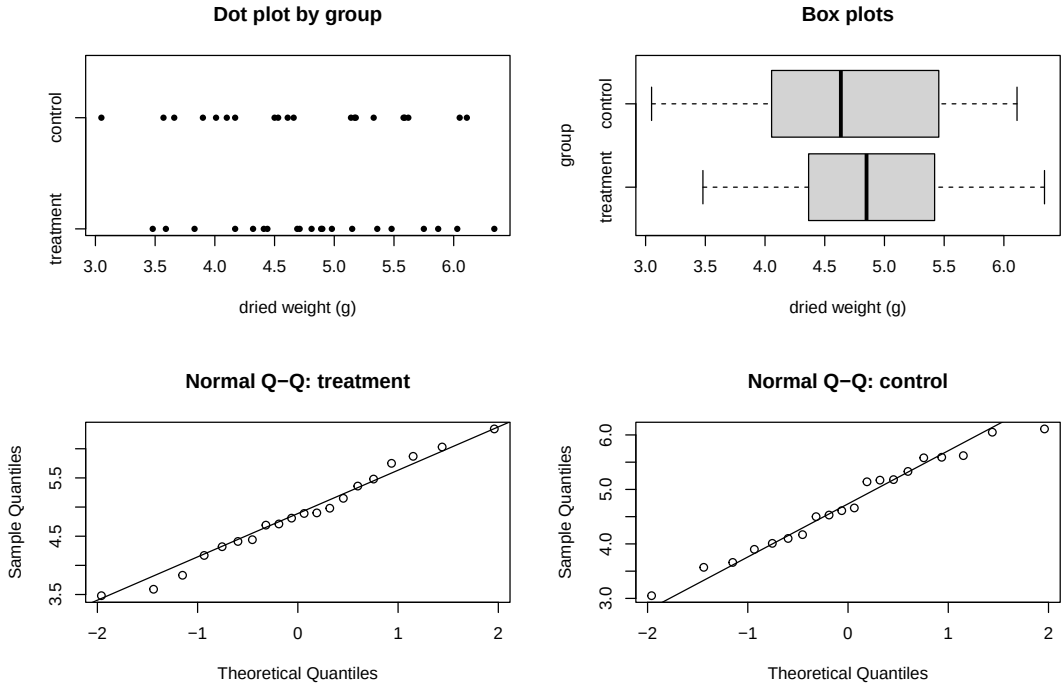
```
           n  mean median    sd  min  max
treatment 20 4.860  4.850 0.791 3.48 6.34
control   20 4.726  4.635 0.864 3.05 6.11
```

(a) **Exploratory analysis.**

```
stem(plants$treatment)
stem(plants$control)
```

```
The decimal point is at the |

3 | 568
4 | 234477899
5 | 024589
6 | 03


The decimal point is at the |

3 | 1679
4 | 0125567
5 | 1223666
6 | 11
```

```
par(mfrow = c(2, 2))
stripchart(weight ~ group, data = plant, method = "stack", pch = 16,
           xlab = "dried weight (g)", main = "Dot plot by group")
boxplot(weight ~ group, data = plant, horizontal = TRUE,
        xlab = "dried weight (g)", main = "Box plots")
for (g in levels(plant$group)) {
  qqnorm(plant$weight[plant$group == g], main = paste("Normal Q-Q:", g))
  qqline(plant$weight[plant$group == g])
}
```




```r
var.test(weight ~ group, data = plant)
```

```
        F test to compare two variances

data:  weight by group
F = 0.83891, num df = 19, denom df = 19, p-value = 0.7057
alternative hypothesis: true ratio of variances is not equal to 1
95 percent confidence interval:
 0.332052 2.119473
sample estimates:
ratio of variances
         0.8389132
```

All values lie in 3.05–6.34 g, so no obvious data-entry errors; both distributions are single-peaked, roughly symmetric, with near-straight Normal probability plots, so Normality is credible. The spreads match ($s_1 = 0.791$, $s_2 = 0.864$; variance-ratio $F_{19,19} = 0.839$, $p = 0.71$), supporting the common-σ^2 assumption. The treatment mean exceeds the control mean by $4.860 - 4.726 = 0.134$ g, an eighth of a standard deviation, with near-complete overlap of the dot plots: any treatment effect is small relative to plant-to-plant variation.

(b) **The unpaired t-test**, pooled-variance to match the common-σ^2 model.

```r
t.test(weight ~ group, data = plant, var.equal = TRUE)
```

```
        Two Sample t-test

data:  weight by group
t = 0.50985, df = 38, p-value = 0.6131
alternative hypothesis: true difference in means between group treatment and group control is
↪  not equal to 0
95 percent confidence interval:
 -0.3965733  0.6635733
sample estimates:
mean in group treatment   mean in group control
                 4.8600                  4.7265
```

The difference is $\overline{y}_1 - \overline{y}_2 = 0.1335$ g with $t = 0.510$ on 38 degrees of freedom, $p = 0.61$: no evidence against H_0. The 95% interval $(-0.397, 0.664)$ contains zero and is wide – the data are consistent with the enriched environment lowering mean dry weight by 0.40 g or raising it by 0.66 g – so the result is inconclusive rather than a demonstration of no effect.

(c) $\widehat{\mu}_j = \overline{Y}_j$ and $\widehat{\mu} = \overline{Y}$, by maximum likelihood and least squares alike. With σ^2 known, $\ell_1 = -\frac{1}{2}N\log(2\pi\sigma^2) - S_1/(2\sigma^2)$ where $S_1 = \sum_j \sum_k (y_{jk} - \mu_j)^2$ and $N = 40$, so the two criteria give the same equations (Equations (2.8) and (2.10)); then

$$\frac{\partial \ell_1}{\partial \mu_j} = \frac{1}{\sigma^2}\sum_{k=1}^{20}(y_{jk} - \mu_j) = 0 \implies \widehat{\mu}_j = \overline{Y}_j,$$
$$\frac{\partial \ell_0}{\partial \mu} = \frac{1}{\sigma^2}\sum_j\sum_k (y_{jk} - \mu) = 0 \implies \widehat{\mu} = \overline{Y},$$

with $\partial^2\ell_1/\partial\mu_j^2 = -20/\sigma^2 < 0$ and $\partial^2\ell_0/\partial\mu^2 = -40/\sigma^2 < 0$, so both are maxima. Numerically $\widehat{\mu}_1 = 4.8600$, $\widehat{\mu}_2 = 4.7265$, $\widehat{\mu} = 4.79325$.
(d) Substituting (c) into the criteria gives $\widehat{S}_1 = \sum\sum(Y_{jk} - \overline{Y}_j)^2$ and $\widehat{S}_0 = \sum\sum(Y_{jk} - \overline{Y})^2$; these are global minima because, the cross-product vanishing by $\sum_k(Y_{jk} - \overline{Y}_j) = 0$,

$$\sum_k (Y_{jk} - \mu_j)^2 = \sum_k (Y_{jk} - \overline{Y}_j)^2 + 20(\overline{Y}_j - \mu_j)^2 \geq \sum_k (Y_{jk} - \overline{Y}_j)^2$$

with equality only at $\mu_j = \overline{Y}_j$, and the same identity over all 40 observations gives $\widehat{S}_0$.
(e) Two printing slips: in the first display the subtracted term is summed over $j = 1, 2$ (not k), and in the third it is $\frac{40}{\sigma^2}(\overline{Y} - \mu)^2$ with no sum over j. Applying Exercise 1.4(b) within group j ($n = 20$, mean μ_j), summing over j and dividing by σ^2,

$$\frac{1}{\sigma^2}\widehat{S}_1 = \frac{1}{\sigma^2}\sum_{j=1}^{2}\sum_{k=1}^{20}(Y_{jk} - \mu_j)^2 - \frac{20}{\sigma^2}\sum_{j=1}^{2}(\overline{Y}_j - \mu_j)^2.$$

Under H_1 the first term is $\chi^2(40)$ and, as $\overline{Y}_j \sim N(\mu_j, \sigma^2/20)$ independently across j, the second is $\chi^2(2)$, independent of $\widehat{S}_1/\sigma^2$ by Exercise 1.4(c); comparing moment generating functions in $\chi^2(40) = \widehat{S}_1/\sigma^2 + \chi^2(2)$ gives $\widehat{S}_1/\sigma^2 \sim \chi^2(38) = \chi^2(40 - 2)$. Likewise with $n = 40$ and the single mean μ,

$$\frac{1}{\sigma^2}\widehat{S}_0 = \frac{1}{\sigma^2}\sum_{j=1}^{2}\sum_{k=1}^{20}(Y_{jk} - \mu)^2 - \frac{40}{\sigma^2}(\overline{Y} - \mu)^2,$$

where the second term is $\chi^2(1)$ (since $\overline{Y} \sim N(\mu, \sigma^2/40)$) and independent of $\widehat{S}_0$, so $\widehat{S}_0/\sigma^2 \sim \chi^2(39)$ under H_0.
(f) Expanding $Y_{jk} - \overline{Y} = (Y_{jk} - \overline{Y}_j) + (\overline{Y}_j - \overline{Y})$ with $\sum_k(Y_{jk} - \overline{Y}_j) = 0$, and using $\overline{Y} = (\overline{Y}_1 + \overline{Y}_2)/2$ for equal group sizes,

$$\widehat{S}_0 - \widehat{S}_1 = 20\sum_{j=1}^{2}(\overline{Y}_j - \overline{Y})^2 = 10(\overline{Y}_1 - \overline{Y}_2)^2.$$

Under H_0, $\overline{Y}_1 - \overline{Y}_2 \sim N(0, \sigma^2/10)$, so $(\widehat{S}_0 - \widehat{S}_1)/\sigma^2 \sim \chi^2(1)$ (Section 2.2.2 with $J = 2$), independent of $\widehat{S}_1$ because the former depends on the group means alone and the latter on the within-group deviations alone. Hence by the definition of the F-distribution (Section 1.4.4),

$$F = \frac{(\widehat{S}_0 - \widehat{S}_1)/\sigma^2}{1} \Big/ \frac{\widehat{S}_1/\sigma^2}{38} = \frac{\widehat{S}_0 - \widehat{S}_1}{\widehat{S}_1/38} \sim F(1, 38).$$

If H_0 is false then $E(\overline{Y}_1 - \overline{Y}_2) = \mu_1 - \mu_2 \neq 0$, the numerator is non-central χ^2 with $\lambda = 10(\mu_1 - \mu_2)^2/\sigma^2$, and F is non-central (Figure 2.5).
(g) Computing the two minima and the statistic from their definitions:

```
y <- plant$weight
S0 <- sum((y - mean(y))^2)
S1 <- sum((y - ave(y, plant$group))^2)
```

```r
Fstat <- (S0 - S1) / (S1 / 38)
c(S0 = S0, S1 = S1, F = Fstat, p = pf(Fstat, 1, 38, lower.tail = FALSE))
```

```
        S0         S1          F          p
26.2316775 26.0534550  0.2599446  0.6131068
```

The same numbers come from the nested model comparison:

```r
anova(lm(weight ~ 1, data = plant), lm(weight ~ group, data = plant))
```

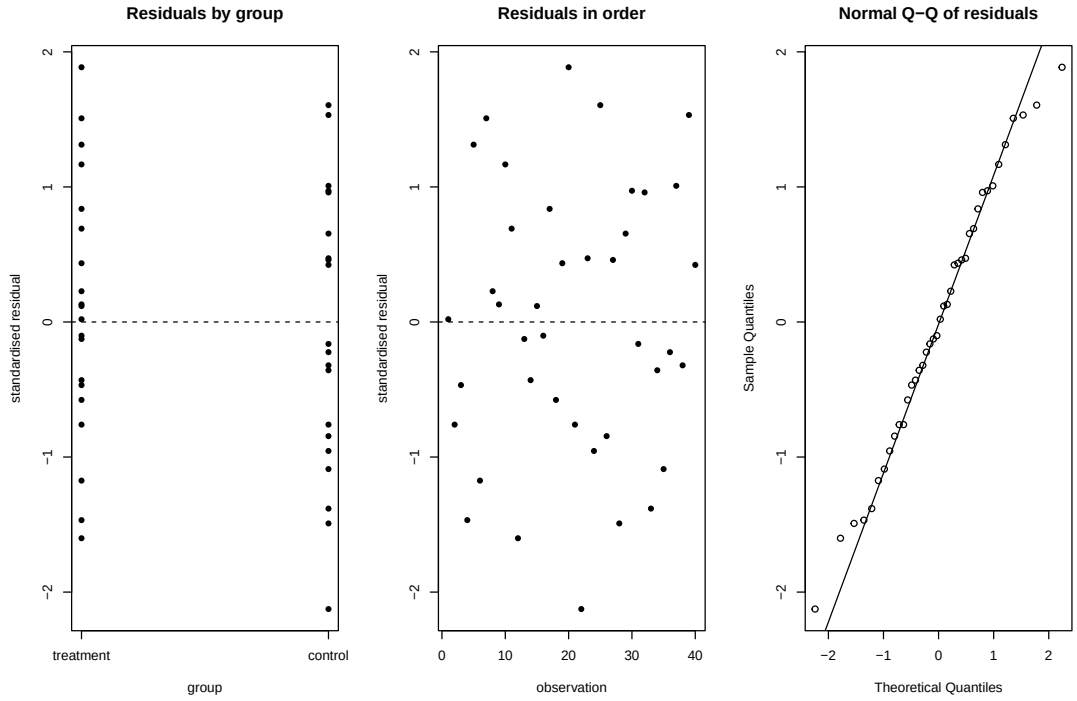
```
Analysis of Variance Table

Model 1: weight ~ 1
Model 2: weight ~ group
  Res.Df    RSS Df Sum of Sq      F Pr(>F)
1     39 26.232
2     38 26.053  1   0.17822 0.2599 0.6131
```

Separate group means reduce the sum of squares from 26.232 to 26.053, an improvement of 0.178 or 0.7% of the total; $F = 0.260$ on $(1, 38)$, $p = 0.61$, far below $F_{0.95}(1, 38) = 4.10$. There is no evidence against H_0, so the single-mean model is preferable and the nutritional enrichment has no demonstrable effect on mean dry weight.

(h) By Section 1.4.4, $T \sim t(n)$ implies $T^2 \sim F(1, n)$; here $t = 0.50985$ gives $t^2 = 0.25994 = F$, and the p-values agree exactly at 0.6131 because the two-sided t-test and the upper-tail F-test reject on the same event $\{|T| > c\}$. The conclusions of (b) and (g) are identical, the t formulation additionally supplying the signed estimate and interval that F discards.

(i) Under H_0 every fitted value is $\overline{y}$, so the residuals are $y_{jk} - \overline{y}$, standardized by $s = \sqrt{\widehat{S}_0/39}$.

```r
r <- (y - mean(y)) / sqrt(S0 / 39)
par(mfrow = c(1, 3))
plot(as.integer(plant$group), r, xaxt = "n", xlab = "group",
     ylab = "standardised residual", main = "Residuals by group", pch = 16)
axis(1, at = 1:2, labels = levels(plant$group)); abline(h = 0, lty = 2)
plot(seq_along(r), r, xlab = "observation", ylab = "standardised residual",
     main = "Residuals in order", pch = 16); abline(h = 0, lty = 2)
qqnorm(r, main = "Normal Q-Q of residuals"); qqline(r)
```




```r
round(c(mean = mean(r), sd = sd(r), min = min(r), max = max(r)), 3)
tapply(r, plant$group, mean)
shapiro.test(r)
```

```
 mean     sd    min    max
0.000  1.000 -2.126  1.886

treatment    control
0.0813899 -0.0813899

        Shapiro-Wilk normality test

data:  r
W = 0.9844, p-value = 0.8457
```

The Normal probability plot is near-straight with no residual beyond ± 2.13 and Shapiro-Wilk $p = 0.85$, and the spread is the same in the two groups, supporting Normality and constant variance. The residual group means are $+0.081$ and -0.081 against a residual standard deviation of 1: no group structure remains, so the H_0 model is adequate.

2.2 Problem 2.2 — The weights, in kilograms, of twenty men before and after participation

Problem 2.2. The weights, in kilograms, of twenty men before and after participation in a "waist loss" program are shown in Table 2.8 (Egger et al. 1999). We want to know if, on average, they retain a weight loss twelve months after the program.

Table 2.8 (Weights of twenty men before and after participation in a "waist loss" program) lists, as (man, before, after): $(1, 100.8, 97.0)$, $(2, 102.0, 107.5)$, $(3, 105.9, 97.0)$, $(4, 108.0, 108.0)$, $(5, 92.0, 84.0)$, $(6, 116.7, 111.5)$, $(7, 110.2, 102.5)$, $(8, 135.0, 127.5)$, $(9, 123.5, 118.5)$, $(10, 95.0, 94.2)$, $(11, 105.0, 105.0)$, $(12, 85.0, 82.4)$, $(13, 107.2, 98.2)$, $(14, 80.0, 83.6)$, $(15, 115.1, 115.0)$, $(16, 103.5, 103.0)$, $(17, 82.0, 80.0)$, $(18, 101.5, 101.5)$, $(19, 103.5, 102.6)$, $(20, 93.0, 93.0)$.

Let Y_{jk} denote the weight of the kth man at the jth time, where $j = 1$ before the program and $j = 2$ twelve months later. Assume the Y_{jk}'s are independent random variables with $Y_{jk} \sim \mathrm{N}(\mu_j, \sigma^2)$ for $j = 1, 2$ and $k = 1, \ldots, 20$.

a. Use an unpaired t-test to test the hypothesis

$$\mathrm{H}_0 : \mu_1 = \mu_2 \qquad \text{versus} \qquad \mathrm{H}_1 : \mu_1 \neq \mu_2.$$

b. Let $D_k = Y_{1k} - Y_{2k}$, for $k = 1, \ldots, 20$. Formulate models for testing H_0 against H_1 using the D_k's. Using analogous methods to Exercise 2.1 above, assuming σ^2 is a known constant, test H_0 against H_1.

c. The analysis in (b) is a paired t-test which uses the natural relationship between weights of the *same* person before and after the program. Are the conclusions the same from (a) and (b)?

d. List the assumptions made for (a) and (b). Which analysis is more appropriate for these data? (difficulty: ⋆⋆)

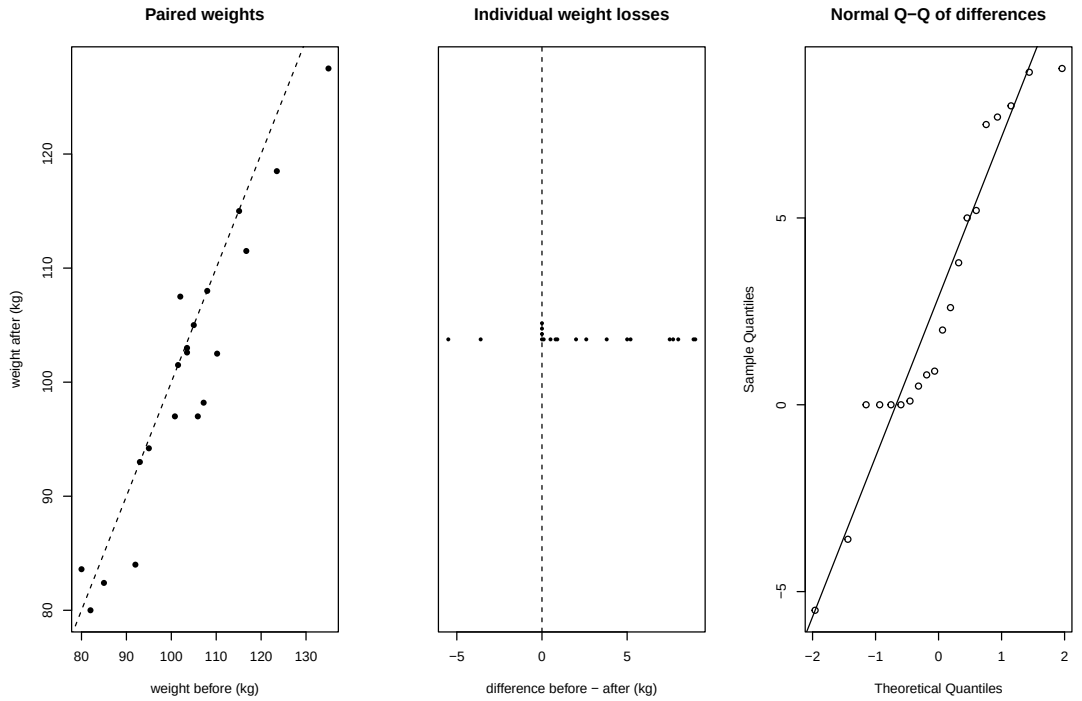
Solution. The paired analysis rejects H_0 and the unpaired one does not; the paired analysis is the correct one, and the men retain a mean loss of 2.645 kg. The data ship in the `dobson` package as `waist`, one row per man.

```r
library(dobson)
data(waist)
w <- data.frame(weight = c(waist$before, waist$after),
                time = factor(rep(c("before", "after"), each = 20),
                              levels = c("before", "after")))
round(t(sapply(split(w$weight, w$time),
       function(v) c(n = length(v), mean = mean(v), sd = sd(v),
                     min = min(v), max = max(v)))), 3)
```

```
       n    mean     sd min   max
before 20 103.245 13.517  80 135.0
after  20 100.600 12.475  80 127.5
```

```r
d <- waist$before - waist$after
par(mfrow = c(1, 3))
```

```r
plot(waist$before, waist$after, pch = 16, xlab = "weight before (kg)",
     ylab = "weight after (kg)", main = "Paired weights")
abline(0, 1, lty = 2)
stripchart(d, method = "stack", pch = 16,
           xlab = "difference before - after (kg)",
           main = "Individual weight losses")
abline(v = 0, lty = 2)
qqnorm(d, main = "Normal Q-Q of differences"); qqline(d)
```



The points lie almost on $y = x$ and nearly all just below it: the men differ enormously from each other (80 to 135 kg) but each changes only a little.

(a) Treating the two sets of 20 weights as independent samples, as the stated model does:

```r
t.test(weight ~ time, data = w, var.equal = TRUE)
```

```
        Two Sample t-test

data:  weight by time
t = 0.64309, df = 38, p-value = 0.524
alternative hypothesis: true difference in means between group before and group after is not
↪  equal to 0
95 percent confidence interval:
 -5.68128 10.97128
sample estimates:
mean in group before  mean in group after
             103.245              100.600
```

The estimated mean loss is $103.245 - 100.600 = 2.645$ kg, but $t = 0.643$ on 38 degrees of freedom gives $p = 0.52$ with wide interval $(-5.68, 10.97)$: no evidence of a retained loss.

(b) With $D_k = Y_{1k} - Y_{2k} \sim \mathrm{N}(\delta, \sigma_D^2)$ independent across men, $\delta = \mu_1 - \mu_2$, and σ_D^2 known, the models are

$$\mathrm{H}_0 : \mathrm{E}(D_k) = 0, \qquad \mathrm{H}_1 : \mathrm{E}(D_k) = \delta, \qquad k = 1, \ldots, 20.$$

As in Exercise 2.1(c), maximizing ℓ_1 is minimizing $S_1 = \sum_k (d_k - \delta)^2$ and gives $\widehat{\delta} = \overline{D}$, so the minimized criteria are $\widehat{S}_0 = \sum_k D_k^2$ (no parameters) and $\widehat{S}_1 = \sum_k (D_k - \overline{D})^2$ (one parameter). Exercise 1.4(b) with $n = 20$ writes $\widehat{S}_1/\sigma_D^2$ as a $\chi^2(20)$ minus an independent $\chi^2(1)$, so $\widehat{S}_1/\sigma_D^2 \sim \chi^2(19)$ regardless of H_0; and under H_0, $\widehat{S}_0 - \widehat{S}_1 = 20\overline{D}^2$ with $\overline{D} \sim \mathrm{N}(0, \sigma_D^2/20)$ is $\sigma_D^2 \chi^2(1)$ independent of $\widehat{S}_1$. Hence

$$F = \frac{\widehat{S}_0 - \widehat{S}_1}{\widehat{S}_1/19} \sim F(1,19) \quad \text{if } \mathrm{H}_0 \text{ is true.}$$

```r
S0 <- sum(d^2); S1 <- sum((d - mean(d))^2)
Fstat <- (S0 - S1) / (S1 / 19)
c(S0 = S0, S1 = S1, diff = S0 - S1, F = Fstat,
  p = pf(Fstat, 1, 19, lower.tail = FALSE))
```

```
          S0           S1         diff            F            p
4.619100e+02 3.219895e+02 1.399205e+02 8.256448e+00 9.730463e-03
```

$F = 8.256$ on $(1, 19)$ gives $p = 0.0097$, beyond $F_{0.95}(1, 19) = 4.38$, so H_0 is rejected. Equivalently, as a t-statistic:

```r
t.test(waist$before, waist$after, paired = TRUE)
```

```
        Paired t-test

data:  waist$before and waist$after
t = 2.8734, df = 19, p-value = 0.00973
alternative hypothesis: true mean difference is not equal to 0
95 percent confidence interval:
 0.718348 4.571652
sample estimates:
mean difference
          2.645
```

Here $t^2 = 2.8734^2 = 8.256 = F$ by the identity of Exercise 2.1(h), and the men retain a mean loss of 2.645 kg with 95% interval $(0.72, 4.57)$ kg.

(c) No — the conclusions are opposite. Both estimate the same 2.645 kg, but the unpaired standard error is 4.11 kg against the paired 0.92 kg, because of the correlation between a man's two weights:

```r
c(cor = cor(waist$before, waist$after),
  se_unpaired = sqrt(var(waist$before)/20 + var(waist$after)/20),
  se_paired = sd(d)/sqrt(20))
```

```
      cor se_unpaired   se_paired
0.9529734   4.1129735   0.9205112
```

With $\rho = 0.953$, $\mathrm{var}(D_k) = 2\sigma^2(1-\rho)$ is about 5% of the $2\sigma^2$ the unpaired analysis assumes: pairing removes the dominant between-man variation, which is irrelevant to the question, so the unpaired test's failure to reject is a Type II error.

(d) For (a): the 40 observations mutually independent, both sets Normal, equal variances, representative sample. Independence is the fatal one, the same 20 men being measured twice. For (b): the 20 differences mutually independent (different men); each D_k Normal with common σ_D^2 (Q-Q acceptably straight, Shapiro-Wilk $p = 0.16$, though with several exact zeros); and a common mean δ, i.e. retained loss independent of initial weight. Nothing is assumed about the between-man weight distribution or about equal variances across times.

```r
shapiro.test(d)
summary(lm(d ~ waist$before))$coefficients
```

```
        Shapiro-Wilk normality test

data:  d
W = 0.93148, p-value = 0.1649

                Estimate Std. Error   t value   Pr(>|t|)
(Intercept)  -9.8004283  6.8611113 -1.428402 0.17029887
waist$before  0.1205427  0.0659201  1.828618 0.08407696
```

Regressing loss on initial weight gives slope 0.121 kg per kg, $p = 0.084$: weak evidence that heavier men retain a larger loss, so the common-δ assumption is not clearly contradicted. The paired analysis of (b) is the appropriate one, the design being before-and-after on the same subjects, and the men retain a mean loss of about 2.6 kg (95% CI 0.7 to 4.6 kg) – though with no control group the program effect cannot be separated from regression to the mean.

2.3 Problem 2.3 — For Model (2.7) for the data on birthweight and gestational age, using

Problem 2.3. For Model (2.7) for the data on birthweight and gestational age, using methods similar to those for Exercise 1.4, show

$$\widehat{S}_1 = \sum_{j=1}^{J}\sum_{k=1}^{K}(Y_{jk} - a_j - b_j x_{jk})^2$$

$$= \sum_{j=1}^{J}\sum_{k=1}^{K}\left[Y_{jk} - (\alpha_j + \beta_j x_{jk})\right]^2 - K\sum_{j=1}^{J}(\overline{Y}_j - \alpha_j - \beta_j \overline{x}_j)^2$$

$$- \sum_{j=1}^{J}(b_j - \beta_j)^2\left(\sum_{k=1}^{K} x_{jk}^2 - K\overline{x}_j^2\right)$$

and that the random variables Y_{jk}, $\overline{Y}_j$ and b_j are all independent and have the following distributions

$$Y_{jk} \sim \mathrm{N}(\alpha_j + \beta_j x_{jk}, \sigma^2),$$

$$\overline{Y}_j \sim \mathrm{N}(\alpha_j + \beta_j \overline{x}_j, \sigma^2/K),$$

$$b_j \sim \mathrm{N}\left(\beta_j,\ \sigma^2 \Big/ \Big(\sum_{k=1}^{K} x_{jk}^2 - K\overline{x}_j^2\Big)\right).$$

Here Model (2.7) is $\mathrm{E}(Y_{jk}) = \mu_{jk} = \alpha_j + \beta_j x_{jk}$ with $Y_{jk} \sim \mathrm{N}(\mu_{jk}, \sigma^2)$ independent, $j = 1, \ldots, J$ indexing the groups (boys and girls, so $J = 2$) and $k = 1, \ldots, K$ the babies within a group ($K = 12$); a_j and b_j are the least squares estimates of α_j and β_j given in Section 2.2.2 by $b_j = \left(K\sum_k x_{jk}Y_{jk} - (\sum_k x_{jk})(\sum_k Y_{jk})\right) / \left(K\sum_k x_{jk}^2 - (\sum_k x_{jk})^2\right)$ and $a_j = \overline{Y}_j - b_j\overline{x}_j$.
(difficulty: ⋆⋆⋆)

Solution. Fix a group j, assume $S_{xx} > 0$, and write $S_{xx} = \sum_k (x_{jk} - \overline{x}_j)^2 = \sum_k x_{jk}^2 - K\overline{x}_j^2$, $S_{xY} = \sum_k (x_{jk} - \overline{x}_j)(Y_{jk} - \overline{Y}_j)$, $S_{YY} = \sum_k (Y_{jk} - \overline{Y}_j)^2$, so that $b_j = S_{xY}/S_{xx}$ and $a_j = \overline{Y}_j - b_j\overline{x}_j$ (Section 2.2.2).
(1) Substituting $a_j = \overline{Y}_j - b_j\overline{x}_j$ gives $Y_{jk} - a_j - b_j x_{jk} = (Y_{jk} - \overline{Y}_j) - b_j(x_{jk} - \overline{x}_j)$, so the group-$j$ contribution to $\widehat{S}_1$ is, using $S_{xY} = b_j S_{xx}$,

$$\widehat{S}_{1j} = S_{YY} - 2b_j S_{xY} + b_j^2 S_{xx} = S_{YY} - b_j^2 S_{xx}. \tag{i}$$

For the right-hand side put $e_{jk} = Y_{jk} - (\alpha_j + \beta_j x_{jk})$, so $\overline{e}_j = \overline{Y}_j - \alpha_j - \beta_j\overline{x}_j$ is the quantity squared in the second term. Exercise 1.4(b) with $n = K$ gives $\sum_k e_{jk}^2 - K\overline{e}_j^2 = \sum_k (e_{jk} - \overline{e}_j)^2$, and since $e_{jk} - \overline{e}_j = (Y_{jk} - \overline{Y}_j) - \beta_j(x_{jk} - \overline{x}_j)$,

$$\sum_k (e_{jk} - \overline{e}_j)^2 = S_{YY} - 2\beta_j b_j S_{xx} + \beta_j^2 S_{xx},$$
$$(b_j - \beta_j)^2 S_{xx} = b_j^2 S_{xx} - 2b_j\beta_j S_{xx} + \beta_j^2 S_{xx},$$

so subtracting cancels every β_j term and leaves $S_{YY} - b_j^2 S_{xx} = \widehat{S}_{1j}$ by (i). Summing over j gives the stated identity, which is purely algebraic: it holds for any α_j, β_j, as a numerical check on the birthweight data with both the Table 2.5 values and arbitrary ones confirms:

```
library(dobson)
data(birthweight)
bw <- data.frame(y   = c(birthweight[[2]], birthweight[[4]]),
                 x   = c(birthweight[[1]], birthweight[[3]]),
```

```
                  sex = rep(c("boys", "girls"), each = 12))
K <- 12
check <- function(alpha, beta) {
  S1 <- 0; A <- 0; B <- 0; C <- 0
  for (j in unique(bw$sex)) {
    yj <- bw$y[bw$sex == j]; xj <- bw$x[bw$sex == j]
    i  <- match(j, unique(bw$sex))
    bj <- cov(xj, yj) / var(xj); aj <- mean(yj) - bj * mean(xj)
    Sxx <- sum(xj^2) - K * mean(xj)^2
    S1 <- S1 + sum((yj - aj - bj * xj)^2)
    A  <- A + sum((yj - (alpha[i] + beta[i] * xj))^2)
    B  <- B + K * (mean(yj) - alpha[i] - beta[i] * mean(xj))^2
    C  <- C + (bj - beta[i])^2 * Sxx
  }
  c(S1 = S1, rhs = A - B - C, A = A, B = B, C = C)
}
round(check(c(-1268.672, -2141.667), c(111.983, 130.400)), 4)
round(check(c(0, 500), c(100, 90)), 4)
```

```
          S1         rhs           A          B         C
652424.5218 652424.5218 652424.5230     0.0011    0.0000

          S1         rhs           A           B        C
  652424.52   652424.52 22475004.00 21757861.67 64717.81
```

The value $\widehat{S}_1 = 652424.5$ agrees with Table 2.5, and `rhs` reproduces it in both cases though the three components differ by orders of magnitude.

(2) $Y_{jk} \sim \mathrm{N}(\alpha_j + \beta_j x_{jk}, \sigma^2)$ is the model assumption (2.7) itself; $\overline{Y}_j$ and b_j are linear in independent Normals, hence Normal, so only the moments are wanted. Immediately

$$\mathrm{E}(\overline{Y}_j) = \alpha_j + \beta_j \overline{x}_j, \qquad \mathrm{var}(\overline{Y}_j) = \frac{1}{K^2}\sum_k \sigma^2 = \frac{\sigma^2}{K},$$

and for the slope, $\sum_k (x_{jk} - \overline{x}_j) = 0$ lets $Y_{jk} - \overline{Y}_j$ be replaced by Y_{jk} in $b_j = S_{xY}/S_{xx} = S_{xx}^{-1}\sum_k (x_{jk} - \overline{x}_j)Y_{jk}$, whence, with $\sum_k (x_{jk} - \overline{x}_j)x_{jk} = S_{xx}$,

$$\mathrm{E}(b_j) = \frac{1}{S_{xx}}\sum_k (x_{jk} - \overline{x}_j)(\alpha_j + \beta_j x_{jk}) = \beta_j,$$
$$\mathrm{var}(b_j) = \frac{\sigma^2}{S_{xx}^2}\sum_k (x_{jk} - \overline{x}_j)^2 = \frac{\sigma^2}{\sum_k x_{jk}^2 - K\overline{x}_j^2}.$$

(3) The stated independence cannot be read literally, $\overline{Y}_j$ being a function of the Y_{jk} of its own group; what holds, and what Section 2.2.2 needs, is that within each group the three **terms of the decomposition** are mutually independent, with independence across groups from disjointness. Rearranged, the identity reads

$$\frac{1}{\sigma^2}\sum_j\sum_k e_{jk}^2 = \frac{\widehat{S}_1}{\sigma^2} + \frac{K}{\sigma^2}\sum_j \overline{e}_j^2 + \frac{1}{\sigma^2}\sum_j (b_j - \beta_j)^2 S_{xx,j}.$$

Fix j, take $\mathbf{e}_j \sim \mathrm{N}_K(\mathbf{0}, \sigma^2\mathbf{I})$, and let $V_j \subset \mathbb{R}^K$ be spanned by the orthonormal $\mathbf{u}_1 = \mathbf{1}/\sqrt{K}$ and $\mathbf{u}_2 = (\mathbf{x}_j - \overline{x}_j\mathbf{1})/\sqrt{S_{xx}}$. Then

$$\mathbf{u}_1^{\mathrm{T}}\mathbf{e}_j = \sqrt{K}\,\overline{e}_j, \qquad \mathbf{u}_2^{\mathrm{T}}\mathbf{e}_j = \frac{S_{xY} - \beta_j S_{xx}}{\sqrt{S_{xx}}} = (b_j - \beta_j)\sqrt{S_{xx}},$$

so the three terms are $\|(\mathbf{I} - \mathbf{P}_j)\mathbf{e}_j\|^2$, $(\mathbf{u}_1^{\mathrm{T}}\mathbf{e}_j)^2$ and $(\mathbf{u}_2^{\mathrm{T}}\mathbf{e}_j)^2$ with $\mathbf{P}_j$ the projection onto V_j; $\mathbf{e}_j$ being spherically Normal, its components along orthogonal directions and in the orthogonal complement are independent, so dividing by σ^2,

$$\frac{\widehat{S}_{1j}}{\sigma^2} \sim \chi^2(K-2), \qquad \frac{K\overline{e}_j^2}{\sigma^2} \sim \chi^2(1), \qquad \frac{(b_j - \beta_j)^2 S_{xx}}{\sigma^2} \sim \chi^2(1),$$

independently, adding to $\chi^2(K)$ as they must. In particular $\overline{Y}_j$ and b_j are jointly Normal with

$$\operatorname{cov}(\overline{Y}_j, b_j) = \frac{\sigma^2}{KS_{xx}} \sum_k (x_{jk} - \overline{x}_j) = 0,$$

hence independent, which is the substantive content of the claim. Summing over j gives $\widehat{S}_1/\sigma^2 \sim \chi^2(JK - 2J)$ as quoted in Section 2.2.2.

2.4 Problem 2.4 — Suppose you have the following data

Problem 2.4. Suppose you have the following data

x	1.0	1.2	1.4	1.6	1.8	2.0
y	3.15	4.85	6.50	7.20	8.25	16.50

and you want to fit a model with

$$\mathrm{E}(Y) = \ln(\beta_0 + \beta_1 x + \beta_2 x^2).$$

Write this model in the form of (2.13) specifying the vectors $\mathbf{y}$ and $\boldsymbol{\beta}$ and the matrix $\mathbf{X}$.
Equation (2.13) of Section 2.4 is $g[\mathrm{E}(\mathbf{y})] = \mathbf{X}\boldsymbol{\beta}$, where $\mathbf{y}$ is the $N \times 1$ vector of responses, $g[\mathrm{E}(\mathbf{y})]$ denotes the vector with elements $g[\mathrm{E}(Y_i)]$ for a single link function g, $\boldsymbol{\beta}$ is the $p \times 1$ vector of parameters and $\mathbf{X}$ is the $N \times p$ design matrix.
(difficulty: $\star$)

Solution. The link is $g(\mu) = e^{\mu}$: exponentiating $\mathrm{E}(Y_i) = \ln(\beta_0 + \beta_1 x_i + \beta_2 x_i^2)$ gives

$$\exp[\mathrm{E}(Y_i)] = \beta_0 + \beta_1 x_i + \beta_2 x_i^2,$$

which is the form $g[\mathrm{E}(Y_i)] = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2}$ of Section 2.4 with $x_{i1} = x_i$, $x_{i2} = x_i^2$ – quadratic in x but linear in the parameters, which is all (2.13) requires. With $N = 6$ and $p = 3$,

$$\mathbf{y} = \begin{bmatrix} 3.15 \\ 4.85 \\ 6.50 \\ 7.20 \\ 8.25 \\ 16.50 \end{bmatrix}, \qquad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}, \qquad \mathbf{X} = \begin{bmatrix} 1 & 1.0 & 1.00 \\ 1 & 1.2 & 1.44 \\ 1 & 1.4 & 1.96 \\ 1 & 1.6 & 2.56 \\ 1 & 1.8 & 3.24 \\ 1 & 2.0 & 4.00 \end{bmatrix},$$

and the model in the form of (2.13) is

$$g[\mathrm{E}(\mathbf{y})] = \begin{bmatrix} \exp[\mathrm{E}(Y_1)] \\ \vdots \\ \exp[\mathrm{E}(Y_6)] \end{bmatrix} = \mathbf{X}\boldsymbol{\beta}.$$

The design matrix:

```r
x <- c(1.0, 1.2, 1.4, 1.6, 1.8, 2.0)
y <- c(3.15, 4.85, 6.50, 7.20, 8.25, 16.50)
X <- cbind(1, x, x^2)
colnames(X) <- c("beta0", "beta1", "beta2")
X
```

```
     beta0 beta1 beta2
[1,]     1   1.0  1.00
[2,]     1   1.2  1.44
[3,]     1   1.4  1.96
[4,]     1   1.6  2.56
[5,]     1   1.8  3.24
[6,]     1   2.0  4.00
```

The logarithm restricts $\boldsymbol{\beta}$ to the region where $\beta_0 + \beta_1 x + \beta_2 x^2 > 0$ over the range of x. Fitting by least squares with a custom link:

```r
explink <- structure(list(
  linkfun  = function(mu)  exp(mu),
  linkinv  = function(eta) log(pmax(eta, .Machine$double.eps)),
  mu.eta   = function(eta) 1 / pmax(eta, .Machine$double.eps),
  valideta = function(eta) all(eta > 0),
  name     = "exp"), class = "link-glm")
fit <- glm(y ~ x + I(x^2), family = gaussian(link = explink),
           start = c(exp(3), 1, 1))
round(coef(fit), 2)
round(cbind(y = y, fitted = fitted(fit)), 3)
```

```
(Intercept)           x      I(x^2)
   60843.03  -111879.21    51059.77

      y fitted
1  3.15  3.161
2  4.85  4.737
3  6.50  8.364
4  7.20  9.437
5  8.25 10.122
6 16.50 10.629
```

The residual sum of squares is 46.47, and a multi-start Nelder-Mead search over the constrained parameter space finds no better optimum, so this is the least squares solution and not a convergence failure: the fit is simply poor, the last observation $y = 16.50$ lying far above what the model can reach.

2.5 Problem 2.5 — The model for two-factor analysis of variance with two levels of one factor,

Problem 2.5. The model for two-factor analysis of variance with two levels of one factor, three levels of the other and no replication is

$$\mathrm{E}(Y_{jk}) = \mu_{jk} = \mu + \alpha_j + \beta_k; \qquad Y_{jk} \sim \mathrm{N}(\mu_{jk}, \sigma^2),$$

where $j = 1, 2$; $k = 1, 2, 3$ and, using the sum-to-zero constraints, $\alpha_1 + \alpha_2 = 0$, $\beta_1 + \beta_2 + \beta_3 = 0$. Also the Y_{jk}'s are assumed to be independent. Write the equation for $\mathrm{E}(Y_{jk})$ in matrix notation. (Hint: Let $\alpha_2 = -\alpha_1$, and $\beta_3 = -\beta_1 - \beta_2$.)
(difficulty: $\star$)

Solution. With g the identity, the model in the form of (2.13) is $\mathrm{E}(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$ with

$$\mathbf{y} = \begin{bmatrix} Y_{11} \\ Y_{12} \\ Y_{13} \\ Y_{21} \\ Y_{22} \\ Y_{23} \end{bmatrix}, \qquad \boldsymbol{\beta} = \begin{bmatrix} \mu \\ \alpha_1 \\ \beta_1 \\ \beta_2 \end{bmatrix}, \qquad \mathbf{X} = \begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & 0 \\ 1 & -1 & 0 & 1 \\ 1 & -1 & -1 & -1 \end{bmatrix}.$$

The unconstrained $\mu + \alpha_j + \beta_k$ carries $1 + 2 + 3 = 6$ parameters for $N = 6$ observations and is not identifiable (Example 2.4.3(b)); the sum-to-zero constraints of Example 2.4.3(d) remove one from each factor, leaving $p = 4$. Substituting $\alpha_2 = -\alpha_1$ and $\beta_3 = -\beta_1 - \beta_2$,

$$\begin{aligned} &\mathrm{E}(Y_{11}) = \mu + \alpha_1 + \beta_1, && \mathrm{E}(Y_{12}) = \mu + \alpha_1 + \beta_2, && \mathrm{E}(Y_{13}) = \mu + \alpha_1 - \beta_1 - \beta_2, \\ &\mathrm{E}(Y_{21}) = \mu - \alpha_1 + \beta_1, && \mathrm{E}(Y_{22}) = \mu - \alpha_1 + \beta_2, && \mathrm{E}(Y_{23}) = \mu - \alpha_1 - \beta_1 - \beta_2, \end{aligned}$$

whose coefficients of $(\mu, \alpha_1, \beta_1, \beta_2)$ are the rows of $\mathbf{X}$ above. This is `contr.sum` coding on both factors:

```r
d <- expand.grid(k = factor(1:3), j = factor(1:2))
```

```r
d <- d[order(d$j, d$k), ]
X <- model.matrix(~ j + k, data = d,
                  contrasts.arg = list(j = "contr.sum", k = "contr.sum"))
colnames(X) <- c("mu", "alpha1", "beta1", "beta2")
rownames(X) <- paste0("Y", d$j, d$k)
X[, ]
c(rank = qr(X)$rank, ncol = ncol(X))
```

```
    mu alpha1 beta1 beta2
Y11  1      1     1     0
Y12  1      1     0     1
Y13  1      1    -1    -1
Y21  1     -1     1     0
Y22  1     -1     0     1
Y23  1     -1    -1    -1

rank ncol
   4    4
```

$\mathbf{X}$ has full column rank 4, so the four parameters are estimable, unlike the unconstrained six; $N - p = 2$ degrees of freedom remain for σ^2, which a $j \times k$ interaction would consume entirely.
The design is balanced, the two factors orthogonal to each other and to the intercept:

```r
t(X) %*% X
```

```
       mu alpha1 beta1 beta2
mu      6      0     0     0
alpha1  0      6     0     0
beta1   0      0     4     2
beta2   0      0     2     4
```

The block-diagonal $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ makes $\widehat{\mu}$, $\widehat{\alpha}_1$ and the pair $(\widehat{\beta}_1, \widehat{\beta}_2)$ mutually uncorrelated, so one factor's estimated effect is unchanged by adding or dropping the other; the off-diagonal 2 reflects only that the two columns coding a three-level factor are not orthogonal to each other under sum-to-zero coding.

3 Exponential Family and Generalized Linear Models

Contents

3.1 Problem 3.1 — The following associations can be described by generalized linear models.

Problem 3.1. The following associations can be described by generalized linear models. For each one, identify the response variable and the explanatory variables, select a probability distribution for the response (justifying your choice) and write down the linear component.
a. The effect of age, sex, height, mean daily food intake and mean daily energy expenditure on a person's weight.
b. The proportions of laboratory mice that became infected after exposure to bacteria when five different exposure levels are used and 20 mice are exposed at each level.
c. The association between the number of trips per week to the supermarket for a household and the number of people in the household, the household income and the distance to the supermarket. (difficulty: $\star$)

Solution. Each part gives the three components of Section 3.4: response distribution, linear component, and link.
(a) Y_i is the weight (kg) of person i: a continuous, roughly symmetric measurement with no hard upper bound, so $Y_i \sim N(\mu_i, \sigma^2)$ (exponential family, Section 3.2.2) with the identity link, giving the normal linear model of Section 3.5.1. With x_{i1} age, x_{i2} sex (dummy), x_{i3} height, x_{i4} mean daily intake and x_{i5} mean daily expenditure,

$$g(\mu_i) = \mu_i = \beta_1 + \beta_2 x_{i1} + \beta_3 x_{i2} + \beta_4 x_{i3} + \beta_5 x_{i4} + \beta_6 x_{i5}.$$

(b) Y_i is the number infected out of $n_i = 20$ at exposure level i ($i = 1, \ldots, 5$), the mice at a level being independent binary trials with common probability, so $Y_i \sim \text{Bin}(20, \pi_i)$ (exponential family with natural parameter $\log[\pi/(1-\pi)]$, Section 3.2.3). Modelling the count rather than the proportion keeps the variance $n_i \pi_i (1 - \pi_i)$. With x_i the exposure level (or log dose) and the natural logit link,

$$g(\pi_i) = \log\left(\frac{\pi_i}{1-\pi_i}\right) = \beta_1 + \beta_2 x_i,$$

a logistic dose-response model, which keeps $\pi_i \in (0, 1)$ for all β_1, β_2, x_i.
(c) Y_i is the number of trips made by household i in a week: an unbounded count of events in a fixed period, so $Y_i \sim \text{Po}(\mu_i)$ (Section 3.2.1). With x_{i1} household size, x_{i2} income and x_{i3} distance, the log link keeps $\mu_i > 0$ and makes effects multiplicative on the rate:

$$g(\mu_i) = \log \mu_i = \beta_1 + \beta_2 x_{i1} + \beta_3 x_{i2} + \beta_4 x_{i3},$$

with $\beta_2 > 0$ and $\beta_4 < 0$ expected. The Poisson assumption $\text{E}(Y) = \text{var}(Y)$ should be checked, a negative binomial (Chapter 9) being preferred if the counts are overdispersed.

3.2 Problem 3.2 — If the random variable Y has the Gamma distribution with a scale param-

Problem 3.2. If the random variable Y has the Gamma distribution with a scale parameter β, which is the parameter of interest, and a known shape parameter α, then its probability density function is

$$f(y; \beta) = \frac{\beta^\alpha}{\Gamma(\alpha)} y^{\alpha-1} e^{-y\beta}.$$

Show that this distribution belongs to the exponential family and find the natural parameter. Also using results in this chapter, find $\text{E}(Y)$ and $\text{var}(Y)$. (difficulty: $\star\star$)

Solution. The natural parameter is $b(\beta) = -\beta$, with $\text{E}(Y) = \alpha/\beta$ and $\text{var}(Y) = \alpha/\beta^2$. Taking logarithms, for $y > 0$,

$$f(y;\beta) = \exp\left[\alpha\log\beta - \log\Gamma(\alpha) + (\alpha-1)\log y - y\beta\right],$$

which is the form (3.3), $f = \exp[a(y)b(\theta) + c(\theta) + d(y)]$, with

$$a(y) = y, \quad b(\beta) = -\beta, \quad c(\beta) = \alpha\log\beta - \log\Gamma(\alpha), \quad d(y) = (\alpha-1)\log y,$$

so the family is exponential and, as $a(y) = y$, in canonical form; the known shape α enters only through c and d, as Section 3.2 permits. Then $b' = -1$, $b'' = 0$, $c' = \alpha/\beta$, $c'' = -\alpha/\beta^2$, so by (3.9) and (3.12),

$$\mathrm{E}(Y) = -\frac{c'(\beta)}{b'(\beta)} = -\frac{\alpha/\beta}{-1} = \frac{\alpha}{\beta},$$
$$\mathrm{var}(Y) = \frac{b''c' - c''b'}{(b')^3} = \frac{0 - (-\alpha/\beta^2)(-1)}{(-1)^3} = \frac{\alpha}{\beta^2}.$$

A numerical check against R's parametrisation (R's `rate` is β):

```r
set.seed(1); a <- 3.5; b <- 2
y <- rgamma(2e6, shape = a, rate = b)
c(mean = mean(y), theory_mean = a/b, var = var(y), theory_var = a/b^2)
```

```
     mean theory_mean         var  theory_var
1.7500115   1.7500000   0.8750181   0.8750000
```

3.3 Problem 3.3 — Show that the following probability density functions belong to the expo-

Problem 3.3. Show that the following probability density functions belong to the exponential family:
a. Pareto distribution $f(y;\theta) = \theta y^{-\theta-1}$.
b. Exponential distribution $f(y;\theta) = \theta e^{-y\theta}$.
c. Negative Binomial distribution

$$f(y;\theta) = \binom{y+r-1}{r-1}\theta^r(1-\theta)^y,$$

where r is known. (difficulty: ⋆⋆)

Solution. In each case take logarithms and read off (3.3), $f(y;\theta) = \exp[a(y)b(\theta) + c(\theta) + d(y)]$; the form is canonical only if $a(y) = y$ (Section 3.2).
(a) Pareto, $y > 1$, $\theta > 0$:

$$f(y;\theta) = \theta y^{-\theta-1} = \exp\left[(\log y)(-\theta) + \log\theta - \log y\right],$$

so (3.3) holds with $a(y) = \log y$, $b(\theta) = -\theta$, $c(\theta) = \log\theta$, $d(y) = -\log y$. Exponential family, but **not** canonical, since $a(y) = \log y \neq y$; equivalently $\log Y \sim \mathrm{Exp}(\theta)$, which is used in Exercises 3.9 and 3.11.
(b) Exponential, $y > 0$:

$$f(y;\theta) = \theta e^{-y\theta} = \exp\left[-y\theta + \log\theta\right],$$

so $a(y) = y$, $b(\theta) = -\theta$, $c(\theta) = \log\theta$, $d(y) = 0$: canonical, with natural parameter $-\theta$. It is the $\alpha = 1$ case of Exercise 3.2's Gamma.
(c) Negative binomial, $y = 0, 1, 2, \ldots$ with r known, so the binomial coefficient depends on y alone:

$$f(y;\theta) = \exp\left[y\log(1-\theta) + r\log\theta + \log\binom{y+r-1}{r-1}\right],$$

giving $a(y) = y$, $b(\theta) = \log(1-\theta)$, $c(\theta) = r\log\theta$, $d(y) = \log\binom{y+r-1}{r-1}$: canonical, with natural parameter $\log(1-\theta)$. Knowing r is essential, since otherwise $d(y)$ would depend on a second parameter and (3.3) would fail.

3.4 Problem 3.4 — Use results (3.9) and (3.12) to verify the following results:

Problem 3.4. Use results (3.9) and (3.12) to verify the following results:
a. For $Y \sim \text{Po}(\theta)$, $\text{E}(Y) = \text{var}(Y) = \theta$.
b. For $Y \sim N(\mu, \sigma^2)$, $\text{E}(Y) = \mu$ and $\text{var}(Y) = \sigma^2$.
c. For $Y \sim \text{Bin}(n, \pi)$, $\text{E}(Y) = n\pi$ and $\text{var}(Y) = n\pi(1-\pi)$. (difficulty: ⋆⋆)

Solution. All three are in canonical form, so $a(Y) = Y$ and (3.9), $\text{E}[a(Y)] = -c'/b'$, and (3.12), $\text{var}[a(Y)] = (b''c' - c''b')/(b')^3$, give the moments of Y directly from the b, c of Table 3.1.
(a) Poisson (Section 3.2.1): $b(\theta) = \log\theta$, $c(\theta) = -\theta$, so $b' = 1/\theta$, $b'' = -1/\theta^2$, $c' = -1$, $c'' = 0$ and

$$\text{E}(Y) = -\frac{-1}{1/\theta} = \theta, \qquad \text{var}(Y) = \frac{(-1/\theta^2)(-1)}{(1/\theta)^3} = \theta.$$

(b) Normal (Section 3.2.2), σ^2 a known nuisance parameter: $b(\mu) = \mu/\sigma^2$, $c(\mu) = -\mu^2/(2\sigma^2) - \frac{1}{2}\log(2\pi\sigma^2)$, so $b' = 1/\sigma^2$, $b'' = 0$, $c' = -\mu/\sigma^2$, $c'' = -1/\sigma^2$ and

$$\text{E}(Y) = -\frac{-\mu/\sigma^2}{1/\sigma^2} = \mu, \qquad \text{var}(Y) = \frac{-(-1/\sigma^2)(1/\sigma^2)}{(1/\sigma^2)^3} = \sigma^2.$$

(c) Binomial (Section 3.2.3): $b(\pi) = \log\pi - \log(1-\pi)$, $c(\pi) = n\log(1-\pi)$, so

$$b'(\pi) = \frac{1}{\pi(1-\pi)}, \quad b''(\pi) = -\frac{1-2\pi}{\pi^2(1-\pi)^2}, \quad c'(\pi) = -\frac{n}{1-\pi}, \quad c''(\pi) = -\frac{n}{(1-\pi)^2},$$

whence $\text{E}(Y) = [n/(1-\pi)]\pi(1-\pi) = n\pi$ and, with denominator $(b')^3 = [\pi(1-\pi)]^{-3}$,

$$\begin{aligned}\text{var}(Y) &= \pi^3(1-\pi)^3\left[\frac{n(1-2\pi)}{\pi^2(1-\pi)^3} + \frac{n}{\pi(1-\pi)^3}\right] \\ &= n\pi(1-2\pi) + n\pi^2 = n\pi(1-\pi).\end{aligned}$$

Applying (3.9) and (3.12) numerically to the same b, c by central differences:

```
ef <- function(b, cc, theta, h = 1e-5) {
  d1 <- function(f, t) (f(t + h) - f(t - h)) / (2 * h)
  d2 <- function(f, t) (f(t + h) - 2 * f(t) + f(t - h)) / h^2
  bp <- d1(b, theta); bpp <- d2(b, theta)
  cp <- d1(cc, theta); cpp <- d2(cc, theta)
  c(mean = -cp / bp, var = (bpp * cp - cpp * bp) / bp^3)
}
th <- 4.3
poi <- ef(function(t) log(t), function(t) -t, th)
sig <- 1.7; mu <- 2.4
nor <- ef(function(t) t / sig^2,
          function(t) -t^2 / (2 * sig^2) - 0.5 * log(2 * pi * sig^2), mu)
n <- 12; pi0 <- 0.3
bin <- ef(function(t) log(t / (1 - t)), function(t) n * log(1 - t), pi0)
round(rbind(Poisson  = c(poi, truth.mean = th,      truth.var = th),
            Normal   = c(nor, truth.mean = mu,      truth.var = sig^2),
            Binomial = c(bin, truth.mean = n * pi0, truth.var = n * pi0 * (1 - pi0))), 6)
```

```
         mean      var truth.mean truth.var
Poisson   4.3 4.300009        4.3      4.30
Normal    2.4 2.889965        2.4      2.89
Binomial  3.6 2.520000        3.6      2.52
```

The discrepancy in the Poisson and Normal variances is truncation error in the numerical second derivative.

3.5 Problem 3.5 — a. For a Negative Binomial distribution Y ∼ NBin(r, θ), find E(Y) and

Problem 3.5. a. For a Negative Binomial distribution $Y \sim \mathrm{NBin}(r, \theta)$, find $\mathrm{E}(Y)$ and $\mathrm{var}(Y)$.
b. Notice that for the Poisson distribution $\mathrm{E}(Y) = \mathrm{var}(Y)$, for the Binomial distribution $\mathrm{E}(Y) > \mathrm{var}(Y)$ and for the Negative Binomial distribution $\mathrm{E}(Y) < \mathrm{var}(Y)$. How might these results affect your choice of a model? (difficulty: ⋆⋆)

Solution. (a) $\mathrm{E}(Y) = r(1-\theta)/\theta$ and $\mathrm{var}(Y) = r(1-\theta)/\theta^2 = \mathrm{E}(Y)/\theta$, so $\mathrm{var}(Y) > \mathrm{E}(Y)$ for $0 < \theta < 1$. From Exercise 3.3(c) the distribution is canonical with $b(\theta) = \log(1-\theta)$, $c(\theta) = r\log\theta$, giving

$$b' = -\frac{1}{1-\theta}, \quad b'' = -\frac{1}{(1-\theta)^2}, \quad c' = \frac{r}{\theta}, \quad c'' = -\frac{r}{\theta^2},$$

so by (3.9) $\mathrm{E}(Y) = -(r/\theta)/(-1/(1-\theta)) = r(1-\theta)/\theta$, while (3.12) has numerator $-r/[\theta(1-\theta)^2] - r/[\theta^2(1-\theta)]$ over $(b')^3 = -1/(1-\theta)^3$, whence

$$\begin{aligned}\mathrm{var}(Y) &= (1-\theta)^3\left[\frac{r}{\theta(1-\theta)^2} + \frac{r}{\theta^2(1-\theta)}\right] \\ &= \frac{r(1-\theta)}{\theta} + \frac{r(1-\theta)^2}{\theta^2} = \frac{r(1-\theta)}{\theta^2}.\end{aligned}$$

```r
r <- 5; th <- 0.35
h <- 1e-5
b  <- function(t) log(1 - t); cc <- function(t) r * log(t)
d1 <- function(f, t) (f(t + h) - f(t - h)) / (2 * h)
d2 <- function(f, t) (f(t + h) - 2 * f(t) + f(t - h)) / h^2
bp <- d1(b, th); bpp <- d2(b, th); cp <- d1(cc, th); cpp <- d2(cc, th)
set.seed(2); y <- rnbinom(2e6, size = r, prob = th)
round(c(mean.3.9 = -cp / bp, formula.mean = r * (1 - th) / th, sim.mean = mean(y),
        var.3.12 = (bpp * cp - cpp * bp) / bp^3, formula.var = r * (1 - th) / th^2,
        sim.var = var(y)), 4)
```

```
mean.3.9 formula.mean     sim.mean     var.3.12  formula.var      sim.var
  9.2857       9.2857       9.2908      26.5306      26.5306      26.5283
```

(b) Choosing the distribution **is** choosing the variance function, since a generalized linear model has no free σ^2 to absorb misspecification. Writing $\mu = \mathrm{E}(Y)$,

$$\text{Binomial: } \mathrm{var}(Y) = \mu(1-\pi) < \mu, \quad \text{Poisson: } \mathrm{var}(Y) = \mu, \quad \text{NBin: } \mathrm{var}(Y) = \mu/\theta > \mu.$$

So: follow the sampling mechanism where there is one – a count out of n independent binary trials is Binomial, its underdispersion being a feature of the design. For unbounded counts the Poisson is the default, but $\mathrm{E}(Y) = \mathrm{var}(Y)$ is testable, e.g. by comparing residual deviance or Pearson X^2 with the residual degrees of freedom. Counts are frequently overdispersed (Section 3.2.1) through unmeasured heterogeneity, clustering or excess zeros, and the negative binomial is the remedy, keeping the log link and the multiplicative interpretation of $\boldsymbol{\beta}$ while estimating the extra parameter (Chapter 9). Ignoring overdispersion damages not the point estimates but the standard errors, understating $\mathrm{var}(\hat{\boldsymbol{\beta}})$ and so giving intervals that are too narrow.

3.6 Problem 3.6 — Do you consider the model suggested in Example 3.5.3 to be adequate for

Problem 3.6. Do you consider the model suggested in Example 3.5.3 to be adequate for the data shown in Figure 3.2? Justify your answer. Use simple linear regression (with suitable transformations of the variables) to obtain a model for the change of death rates with age. How well does the model

fit the data? (Hint: Compare observed and expected numbers of deaths in each group.)
Table 3.2 gives numbers of deaths from coronary heart disease and population sizes by 5-year age groups for men in the Hunter region of New South Wales, Australia in 1991: age group 30-34, $y = 1$ death, $n = 17{,}742$, rate 5.6 per 100,000 men per year; 35-39, $y = 5$, $n = 16{,}554$, rate 30.2; 40-44, $y = 5$, $n = 16{,}059$, rate 31.1; 45-49, $y = 12$, $n = 13{,}083$, rate 91.7; 50-54, $y = 25$, $n = 10{,}784$, rate 231.8; 55-59, $y = 38$, $n = 9{,}645$, rate 394.0; 60-64, $y = 54$, $n = 10{,}706$, rate 504.4; 65-69, $y = 65$, $n = 9{,}933$, rate 654.4. Figure 3.2 plots the logarithm of the death rate per 100,000 against age group; the eight points rise steadily and are approximately linear, apart from the second and third groups (35-39 and 40-44), which have almost the same log rate.
The model suggested in Example 3.5.3 is $\mathrm{E}(Y_i) = \mu_i = n_i e^{\theta i}$ with $Y_i \sim \mathrm{Po}(\mu_i)$, where $i = 1$ for the age group 30-34 up to $i = 8$ for 65-69; equivalently $g(\mu_i) = \log \mu_i = \log n_i + \theta i$, a generalized linear model with $\mathbf{x}_i^T = [\log n_i \;\; i]$ and $\boldsymbol{\beta}^T = [1 \;\; \theta]$. (difficulty: ⋆⋆⋆)

Solution. No: the model of Example 3.5.3 is inadequate, because $\log n_i$ enters as an offset with **no intercept**, forcing the fitted log rate through the origin at $i = 0$.

```
library(dobson)
data(mortality)
d <- as.data.frame(mortality)
names(d) <- c("agegroup", "deaths", "population")
d$i <- 1:8
d$rate <- d$deaths / d$population * 1e5
d
```

```
  agegroup deaths population i       rate
1    30-34      1      17742 1   5.636343
2    35-39      5      16554 2  30.204180
3    40-44      5      16059 3  31.135189
4    45-49     12      13083 4  91.722082
5    50-54     25      10784 5 231.824926
6    55-59     38       9645 6 393.986522
7    60-64     54      10706 7 504.390062
8    65-69     65       9933 8 654.384375
```

The `poisson` family object is masked by a `dobson` data set of the same name, hence `stats::poisson` below.

```
m1 <- glm(deaths ~ i - 1 + offset(log(population)), family = stats::poisson, data = d)
summary(m1)
```

```
Call:
glm(formula = deaths ~ i - 1 + offset(log(population)), family = stats::poisson,
    data = d)

Coefficients:
  Estimate Std. Error z value Pr(>|z|)
i -2.72150    0.02583  -105.4   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for poisson family taken to be 1)

    Null deviance: 206303.6  on 8  degrees of freedom
Residual deviance:   6990.4  on 7  degrees of freedom
AIC: 7028.1

Number of Fisher Scoring iterations: 8
```

The residual deviance is 6990.4 on 7 degrees of freedom, against a $\chi^2(7)$ mean of 7, and $\hat{\theta} = -2.72 < 0$ makes the fitted rate $e^{\hat{\theta} i}$ **decrease** with age, contradicting Figure 3.2. Without an intercept no single θ can make $e^{\theta i}$ both start near e^{θ} and pass through rates running from 5.6×10^{-5} to 6.5×10^{-3}; the exponential shape is not at fault.
Following the hint, regress the log rate on the age-group index by least squares, Figure 3.2 being

approximately linear in i (equally spaced indices being the group midpoints up to a linear rescaling).

```r
d$lograte <- log(d$deaths / d$population)
ols <- lm(lograte ~ i, data = d)
summary(ols)
```

```
Call:
lm(formula = lograte ~ i, data = d)

Residuals:
     Min       1Q   Median       3Q      Max
-0.59459 -0.28691  0.05263  0.34854  0.46029

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -9.85457    0.34698 -28.401 1.26e-07 ***
i            0.66547    0.06871   9.685 6.95e-05 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.4453 on 6 degrees of freedom
Multiple R-squared:  0.9399,        Adjusted R-squared:  0.9299
F-statistic:  93.8 on 1 and 6 DF,  p-value: 6.95e-05
```

The line explains 94% of the variation, with $\hat{\beta}_2 = 0.665$ multiplying the death rate by $e^{0.665} = 1.95$ per five-year band. But least squares assumes constant variance on the log-rate scale, whereas $\operatorname{var}[\log(y_i/n_i)] \approx 1/y_i$ ranges from 1 to 0.015 across the groups. The correct version keeps the offset and adds an intercept,

$$\log \mu_i = \log n_i + \beta_1 + \beta_2 i.$$

```r
m2 <- glm(deaths ~ i + offset(log(population)), family = stats::poisson, data = d)
summary(m2)
```

```
Call:
glm(formula = deaths ~ i + offset(log(population)), family = stats::poisson,
    data = d)

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -9.01688    0.26188  -34.43   <2e-16 ***
i            0.52219    0.03905   13.37   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for poisson family taken to be 1)

    Null deviance: 257.51  on 7  degrees of freedom
Residual deviance:  14.69  on 6  degrees of freedom
AIC: 54.376

Number of Fisher Scoring iterations: 4
```

The Poisson slope $\hat{\beta}_2 = 0.522$ (standard error 0.039) is smaller than the OLS 0.665 because the poorly determined early groups no longer dominate the weighting; the rate ratio per five-year band is $e^{0.522} = 1.69$, 95% interval $\exp(0.522 \pm 1.96 \times 0.039) = (1.56, 1.82)$.

Comparing observed and expected deaths group by group, as the hint asks:

```r
m3 <- glm(deaths ~ i + I(i^2) + offset(log(population)), family = stats::poisson, data = d)
data.frame(agegroup = d$agegroup, observed = d$deaths,
           exp.Ex353 = round(fitted(m1), 2),
           exp.OLS   = round(d$population * exp(predict(ols)), 2),
           exp.m2    = round(fitted(m2), 2),
           exp.m3    = round(fitted(m3), 2),
           pearson.m2 = round(residuals(m2, type = "pearson"), 2))
```

```
  agegroup observed exp.Ex353 exp.OLS exp.m2 exp.m3 pearson.m2
```

```
1    30–34        1   1167.00    1.81   3.63   1.01      -1.38
2    35–39        5     71.62    3.29   5.71   2.94      -0.30
3    40–44        5      4.57    6.21   9.33   7.61      -1.42
4    45–49       12      0.24    9.84  12.82  14.23      -0.23
5    50–54       25      0.01   15.78  17.81  23.09       1.70
6    55–59       38      0.00   27.45  26.86  34.91       2.15
7    60–64       54      0.00   59.28  50.25  56.23       0.53
8    65–69       65      0.00  107.00  78.59  64.99      -1.53
```

The Example 3.5.3 model predicts 1167 deaths in the youngest group, where one occurred, and essentially zero in the oldest, where 65 occurred. The OLS expectations are better but poor at the extremes (107 against 65 observed in the oldest group) and sum to 230.7 against 205 observed, whereas the Poisson fit with an intercept reproduces the total exactly, its intercept score equation forcing $\sum \hat{\mu}_i = \sum y_i$. That fit has deviance 14.69 on 6 degrees of freedom, $p = 0.023$, and Pearson residuals negative at both ends and positive in the middle – the signature of curvature in log(rate) against i, which a quadratic term removes.

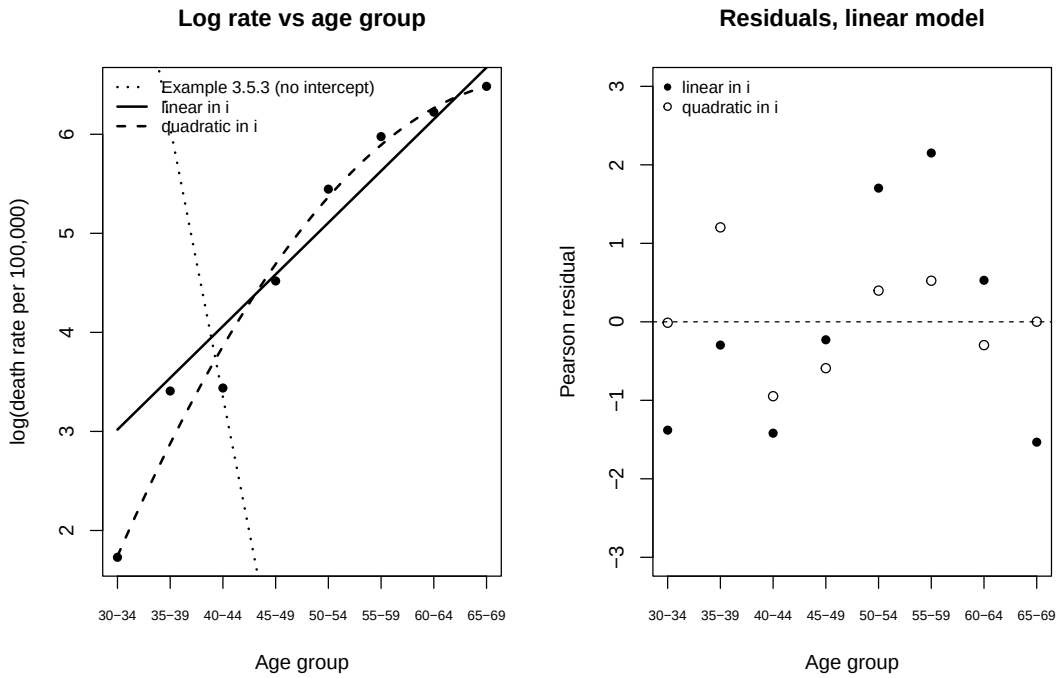
```r
anova(m2, m3, test = "Chisq")
```

```
Analysis of Deviance Table

Model 1: deaths ~ i + offset(log(population))
Model 2: deaths ~ i + I(i^2) + offset(log(population))
  Resid. Df Resid. Dev Df Deviance  Pr(>Chi)
1         6    14.6899
2         5     3.0938  1   11.596 0.0006609 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```r
gof <- function(m) c(deviance = deviance(m), df = df.residual(m),
                     p = pchisq(deviance(m), df.residual(m), lower.tail = FALSE),
                     AIC = AIC(m))
round(rbind(Ex353 = gof(m1), linear = gof(m2), quadratic = gof(m3)), 4)
```

```
           deviance df      p       AIC
Ex353     6990.4444  7 0.0000 7028.1303
linear      14.6899  6 0.0228   54.3758
quadratic    3.0938  5 0.6855   44.7797
```

```r
par(mfrow = c(1, 2))
plot(d$i, log(d$rate), pch = 16, xaxt = "n",
     xlab = "Age group", ylab = "log(death rate per 100,000)",
     main = "Log rate vs age group")
axis(1, at = d$i, labels = d$agegroup, cex.axis = 0.7)
g <- seq(1, 8, length = 100)
lines(g, coef(m1)[1] * g + log(1e5), lty = 3, lwd = 2)
lines(g, coef(m2)[1] + coef(m2)[2] * g + log(1e5), lty = 1, lwd = 2)
lines(g, coef(m3)[1] + coef(m3)[2] * g + coef(m3)[3] * g^2 + log(1e5), lty = 2, lwd = 2)
legend("topleft", c("Example 3.5.3 (no intercept)", "linear in i", "quadratic in i"),
       lty = c(3, 1, 2), lwd = 2, bty = "n", cex = 0.8)
plot(d$i, residuals(m2, type = "pearson"), pch = 16, xaxt = "n", ylim = c(-3, 3),
     xlab = "Age group", ylab = "Pearson residual", main = "Residuals, linear model")
axis(1, at = d$i, labels = d$agegroup, cex.axis = 0.7)
abline(h = 0, lty = 2); points(d$i, residuals(m3, type = "pearson"), pch = 1)
legend("topleft", c("linear in i", "quadratic in i"), pch = c(16, 1), bty = "n", cex = 0.8)
```



So the Example 3.5.3 model as written is inadequate – off by three orders of magnitude, with a slope of the wrong sign – though its exponential shape is right: with an intercept, $\log \mu_i = \log n_i + \beta_1 + \beta_2 i$ describes the data reasonably, the coronary death rate rising by about 1.69 per five-year band. The quadratic model, deviance 3.09 on 5 df ($p = 0.69$) and AIC lower by nearly 10, is preferred.

3.7 Problem 3.7 — Consider N independent binary random variables Y1 , . . . ,YN with

Problem 3.7. Consider N independent binary random variables $Y_1, \ldots, Y_N$ with

$$P(Y_i = 1) = \pi_i \quad \text{and} \quad P(Y_i = 0) = 1 - \pi_i.$$

The probability function of Y_i, the Bernoulli distribution $\mathrm{B}(\pi)$, can be written as

$$\pi_i^{y_i}(1 - \pi_i)^{1-y_i},$$

where $y_i = 0$ or 1.

a. Show that this probability function belongs to the exponential family of distributions.

b. Show that the natural parameter is

$$\log\left(\frac{\pi_i}{1 - \pi_i}\right).$$

This function, the logarithm of the odds $\pi_i/(1 - \pi_i)$, is called the logit function.

c. Show that $\mathrm{E}(Y_i) = \pi_i$.

d. If the link function is

$$g(\pi) = \log\left(\frac{\pi}{1 - \pi}\right) = \mathbf{x}^T\boldsymbol{\beta},$$

show that this is equivalent to modelling the probability π as

$$\pi = \frac{e^{\mathbf{x}^T\boldsymbol{\beta}}}{1 + e^{\mathbf{x}^T\boldsymbol{\beta}}}.$$

e. In the particular case where $\mathbf{x}^T\boldsymbol{\beta} = \beta_1 + \beta_2 x$, this gives

$$\pi = \frac{e^{\beta_1+\beta_2 x}}{1 + e^{\beta_1+\beta_2 x}},$$

which is the logistic function. Sketch the graph of π against x in this case, taking β_1 and β_2 as constants. How would you interpret this graph if x is the dose of an insecticide and π is the probability of an insect dying? (difficulty: ⋆⋆)

Solution. (a) Taking logarithms,

$$f(y_i;\pi_i) = \pi_i^{y_i}(1-\pi_i)^{1-y_i} = \exp\left[y_i \log\left(\frac{\pi_i}{1-\pi_i}\right) + \log(1-\pi_i)\right],$$

which is (3.3) with $a(y_i) = y_i$, $b(\pi_i) = \log[\pi_i/(1-\pi_i)]$, $c(\pi_i) = \log(1-\pi_i)$, $d(y_i) = 0$: the Bernoulli is in the exponential family, being the $n = 1$ case of Section 3.2.3.
(b) $a(y_i) = y_i$, so the form is canonical and the natural parameter is $b(\pi_i) = \log[\pi_i/(1-\pi_i)]$, the logit – whence the logit is the natural link for binary data, the linear predictor then being the natural parameter itself.
(c) $\mathrm{E}(Y_i) = 1\cdot\pi_i + 0\cdot(1-\pi_i) = \pi_i$; by (3.9), with $b'(\pi_i) = [\pi_i(1-\pi_i)]^{-1}$ and $c'(\pi_i) = -(1-\pi_i)^{-1}$,

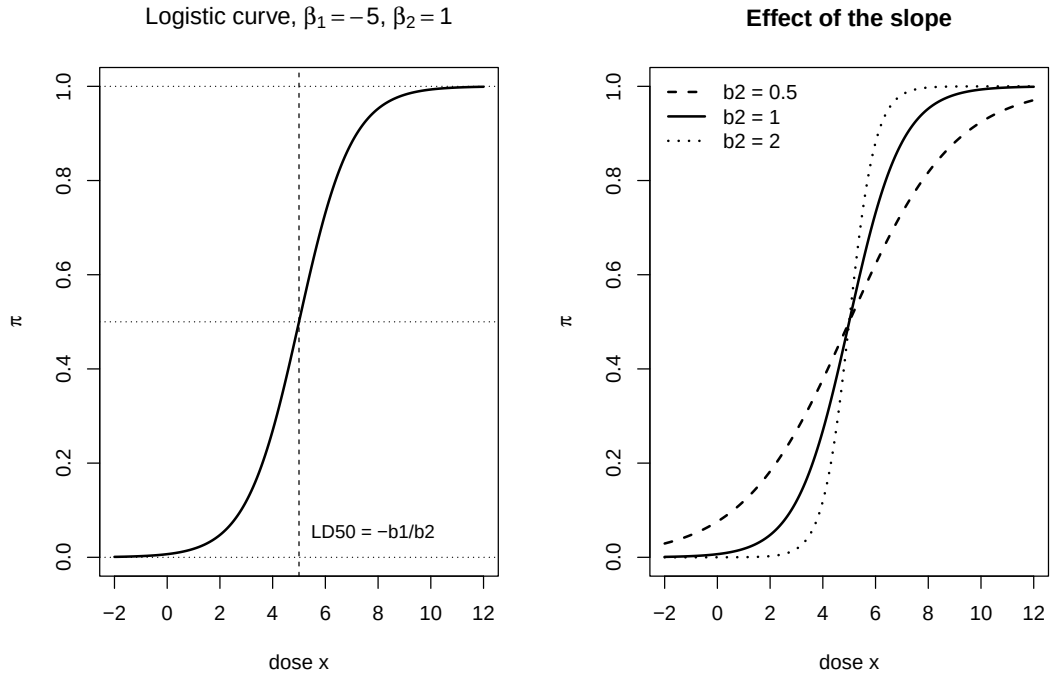
$$\mathrm{E}(Y_i) = -\frac{c'(\pi_i)}{b'(\pi_i)} = \frac{1/(1-\pi_i)}{1/[\pi_i(1-\pi_i)]} = \pi_i,$$

which is Exercise 3.4(c) with $n = 1$.
(d) Exponentiating $\log[\pi/(1-\pi)] = \mathbf{x}^T\boldsymbol{\beta}$ gives $\pi = (1-\pi)e^{\mathbf{x}^T\boldsymbol{\beta}}$, so

$$\pi = \frac{e^{\mathbf{x}^T\boldsymbol{\beta}}}{1+e^{\mathbf{x}^T\boldsymbol{\beta}}} = \frac{1}{1+e^{-\mathbf{x}^T\boldsymbol{\beta}}},$$

the logit being a strictly increasing bijection $(0,1) \to \mathbb{R}$ with this inverse; whatever real value $\mathbf{x}^T\boldsymbol{\beta}$ takes, π lies in $(0,1)$.
(e) The graph of $\pi(x) = e^{\beta_1+\beta_2 x}/(1+e^{\beta_1+\beta_2 x})$ is the sigmoid logistic curve. For $\beta_2 > 0$ it is strictly increasing, $d\pi/dx = \beta_2\pi(1-\pi) > 0$, with asymptotes $\pi \to 0$ and $\pi \to 1$, passing through $\pi = 1/2$ at $x = -\beta_1/\beta_2$, symmetric about that point, where the slope is steepest at $\beta_2/4$. For $\beta_2 < 0$ it decreases; $\beta_2 = 0$ gives the horizontal line $\pi = e^{\beta_1}/(1+e^{\beta_1})$; larger $|\beta_2|$ sharpens the transition.

```r
x <- seq(-2, 12, length = 400)
logistic <- function(x, b1, b2) exp(b1 + b2 * x) / (1 + exp(b1 + b2 * x))
par(mfrow = c(1, 2))
plot(x, logistic(x, -5, 1), type = "l", lwd = 2, ylim = c(0, 1),
     xlab = "dose x", ylab = expression(pi),
     main = expression(paste("Logistic curve, ", beta[1] == -5, ", ", beta[2] == 1)))
abline(h = c(0, 0.5, 1), lty = 3); abline(v = 5, lty = 2)
text(5, 0.05, "LD50 = -b1/b2", pos = 4, cex = 0.9)
plot(x, logistic(x, -5, 1), type = "l", lwd = 2, ylim = c(0, 1),
     xlab = "dose x", ylab = expression(pi), main = "Effect of the slope")
lines(x, logistic(x, -2.5, 0.5), lwd = 2, lty = 2)
lines(x, logistic(x, -10, 2), lwd = 2, lty = 3)
legend("topleft", c("b2 = 0.5", "b2 = 1", "b2 = 2"), lty = c(2, 1, 3), lwd = 2, bty = "n")
```



With x an insecticide dose and π the probability of death, this is the classical dose-response curve: almost no insects die at low doses and almost all at high ones, neither extreme reached exactly, with a steep rise over a narrow middle band beyond which extra dose buys little. The dose $x = -\beta_1/\beta_2$ at which $\pi = 1/2$ is the median lethal dose LD50, the standard measure of potency (5 in the left panel, with maximum slope $\beta_2/4 = 0.25$ per unit dose). The slope β_2 multiplies the odds of death by e^{β_2} per unit dose, constantly across the range, whereas the effect on the **probability** is largest near LD50.

3.8 Problem 3.8 — Is the extreme value (Gumbel) distribution, with probability density

Problem 3.8. Is the extreme value (Gumbel) distribution, with probability density function

$$f(y;\theta) = \frac{1}{\phi}\exp\left\{\frac{(y-\theta)}{\phi} - \exp\left[\frac{(y-\theta)}{\phi}\right]\right\}$$

(where $\phi > 0$ is regarded as a nuisance parameter) a member of the exponential family? (difficulty: ⋆⋆)

Solution. Yes, though not in canonical form. Taking logarithms with ϕ known,

$$\log f(y;\theta) = -\log\phi + \frac{y}{\phi} - \frac{\theta}{\phi} - e^{y/\phi}e^{-\theta/\phi},$$

whose last term is the only one mixing y and θ and already factorises, so (3.3) holds with

$$a(y) = e^{y/\phi}, \quad b(\theta) = -e^{-\theta/\phi}, \quad c(\theta) = -\frac{\theta}{\phi} - \log\phi, \quad d(y) = \frac{y}{\phi}.$$

The support is all of $\mathbb{R}$ and free of θ, as Section 3.3 requires; and ϕ must genuinely be known, since otherwise a and d depend on it and the family is two-parameter. Since $a(y) = e^{y/\phi} \neq y$ the form is not canonical – it is $e^{Y/\phi}$ that is canonical, the display showing $e^{(Y-\theta)/\phi} \sim \text{Exp}(1)$ – so (3.9) and (3.12) give the moments of $a(Y)$, not of Y. With $b' = \phi^{-1}e^{-\theta/\phi}$, $b'' = -\phi^{-2}e^{-\theta/\phi}$, $c' = -1/\phi$, $c'' = 0$,

$$\mathrm{E}\left(e^{Y/\phi}\right) = -\frac{c'}{b'} = \frac{1/\phi}{e^{-\theta/\phi}/\phi} = e^{\theta/\phi},$$

$$\operatorname{var}\left(e^{Y/\phi}\right) = \frac{b''c' - c''b'}{(b')^3} = \frac{\left(-\phi^{-2}e^{-\theta/\phi}\right)\left(-\phi^{-1}\right)}{\phi^{-3}e^{-3\theta/\phi}} = e^{2\theta/\phi}.$$

Confirmed by simulation, generating via $e^{(Y-\theta)/\phi} \sim \text{Exp}(1)$:

```
set.seed(7); theta <- 1.3; phi <- 0.7
u <- rexp(2e6)
y <- theta + phi * log(u)
a <- exp(y / phi)
round(c(mean.a = mean(a), theory.mean = exp(theta / phi),
        var.a = var(a),  theory.var = exp(2 * theta / phi)), 4)
```

```
mean.a theory.mean       var.a  theory.var
6.4100      6.4054     41.0751     41.0293
```

3.9 Problem 3.9 — Suppose Y1 , . . . ,YN are independent random variables each with the Pareto

Problem 3.9. Suppose $Y_1, \ldots, Y_N$ are independent random variables each with the Pareto distribution and

$$\text{E}(Y_i) = (\beta_0 + \beta_1 x_i)^2.$$

Is this a generalized linear model? Give reasons for your answer. (difficulty: ⋆⋆)

Solution. Yes, with link $g(\mu) = \mu^{1/2}$ and linear predictor $\beta_0 + \beta_1 x_i$, checking the three components of Section 3.4.
(i) **Distribution.** The Y_i are independent Pareto, which is in the exponential family with $a(y) = \log y$, $b(\theta_i) = -\theta_i$, $c(\theta_i) = \log\theta_i$, $d(y) = -\log y$ (Exercise 3.3(a)), each depending on one parameter. Strictly, Section 3.4 asks for the **canonical** form $\exp[y_i b(\theta_i) + c(\theta_i) + d(y_i)]$, which the Pareto misses since $a(y) = \log y$; but a is a fixed known transformation and $\log Y_i \sim \text{Exp}(\theta_i)$ is canonical, so the model is a generalized linear model for the transformed response.
(ii) **Linear component.** $\beta_0 + \beta_1 x_i = \mathbf{x}_i^T\boldsymbol{\beta}$ with $\mathbf{x}_i^T = [1 \quad x_i]$; linearity in $\boldsymbol{\beta}$, not in x_i, is what is required.
(iii) **Link.** $\mu_i = (\beta_0 + \beta_1 x_i)^2$ inverts to $g(\mu) = \mu^{1/2}$, strictly increasing and differentiable on $\mu > 0$.
Two restrictions on the parameter space follow. The square root inverts $\mu \mapsto \mu^2$ on one branch only, so (β_0, β_1) and $(-\beta_0, -\beta_1)$ give identical means and identifiability needs $\beta_0 + \beta_1 x_i > 0$ throughout. And $\text{E}(Y) = \theta/(\theta - 1) > 1$ for every admissible $\theta > 1$ (the mean not existing for $\theta \le 1$), so coherence needs $\beta_0 + \beta_1 x_i > 1$ at every observed x_i.

3.10 Problem 3.10 — Let Y1 , . . . ,YN be independent random variables with

Problem 3.10. Let $Y_1, \ldots, Y_N$ be independent random variables with

$$\text{E}(Y_i) = \mu_i = \beta_0 + \log(\beta_1 + \beta_2 x_i); \qquad Y_i \sim N(\mu, \sigma^2)$$

for all $i = 1, \ldots, N$. Is this a generalized linear model? Give reasons for your answer. (difficulty: ⋆)

Solution. No: it is a nonlinear regression model. The distribution is fine – independent Normals, canonical exponential family (Section 3.2.2) – but the systematic part is not $g(\mu_i) = \mathbf{x}_i^T\boldsymbol{\beta}$ for any link. Rearranging,

$$e^{\mu_i - \beta_0} = \beta_1 + \beta_2 x_i,$$

whose right side is linear in (β_1, β_2); so if β_0 were known this would be a generalized linear model with link $g(\mu) = e^{\mu - \beta_0}$. But β_0 must be estimated, and a link is a **fixed known** function of μ alone. Equivalently, β_0 enters outside the logarithm and β_1, β_2 inside it, so no g puts all three into one linear form. (The three are in any case unidentified without a constraint, since adding $\log k$ to

β_0 and dividing β_1, β_2 by k leaves μ_i unchanged; imposing $\beta_0 = 0$ does make it a generalized linear model with $g(\mu) = e^{\mu}$.) As written the model needs nonlinear least squares, and $\beta_1 + \beta_2 x_i > 0$ at every observation.

3.11 Problem 3.11 — For the Pareto distribution, find the score statistics U and the information

Problem 3.11. For the Pareto distribution, find the score statistics U and the information $\mathfrak{I} = \text{var}(U)$. Verify that $\text{E}(U) = 0$. (difficulty: ⋆⋆)

Solution. $U = 1/\theta - \log Y$ and $\mathfrak{I} = 1/\theta^2$. From Exercise 3.3(a) the Pareto has $a(y) = \log y$, $b(\theta) = -\theta$, $c(\theta) = \log\theta$, $d(y) = -\log y$, so $l(\theta; y) = -\theta \log y + \log\theta - \log y$ and, by (3.13) with $b' = -1$, $c' = 1/\theta$,

$$U = \frac{dl}{d\theta} = \frac{1}{\theta} - \log Y.$$

By (3.9), $\text{E}(\log Y) = -c'/b' = 1/\theta$ (directly, $\log Y \sim \text{Exp}(\theta)$), so $\text{E}(U) = 1/\theta - 1/\theta = 0$, the general result (3.14). For the information, Section 3.3 gives $\mathfrak{I} = (b')^2 \text{var}[a(Y)] = \text{var}(\log Y) = 1/\theta^2$, the same as (3.15) with $b'' = 0$ and $c'' = -1/\theta^2$,

$$\text{var}(U) = \frac{b''(\theta)c'(\theta)}{b'(\theta)} - c''(\theta) = 0 + \frac{1}{\theta^2},$$

and as (3.16), $U' = -1/\theta^2$ being non-random. For N independent observations the log-likelihoods add, so $U = N/\theta - \sum_i \log Y_i$ and $\mathfrak{I} = N/\theta^2$, giving $\hat\theta = N/\sum \log Y_i$ with asymptotic standard error $\theta/\sqrt{N}$. Simulation for a single observation:

```
set.seed(11); theta <- 2.5
y <- exp(rexp(2e6, rate = theta))
U <- 1 / theta - log(y)
round(c(mean.U = mean(U), theory = 0,
        var.U = var(U), information = 1 / theta^2,
        mean.logY = mean(log(y)), theory.logY = 1 / theta), 5)
```

```
  mean.U      theory       var.U information   mean.logY theory.logY
-0.0002      0.0000      0.1603      0.1600      0.4002      0.4000
```

3.12 Problem 3.12 — See some more relationships between distributions in Figure 3.3.

Problem 3.12. See some more relationships between distributions in Figure 3.3.
Figure 3.3 shows eight boxes joined by arrows, dotted lines indicating an asymptotic relationship and solid lines a transformation. Reading the figure edge by edge: Binomial $\text{Bin}(n, \pi)$ and Bernoulli $\text{B}(\pi)$ are joined by a solid double-headed arrow, labelled $n = 1$ in the direction Binomial to Bernoulli and $X_1 + \cdots + X_n$ in the direction Bernoulli to Binomial; a dotted arrow runs from Binomial to Poisson $\text{Po}(\mu)$ labelled $\mu = n\pi$, $n \to \infty$; a dotted arrow runs from Negative Binomial $\text{NBin}(r, \theta)$ to Poisson labelled $\mu = r(1-\theta)$, $r \to \infty$; a dotted arrow runs from Poisson to Normal $N(\mu, \sigma^2)$ labelled $\sigma^2 = \mu$, $\mu > 15$; a dotted arrow runs from Binomial to Normal labelled $\mu = n\pi$, $\sigma^2 = n\pi(1-\pi)$, $n\pi > 5$, $n\pi(1-\pi) > 5$; a dotted arrow runs from Gamma $G(\alpha, \beta)$ to Normal labelled $\mu = \alpha/\beta$, $\sigma^2 = \alpha/\beta^2$, $\alpha \to \infty$; a solid arrow runs from Gamma to Exponential $\text{Exp}(\theta)$ labelled $\alpha = \theta$, $\beta = 1$; and a solid arrow runs from Standard Uniform $U(0, 1)$ to Exponential labelled $-\theta \log X$. The Negative Binomial box is joined only to the Poisson box; there is no edge from it to the Normal.
a. Show that the Exponential distribution $\text{Exp}(\theta)$ is a special case of the Gamma distribution $G(\alpha, \beta)$.
b. If X has the Uniform distribution $U[0, 1]$, that is, $f(x) = 1$ for $0 < x < 1$, show that $Y = -\theta \log X$ has the distribution $\text{Exp}(\theta)$.
c. Use the moment generating functions (or other methods) to show

i. $\mathrm{Bin}(n,\pi) \to \mathrm{Po}(\lambda)$ as $n \to \infty$.
ii. $\mathrm{NBin}(r,\theta) \to \mathrm{Po}(r(1-\theta))$ as $r \to \infty$.
d. Use the Central Limit Theorem to show
i. $\mathrm{Po}(\lambda) \to N(\mu,\mu)$ for large μ.
ii. $\mathrm{Bin}(n,\pi) \to N(n\pi, n\pi(1-\pi))$ for large n, provided neither $n\pi$ nor $n\pi(1-\pi)$ is too small.
iii. $G(\alpha,\beta) \to N(\alpha/\beta, \alpha/\beta^2)$ for large α. (difficulty: ⋆⋆⋆)

Solution. (a) $\mathrm{Exp}(\theta) = G(1,\theta)$: putting $\alpha = 1$, $\beta = \theta$ in the Gamma density of Exercise 3.2, with $\Gamma(1) = 1$,

$$f(y;1,\theta) = \frac{\theta^1}{\Gamma(1)} y^0 e^{-y\theta} = \theta e^{-y\theta},$$

the exponential density of Exercise 3.3(b); the moments agree, $\alpha/\beta = 1/\theta$ and $\alpha/\beta^2 = 1/\theta^2$. (Figure 3.3's label $\alpha = \theta$, $\beta = 1$ interchanges the substitutions: $G(\theta,1)$ is exponential only at $\theta = 1$.)
(b) For $X \sim U[0,1]$ and $Y = -\theta \log X$, we have $Y > 0$ and, for $y > 0$,

$$P(Y > y) = P\left(X < e^{-y/\theta}\right) = e^{-y/\theta},$$

since $P(X < x) = x$ on $(0,1)$; differentiating, $f_Y(y) = \theta^{-1} e^{-y/\theta}$, exponential with **mean** θ. Under the book's rate parametrisation $f(y;\theta) = \theta e^{-y\theta}$ the printed statement reads $-\theta \log X \sim \mathrm{Exp}(1/\theta)$; the transformation giving $\mathrm{Exp}(\theta)$ exactly is $Y = -\theta^{-1} \log X$.
(c)(i) For $Y \sim \mathrm{Bin}(n,\pi)$, $M_Y(t) = (1 - \pi + \pi e^t)^n$, so with $\lambda = n\pi$ fixed and $n \to \infty$,

$$M_Y(t) = \left[1 + \frac{\lambda(e^t - 1)}{n}\right]^n \longrightarrow \exp\left[\lambda\left(e^t - 1\right)\right],$$

which is the moment generating function of $\mathrm{Po}(\lambda)$; the continuity theorem gives $\mathrm{Bin}(n, \lambda/n) \to \mathrm{Po}(\lambda)$.
(ii) For $Y \sim \mathrm{NBin}(r,\theta)$, the negative binomial series $\sum_y \binom{y+r-1}{r-1} u^y = (1-u)^{-r}$ gives $M_Y(t) = [\theta/(1 - (1-\theta)e^t)]^r$ for $(1-\theta)e^t < 1$, so with $\lambda = r(1-\theta)$ fixed and $r \to \infty$,

$$\begin{aligned} \log M_Y(t) &= r\left[\log\left(1 - \frac{\lambda}{r}\right) - \log\left(1 - \frac{\lambda e^t}{r}\right)\right] \\ &= r\left[-\frac{\lambda}{r} + \frac{\lambda e^t}{r} + O(r^{-2})\right] \longrightarrow \lambda(e^t - 1), \end{aligned}$$

so $\mathrm{NBin}(r,\theta) \to \mathrm{Po}(r(1-\theta))$ – consistent with Exercise 3.5, where $\mathrm{var}(Y)/\mathrm{E}(Y) = 1/\theta \to 1$ as $\theta \to 1$. Both limits checked by the largest absolute discrepancy between probability functions, $\lambda = 3$:

```
lam <- 3
k <- 0:30
bin.err <- sapply(c(10, 50, 200, 5000),
                  function(n) max(abs(dbinom(k, n, lam / n) - dpois(k, lam))))
nb.err  <- sapply(c(5, 25, 100, 2000),
                  function(r) max(abs(dnbinom(k, size = r, prob = 1 - lam / r) - dpois(k,
                  ↪  lam))))
out <- rbind(Bin.to.Po = bin.err, NBin.to.Po = nb.err)
colnames(out) <- c("n or r = 10/5", "50/25", "200/100", "5000/2000")
signif(out, 3)
```

```
           n or r = 10/5   50/25 200/100 5000/2000
Bin.to.Po         0.0428 0.00702 0.00170  6.72e-05
NBin.to.Po        0.1690 0.03250 0.00792  3.92e-04
```

(d) Each family is closed under convolution, so each distribution is a sum of independent identically distributed pieces and the Central Limit Theorem applies.
(i) **Poisson.** For integer μ, $Y \sim \mathrm{Po}(\mu)$ is the sum of μ independent $\mathrm{Po}(1)$ variables, each of mean and variance 1 (Exercise 3.4(a)), so Y is asymptotically $N(\mu,\mu)$; for non-integer μ, write Y as a sum of n independent $\mathrm{Po}(\mu/n)$ variables. Figure 3.3's rule of thumb is $\mu > 15$.

(ii) **Binomial.** $Y \sim \text{Bin}(n, \pi)$ is a sum of n independent Bernoulli variables with mean π and variance $\pi(1-\pi)$ (Exercise 3.7), so Y is asymptotically $N(n\pi, n\pi(1-\pi))$. The summands are skew unless $\pi = 1/2$, the standardised skewness of Y being $(1-2\pi)/\sqrt{n\pi(1-\pi)}$, small only when $n\pi(1-\pi)$ is large; for very small π the boundary at 0 truncates the Normal shape and the Poisson limit of (c)(i) applies instead. Hence $n\pi > 5$ and $n\pi(1-\pi) > 5$.
(iii) **Gamma.** For integer α, $Y \sim G(\alpha, \beta)$ is a sum of α independent $\text{Exp}(\beta)$ variables by (a), each of mean $1/\beta$ and variance $1/\beta^2$, so Y is asymptotically $N(\alpha/\beta, \alpha/\beta^2)$, matching Exercise 3.2; for real $\alpha > 0$ use $G(\alpha, \beta) = \sum_{j=1}^{n} G(\alpha/n, \beta)$ independently.
Checked by the largest absolute difference between exact and Normal distribution functions, with a continuity correction in the discrete cases:

```r
cc <- function(q, m, v) pnorm(q + 0.5, m, sqrt(v))
po <- sapply(c(5, 20, 100), function(mu) { k <- 0:ceiling(mu + 10 * sqrt(mu))
                max(abs(ppois(k, mu) - cc(k, mu, mu))) })
bi <- sapply(c(10, 50, 500), function(n) { k <- 0:n
                max(abs(pbinom(k, n, 0.3) - cc(k, n * 0.3, n * 0.3 * 0.7))) })
ga <- sapply(c(2, 10, 100), function(a) { q <- seq(0, a + 10 * sqrt(a), length = 2000)
                max(abs(pgamma(q, shape = a, rate = 1) - pnorm(q, a, sqrt(a)))) })
out <- rbind(Po.mu = po, Bin.n = bi, Gamma.alpha = ga)
colnames(out) <- c("small", "medium", "large")
round(out, 4)
```

```
             small medium  large
Po.mu       0.0290 0.0148 0.0066
Bin.n       0.0177 0.0081 0.0026
Gamma.alpha 0.0945 0.0421 0.0133
```

The parameters are $\mu = 5, 20, 100$; $n = 10, 50, 500$ with $\pi = 0.3$; and $\alpha = 2, 10, 100$ with $\beta = 1$. Every row falls roughly as the square root of the parameter, the Berry-Esseen rate, with maximum error at or below about 1.5% by $\mu = 20$, $n = 50$, $\alpha = 100$ – which is where Figure 3.3's rules of thumb sit.

4 Estimation

Contents

4.1 Problem 4.1 — The data in Table 4.5 show the numbers of cases of AIDS in Australia

Problem 4.1. The data in Table 4.5 show the numbers of cases of AIDS in Australia by date of diagnosis for successive 3-month periods from 1984 to 1988. (Data from National Centre for HIV Epidemiology and Clinical Research, 1994.)
Table 4.5 gives, for each year 1984–1988, the number of cases in quarters 1, 2, 3 and 4 respectively: 1984: 1, 6, 16, 23; 1985: 27, 39, 31, 30; 1986: 43, 51, 63, 70; 1987: 88, 97, 91, 104; 1988: 110, 113, 149, 159. Reading across rows gives the $N = 20$ successive quarterly counts $y_1, \ldots, y_{20}$.
In this early phase of the epidemic, the numbers of cases seemed to be increasing exponentially.

(a) Plot the number of cases y_i against time period i $(i = 1, \ldots, 20)$.

(b) A possible model is the Poisson distribution with parameter $\lambda_i = i^\theta$, or equivalently

$$\log \lambda_i = \theta \log i.$$

Plot $\log y_i$ against $\log i$ to examine this model.

(c) Fit a generalized linear model to these data using the Poisson distribution, the log-link function and the equation

$$g(\lambda_i) = \log \lambda_i = \beta_1 + \beta_2 x_i,$$

where $x_i = \log i$. Firstly, do this from first principles, working out expressions for the weight matrix $\mathbf{W}$ and other terms needed for the iterative equation

$$\mathbf{X}^T\mathbf{W}\mathbf{X}\mathbf{b}^{(m)} = \mathbf{X}^T\mathbf{W}\mathbf{z}$$

and using software which can perform matrix operations to carry out the calculations.

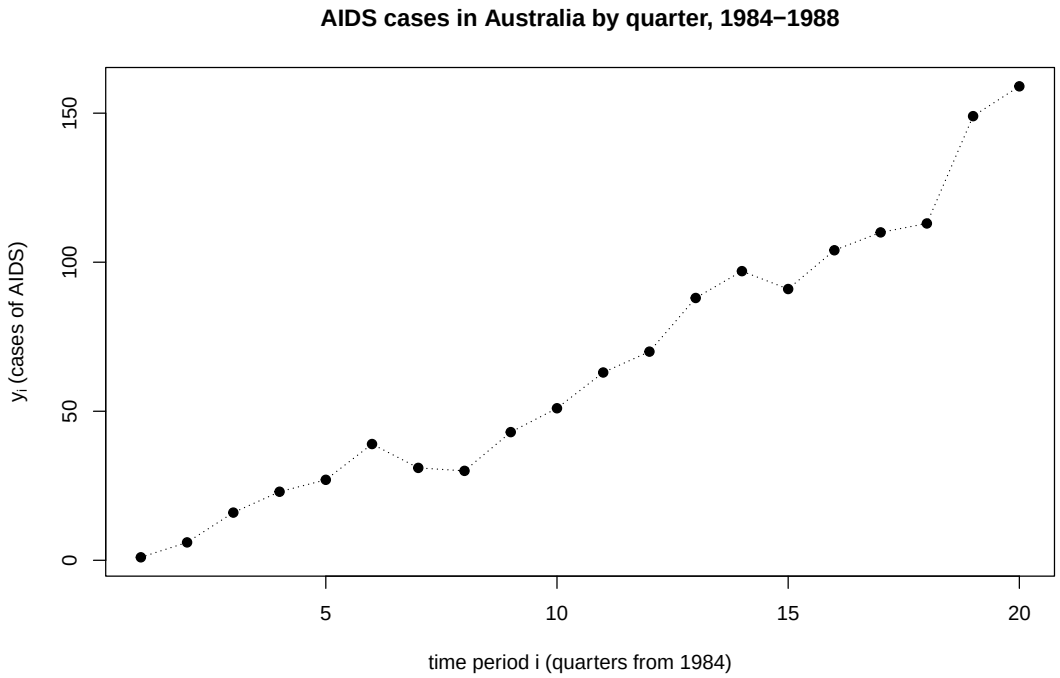
(d) Fit the model described in (c) using statistical software which can perform Poisson regression. Compare the results with those obtained in (c).

(difficulty: ⋆⋆)

Solution. The fitted model is $\widehat{\lambda}_i = e^{0.996} i^{1.327}$, obtained identically by hand-coded iterative weighted least squares and by `glm`.

(a) **The raw series.**

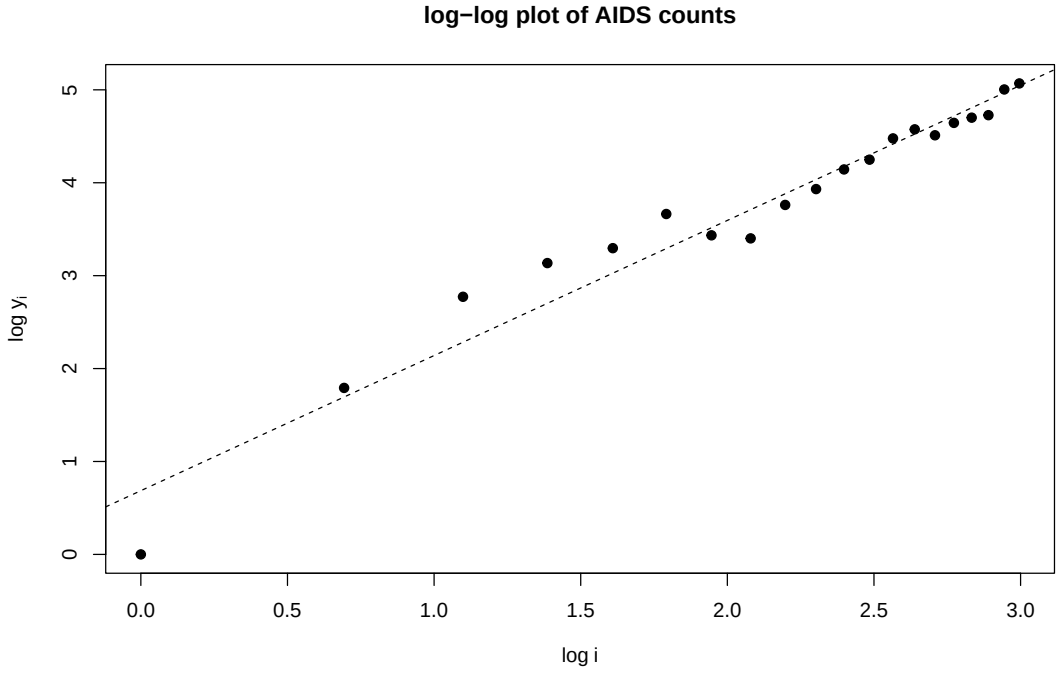
```
library(dobson)
data(aids)
y <- aids$cases
i <- seq_along(y)
plot(i, y, pch = 19, xlab = "time period i (quarters from 1984)",
     ylab = expression(y[i]~"(cases of AIDS)"),
     main = "AIDS cases in Australia by quarter, 1984–1988")
lines(i, y, lty = 3)
```



The counts rise monotonically apart from wobbles at $i = 7, 8$ and $i = 15$, and not linearly: the increment per quarter is about 5 cases early and 15 at the end. The scatter widens with the level, the mean-variance behaviour $\text{var}(Y_i) = \text{E}(Y_i)$ that motivates the Poisson model.

(b) **The log-log plot.** Under $\lambda_i = i^\theta$, $\log \lambda_i = \theta \log i$, so $\log y_i$ against $\log i$ should be a straight line through the origin with slope θ.

```
plot(log(i), log(y), pch = 19, xlab = expression(log~i),
     ylab = expression(log~y[i]), main = "log-log plot of AIDS counts")
abline(lm(log(y) ~ log(i)), lty = 2)
```



The points lie close to a line, so the power law is a reasonable description; least squares through the log-log points gives slope 1.454 and intercept 0.686. The intercept is not zero, which is why (c) generalises to $\log \lambda_i = \beta_1 + \beta_2 x_i$, $x_i = \log i$, of which $\lambda_i = i^\theta$ is the case $\beta_1 = 0$.

(c) **Iterative weighted least squares from first principles.** With $Y_i \sim \text{Po}(\mu_i)$ independent and

$\eta_i = \log \mu_i = \mathbf{x}_i^T \boldsymbol{\beta}$,

$$\mu_i = e^{\eta_i}, \qquad \frac{\partial \mu_i}{\partial \eta_i} = e^{\eta_i} = \mu_i, \qquad \operatorname{var}(Y_i) = \mu_i.$$

From equation (4.23) the diagonal weights are

$$w_{ii} = \frac{1}{\operatorname{var}(Y_i)} \left(\frac{\partial \mu_i}{\partial \eta_i} \right)^2 = \frac{\mu_i^2}{\mu_i} = \mu_i,$$

so $\mathbf{W} = \operatorname{diag}(\mu_1, \ldots, \mu_N)$, the weights reducing to the variance function because the log link is canonical for the Poisson. From equation (4.24) the working response is

$$z_i = \sum_{k=1}^{p} x_{ik} b_k^{(m-1)} + (y_i - \mu_i) \frac{\partial \eta_i}{\partial \mu_i} = \eta_i + \frac{y_i - \mu_i}{\mu_i},$$

with η_i, μ_i at $\mathbf{b}^{(m-1)}$. With $\mathbf{X}$ having rows $(1, \log i)$, the information matrix $\mathfrak{I} = \mathbf{X}^T \mathbf{W} \mathbf{X}$ has entries

$$\mathfrak{I} = \begin{bmatrix} \sum_i \mu_i & \sum_i \mu_i x_i \\ \sum_i \mu_i x_i & \sum_i \mu_i x_i^2 \end{bmatrix}, \qquad \mathbf{X}^T \mathbf{W} \mathbf{z} = \begin{bmatrix} \sum_i [\mu_i \eta_i + (y_i - \mu_i)] \\ \sum_i x_i [\mu_i \eta_i + (y_i - \mu_i)] \end{bmatrix}.$$

Solving $\mathbf{X}^T \mathbf{W} \mathbf{X} \mathbf{b}^{(m)} = \mathbf{X}^T \mathbf{W} \mathbf{z}$ repeatedly, from the log-log fit of (b):

```
x <- log(i)
X <- cbind(1, x)
b <- c(0.5, 1.5)                          # rough start suggested by the log-log plot
for (m in 1:6) {
  eta <- X %*% b
  mu  <- exp(eta)                         # inverse log link
  W   <- diag(as.vector(mu))              # w_ii = (dmu/deta)^2 / var(Y) = mu_i
  z   <- eta + (y - mu)/mu                # z_i = eta_i + (y_i - mu_i) deta/dmu
  b   <- solve(t(X) %*% W %*% X, t(X) %*% W %*% z)
  cat(sprintf("m = %d   b1 = %.6f   b2 = %.6f\n", m, b[1], b[2]))
}
```

```
m = 1   b1 = 1.054285   b2 = 1.305697
m = 2   b1 = 0.996735   b2 = 1.326344
m = 3   b1 = 0.995998   b2 = 1.326610
m = 4   b1 = 0.995998   b2 = 1.326610
m = 5   b1 = 0.995998   b2 = 1.326610
m = 6   b1 = 0.995998   b2 = 1.326610
```

Convergence is complete after three iterations, as in Table 4.4, giving $\widehat{\beta}_1 = 0.99600$ and $\widehat{\beta}_2 = 1.32661$. The inverse information matrix at the estimates gives the standard errors, by (4.12) in vector form:

```
I <- t(X) %*% diag(as.vector(exp(X %*% b))) %*% X
I
solve(I)
sqrt(diag(solve(I)))
```

```
                  x
  1311.000 3396.379
x 3396.379 9038.301
                         x
   0.02880067 -0.01082261
x -0.01082261  0.00417752
                    x
0.16970761 0.06463374
```

(d) **The same model via Poisson regression software.**

```
aids$i <- seq_len(nrow(aids))
res.p <- glm(cases ~ log(i), family = poisson(link = "log"), data = aids)
summary(res.p)
```

```
Call:
glm(formula = cases ~ log(i), family = poisson(link = "log"),
    data = aids)
```

```
Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept)  0.99600    0.16971   5.869 4.39e-09 ***
log(i)       1.32661    0.06463  20.525  < 2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for poisson family taken to be 1)

    Null deviance: 677.264  on 19  degrees of freedom
Residual deviance:  21.755  on 18  degrees of freedom
AIC: 138.05

Number of Fisher Scoring iterations: 4
```

(The explicit `poisson(link = "log")` is needed because after `library(dobson)` the bare name `poisson` is the package's Table 4.3 data set.)

Estimates and standard errors agree with (c) to every printed digit, $b_1 = 0.99600\,(0.16971)$ and $b_2 = 1.32661\,(0.06463)$, since `glm` runs the algorithm of (4.25) and Fisher scoring coincides with Newton-Raphson for the canonical link.

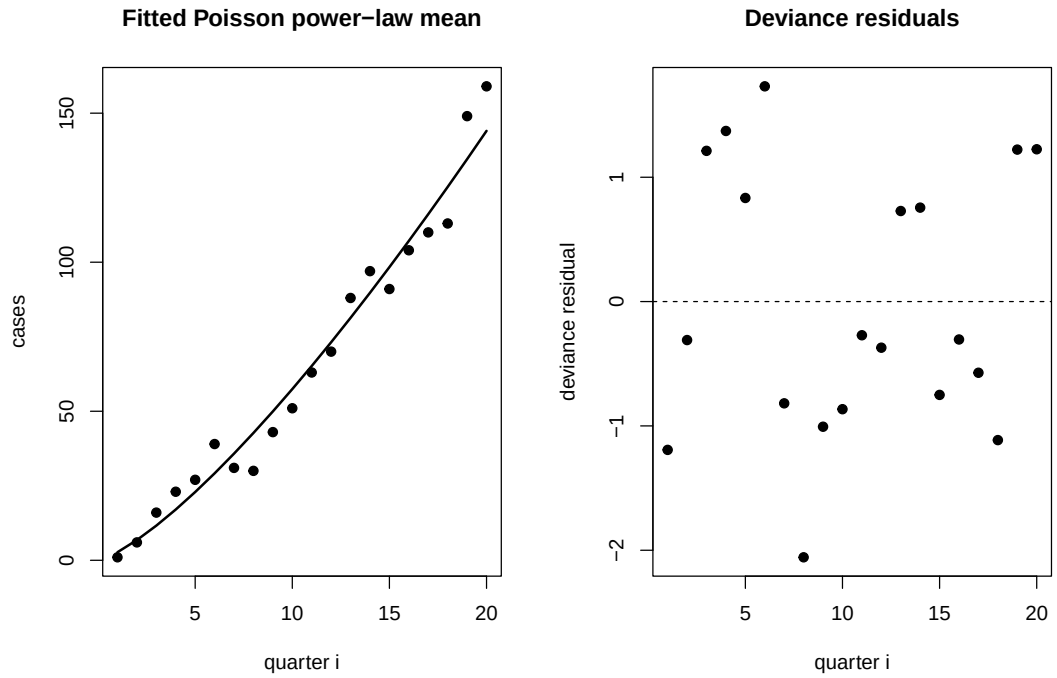
The fitted mean $\widehat{\lambda}_i = 2.71\, i^{1.327}$ grows as a power of time with exponent about 1.33, not exponentially in i; the approximate 95% interval $1.3266 \pm 1.96 \times 0.0646 = (1.200, 1.453)$ excludes 1, so growth is faster than linear but far short of doubling behaviour, and the one-parameter model $\beta_1 = 0$ of (b) is rejected ($z = 5.87$). The residual deviance 21.755 on 18 degrees of freedom gives $p = 0.243$: no evidence of lack of fit or overdispersion. Against the literal exponential-growth model $\log \lambda_i = \beta_1 + \beta_2 i$:

```r
m.pow <- glm(cases ~ log(i), family = poisson(link = "log"), data = aids)
m.exp <- glm(cases ~ i,      family = poisson(link = "log"), data = aids)
c(power.dev = deviance(m.pow), power.AIC = AIC(m.pow),
  exp.dev = deviance(m.exp), exp.AIC = AIC(m.exp))
```

```
power.dev power.AIC   exp.dev   exp.AIC
 21.75511 138.05303  53.02000 169.31792
```

The power-law model is far better: deviance 21.8 against 53.0 on the same 18 degrees of freedom, the exponential model having $p = 2.6 \times 10^{-5}$ for lack of fit and AIC 31 units worse. The epidemic was already decelerating on the log scale by 1988.

```r
par(mfrow = c(1, 2))
plot(aids$i, aids$cases, pch = 19, xlab = "quarter i", ylab = "cases",
     main = "Fitted Poisson power-law mean")
lines(aids$i, fitted(m.pow), lwd = 2)
plot(aids$i, residuals(m.pow, type = "deviance"), pch = 19,
     xlab = "quarter i", ylab = "deviance residual", main = "Deviance residuals")
abline(h = 0, lty = 2)
```



The fitted curve tracks the counts closely and the deviance residuals show no trend or funnelling, running from -2.06 (at $i = 8$, where the series briefly flattens) to 1.73. The model is adequate.

4.2 Problem 4.2 — The data in Table 4.6 are times to death, yi , in weeks from diagnosis and

Problem 4.2. The data in Table 4.6 are times to death, y_i, in weeks from diagnosis and $\log_{10}$ (initial white blood cell count), x_i, for seventeen patients suffering from leukemia. (This is Example U from Cox and Snell, 1981.)
Table 4.6 lists the seventeen pairs (y_i, x_i) as: $(65, 3.36)$, $(156, 2.88)$, $(100, 3.63)$, $(134, 3.41)$, $(16, 3.78)$, $(108, 4.02)$, $(121, 4.00)$, $(4, 4.23)$, $(39, 3.73)$, $(143, 3.85)$, $(56, 3.97)$, $(26, 4.51)$, $(22, 4.54)$, $(1, 5.00)$, $(1, 5.00)$, $(5, 4.72)$, $(65, 5.00)$.

(a) Plot y_i against x_i. Do the data show any trend?

(b) A possible specification for $\mathrm{E}(Y)$ is

$$\mathrm{E}(Y_i) = \exp(\beta_1 + \beta_2 x_i),$$

which will ensure that $\mathrm{E}(Y)$ is non-negative for all values of the parameters and all values of x. Which link function is appropriate in this case?

(c) The Exponential distribution is often used to describe survival times. The probability distribution is $f(y;\theta) = \theta e^{-y\theta}$. This is a special case of the Gamma distribution with shape parameter $\phi = 1$ (see Exercise 3.12(a)). Show that $\mathrm{E}(Y) = 1/\theta$ and $\mathrm{var}(Y) = 1/\theta^2$.

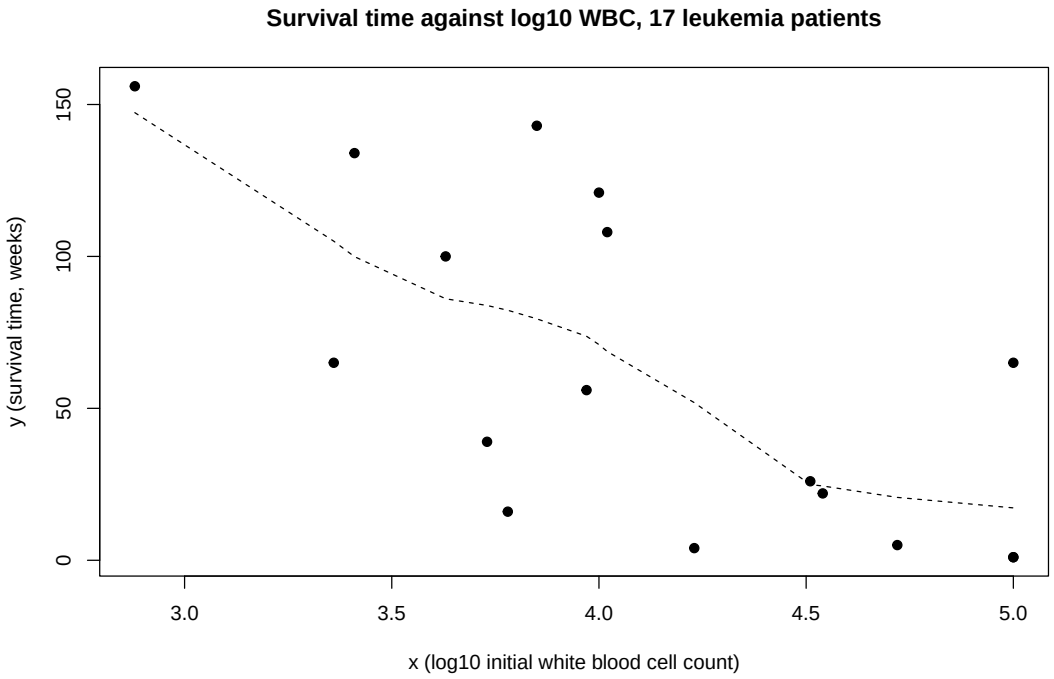
(d) Fit a model with the equation for $\mathrm{E}(Y_i)$ given in (b) and the Exponential distribution using appropriate statistical software.

(e) For the model fitted in (d), compare the observed values y_i and fitted values $\widehat{y}_i = \exp(\widehat{\beta}_1 + \widehat{\beta}_2 x_i)$, and use the standardized residuals $r_i = (y_i - \widehat{y}_i)/\widehat{y}_i$ to investigate the adequacy of the model. (Note: $\widehat{y}_i$ is used as the denominator of r_i because it is an estimate of the standard deviation of Y_i — see (c) above.)

(difficulty: ⋆⋆)

Solution. The fitted exponential model is $\widehat{y}_i = \exp(8.478 - 1.109 x_i)$, which is adequate. Each y_i is a leukemia patient's time to death in weeks; the x_i are $\log_{10}$ initial white blood cell counts.
(a) **Scatter plot.**

```r
library(dobson)
data(leukemia)
x <- leukemia$wbc
y <- leukemia$time
plot(x, y, pch = 19, xlab = "x (log10 initial white blood cell count)",
     ylab = "y (survival time, weeks)",
     main = "Survival time against log10 WBC, 17 leukemia patients")
lines(lowess(x, y), lty = 2)
```




```r
length(x)  # 17 patients
```

```
[1] 17
```

The trend is clearly negative: survival falls as the initial white cell count rises. The spread of y also shrinks with x – at $x \approx 3$ survival ranges from 16 to 156 weeks, while at $x = 5$ the three patients survived 1, 1 and 65 weeks – so variability scales with level, ruling out constant-variance least squares; and the decline is curved, consistent with a multiplicative effect of x.

(b) The log link, $g(\mu) = \log \mu$, since

$$\mathrm{E}(Y_i) = \exp(\beta_1 + \beta_2 x_i) \iff \log \mathrm{E}(Y_i) = \beta_1 + \beta_2 x_i,$$

which is the form $g(\mu_i) = \mathbf{x}_i^T \boldsymbol{\beta}$ of equation (4.16). It keeps $\mathrm{E}(Y) > 0$ for every β and x, accommodates the mean-dependent variance, and makes a unit increase in x_i multiply $\mathrm{E}(Y)$ by e^{β_2}; the trend in (a) implies $\beta_2 < 0$.

(c) For $f(y;\theta) = \theta e^{-y\theta}$, $y > 0$, integrating by parts with $u = y$,

$$\mathrm{E}(Y) = \left[-ye^{-y\theta}\right]_0^\infty + \int_0^\infty e^{-y\theta}\,\mathrm{d}y = 0 + \left[-\theta^{-1}e^{-y\theta}\right]_0^\infty = \frac{1}{\theta},$$

while the Gamma integral $\int_0^\infty y^n e^{-y\theta}\,\mathrm{d}y = n!/\theta^{n+1}$ gives $\mathrm{E}(Y^2) = \theta \cdot 2!/\theta^3 = 2/\theta^2$, so

$$\mathrm{var}(Y) = \frac{2}{\theta^2} - \frac{1}{\theta^2} = \frac{1}{\theta^2} = [\mathrm{E}(Y)]^2,$$

the Gamma variance $\phi[\mathrm{E}(Y)]^2$ with $\phi = 1$: the standard deviation equals the mean, which (e) exploits.

(d) **Fitting the model.**

```r
fit <- glm(y ~ x, family = Gamma(link = "log"), data = data.frame(x, y))
summary(fit)
```

```
Call:
glm(formula = y ~ x, family = Gamma(link = "log"), data = data.frame(x,
    y))

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   8.4775     1.6034   5.287 9.13e-05 ***
x            -1.1093     0.3872  -2.865   0.0118 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for Gamma family taken to be 0.9388638)

    Null deviance: 26.282  on 16  degrees of freedom
Residual deviance: 19.457  on 15  degrees of freedom
AIC: 173.97

Number of Fisher Scoring iterations: 8
```

`Gamma(link = "log")` is used because the exponential is the Gamma with $\phi = 1$. The estimates of $\boldsymbol{\beta}$ are the exponential-model ones, ϕ cancelling from the score equations (4.18) as a constant multiplier of $\mathrm{var}(Y_i)$; only the standard errors are affected, and `glm` estimates ϕ by default. Imposing $\phi = 1$:

```r
summary(fit, dispersion = 1)$coefficients
```

```
             Estimate Std. Error   z value     Pr(>|z|)
(Intercept)  8.477494  1.6548077  5.122948 3.007955e-07
x           -1.109297  0.3996545 -2.775640 5.509317e-03
```

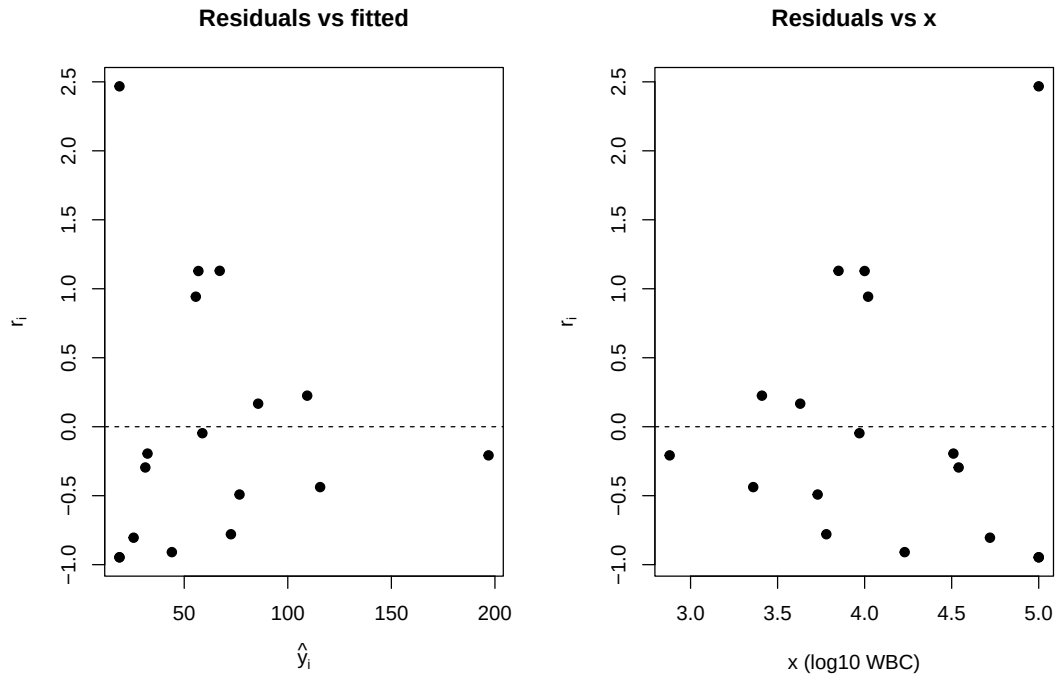
The standard errors change little (1.603 to 1.655, 0.387 to 0.400) because $\widehat{\phi} = 0.939$ is already near 1. Here $\widehat{\beta}_2 = -1.109$, so a tenfold increase in white cell count multiplies expected survival by $e^{-1.109} = 0.33$; the 95% interval $-1.109 \pm 1.96 \times 0.400 = (-1.893, -0.326)$ gives a factor between 0.15 and 0.72, the direction clear but the size imprecise with 17 patients. Fitted mean survival runs from 197 weeks at $x = 2.88$ to 19 weeks at $x = 5.00$.

(e) By (c), $\mathrm{sd}(Y_i) = \mathrm{E}(Y_i)$ under the exponential model, so dividing by $\widehat{y}_i$ divides by the estimated standard deviation and

$$r_i = \frac{y_i - \widehat{y}_i}{\widehat{y}_i}, \qquad \widehat{y}_i = \exp(\widehat{\beta}_1 + \widehat{\beta}_2 x_i)$$

is genuinely standardized – these are the Pearson residuals for the Gamma family.

```r
b1 <- coef(fit)[1]
b2 <- coef(fit)[2]

yhat <- exp(b1 + b2*x)     # equivalently fitted(fit)
r    <- (y - yhat) / yhat  # equivalently residuals(fit, type = "pearson")

par(mfrow = c(1, 2))
plot(yhat, r, xlab = expression(hat(y)[i]), ylab = expression(r[i]),
     main = "Residuals vs fitted", pch = 19); abline(h = 0, lty = 2)
plot(x, r, xlab = "x (log10 WBC)", ylab = expression(r[i]),
     main = "Residuals vs x", pch = 19); abline(h = 0, lty = 2)
```




```r
data.frame(x, y, yhat = round(yhat, 2), r = round(r, 3))
```

```
      x   y   yhat      r
1  3.36  65 115.61 -0.438
2  2.88 156 196.90 -0.208
3  3.63 100  85.69  0.167
4  3.41 134 109.38  0.225
5  3.78  16  72.56 -0.779
6  4.02 108  55.60  0.943
7  4.00 121  56.84  1.129
8  4.23   4  44.04 -0.909
9  3.73  39  76.69 -0.491
10 3.85 143  67.13  1.130
11 3.97  56  58.77 -0.047
12 4.51  26  32.28 -0.195
13 4.54  22  31.23 -0.295
14 5.00   1  18.75 -0.947
15 5.00   1  18.75 -0.947
16 4.72   5  25.57 -0.804
17 5.00  65  18.75  2.467
```

The model is adequate. The residuals are centred near zero with $\text{sd}(r_i) = 0.938$, and since the model implies $\text{sd}(Y_i) = \text{E}(Y_i)$ a typical magnitude near 1 is expected; all but one fall in $(-0.95, 1.13)$, and the right skew is a property of r_i being bounded below by -1 and unbounded above. Being Pearson residuals, $\widehat{\phi} = \frac{1}{15}\sum r_i^2 = 0.939$ matches part (d) and supports $\phi = 1$. The residual deviance $D = 19.457$ on 15 degrees of freedom is already the scaled deviance when $\phi = 1$, giving $p = 0.194$ against $\chi^2(15)$: no lack of fit. Neither plot shows funnelling or curvature, so the log link and mean function are appropriate. The one outlier, $r_{17} = 2.47$ at $x = 5.00$, $y = 65$, reflects three patients sharing the highest count with survivals 1, 1 and 65 against a common $\widehat{y} = 18.75$; since $\Pr(Y > 3.47\mu) = e^{-3.47} = 0.031$, a residual this large among 17 is unusual but not extraordinary.

4.3 Problem 4.3 — Let Y1 , . . . ,YN be a random sample from the Normal distribution Yi ∼

Problem 4.3. Let $Y_1, \ldots, Y_N$ be a random sample from the Normal distribution $Y_i \sim N(\log\beta, \sigma^2)$ where σ^2 is known. Find the maximum likelihood estimator of β from first principles. Also verify Equations (4.18) and (4.25) in this case. (difficulty: ⋆⋆)

Solution. $\widehat{\beta} = \exp(\overline{Y})$, with $\overline{Y} = N^{-1}\sum_i Y_i$. From first principles:

$$l(\beta;\mathbf{y}) = -\frac{1}{2\sigma^2}\sum_{i=1}^{N}(y_i - \log\beta)^2 - N\log\left(\sigma\sqrt{2\pi}\right),$$

$$U = \frac{\mathrm{d}l}{\mathrm{d}\beta} = \frac{1}{\beta\sigma^2}\sum_{i=1}^{N}(Y_i - \log\beta) = \frac{N}{\beta\sigma^2}\left(\overline{Y} - \log\beta\right),$$

$$U' = -\frac{N}{\beta^2\sigma^2}\left[1 + \overline{Y} - \log\beta\right].$$

Since $\beta > 0$ the factor $N/(\beta\sigma^2)$ never vanishes, so $U = 0$ forces $\log\beta = \overline{y}$; and $U'(\widehat{\beta}) = -N/(\widehat{\beta}^2\sigma^2) < 0$, a maximum. (Equivalently, by invariance under reparametrisation: $\mu = \log\beta$ has $\widehat{\mu} = \overline{Y}$.) Since $\mathrm{E}(\overline{Y}) = \log\beta$,

$$\mathfrak{I} = \mathrm{E}(-U') = \frac{N}{\beta^2\sigma^2}, \qquad s.e.(\widehat{\beta}) = \sqrt{1/\mathfrak{I}} = \widehat{\beta}\sigma/\sqrt{N}$$

by equation (4.12).

Equation (4.18). As a generalized linear model: $p = 1$, $\mathbf{X} = \mathbf{1}_N$, $\eta_i = \beta$, $\mu_i = \log\beta$, so the link required by (4.16) is $g(\mu) = e^{\mu}$, the inverse of the mean function $\mu = \log\eta$. With $\mathrm{var}(Y_i) = \sigma^2$ and $\partial\mu_i/\partial\eta_i = 1/\beta$,

$$U_1 = \sum_{i=1}^{N}\frac{(Y_i - \mu_i)}{\mathrm{var}(Y_i)}x_{i1}\frac{\partial\mu_i}{\partial\eta_i} = \frac{N}{\beta\sigma^2}\left(\overline{Y} - \log\beta\right),$$

$$\mathfrak{I}_{11} = \sum_{i=1}^{N}\frac{x_{i1}^2}{\mathrm{var}(Y_i)}\left(\frac{\partial\mu_i}{\partial\eta_i}\right)^2 = \frac{N}{\beta^2\sigma^2},$$

matching the score and information above, which verifies (4.18) and (4.20).

Equation (4.25). The weights of (4.23) are $w_{ii} = 1/(\sigma^2\beta^2)$, so $\mathbf{W} = (\sigma^2\beta^2)^{-1}\mathbf{I}_N$ and $\mathbf{X}^T\mathbf{W}\mathbf{X} = N/(\sigma^2\beta^2) = \mathfrak{I}$. Writing $b = b^{(m-1)}$, the working response (4.24) is $z_i = b + (y_i - \log b)b$, since $\partial\eta_i/\partial\mu_i = \beta$ evaluated at b. Hence

$$\mathbf{X}^T\mathbf{W}\mathbf{z} = \frac{1}{\sigma^2 b^2}\sum_{i=1}^{N}\left[b + b(y_i - \log b)\right] = \frac{N}{\sigma^2 b}\left[1 + \overline{y} - \log b\right],$$

$$b^{(m)} = b^{(m-1)}\left[1 + \overline{y} - \log b^{(m-1)}\right],$$

the second line solving $\mathbf{X}^T\mathbf{W}\mathbf{X}b^{(m)} = \mathbf{X}^T\mathbf{W}\mathbf{z}$. This is exactly the method of scoring (4.21), $b + \mathfrak{I}^{-1}U = b[1 + \overline{y} - \log b]$, and its fixed point is $\log b = \overline{y}$, i.e. $b = \widehat{\beta}$. Note the step is genuinely iterative despite the Normal response, because g is not the identity, so $\mathbf{W}$ and $\mathbf{z}$ depend on b.

Numerically, with $N = 40$, $\beta = 3$, $\sigma = 0.5$:

```r
set.seed(4)
N <- 40; beta.true <- 3; sigma <- 0.5
y <- rnorm(N, mean = log(beta.true), sd = sigma)

cat("closed form  exp(ybar) =", exp(mean(y)), "\n")
loglik <- function(b) sum(dnorm(y, mean = log(b), sd = sigma, log = TRUE))
cat("optimise     =", optimise(loglik, c(0.1, 20), maximum = TRUE)$maximum, "\n")
```

```r

b <- 1                                   # IRLS recursion from (4.25)
for (m in 1:6) {
  b <- b * (1 + mean(y) - log(b))
  cat(sprintf("m = %d  b = %.8f\n", m, b))
}
cat("score (4.18) at b:", sum((y - log(b))/sigma^2) * (1/b), "\n")
cat("s.e. = sqrt(1/I):", sqrt(b^2 * sigma^2 / N), "\n")
```

```
closed form  exp(ybar) = 3.557892
optimise     = 3.557885
m = 1  b = 2.26916826
m = 2  b = 3.28973781
m = 3  b = 3.54752296
m = 4  b = 3.55787697
m = 5  b = 3.55789210
m = 6  b = 3.55789210
score (4.18) at b: 8.737265e-16
s.e. = sqrt(1/I): 0.2812761
```

From $b^{(0)} = 1$ the recursion converges to $3.5578921 = e^{\overline{y}}$, the score (4.18) vanishes there to machine precision, and $\widehat{\beta}\sigma/\sqrt{N} = 0.281$ confirms the information calculation.

5 Inference

Contents

5.1 Problem 5.1 — Consider the single response variable Y with Y ∼ Bin(n, π).

Problem 5.1. Consider the single response variable Y with $Y \sim \text{Bin}(n, \pi)$.
a. Find the Wald statistic $(\hat{\pi} - \pi)^T \mathcal{I}(\hat{\pi} - \pi)$, where $\hat{\pi}$ is the maximum likelihood estimator of π and $\mathcal{I}$ is the information. b. Verify that the Wald statistic is the same as the score statistic $U^T \mathcal{I}^{-1} U$ in this case (see Example 5.2.2). c. Find the deviance

$$2[l(\hat{\pi}; y) - l(\pi; y)].$$

d. For large samples, both the Wald/score statistic and the deviance approximately have the $\chi^2(1)$ distribution. For $n = 10$ and $y = 3$, use both statistics to assess the adequacy of the models: (i) $\pi = 0.1$; (ii) $\pi = 0.3$; (iii) $\pi = 0.5$. Do the two statistics lead to the same conclusions?
(difficulty: ⋆⋆)

Solution. a. The Wald statistic is $(Y - n\pi)^2/\{n\pi(1-\pi)\}$. From Example 5.2.2,

$$l(\pi; y) = y \log \pi + (n - y) \log(1 - \pi) + \log \binom{n}{y},$$
$$U = \frac{Y}{\pi} - \frac{n - Y}{1 - \pi} = \frac{Y - n\pi}{\pi(1 - \pi)}, \qquad \mathcal{I} = \text{var}(U) = \frac{n}{\pi(1 - \pi)},$$

and $U = 0$ gives $\hat{\pi} = Y/n$. With one parameter the quadratic form (5.7) is a scalar:

$$(\hat{\pi} - \pi)^T \mathcal{I}(\hat{\pi} - \pi) = \left(\frac{Y}{n} - \pi\right)^2 \frac{n}{\pi(1 - \pi)} = \frac{(Y - n\pi)^2}{n\pi(1 - \pi)},$$

the square of $(Y - n\pi)/\sqrt{n\pi(1-\pi)}$, which is asymptotically $N(0, 1)$ by Example 5.2.2; hence the statistic is asymptotically $\chi^2(1)$. The information is evaluated at π rather than at $\hat{\pi}$: the two agree asymptotically but differ in finite samples, and only $\mathcal{I}(\pi)$ gives the identity of part (b).
b. With one parameter,

$$U^T \mathcal{I}^{-1} U = \frac{U^2}{\mathcal{I}} = \left[\frac{Y - n\pi}{\pi(1 - \pi)}\right]^2 \cdot \frac{\pi(1 - \pi)}{n} = \frac{(Y - n\pi)^2}{n\pi(1 - \pi)},$$

exactly the Wald statistic of (a). The equality is identical, not asymptotic, because for the one-parameter exponential family in its mean-value parameter $U(\pi) = \mathcal{I}(\pi)(\hat{\pi} - \pi)$ holds exactly, so (5.5) is exact here rather than a Taylor approximation.
c. The saturated model for a single observation has $\hat{\pi} = y/n$, so the $\log \binom{n}{y}$ terms cancel and, by Section 5.6.1,

$$D = 2[l(\hat{\pi}; y) - l(\pi; y)] = 2\left[y \log \frac{\hat{\pi}}{\pi} + (n - y) \log \frac{1 - \hat{\pi}}{1 - \pi}\right]$$
$$= 2\left[y \log \frac{y}{n\pi} + (n - y) \log \frac{n - y}{n - n\pi}\right] = 2 \sum o \log(o/e),$$

summed over the cells "success" and "failure". With $m = 1$ and $p = 0$, $D \sim \chi^2(1)$ approximately.
d. Here $n = 10$, $y = 3$, so $\hat{\pi} = 0.3$.

```r
n <- 10; y <- 3; pi0 <- c(0.1, 0.3, 0.5)
pihat <- y/n
W <- (pihat - pi0)^2 * n/(pi0*(1-pi0))              # Wald = score statistic
D <- 2*(y*log(pihat/pi0) + (n-y)*log((1-pihat)/(1-pi0)))   # deviance
data.frame(pi = pi0, W = round(W,4), p_W = round(pchisq(W,1,lower.tail=FALSE),4),
           D = round(D,4), p_D = round(pchisq(D,1,lower.tail=FALSE),4))
```

```
  pi      W    p_W      D    p_D
1 0.1 4.4444 0.0350 3.0733 0.0796
2 0.3 0.0000 1.0000 0.0000 1.0000
3 0.5 1.6000 0.2059 1.6457 0.1996
```

The 5% critical value of $\chi^2(1)$ is 3.8415.

- (i) $\pi = 0.1$: Wald/score = 4.444 exceeds 3.84 ($p = 0.035$), so this model is rejected. The deviance is 3.073 ($p = 0.080$), which does **not** reach the critical value. **The two statistics disagree.**
- (ii) $\pi = 0.3$: both statistics are exactly 0, because π coincides with $\hat{\pi} = 3/10$ and the model of interest is then the saturated model. Both accept.
- (iii) $\pi = 0.5$: Wald/score = 1.600, deviance = 1.646; both well below 3.84, both accept.

So the statistics agree on (ii) and (iii) but conflict on (i). The two are asymptotically equivalent — a second-order expansion of D about $\hat{\pi}$ returns the Wald statistic, by Equation (5.4) — but $n\pi = 1$ is far from asymptotic and the Binomial is badly skewed there, so the quadratic approximation behind the Wald statistic is poor. The deviance uses the actual log-likelihood and is the more trustworthy in small samples; on that basis $\pi = 0.1$ is borderline rather than rejected.

5.2 Problem 5.2 — Consider a random sample Y1 , . . . ,YN with the exponential distribution

Problem 5.2. Consider a random sample $Y_1, \ldots, Y_N$ with the exponential distribution

$$f(y_i; \theta_i) = \theta_i \exp(-y_i \theta_i).$$

Derive the deviance by comparing the maximal model with different values of θ_i for each Y_i and the model with $\theta_i = \theta$ for all i. (difficulty: ⋆⋆)

Solution. $D = 2\sum_{i=1}^{N} \log(\bar{y}/y_i)$. The Y_i are independent, so

$$l(\boldsymbol{\theta}; \mathbf{y}) = \sum_{i=1}^{N} (\log \theta_i - y_i \theta_i),$$

with $E(Y_i) = 1/\theta_i = \mu_i$ (Exercise 4.2(c)).

- (i) Maximal model, $m = N$ free parameters: $\partial l/\partial \theta_i = 1/\theta_i - y_i = 0$ gives $\hat{\theta}_i = 1/y_i$, a maximum since $\partial^2 l/\partial \theta_i^2 = -1/\theta_i^2 < 0$, so $l(\mathbf{b}_{\max}; \mathbf{y}) = -\sum_i \log y_i - N$.
- (ii) Model of interest, $p = 1$: $dl/d\theta = N/\theta - \sum y_i = 0$ gives $\hat{\theta} = 1/\bar{y}$, i.e. fitted mean $\hat{\mu}_i = \bar{y}$, so $l(b; \mathbf{y}) = -N \log \bar{y} - N$.

Subtracting as in Section 5.5, the two $-N$ terms cancel:

$$\begin{aligned} D = 2\left[l(\mathbf{b}_{\max}; \mathbf{y}) - l(b; \mathbf{y})\right] &= 2\left[N \log \bar{y} - \sum_{i=1}^{N} \log y_i\right] \\ &= 2\sum_{i=1}^{N} \log \frac{\bar{y}}{y_i} = -2\sum_{i=1}^{N} \log \frac{y_i}{\hat{\mu}_i}. \end{aligned}$$

Since $m - p = N - 1$, Section 5.6 gives $D \sim \chi^2(N-1)$ approximately; no nuisance parameter appears, so D is a goodness-of-fit statistic computable from the data alone.

The exponential is Gamma with shape 1 (Exercise 3.3(b)), so an intercept-only Gamma fit in R must return $2\sum \log(\bar{y}/y_i)$.

```r
set.seed(1); y <- rexp(20, rate = 0.5)
D_formula <- 2*sum(log(mean(y)/y))
D_glm <- deviance(glm(y ~ 1, family = Gamma(link = "log")))
c(formula = D_formula, glm = D_glm)
```

```
 formula      glm
14.84745 14.84745
```

The two agree, as they must.

5.3 Problem 5.3 — Suppose Y1 , . . . ,YN are independent identically distributed random vari-

Problem 5.3. Suppose $Y_1, \ldots, Y_N$ are independent identically distributed random variables with the Pareto distribution with parameter θ.
a. Find the maximum likelihood estimator $\hat{\theta}$ of θ. b. Find the Wald statistic for making inferences about θ (Hint: Use the results from Exercise 3.10). c. Use the Wald statistic to obtain an expression for an approximate 95% confidence interval for θ. d. Random variables Y with the Pareto distribution with the parameter θ can be generated from random numbers U, which are uniformly distributed between 0 and 1 using the relationship $Y = (1/U)^{1/\theta}$ (Evans et al. 2000). Use this relationship to generate a sample of 100 values of Y with $\theta = 2$. From these data calculate an estimate $\hat{\theta}$. Repeat this process 20 times and also calculate 95% confidence intervals for θ. Compare the average of the estimates $\hat{\theta}$ with $\theta = 2$. How many of the confidence intervals contain θ?
(difficulty: ⋆⋆)

Solution. The printed hint cites Exercise 3.10, which in this edition is about a different model; the Pareto score and information are Exercise 3.11, derived below. The book's density (Exercise 3.3(a)) is $f(y;\theta) = \theta y^{-\theta-1}$ for $y > 1$, $\theta > 0$, consistent with part (d): $Y = (1/U)^{1/\theta}$ has $\Pr(Y > y) = \Pr(U < y^{-\theta}) = y^{-\theta}$.
a. $\hat{\theta} = N/\sum_{i=1}^{N} \log y_i$, the reciprocal of the mean of the $\log y_i$. Indeed

$$l(\theta;\mathbf{y}) = N\log\theta - (\theta+1)\sum_{i=1}^{N}\log y_i, \qquad U = \frac{N}{\theta} - \sum_{i=1}^{N}\log Y_i,$$

and $U = 0$ gives $\hat{\theta}$, a maximum since $U' = -N/\theta^2 < 0$.
b. $\log Y$ is exponential with parameter θ, since $\Pr(\log Y > t) = \Pr(Y > e^t) = e^{-\theta t}$; hence $E(\log Y_i) = 1/\theta$ and $\operatorname{var}(\log Y_i) = 1/\theta^2$, so $E(U) = 0$ as Equation (5.2) requires and

$$\mathcal{I} = \operatorname{var}(U) = \sum_{i=1}^{N}\operatorname{var}(\log Y_i) = \frac{N}{\theta^2} = -E(U'),$$

the two definitions agreeing (Exercise 3.11). Evaluating the information at the estimator, Equation (5.7) gives the Wald statistic

$$(\hat{\theta}-\theta)^T\mathcal{I}(\hat{\theta})(\hat{\theta}-\theta) = \frac{N(\hat{\theta}-\theta)^2}{\hat{\theta}^2} \sim \chi^2(1)$$

approximately, equivalently $\hat{\theta} \sim N(\theta, \theta^2/N)$ in the form of Equation (5.8).
c. Inverting $|\sqrt{N}(\hat{\theta}-\theta)/\hat{\theta}| \le 1.96$,

$$\hat{\theta}\left(1 - \frac{1.96}{\sqrt{N}}\right) \le \theta \le \hat{\theta}\left(1 + \frac{1.96}{\sqrt{N}}\right).$$

The standard error is proportional to $\hat{\theta}$, so the relative width is the constant $2 \times 1.96/\sqrt{N}$ — at $N = 100$, $\pm 19.6\%$ of the estimate.
d. Twenty independent samples of $N = 100$, generated by the inversion rule with $\theta = 2$.

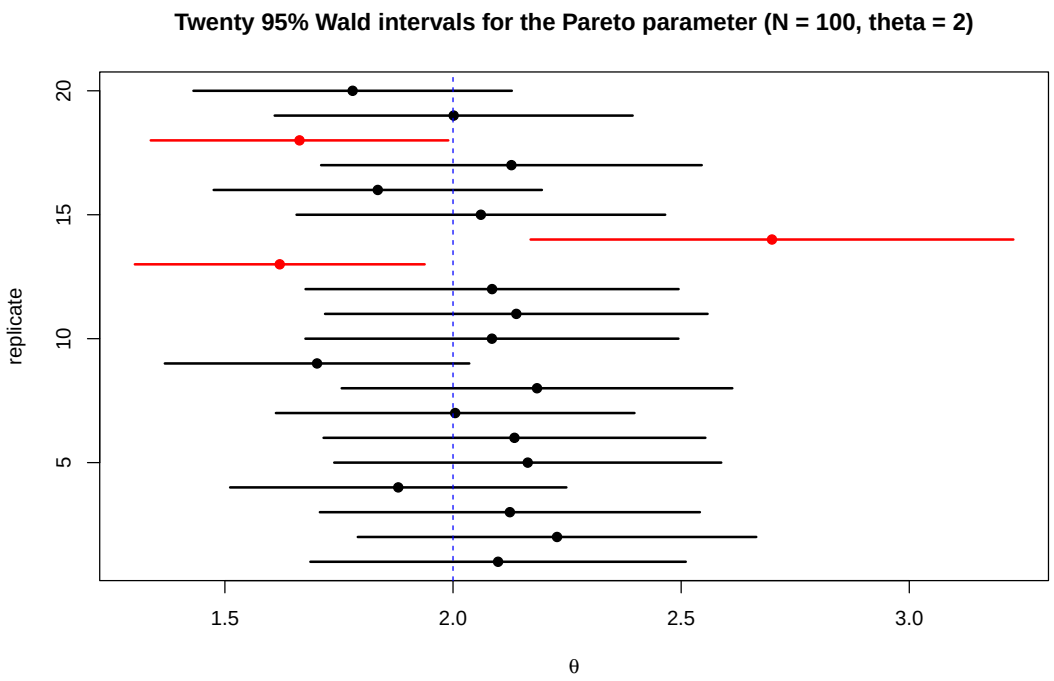
```r
set.seed(5003)
theta <- 2; N <- 100; R <- 20
sim <- t(sapply(1:R, function(r) {
  u  <- runif(N)
  y  <- (1/u)^(1/theta)          # Pareto(theta), support y > 1
  th <- N/sum(log(y))            # MLE from part (a)
  se <- th/sqrt(N)               # estimated standard error from part (b)
  c(theta_hat = th, lower = th - 1.96*se, upper = th + 1.96*se)
}))
sim <- as.data.frame(sim)
sim$covers <- sim$lower <= theta & theta <= sim$upper
round(sim[,1:3], 4)
```

```
   theta_hat  lower  upper
1     2.0987 1.6874 2.5101
2     2.2280 1.7913 2.6646
3     2.1246 1.7082 2.5410
4     1.8799 1.5115 2.2484
5     2.1638 1.7397 2.5879
6     2.1347 1.7163 2.5531
7     2.0047 1.6118 2.3977
8     2.1841 1.7560 2.6121
9     1.7020 1.3684 2.0356
10    2.0853 1.6765 2.4940
11    2.1387 1.7195 2.5579
12    2.0856 1.6768 2.4944
13    1.6202 1.3027 1.9378
14    2.6990 2.1700 3.2281
15    2.0610 1.6571 2.4650
16    1.8351 1.4754 2.1947
17    2.1280 1.7109 2.5451
18    1.6635 1.3375 1.9896
19    2.0014 1.6091 2.3937
20    1.7800 1.4311 2.1288
```

```r
c(mean_theta_hat = mean(sim$theta_hat), sd_theta_hat = sd(sim$theta_hat),
  asymptotic_se = theta/sqrt(N), n_covering = sum(sim$covers))
```

```
mean_theta_hat   sd_theta_hat  asymptotic_se     n_covering
      2.030913       0.242346       0.200000      17.000000
```

```r
cov <- sim$covers
plot(sim$theta_hat, 1:R, xlim = range(sim[,2:3]), pch = 19,
     col = ifelse(cov, "black", "red"),
     xlab = expression(theta), ylab = "replicate",
     main = "Twenty 95% Wald intervals for the Pareto parameter (N = 100, theta = 2)")
segments(sim$lower, 1:R, sim$upper, 1:R, col = ifelse(cov, "black", "red"), lwd = 2)
abline(v = theta, lty = 2, col = "blue")
```



Interpretation.

- The average of the estimates is 2.031, against $\theta = 2$. The estimator is slightly biased upwards: $\sum \log Y_i \sim \text{Gamma}(N, \theta)$, so $E(\hat{\theta}) = N\theta/(N-1) = 2.0202$ exactly, and the bias is $O(1/N)$.
- Their standard deviation is 0.242 against the asymptotic $\theta/\sqrt{N} = 0.2$; with twenty replicates the sample standard deviation has relative standard error about $1/\sqrt{2 \times 19} \approx 16\%$, so this is ordinary

sampling noise.

- Seventeen of the twenty intervals contain $\theta = 2$ (the failures, red in the figure, are replicates 13, 14, 18) against a nominal 19. Under exact 95% coverage the misses are $\text{Bin}(20, 0.05)$ with $\Pr(\geq 3) = 0.075$, so this is no evidence against the method. A longer run:

```
set.seed(99)
M <- 20000
cover <- replicate(M, { y <- (1/runif(N))^(1/theta); th <- N/sum(log(y))
                        abs(th - theta) <= 1.96*th/sqrt(N) })
mean(cover)
```

```
[1] 0.94975
```

Empirical coverage 0.94975 against a nominal 0.95: the interval of part (c) is essentially exact at $N = 100$, so the shortfall in the run of twenty is chance alone.

5.4 Problem 5.4 — For the leukemia survival data in Exercise 4.2:

Problem 5.4. For the leukemia survival data in Exercise 4.2:
a. Use the Wald statistic to obtain an approximate 95% confidence interval for the parameter β_1. b. By comparing the deviances for two appropriate models, test the null hypothesis $\beta_2 = 0$ against the alternative hypothesis $\beta_2 \neq 0$. What can you conclude about the use of the initial white blood cell count as a predictor of survival time?
(For reference, Exercise 4.2 gives times to death y_i in weeks from diagnosis and $\log_{10}$ of the initial white blood cell count x_i, for seventeen patients suffering from leukemia — Example U of Cox and Snell, 1981. Table 4.6 reads: $y = 65, 156, 100, 134, 16, 108, 121, 4, 39, 143, 56, 26, 22, 1, 1, 5, 65$ with corresponding $x = 3.36, 2.88, 3.63, 3.41, 3.78, 4.02, 4.00, 4.23, 3.73, 3.85, 3.97, 4.51, 4.54, 5.00, 5.00, 4.72, 5.00$. The model is $E(Y_i) = \exp(\beta_1 + \beta_2 x_i)$ with Y_i exponentially distributed, $f(y;\theta) = \theta e^{-y\theta}$, i.e. a Gamma model with shape parameter 1, equivalently dispersion $\phi = 1$, and a log link.)
(difficulty: ⋆⋆)

Solution. The interval is $\beta_1 \in (5.234, 11.721)$ and $H_0 : \beta_2 = 0$ is rejected. Carry over the Exercise 4.2(d) fit, but with the dispersion held at $\phi = 1$, which is what the exponential distribution asserts: Equation (5.7) needs the information implied by the assumed model, whereas R's default estimates ϕ from the Pearson statistic ($\hat{\phi} = 0.939$).

```
library(dobson)
data(leukemia)
leuk <- as.data.frame(leukemia)
names(leuk) <- c("y", "x")     # y = survival weeks, x = log10 initial WBC
fit1 <- glm(y ~ x, family = Gamma(link = "log"), data = leuk)
summary(fit1, dispersion = 1)
```

```
Call:
glm(formula = y ~ x, family = Gamma(link = "log"), data = leuk)

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept)   8.4775     1.6548   5.123 3.01e-07 ***
x            -1.1093     0.3997  -2.776  0.00551 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for Gamma family taken to be 1)

    Null deviance: 26.282  on 16  degrees of freedom
Residual deviance: 19.457  on 15  degrees of freedom
AIC: 173.97

Number of Fisher Scoring iterations: 8
```

So $b_1 = 8.4775$ and $b_2 = -1.1093$.

a. By Equation (5.8), $b \sim N(\beta, \mathcal{I}^{-1})$ approximately with $\mathcal{I}^{-1} = (X^T W X)^{-1}$ at the estimates, so the interval for the single component β_1 is $b_1 \pm 1.96\sqrt{(\mathcal{I}^{-1})_{11}}$, where $\sqrt{(\mathcal{I}^{-1})_{11}} = 1.6548$.

```
b  <- coef(fit1)
se <- sqrt(diag(summary(fit1, dispersion = 1)$cov.scaled))
round(cbind(estimate = b, se = se, lower = b - 1.96*se, upper = b + 1.96*se), 4)
```

```
            estimate     se   lower   upper
(Intercept)   8.4775 1.6548  5.2341 11.7209
x            -1.1093 0.3997 -1.8926 -0.3260
```

The approximate 95% confidence interval for β_1 is

$$8.4775 \pm 1.96 \times 1.6548 = (5.234,\ 11.721).$$

Here β_1 is $\log E(Y)$ at $x = 0$, a count of $10^0 = 1$, far outside the observed range 2.88 to 5.00; hence the width, $e^{5.234} = 188$ to $e^{11.721} \approx 1.2 \times 10^5$ weeks about $e^{8.478} \approx 4805$. It is a statement about the intercept of the fitted line on the log scale, not a survival prediction.

b. Following Section 5.7, compare two nested models with the same distribution and link:

- M_0: $E(Y_i) = \exp(\beta_1)$, a single common mean, $q = 1$ parameter, deviance D_0;
- M_1: $E(Y_i) = \exp(\beta_1 + \beta_2 x_i)$, $p = 2$ parameters, deviance D_1.

```
fit0 <- glm(y ~ 1, family = Gamma(link = "log"), data = leuk)
anova(fit0, fit1, test = "Chisq", dispersion = 1)
```

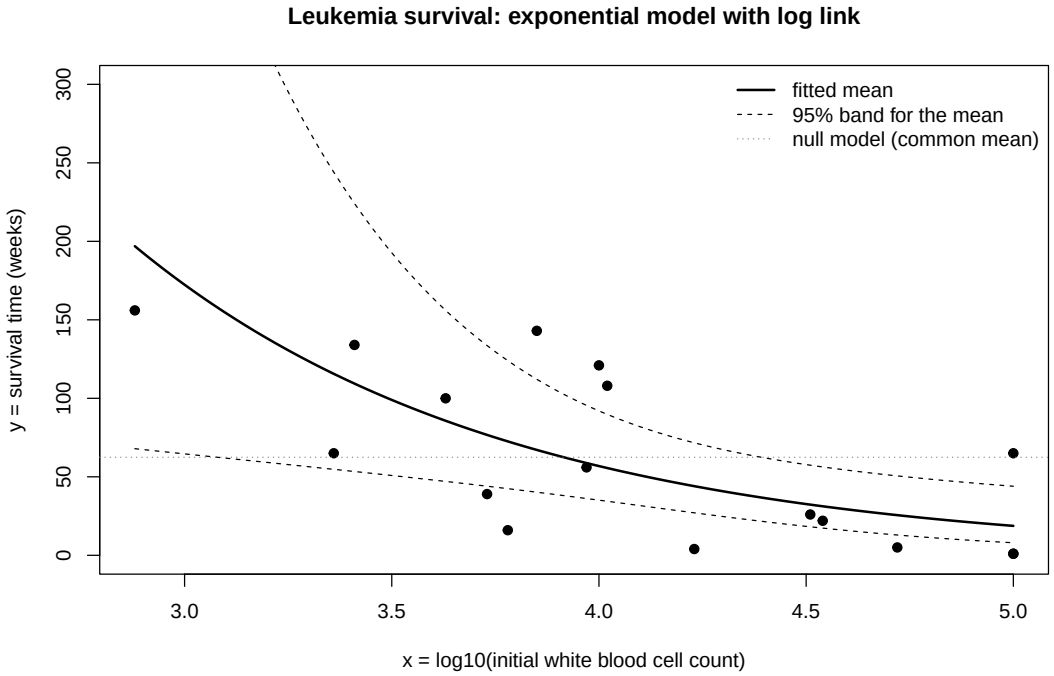
```
Analysis of Deviance Table

Model 1: y ~ 1
Model 2: y ~ x
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
1        16     26.282
2        15     19.456  1   6.8256 0.008986 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

So $D_0 = 26.282$ on $N - q = 16$ degrees of freedom, $D_1 = 19.456$ on $N - p = 15$, and

$$\triangle D = D_0 - D_1 = 26.282 - 19.456 = 6.826 \sim \chi^2(p - q) = \chi^2(1)$$

under H_0. Since $6.826 > \chi^2_{0.95}(1) = 3.841$ ($p = 0.0090$), reject H_0: $\beta_2 \neq 0$. No F ratio is needed here, unlike Section 5.7's Normal case, because the exponential deviance of Exercise 5.2 carries no nuisance parameter. The residual deviance $D_1 = 19.456$ against $\chi^2(15)$ gives $p = 0.19$, so M_1 itself fits adequately.

```
xs <- seq(min(leuk$x), max(leuk$x), length = 200)
p  <- predict(fit1, newdata = data.frame(x = xs), se.fit = TRUE, dispersion = 1)
plot(leuk$x, leuk$y, pch = 19, ylim = c(0, 300),
     xlab = "x = log10(initial white blood cell count)",
     ylab = "y = survival time (weeks)",
     main = "Leukemia survival: exponential model with log link")
lines(xs, exp(p$fit), lwd = 2)
lines(xs, exp(p$fit - 1.96*p$se.fit), lty = 2)
lines(xs, exp(p$fit + 1.96*p$se.fit), lty = 2)
abline(h = mean(leuk$y), col = "grey50", lty = 3)
legend("topright", c("fitted mean", "95% band for the mean", "null model (common mean)"),
       lty = c(1,2,3), lwd = c(2,1,1), col = c("black","black","grey50"), bty = "n")
```



So the initial white blood cell count is a useful predictor of survival time: $b_2 = -1.109$ with 95% Wald interval $(-1.893, -0.326)$, so a unit increase in x — a tenfold increase in the count — multiplies expected survival by $e^{-1.109} = 0.33$, with interval $(0.15, 0.72)$. The figure shows the fitted mean falling from about 200 weeks at the lowest observed count to under 20 weeks at the highest, well clear of the null model's flat line over most of the range.

6 Normal Linear Models

Contents

6.1 Problem 6.1 — Table 6.22 shows the average apparent per capita consumption of sugar

Problem 6.1. Table 6.22 shows the average apparent per capita consumption of sugar (in kg per year) in Australia, as refined sugar and in manufactured foods (from Australian Bureau of Statistics, 1998).
Table 6.22 Australian sugar consumption. The columns are period, refined sugar, and sugar in manufactured food: 1936–39, 32.0, 16.3; 1946–49, 31.2, 23.1; 1956–59, 27.0, 23.6; 1966–69, 21.0, 27.7; 1976–79, 14.9, 34.6; 1986–89, 8.8, 33.9.
a. Plot sugar consumption against time separately for refined sugar and sugar in manufactured foods. Fit simple linear regression models to summarize the pattern of consumption of each form of sugar. Calculate 95% confidence intervals for the average annual change in consumption for each form.
b. Calculate the total average sugar consumption for each period and plot these data against time. Using suitable models, test the hypothesis that total sugar consumption did not change over time. (difficulty: ⋆⋆)

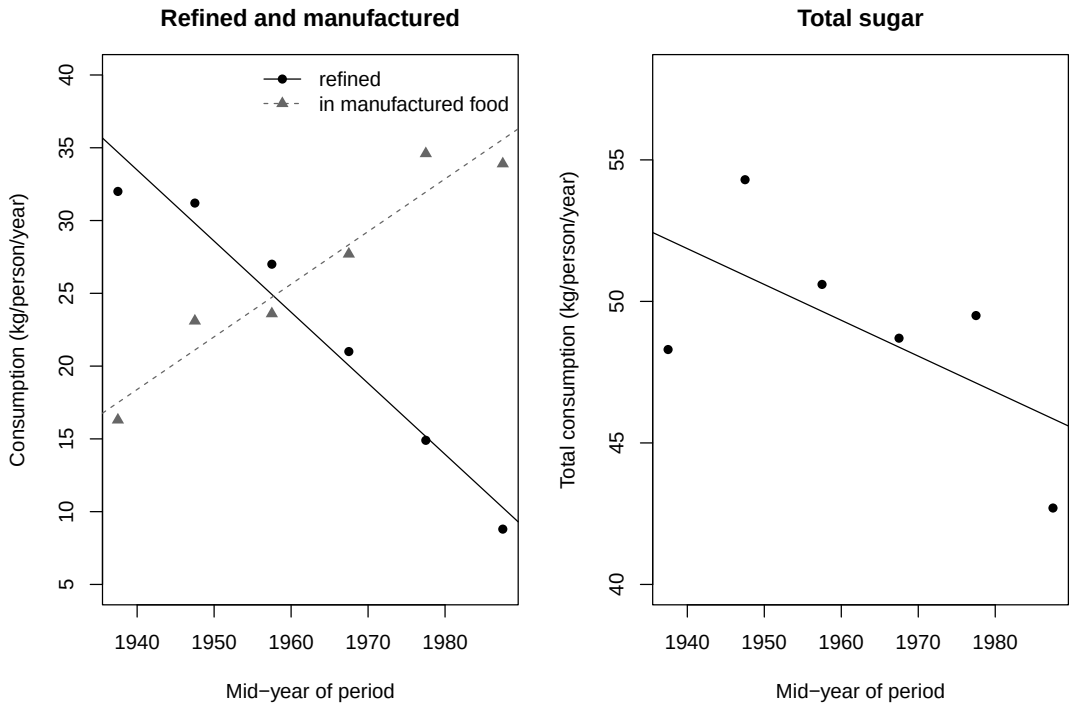
Solution. Take the mid-year of each period as covariate, $x = 1937.5, 1947.5, \ldots, 1987.5$, so that the slope is the average change in consumption per year, which is what part (a) asks for. (The `dobson` package ships `sugar` with `1046–49` in row 2, a typo in the label only; the numeric columns are correct.)

```
library(dobson)
data(sugar)
sugar <- as.data.frame(sugar)
sugar$period[2] <- "1946–49"   # package ships a typo, 1046–49
sugar$year  <- c(1937.5, 1947.5, 1957.5, 1967.5, 1977.5, 1987.5)
sugar$total <- sugar$refined + sugar$manufactured
sugar
```

```
   period refined manufactured   year total
1 1936–39    32.0         16.3 1937.5  48.3
2 1946–49    31.2         23.1 1947.5  54.3
3 1956–59    27.0         23.6 1957.5  50.6
4 1966–69    21.0         27.7 1967.5  48.7
5 1976–79    14.9         34.6 1977.5  49.5
6 1986–89     8.8         33.9 1987.5  42.7
```

Part (a) — the two forms separately.

```
par(mfrow = c(1,2), mar = c(4.5,4.5,3,1))
plot(sugar$year, sugar$refined, pch = 16, ylim = c(5,40),
     xlab = "Mid-year of period", ylab = "Consumption (kg/person/year)",
     main = "Refined and manufactured")
abline(lm(refined ~ year, data = sugar), lty = 1)
points(sugar$year, sugar$manufactured, pch = 17, col = "grey40")
abline(lm(manufactured ~ year, data = sugar), lty = 2, col = "grey40")
legend("topright", c("refined","in manufactured food"), pch = c(16,17),
       lty = c(1,2), col = c("black","grey40"), bty = "n")
plot(sugar$year, sugar$total, pch = 16, ylim = c(40,58),
     xlab = "Mid-year of period", ylab = "Total consumption (kg/person/year)",
     main = "Total sugar")
abline(lm(total ~ year, data = sugar), lty = 1)
```



Refined sugar falls steadily and sugar in manufactured food rises steadily, both close to linear over this span, so the Section 6.2 model $E(Y_i) = \beta_0 + \beta_1 x_i$ with $Y_i \sim N(\mu_i, \sigma^2)$ suits each series.

```
fit.r <- lm(refined ~ year, data = sugar)
fit.m <- lm(manufactured ~ year, data = sugar)
summary(fit.r)
```

```
Call:
lm(formula = refined ~ year, data = sugar)

Residuals:
      1       2       3       4       5       6
-2.6905  1.3924  2.0752  0.9581 -0.2590 -1.4762

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 980.74405   95.71073   10.25 0.000511 ***
year         -0.48829    0.04877  -10.01 0.000559 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 2.04 on 4 degrees of freedom
Multiple R-squared:  0.9616,        Adjusted R-squared:  0.952
F-statistic: 100.2 on 1 and 4 DF,  p-value: 0.0005593
```

```
summary(fit.m)
```

```
Call:
lm(formula = manufactured ~ year, data = sugar)

Residuals:
      1       2       3       4       5       6
-1.1905  1.9924 -1.1248 -0.6419  2.6410 -1.6762

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept) -683.33095   96.28391  -7.097  0.00208 **
year           0.36171    0.04906   7.373  0.00180 **
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 2.052 on 4 degrees of freedom
```

```
Multiple R-squared:  0.9315,        Adjusted R-squared:  0.9143
F-statistic: 54.36 on 1 and 4 DF,  p-value: 0.001804
```

```
rbind(refined = confint(fit.r)["year",],
      manufactured = confint(fit.m)["year",])
```

```
                2.5 %     97.5 %
refined      -0.6236872 -0.3528842
manufactured  0.2255019  0.4979267
```

Refined-sugar consumption fell by 0.488 kg per person per year, 95% CI $(-0.624, -0.353)$, a drop of some 24 kg over the half-century, with $R^2 = 0.96$; sugar inside manufactured food rose by 0.362 kg per person per year, 95% CI $(0.226, 0.498)$. Neither interval contains zero. The slopes are of similar magnitude and opposite sign, so the composition of consumption changed more than the amount.

Part (b) — total consumption.

The total, in the right-hand panel above, hovers near 50 kg. To test $H_0 : \beta_1 = 0$, compare the straight line with the intercept-only model $E(Y_i) = \beta_0$ as in Section 6.2.4; σ^2 being unknown, the statistic is in residual sums of squares,

$$F = \frac{(S_0 - S_1)/(p - q)}{S_1/(N - p)} \sim F(1, 4)$$

under H_0, where $S_0 = y^T y - b_0^T X_0^T y$ and $S_1 = y^T y - b_1^T X_1^T y$, with $q = 1$, $p = 2$ and $N = 6$.

```
fit.t <- lm(total ~ year, data = sugar)
anova(lm(total ~ 1, data = sugar), fit.t)
```

```
Analysis of Variance Table

Model 1: total ~ 1
Model 2: total ~ year
  Res.Df    RSS Df Sum of Sq      F Pr(>F)
1      5 71.168
2      4 43.133  1    28.036 2.5999 0.1822
```

```
summary(fit.t)$coefficients
confint(fit.t)["year",]
```

```
               Estimate   Std. Error   t value  Pr(>|t|)
(Intercept) 297.4130952 154.05674704  1.930542 0.1257369
year         -0.1265714   0.07849728 -1.612431 0.1821628
      2.5 %      97.5 %
-0.34451482  0.09137196
```

$F = 2.60$ on 1 and 4 degrees of freedom, $p = 0.18$ (equivalently $F = t^2 = (-1.612)^2$), so there is no evidence against the hypothesis that total sugar consumption did not change. The point estimate is a decline of 0.127 kg per person per year with 95% CI $(-0.345, 0.091)$, so a modest decline is not ruled out — with $N = 6$ the test has little power. What is firmly established is the substitution: total intake changed little while its source shifted from refined sugar to sugar in manufactured food.

6.2 Problem 6.2 — Table 6.23 shows response of a grass and legume pasture system to vari-

Problem 6.2. Table 6.23 shows response of a grass and legume pasture system to various quantities of phosphorus fertilizer (data from D. F. Sinclair; the results were reported in Sinclair and Probert, 1986). The total yield, of grass and legume together, and amount of phosphorus (K) are both given in kilograms per hectare. Find a suitable model for describing the association between yield and quantity of fertilizer.

a. Plot yield against phosphorus to obtain an approximately linear association (you may need to try several transformations of either or both variables in order to achieve approximate linearity).

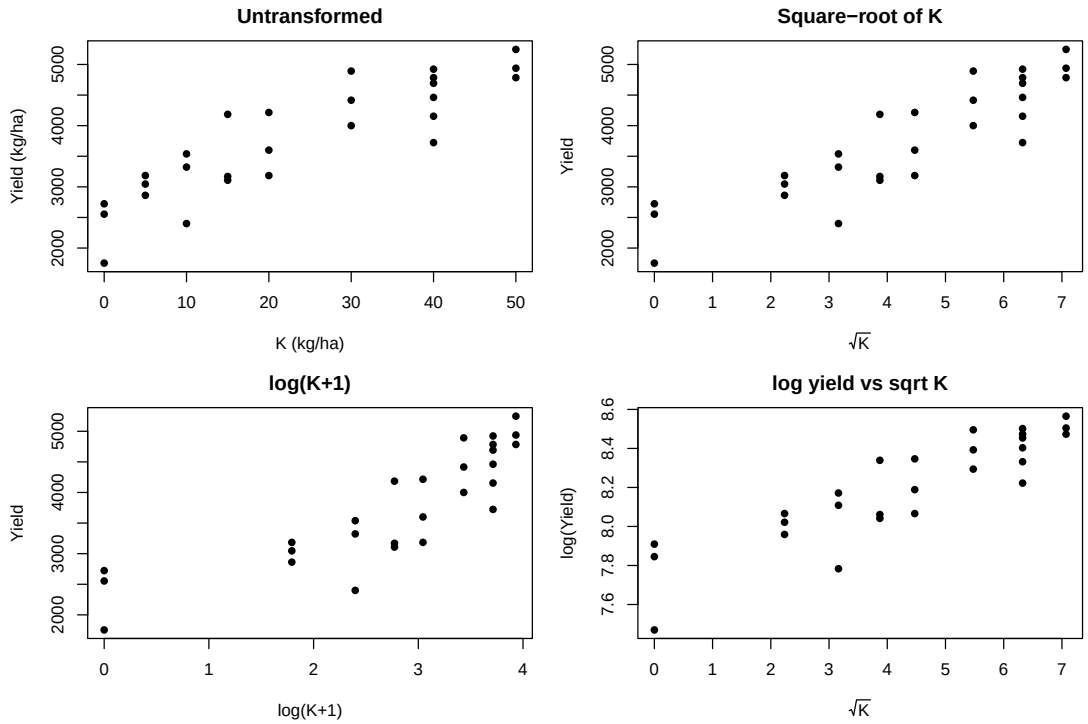
b. Use the results of (a) to specify a possible model. Fit the model.

c. Calculate the standardized residuals for the model and use appropriate plots to check for any systematic effects that might suggest alternative models and to investigate the validity of any assumptions made.

Table 6.23 Yield of grass and legume pasture and phosphorus levels (K), read as (K, yield) pairs down three columns: $(0, 1753.9)$, $(40, 4923.1)$, $(50, 5246.2)$, $(5, 3184.6)$, $(10, 3538.5)$, $(30, 4000.0)$, $(15, 4184.6)$, $(40, 4692.3)$, $(20, 3600.0)$; $(15, 3107.7)$, $(30, 4415.4)$, $(50, 4938.4)$, $(5, 3046.2)$, $(0, 2553.8)$, $(10, 3323.1)$, $(40, 4461.5)$, $(20, 4215.4)$, $(40, 4153.9)$; $(10, 2400.0)$, $(5, 2861.6)$, $(40, 3723.0)$, $(30, 4892.3)$, $(40, 4784.6)$, $(20, 3184.6)$, $(0, 2723.1)$, $(50, 4784.6)$, $(15, 3169.3)$. (difficulty: ⋆⋆)

Solution. Part (a) — finding a linearizing transformation.
Yield rises with phosphorus but must saturate, so the association is concave; the candidates are $\sqrt{K}$, $\log(K+1)$ (shifted because $K = 0$ occurs), and a quadratic in K.

```
library(dobson)
data(pasture)
pasture <- as.data.frame(pasture)
par(mfrow = c(2,2), mar = c(4.2,4.2,2.5,1))
plot(pasture$K, pasture$yield, pch = 16, xlab = "K (kg/ha)",
     ylab = "Yield (kg/ha)", main = "Untransformed")
plot(sqrt(pasture$K), pasture$yield, pch = 16, xlab = expression(sqrt(K)),
     ylab = "Yield", main = "Square-root of K")
plot(log(pasture$K + 1), pasture$yield, pch = 16, xlab = "log(K+1)",
     ylab = "Yield", main = "log(K+1)")
plot(sqrt(pasture$K), log(pasture$yield), pch = 16, xlab = expression(sqrt(K)),
     ylab = "log(Yield)", main = "log yield vs sqrt K")
```



Against raw K the cloud bends — the jump from $K = 0$ to $K = 10$ far exceeds that from $K = 40$ to $K = 50$ — and $\sqrt{K}$ straightens it, while $\log(K+1)$ over-corrects, bunching the high-K points and stranding $K = 0$. The spread of yields is roughly constant across K, so the response needs no transformation. Residual sums of squares confirm the reading (the last row is on a different response scale, so only its R^2 is comparable):

```
cand <- list("yield ~ K"        = lm(yield ~ K, data = pasture),
             "yield ~ sqrt(K)"  = lm(yield ~ sqrt(K), data = pasture),
             "yield ~ log(K+1)" = lm(yield ~ log(K + 1), data = pasture),
             "yield ~ K + K^2"  = lm(yield ~ K + I(K^2), data = pasture),
             "log(yield) ~ K"   = lm(log(yield) ~ K, data = pasture))
round(data.frame(RSS = sapply(cand, deviance),
                 R2  = sapply(cand, function(m) summary(m)$r.squared),
                 AIC = sapply(cand, AIC)), 4)
```

```
                          RSS     R2      AIC
yield ~ K        4952793.4931 0.7763 409.8526
yield ~ sqrt(K)  4822052.9000 0.7822 409.1303
yield ~ log(K+1) 6465532.7633 0.7080 417.0490
yield ~ K + K^2  4616095.2576 0.7915 409.9517
log(yield) ~ K         0.5135 0.7240 -24.3584
```

The quadratic buys a slightly smaller RSS for an extra parameter and has the worse AIC; $\sqrt{K}$ is the parsimonious choice and stays monotone increasing, whereas the fitted quadratic must eventually turn down.

Part (b) — the model.

Take the Normal linear model of equation (6.2),

$$E(Y_i) = \beta_0 + \beta_1\sqrt{K_i}, \qquad Y_i \sim N(\mu_i, \sigma^2) \text{ independent},$$

with $N = 27$ and $p = 2$.

```r
fit <- lm(yield ~ sqrt(K), data = pasture)
summary(fit)
```

```
Call:
lm(formula = yield ~ sqrt(K), data = pasture)

Residuals:
    Min      1Q  Median      3Q     Max
-938.37 -295.34   53.25  327.71  690.59

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  2159.03     190.10  11.357 2.32e-11 ***
sqrt(K)       372.94      39.35   9.476 9.39e-10 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 439.2 on 25 degrees of freedom
Multiple R-squared:  0.7822,        Adjusted R-squared:  0.7735
F-statistic:  89.8 on 1 and 25 DF,  p-value: 9.386e-10
```

```r
round(confint(fit), 2)
```

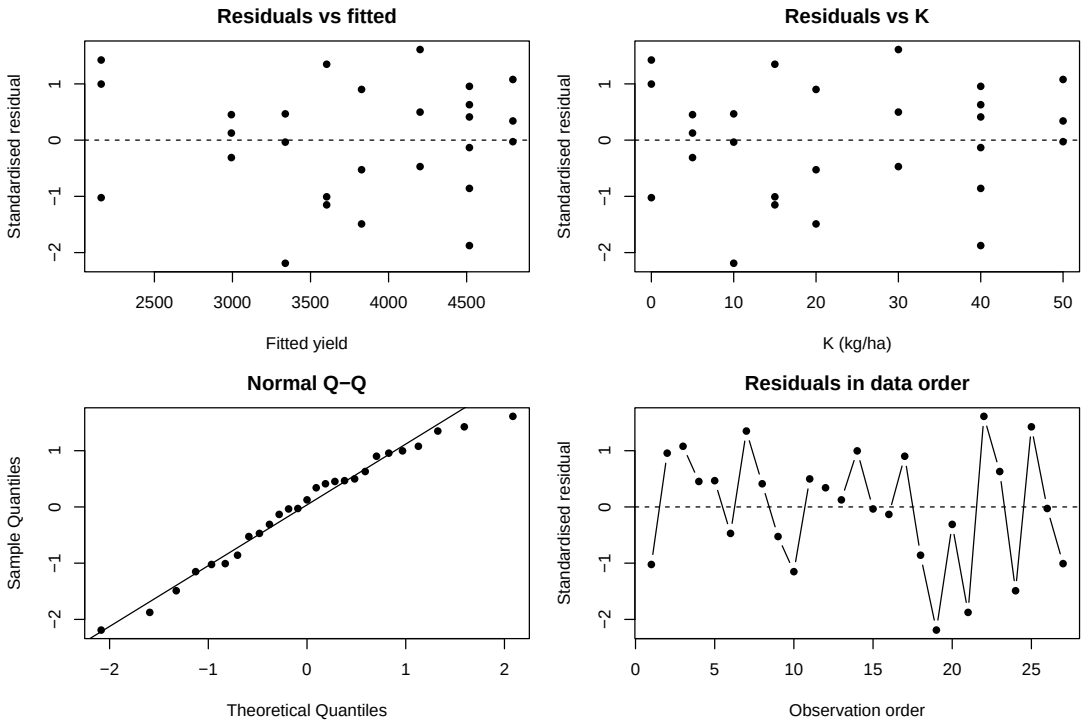
```
              2.5 %  97.5 %
(Intercept) 1767.51 2550.55
sqrt(K)      291.89  453.99
```

With no phosphorus the pasture yields 2159 kg/ha (95% CI 1768 to 2551), and yield then grows like $373\sqrt{K}$: $K = 0$ to $K = 10$ adds $373\sqrt{10} \approx 1179$ kg/ha, whereas $K = 40$ to $K = 50$ adds only $373(\sqrt{50} - \sqrt{40}) \approx 279$ kg/ha — the diminishing returns the square root encodes. The residual standard deviation is 439 kg/ha, about 10% of a typical yield.

Part (c) — standardized residuals and diagnostics.

Standardized residuals are those of Section 6.2.6, $r_i = (y_i - \hat{\mu}_i)/\{\hat{\sigma}\sqrt{1 - h_{ii}}\}$, obtained in R with `rstandard`.

```r
r <- rstandard(fit)
par(mfrow = c(2,2), mar = c(4.2,4.2,2.5,1))
plot(fitted(fit), r, pch = 16, xlab = "Fitted yield",
     ylab = "Standardised residual", main = "Residuals vs fitted"); abline(h = 0, lty = 2)
plot(pasture$K, r, pch = 16, xlab = "K (kg/ha)",
     ylab = "Standardised residual", main = "Residuals vs K"); abline(h = 0, lty = 2)
qqnorm(r, pch = 16, main = "Normal Q-Q"); qqline(r)
plot(seq_along(r), r, type = "b", pch = 16, xlab = "Observation order",
     ylab = "Standardised residual", main = "Residuals in data order"); abline(h = 0, lty =
     ↪  2)
```



The residuals scatter about zero with no funnel against the fitted values (homoscedasticity is tenable) and no arch or sag against K (the bend is right), and the Q-Q plot is close to the line. Since K takes only eight distinct levels with replication, a lack-of-fit test is available: compare the fitted line with the one-way model giving each level its own mean, so the extra sum of squares measures curvature missed by $\sqrt{K}$ against pure error.

```
anova(fit, lm(yield ~ factor(K), data = pasture))
```

```
Analysis of Variance Table

Model 1: yield ~ sqrt(K)
Model 2: yield ~ factor(K)
  Res.Df     RSS Df Sum of Sq      F Pr(>F)
1     25 4822053
2     19 4109224  6    712829 0.5493 0.7645
```

```
shapiro.test(rstandard(fit))
```

```
        Shapiro-Wilk normality test

data:  rstandard(fit)
W = 0.96755, p-value = 0.5384
```

$F = 0.55$ on 6 and 19 degrees of freedom ($p = 0.76$): no detectable systematic departure from the square-root curve, so nothing is left for a more elaborate model to explain. Normality is not contradicted ($p = 0.54$). The model

$$\widehat{\text{yield}} = 2159 + 373\sqrt{K}$$

is an adequate summary of the fertilizer response.

6.3 Problem 6.3 — Analyze the carbohydrate data in Table 6.3 using appropriate software (or,

Problem 6.3. Analyze the carbohydrate data in Table 6.3 using appropriate software (or, preferably, repeat the analyses using several different regression programs and compare the results).
a. Plot the responses y against each of the explanatory variables x_1, x_2 and x_3 to see if y appears to be linearly related to them.
b. Fit the Model (6.6) and examine the residuals to assess the adequacy of the model and the

assumptions.
c. Fit the models

$$E(Y_i) = \beta_0 + \beta_1 x_{i1} + \beta_3 x_{i3}$$

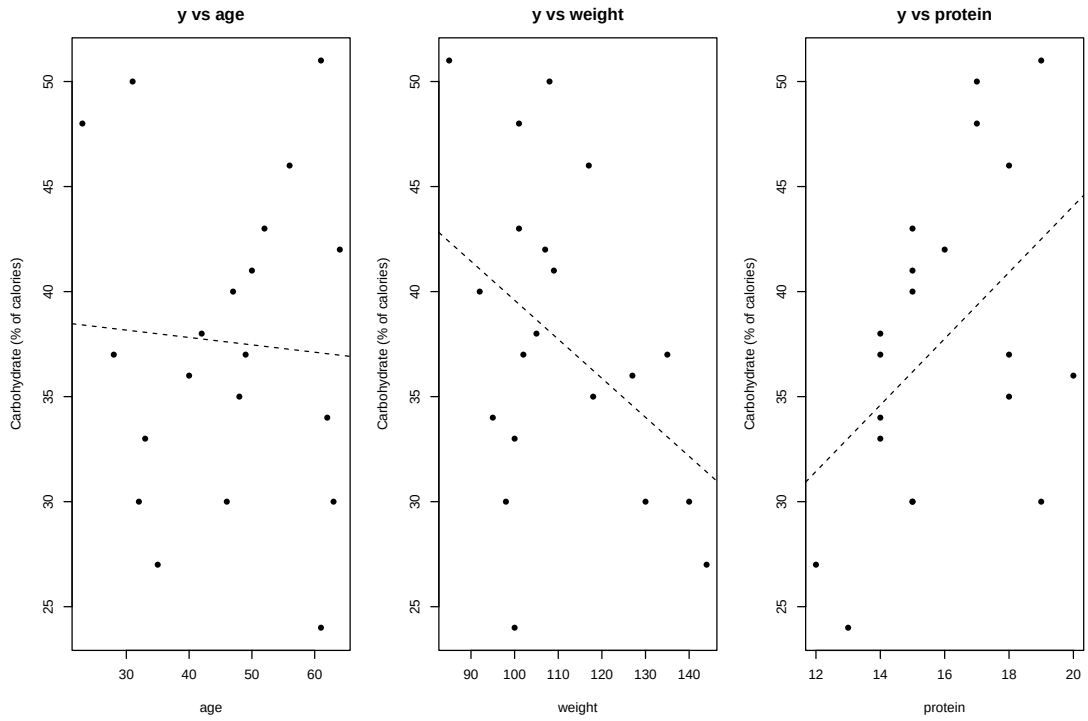
and

$$E(Y_i) = \beta_0 + \beta_3 x_{i3}$$

(note the variable x_2, relative weight, is omitted from both models), and use these to test the hypothesis: $\beta_1 = 0$. Compare your results with Table 6.5.
Table 6.3 gives, for twenty male insulin-dependent diabetics, carbohydrate y (percentage of total calories from complex carbohydrates), age x_1 (years), relative weight x_2 and protein x_3 (percentage of calories), as rows (y, x_1, x_2, x_3): $(33, 33, 100, 14)$, $(40, 47, 92, 15)$, $(37, 49, 135, 18)$, $(27, 35, 144, 12)$, $(30, 46, 140, 15)$, $(43, 52, 101, 15)$, $(34, 62, 95, 14)$, $(48, 23, 101, 17)$, $(30, 32, 98, 15)$, $(38, 42, 105, 14)$, $(50, 31, 108, 17)$, $(51, 61, 85, 19)$, $(30, 63, 130, 19)$, $(36, 40, 127, 20)$, $(41, 50, 109, 15)$, $(42, 64, 107, 16)$, $(46, 56, 117, 18)$, $(24, 61, 100, 13)$, $(35, 48, 118, 18)$, $(37, 28, 102, 14)$. (difficulty: ⋆⋆)

Solution. Model (6.6) is adequate and $H_0 : \beta_1 = 0$ is not rejected, but with a different sum of squares from Table 6.5, because the design is not orthogonal.
Part (a) — marginal plots.

```
library(dobson)
data(carbohydrate)
carbohydrate <- as.data.frame(carbohydrate)
par(mfrow = c(1,3), mar = c(4.5,4.5,3,1))
for (v in c("age","weight","protein")) {
  plot(carbohydrate[[v]], carbohydrate$carbohydrate, pch = 16, xlab = v,
       ylab = "Carbohydrate (% of calories)", main = paste("y vs", v))
  abline(lm(carbohydrate$carbohydrate ~ carbohydrate[[v]]), lty = 2)
}
```




```
round(cor(carbohydrate), 3)
```

```
             carbohydrate    age weight protein
carbohydrate        1.000 -0.059 -0.407   0.463
age                -0.059  1.000 -0.043   0.193
weight             -0.407 -0.043  1.000   0.147
protein             0.463  0.193  0.147   1.000
```

Marginally y is essentially unassociated with age ($r = -0.06$), moderately negatively with relative

weight ($r = -0.41$) and moderately positively with protein ($r = 0.46$); a straight line is defensible in each panel. The explanatory variables are only weakly intercorrelated (largest $|r| = 0.19$), so the design is close to but not exactly orthogonal — which part (c) probes.

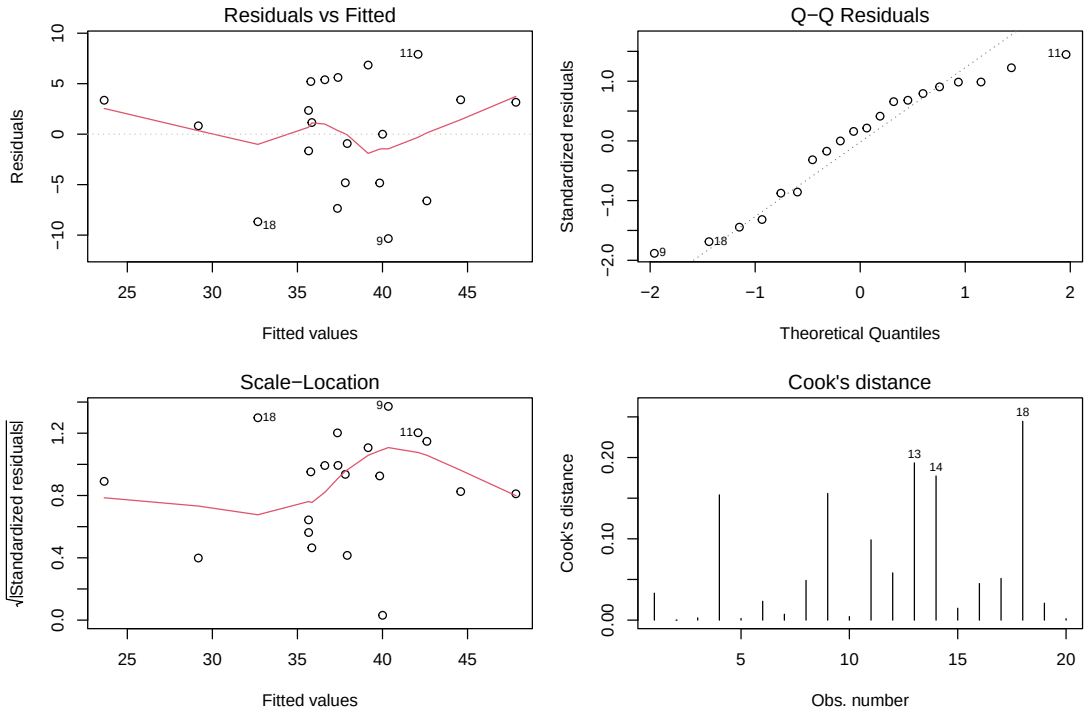
Part (b) — Model (6.6) and its residuals.

```
m66 <- lm(carbohydrate ~ age + weight + protein, data = carbohydrate)
summary(m66)
```

```
Call:
lm(formula = carbohydrate ~ age + weight + protein, data = carbohydrate)

Residuals:
     Min       1Q   Median       3Q      Max
-10.3424  -4.8203   0.9897   3.8553   7.9087

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 36.96006   13.07128   2.828  0.01213 *
age         -0.11368    0.10933  -1.040  0.31389
weight      -0.22802    0.08329  -2.738  0.01460 *
protein      1.95771    0.63489   3.084  0.00712 **
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 5.956 on 16 degrees of freedom
Multiple R-squared:  0.4805,        Adjusted R-squared:  0.3831
F-statistic: 4.934 on 3 and 16 DF,  p-value: 0.01297
```

This reproduces the book exactly: $b = (36.960, -0.114, -0.228, 1.958)^T$ and the standard errors of Table 6.4, with residual sum of squares 567.663 on 16 degrees of freedom and $\hat{\sigma}^2 = 35.48$.

```
par(mfrow = c(2,2), mar = c(4.2,4.2,2.5,1))
plot(m66, which = 1:4)
```




```
round(data.frame(y = carbohydrate$carbohydrate, fitted = fitted(m66),
                 std.res = rstandard(m66), leverage = hatvalues(m66),
                 cooks = cooks.distance(m66)), 3)
```

```
    y fitted std.res leverage cooks
1  33 37.815  -0.876    0.148 0.033
2  40 40.005  -0.001    0.120 0.000
3  37 35.846   0.215    0.192 0.003
```

```
4  27 23.639   0.794    0.495 0.154
5  30 29.174   0.159    0.239 0.002
6  43 37.385   0.987    0.087 0.023
7  34 35.658  -0.316    0.224 0.007
8  48 44.597   0.681    0.296 0.049
9  30 40.342  -1.883    0.149 0.156
10 38 35.652   0.414    0.093 0.004
11 50 42.091   1.448    0.159 0.099
12 51 47.841   0.658    0.349 0.058
13 30 37.353  -1.445    0.270 0.193
14 36 42.609  -1.317    0.290 0.177
15 41 35.788   0.906    0.067 0.015
16 42 36.610   0.985    0.156 0.045
17 46 39.155   1.225    0.120 0.051
18 24 32.674  -1.688    0.256 0.245
19 35 39.836  -0.857    0.102 0.021
20 37 37.927  -0.173    0.188 0.002
```

This is Table 6.6 and Figure 6.1 of the text:

- Residuals versus fitted values show no trend and no funnel, so linearity in the mean and constant variance are tenable.
- The standardized residuals lie inside $(-1.9, 1.5)$, unremarkable for $N = 20$, and the Q-Q plot is close to straight, so Normality is not contradicted.
- Observation 4 has the largest leverage, $h_{44} = 0.495$ against the average $p/N = 0.2$: highest relative weight (144), lowest protein (12), so at the edge of the covariate space. Its residual is small, so Cook's distance is only 0.154.
- The largest Cook's distance is 0.245 (observation 18), far below the conventional 1.

So there is little evidence against the assumptions and no unduly influential observation.

Part (c) — testing $\beta_1 = 0$ with x_2 omitted.

```r
m13 <- lm(carbohydrate ~ age + protein, data = carbohydrate)
m3  <- lm(carbohydrate ~ protein, data = carbohydrate)
anova(m3, m13)
```

```
Analysis of Variance Table

Model 1: carbohydrate ~ protein
Model 2: carbohydrate ~ age + protein
  Res.Df    RSS Df Sum of Sq      F Pr(>F)
1     18 858.65
2     17 833.57  1    25.079 0.5115 0.4842
```

Adding age to the protein-only model improves the fit by $858.650 - 833.571 = 25.079$, so

$$F = \frac{25.079/1}{833.571/17} = \frac{25.079}{49.033} = 0.51 \sim F(1, 17),$$

which is not significant ($p = 0.48$): no evidence that carbohydrate depends on age, agreeing with the text. The numbers, however, differ from Table 6.5, where with weight in the model the improvement due to age was $606.022 - 567.663 = 38.359$ and $F = 38.359/35.489 = 1.08$ on 1 and 16 degrees of freedom:

```r
anova(lm(carbohydrate ~ weight + protein, data = carbohydrate), m66)
```

```
Analysis of Variance Table

Model 1: carbohydrate ~ weight + protein
Model 2: carbohydrate ~ age + weight + protein
  Res.Df    RSS Df Sum of Sq      F Pr(>F)
1     17 606.02
2     16 567.66  1    38.359 1.0812 0.3139
```

So both parts of the F ratio move: the sum of squares for age is 25.079 without weight but 38.359 with it, and the residual mean square falls from 49.03 to 35.49. This is the lack of orthogonality of Section 6.2.5: were X orthogonal, $X^T X$ would be block diagonal and neither b_1 nor its sum of squares would depend on which other columns were fitted. Here age and protein correlate at $r = 0.19$ and weight and protein at $r = 0.15$, so the contribution of age depends on the order of fitting — as does

the protein coefficient, 1.958 in Model (6.6) against 1.682 without weight. A sum of squares for age therefore means nothing until one says what else was in the model.

6.4 Problem 6.4 — It is well known that the concentration of cholesterol in blood serum in-

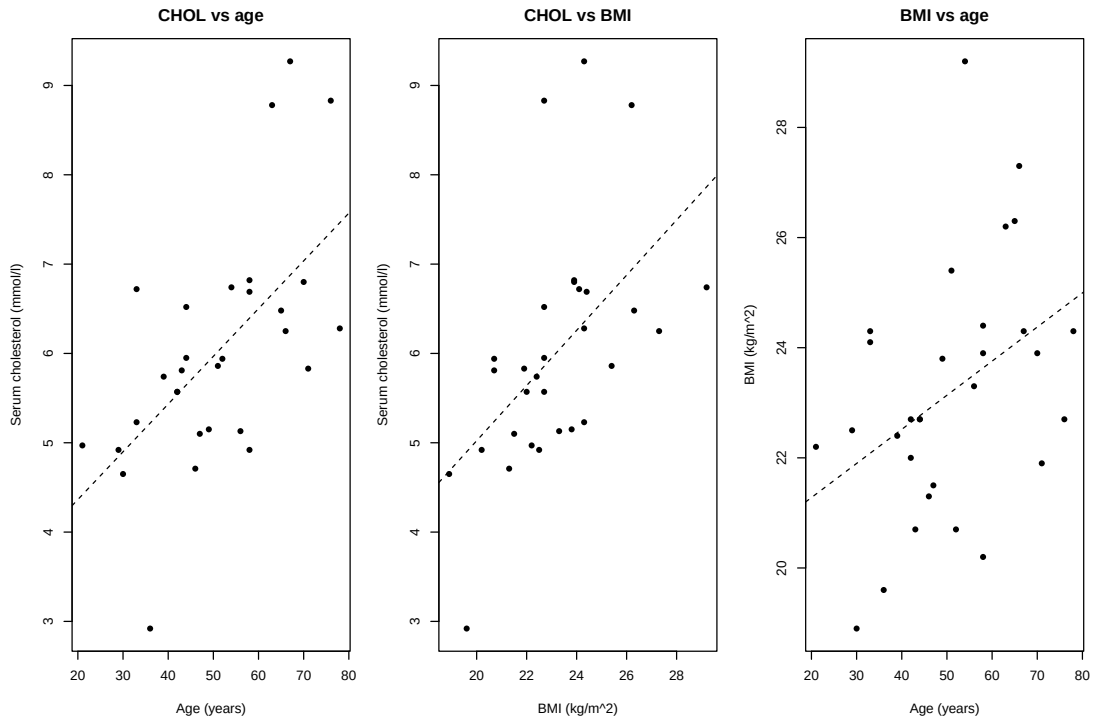
Problem 6.4. It is well known that the concentration of cholesterol in blood serum increases with age, but it is less clear whether cholesterol level is also associated with body weight. Table 6.24 shows for thirty women serum cholesterol (millimoles per liter), age (years) and body mass index (weight divided by height squared, where weight was measured in kilograms and height in meters). Use multiple regression to test whether serum cholesterol is associated with body mass index when age is already included in the model.
Table 6.24 Cholesterol (CHOL), age and body mass index (BMI) for thirty women, as triples (CHOL, Age, BMI): $(5.94, 52, 20.7)$, $(4.71, 46, 21.3)$, $(5.86, 51, 25.4)$, $(6.52, 44, 22.7)$, $(6.80, 70, 23.9)$, $(5.23, 33, 24.3)$, $(4.97, 21, 22.2)$, $(8.78, 63, 26.2)$, $(5.13, 56, 23.3)$, $(6.74, 54, 29.2)$, $(5.95, 44, 22.7)$, $(5.83, 71, 21.9)$, $(5.74, 39, 22.4)$, $(4.92, 58, 20.2)$, $(6.69, 58, 24.4)$, $(6.48, 65, 26.3)$, $(8.83, 76, 22.7)$, $(5.10, 47, 21.5)$, $(5.81, 43, 20.7)$, $(4.65, 30, 18.9)$, $(6.82, 58, 23.9)$, $(6.28, 78, 24.3)$, $(5.15, 49, 23.8)$, $(2.92, 36, 19.6)$, $(9.27, 67, 24.3)$, $(5.57, 42, 22.0)$, $(4.92, 29, 22.5)$, $(6.72, 33, 24.1)$, $(5.57, 42, 22.7)$, $(6.25, 66, 27.3)$. (difficulty: ⋆⋆)

Solution. Yes: BMI is associated with serum cholesterol after adjusting for age ($F = 5.15$ on 1 and 27 degrees of freedom, $p = 0.031$). The question is conditional, so it is a comparison of two nested Normal linear models,

$$M_1: \; E(Y_i) = \beta_0 + \beta_1 \text{age}_i, \qquad M_2: \; E(Y_i) = \beta_0 + \beta_1 \text{age}_i + \beta_2 \text{BMI}_i,$$

with $Y_i \sim N(\mu_i, \sigma^2)$, tested by $H_0 : \beta_2 = 0$ using the F statistic of Section 6.2.4.

```
library(dobson)
data(cholesterol)
chol <- as.data.frame(cholesterol)
par(mfrow = c(1,3), mar = c(4.5,4.5,3,1))
plot(chol$age, chol$chol, pch = 16, xlab = "Age (years)",
     ylab = "Serum cholesterol (mmol/l)", main = "CHOL vs age")
abline(lm(chol ~ age, data = chol), lty = 2)
plot(chol$bmi, chol$chol, pch = 16, xlab = "BMI (kg/m^2)",
     ylab = "Serum cholesterol (mmol/l)", main = "CHOL vs BMI")
abline(lm(chol ~ bmi, data = chol), lty = 2)
plot(chol$age, chol$bmi, pch = 16, xlab = "Age (years)",
     ylab = "BMI (kg/m^2)", main = "BMI vs age")
abline(lm(bmi ~ age, data = chol), lty = 2)
```




```
round(cor(chol), 3)
```

```
      chol   age   bmi
chol 1.000 0.603 0.535
age  0.603 1.000 0.403
bmi  0.535 0.403 1.000
```

The third panel shows why the question is worth asking: age and BMI are themselves correlated ($r = 0.40$), so the marginal cholesterol–BMI association ($r = 0.54$) is partly borrowed from age, and only a multiple regression separates them.

```
m1 <- lm(chol ~ age, data = chol)
m2 <- lm(chol ~ age + bmi, data = chol)
summary(m1)
```

```
Call:
lm(formula = chol ~ age, data = chol)

Residuals:
     Min       1Q   Median       3Q      Max
-2.29944 -0.67361  0.02992  0.40873  2.39393

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  3.29561    0.70480   4.676 6.72e-05 ***
age          0.05344    0.01336   3.999 0.000422 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 1.063 on 28 degrees of freedom
Multiple R-squared:  0.3635,        Adjusted R-squared:  0.3408
F-statistic: 15.99 on 1 and 28 DF,  p-value: 0.0004216
```

```
summary(m2)
```

```
Call:
lm(formula = chol ~ age + bmi, data = chol)

Residuals:
    Min      1Q  Median      3Q     Max
-1.7619 -0.7353 -0.0205  0.3772  2.3717

Coefficients:
```

```
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -0.73983    1.89641  -0.390  0.69951
age          0.04097    0.01363   3.006  0.00567 **
bmi          0.20137    0.08876   2.269  0.03149 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.992 on 27 degrees of freedom
Multiple R-squared:  0.4654,        Adjusted R-squared:  0.4258
F-statistic: 11.75 on 2 and 27 DF,  p-value: 0.000213
```

```r
anova(m1, m2)
```

```
Analysis of Variance Table

Model 1: chol ~ age
Model 2: chol ~ age + bmi
  Res.Df    RSS Df Sum of Sq      F  Pr(>F)
1     28 31.636
2     27 26.571  1    5.0655 5.1474 0.03149 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

```r
round(confint(m2), 4)
```

```
              2.5 % 97.5 %
(Intercept) -4.6309 3.1513
age          0.0130 0.0689
bmi          0.0193 0.3835
```

Adding BMI reduces the residual sum of squares from 31.636 to 26.571, an improvement of 5.066 on one degree of freedom, so with $\hat{\sigma}^2 = 26.571/27 = 0.984$,

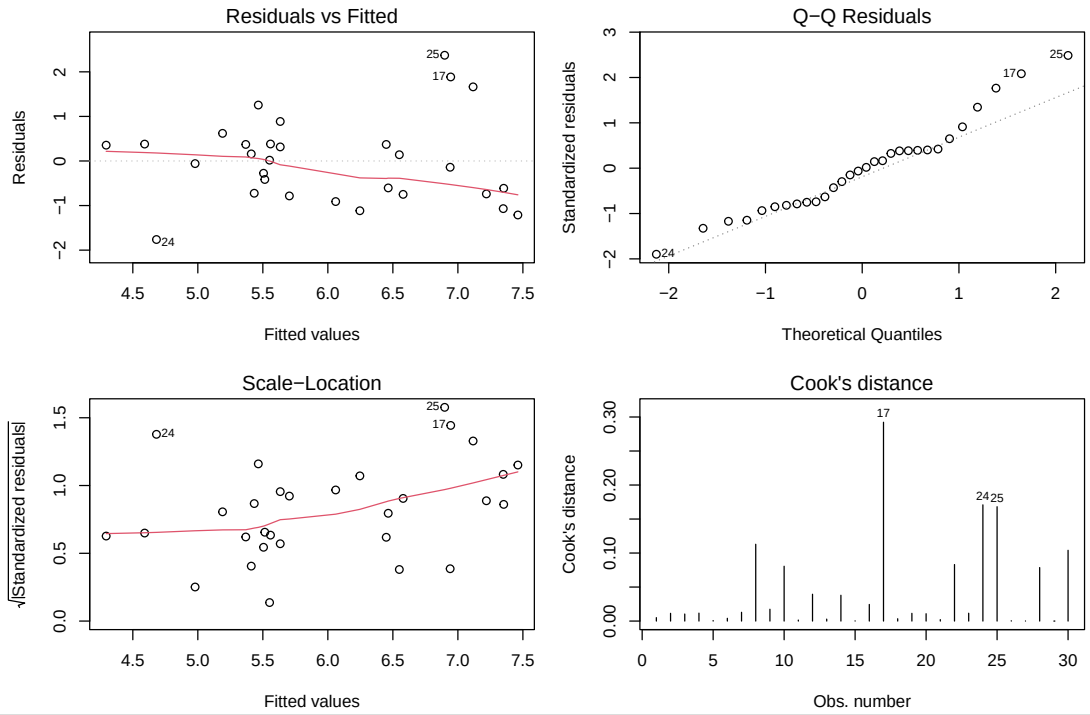
$$F = \frac{5.066/1}{26.571/27} = 5.15 \sim F(1, 27) \text{ under } H_0,$$

giving $p = 0.031$ (equivalently $t = 2.269$ on the BMI coefficient, $t^2 = 5.15$), so $H_0 : \beta_2 = 0$ is rejected at the 5% level.

Holding age fixed, each additional kg/m^2 of BMI carries 0.201 mmol/l more cholesterol, 95% CI $(0.019, 0.384)$ — wide and only just clear of zero, so with $N = 30$ the evidence is moderate rather than decisive. The unadjusted BMI slope of 0.309 shrinks to 0.201 on adjustment, so about a third of the apparent BMI effect is age acting through the age–BMI correlation. Age survives adjustment (0.041 mmol/l per year, $p = 0.006$), and the two covariates together explain 47% of the variance.

Checking the model.

```r
par(mfrow = c(2,2), mar = c(4.2,4.2,2.5,1))
plot(m2, which = 1:4)
```




```
round(head(sort(cooks.distance(m2), decreasing = TRUE), 4), 3)
anova(m2, lm(chol ~ age * bmi, data = chol))
```

```
   17    24    25     8
0.292 0.171 0.168 0.113

Analysis of Variance Table

Model 1: chol ~ age + bmi
Model 2: chol ~ age * bmi
  Res.Df    RSS Df Sum of Sq      F Pr(>F)
1     27 26.571
2     26 26.127  1   0.44352 0.4414 0.5123
```

Residuals show no pattern against fitted values and follow the Normal Q-Q line reasonably, and the largest Cook's distance is 0.29 (woman 17, aged 76, cholesterol 8.83 on average BMI), well short of 1. Adding an age-by-BMI interaction gives $F = 0.44$, $p = 0.51$, so the additive model is adequate.

6.5 Problem 6.5 — Table 6.25 shows plasma inorganic phosphate levels (mg/dl) one hour af-

Problem 6.5. Table 6.25 shows plasma inorganic phosphate levels (mg/dl) one hour after a standard glucose tolerance test for obese subjects, with or without hyperinsulinemia, and controls (data from Jones, 1987).

Table 6.25 Plasma phosphate levels in obese and control subjects. Hyperinsulinemic obese ($n = 11$): $2.3, 4.1, 4.2, 4.0, 4.6, 4.6, 3.8, 5.2, 3.1, 3.7, 3.8$. Non-hyperinsulinemic obese ($n = 8$): $3.0, 4.1, 3.9, 3.1, 3.3, 2.9, 3.3, 3.9$. Controls ($n = 12$): $3.0, 2.6, 3.1, 2.2, 2.1, 2.4, 2.8, 3.4, 2.9, 2.6, 3.1, 3.2$.

a. Perform a one-factor analysis of variance to test the hypothesis that there are no mean differences among the three groups. What conclusions can you draw?

b. Obtain a 95% confidence interval for the difference in means between the two obese groups.

c. Using an appropriate model, examine the standardized residuals for all the observations to look for any systematic effects and to check the Normality assumption. (difficulty: ⋆⋆)

Solution. The group means differ ($F = 11.65$, $p = 0.0002$), though the two obese groups are not separated. This is the one-factor analysis of variance of Section 6.4.1, with $J = 3$ groups of sizes

$n_1 = 12$, $n_2 = 8$, $n_3 = 11$ and $N = 31$:

$$E(Y_{jk}) = \mu + \alpha_j, \qquad Y_{jk} \sim N(\mu + \alpha_j, \sigma^2),$$

$j = 1, 2, 3$, with the corner-point constraint $\alpha_1 = 0$ (controls as reference). The null hypothesis is $H_0 : \alpha_1 = \alpha_2 = \alpha_3$, equivalently $E(Y_{jk}) = \mu$ for all groups.

```
library(dobson)
data(plasma)
pl <- as.data.frame(plasma)
pl$Group <- factor(pl$Group, levels = c("C","N-O","H-O"),
                   labels = c("control","non-hyperinsulinemic obese",
                              "hyperinsulinemic obese"))
aggregate(phosphate ~ Group, data = pl,
          function(z) c(n = length(z), mean = round(mean(z),3), sd = round(sd(z),3)))
```

```
                      Group phosphate.n phosphate.mean phosphate.sd
1                   control      12.000          2.783        0.409
2 non-hyperinsulinemic obese       8.000          3.438        0.463
3     hyperinsulinemic obese      11.000          3.945        0.778
```

Part (a) — the analysis of variance.

```
fit <- lm(phosphate ~ Group, data = pl)
anova(fit)
```

```
Analysis of Variance Table

Response: phosphate
          Df Sum Sq Mean Sq F value    Pr(>F)
Group      2 7.8083  3.9041  11.651 0.0002082 ***
Residuals 28 9.3827  0.3351
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

```
summary(fit)
```

```
Call:
lm(formula = phosphate ~ Group, data = pl)

Residuals:
     Min       1Q   Median       3Q      Max
-1.64545 -0.29148  0.01667  0.36667  1.25455

Coefficients:
                               Estimate Std. Error t value Pr(>|t|)
(Intercept)                      2.7833     0.1671  16.656 4.63e-16 ***
Groupnon-hyperinsulinemic obese  0.6542     0.2642   2.476   0.0196 *
Grouphyperinsulinemic obese      1.1621     0.2416   4.809 4.67e-05 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.5789 on 28 degrees of freedom
Multiple R-squared:  0.4542,        Adjusted R-squared:  0.4152
F-statistic: 11.65 on 2 and 28 DF,  p-value: 0.0002082
```

The between-groups sum of squares is 7.808 on 2 degrees of freedom and the residual sum of squares 9.383 on 28, so

$$F = \frac{7.8083/2}{9.3827/28} = \frac{3.904}{0.335} = 11.65 \sim F(2, 28)$$

under H_0, with $p = 0.0002$; reject H_0 decisively. The means are ordered controls 2.78 < non-hyperinsulinemic obese 3.44 < hyperinsulinemic obese 3.94 mg/dl, both obese groups above the controls by +0.65 (95% CI 0.11 to 1.20) and +1.16 (95% CI 0.67 to 1.66) mg/dl respectively, with group membership accounting for 45% of the variance. Obesity is thus associated with higher post-glucose-load phosphate, and hyperinsulinemia appears to raise it further — though part (b) shows the second step is the less well established.

Part (b) — difference between the two obese groups.

The contrast $\alpha_3 - \alpha_2$ has estimated standard error $\hat{\sigma}\sqrt{1/n_2 + 1/n_3}$ from the pooled residual mean square.

```
s2 <- summary(fit)$sigma^2
n2 <- 8; n3 <- 11
d  <- diff(tapply(pl$phosphate, pl$Group, mean)[2:3])
se <- sqrt(s2 * (1/n2 + 1/n3))
tc <- qt(0.975, df.residual(fit))
round(c(difference = unname(d), se = se,
        lower = unname(d) - tc*se, upper = unname(d) + tc*se), 4)
```

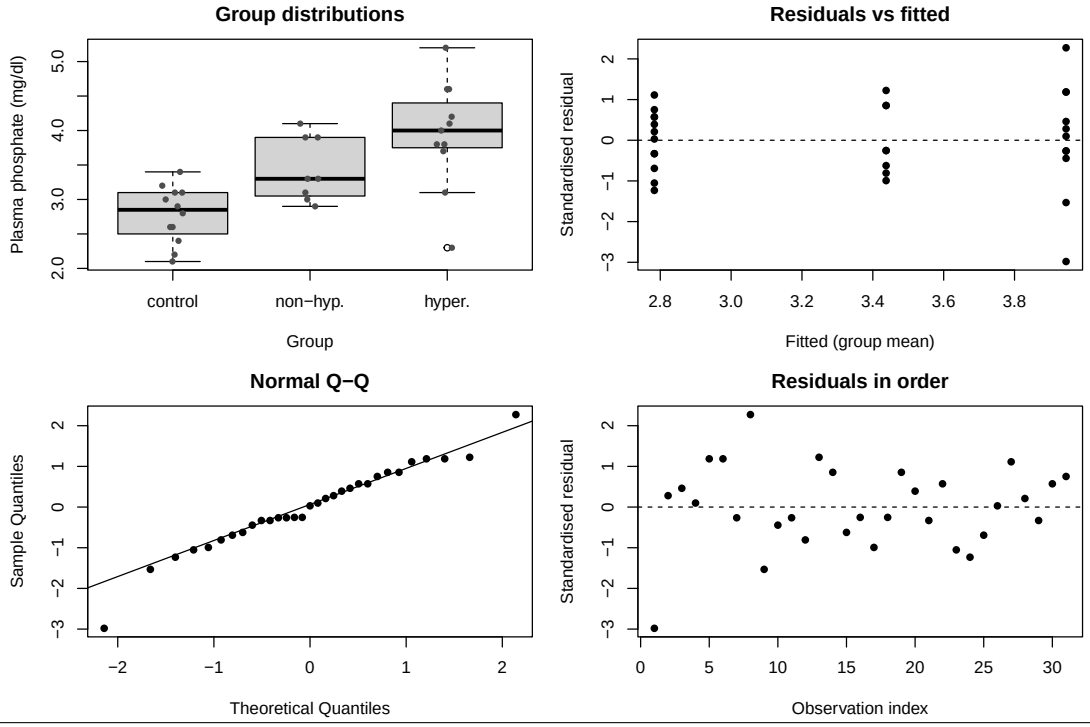
```
difference         se      lower      upper
    0.5080     0.2690    -0.0430     1.0589
```

The hyperinsulinemic obese average 0.508 mg/dl above the non-hyperinsulinemic obese, 95% CI $(-0.043, 1.059)$. The interval just includes zero, so the two obese groups are not separated at the 5% level ($t = 1.89$, $p = 0.069$): the overall F test is driven mainly by obese versus control. The interval uses the pooled $\hat{\sigma}^2 = 0.335$ on 28 degrees of freedom, legitimate only under the equal-variance assumption checked in part (c).

Part (c) — residuals.

The fitted value is the group mean, so the residuals $y_{jk} - \bar{y}_j$ carry the within-group information; standardize as in Section 6.2.6, $r_i = (y_i - \hat{\mu}_i)/\{\hat{\sigma}\sqrt{1 - h_{ii}}\}$.

```
par(mfrow = c(2,2), mar = c(4.2,4.2,2.5,1))
boxplot(phosphate ~ Group, data = pl, ylab = "Plasma phosphate (mg/dl)",
        names = c("control","non-hyp.","hyper."), main = "Group distributions")
stripchart(phosphate ~ Group, data = pl, vertical = TRUE, add = TRUE,
           pch = 16, col = "grey30", method = "jitter", jitter = 0.08)
r <- rstandard(fit)
plot(fitted(fit), r, pch = 16, xlab = "Fitted (group mean)",
     ylab = "Standardised residual", main = "Residuals vs fitted"); abline(h = 0, lty = 2)
qqnorm(r, pch = 16, main = "Normal Q-Q"); qqline(r)
plot(seq_along(r), r, pch = 16, xlab = "Observation index",
     ylab = "Standardised residual", main = "Residuals in order"); abline(h = 0, lty = 2)
```




```
bartlett.test(phosphate ~ Group, data = pl)
shapiro.test(rstandard(fit))
round(sort(rstandard(fit))[1:3], 3)
```

```
        Bartlett test of homogeneity of variances
```

```
data:  phosphate by Group
Bartlett's K-squared = 4.663, df = 2, p-value = 0.09715

        Shapiro-Wilk normality test

data:  rstandard(fit)
W = 0.96994, p-value = 0.5174

     1      9     24
-2.981 -1.532 -1.233
```

- Residuals versus fitted: the group with the largest mean has the widest spread, within-group standard deviations 0.41, 0.46, 0.78. Bartlett gives $p = 0.097$, not formally significant, but this is the one visible systematic effect and it strains the pooled-variance interval of part (b).
- Normal Q-Q: straight but for observation 1, the hyperinsulinemic subject with phosphate 2.3, standardized residual -2.98 — the outlier inflating the third group's variance. Shapiro–Wilk over all 31 residuals gives $p = 0.52$, so Normality is not rejected; excluding the point would sharpen the obese contrast, not weaken it.
- No trend against observation index, consistent with independence.

So the one-factor Normal model is acceptable, though the hyperinsulinemic-versus-non-hyperinsulinemic comparison rests on the equal-variance assumption and the one aberrant reading.

6.6 Problem 6.6 — The weights (in grams) of machine components of a standard size made

Problem 6.6. The weights (in grams) of machine components of a standard size made by four different workers on two different days are shown in Table 6.26; five components were chosen randomly from the output of each worker on each day. Perform an analysis of variance to test for differences among workers, among days, and possible interaction effects. What are your conclusions?
Table 6.26 Weights of machine components made by workers on different days. Day 1, worker 1: $35.7, 37.1, 36.7, 37.7, 35.3$; worker 2: $38.4, 37.2, 38.1, 36.9, 37.2$; worker 3: $34.9, 34.3, 34.5, 33.7, 36.2$; worker 4: $37.1, 35.5, 36.5, 36.0, 33.8$. Day 2, worker 1: $34.7, 35.2, 34.6, 36.4, 35.2$; worker 2: $36.9, 38.5, 36.4, 37.8, 36.1$; worker 3: $32.0, 35.2, 33.5, 32.9, 33.3$; worker 4: $35.8, 32.9, 35.7, 38.0, 36.1$. (difficulty: ⋆⋆)

Solution. Workers differ strongly, days mildly, and there is no interaction. This is the balanced two-factor analysis of variance of Section 6.4.2, with factor A = worker ($J = 4$), factor B = day ($K = 2$) and $L = 5$ replicates in each of the $JK = 8$ subgroups, so $N = 40$: fit the saturated Model (6.9) and the reduced Models (6.10) to (6.12) with corner-point constraints, and compare by F tests on differences in the scaled deviance $\sigma^2 D = y^T y - b^T X^T y$. (Two faults in the `dobson` copy of Table 6.26 need repair first: four all-missing rows 41–44, and 332.9 for worker 4 on day 2 where the table prints 32.9.)

```r
library(dobson)
data(machine)
mc <- as.data.frame(machine)
mc <- mc[!is.na(mc$weight), ]      # drop 4 empty rows shipped in the package
mc$weight[mc$weight > 100] <- 32.9 # 332.9 is a typo for 32.9
mc$day <- factor(mc$day); mc$worker <- factor(mc$worker)
tapply(mc$weight, list(mc$day, mc$worker), mean)
```

```
      1     2     3     4
1 36.50 37.56 34.72 35.78
2 35.22 37.14 33.38 35.70
```

The sequence of model comparisons.

```r
sat <- lm(weight ~ day * worker, data = mc)   # Model (6.9)
add <- lm(weight ~ day + worker, data = mc)   # Model (6.10)
mW  <- lm(weight ~ worker, data = mc)         # Model (6.11), B omitted
mD  <- lm(weight ~ day, data = mc)            # Model (6.12), A omitted
```

```
anova(add, sat)
```

```
Analysis of Variance Table

Model 1: weight ~ day + worker
Model 2: weight ~ day * worker
  Res.Df    RSS Df Sum of Sq     F Pr(>F)
1     35 43.154
2     32 40.196  3     2.958 0.785 0.5112
```

H_I (no interaction): $F = (2.958/3)/(40.196/32) = 0.79$ on 3 and 32 degrees of freedom, $p = 0.51$, so the day-to-day difference is the same for every worker and we proceed to the main effects.

```
anova(mW, add)   # HB: no day effect
```

```
Analysis of Variance Table

Model 1: weight ~ worker
Model 2: weight ~ day + worker
  Res.Df    RSS Df Sum of Sq      F  Pr(>F)
1     36 49.238
2     35 43.154  1     6.084 4.9344 0.03289 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

```
anova(mD, add)   # HA: no worker effect
```

```
Analysis of Variance Table

Model 1: weight ~ day
Model 2: weight ~ day + worker
  Res.Df    RSS Df Sum of Sq      F    Pr(>F)
1     38 97.776
2     35 43.154  3    54.622 14.767 2.236e-06 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

The full table collects this. The design being balanced, X can be made orthogonal (Section 6.2.5), so the sums of squares do not depend on the order of fitting and the sequential table matches the comparisons above.

```
anova(sat)
```

```
Analysis of Variance Table

Response: weight
           Df Sum Sq Mean Sq F value    Pr(>F)
day         1  6.084  6.0840  4.8435   0.03508 *
worker      3 54.622 18.2073 14.4948 3.895e-06 ***
day:worker  3  2.958  0.9860  0.7850   0.51117
Residuals  32 40.196  1.2561
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

The fitted additive model.

```
summary(add)
```

```
Call:
lm(formula = weight ~ day + worker, data = mc)

Residuals:
    Min      1Q  Median      3Q     Max
-2.4500 -0.6575 -0.1350  0.6825  2.6500

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  36.2500     0.3926  92.337  < 2e-16 ***
day2         -0.7800     0.3511  -2.221  0.03289 *
worker2       1.4900     0.4966   3.001  0.00494 **
worker3      -1.8100     0.4966  -3.645  0.00086 ***
```

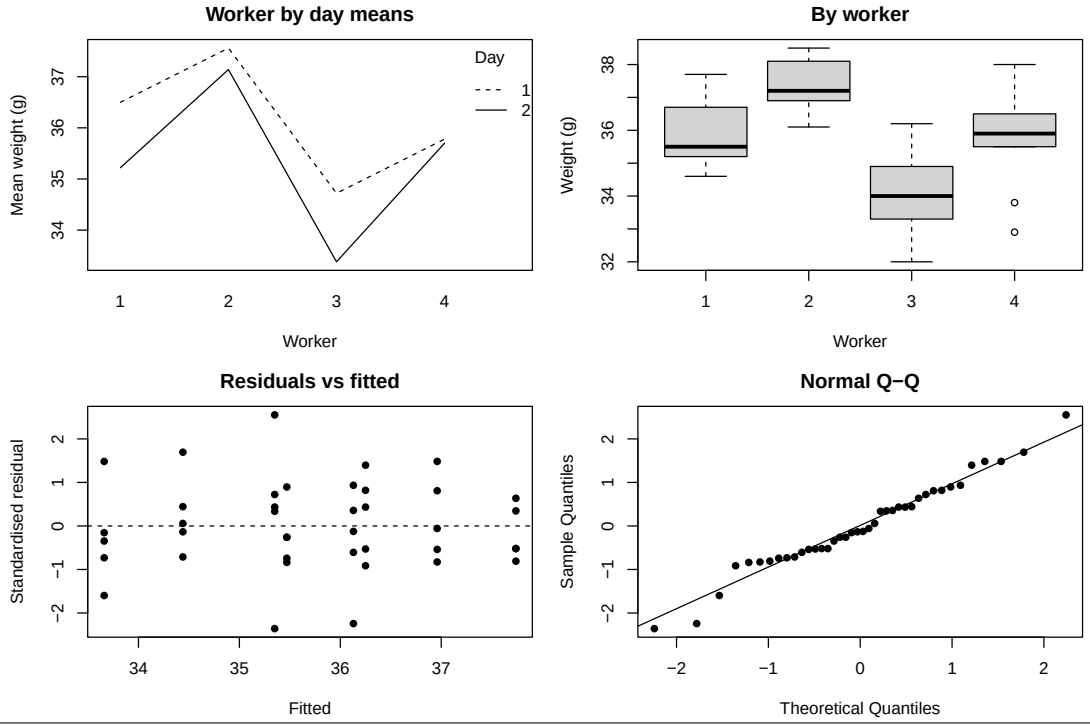
```
worker4      -0.1200     0.4966  -0.242  0.81046
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 1.11 on 35 degrees of freedom
Multiple R-squared:  0.5845,        Adjusted R-squared:  0.537
F-statistic: 12.31 on 4 and 35 DF,  p-value: 2.373e-06
```

```r
round(TukeyHSD(aov(weight ~ day + worker, data = mc))$worker, 4)
```

```
     diff     lwr     upr  p adj
2-1  1.49  0.1508  2.8292 0.0243
3-1 -1.81 -3.1492 -0.4708 0.0046
4-1 -0.12 -1.4592  1.2192 0.9949
3-2 -3.30 -4.6392 -1.9608 0.0000
4-2 -1.61 -2.9492 -0.2708 0.0133
4-3  1.69  0.3508  3.0292 0.0087
```

Diagnostics.

```r
par(mfrow = c(2,2), mar = c(4.2,4.2,2.5,1))
with(mc, interaction.plot(worker, day, weight, ylab = "Mean weight (g)",
     xlab = "Worker", trace.label = "Day", main = "Worker by day means"))
boxplot(weight ~ worker, data = mc, xlab = "Worker", ylab = "Weight (g)",
        main = "By worker")
r <- rstandard(add)
plot(fitted(add), r, pch = 16, xlab = "Fitted",
     ylab = "Standardised residual", main = "Residuals vs fitted"); abline(h = 0, lty = 2)
qqnorm(r, pch = 16, main = "Normal Q–Q"); qqline(r)
```




```r
shapiro.test(rstandard(add))
```

```
        Shapiro-Wilk normality test

data:  rstandard(add)
W = 0.97626, p-value = 0.5533
```

The interaction plot shows four near-parallel day-to-day drops, which is the picture behind $p = 0.51$ for H_I. Residuals are patternless against fitted values and close to Normal ($p = 0.55$).

Conclusions.

- Interaction: none ($F = 0.79$ on $3, 32$, $p = 0.51$); the additive model suffices.
- Workers: strong differences ($F = 14.77$ on $3, 35$, $p = 2 \times 10^{-6}$). Against worker 1, worker 2 runs 1.49 g heavy and worker 3 runs 1.81 g light, worker 4 indistinguishable. Tukey intervals separate

worker 2 from 1, 3, 4 and worker 3 from 1, 2, 4, but not 1 from 4. The spread from worker 3 to worker 2 is 3.3 g, about three residual standard deviations.

- Days: borderline ($F = 4.93$ on $1, 35$, $p = 0.033$); day 2 averages 0.78 g lighter, a modest shift smaller than the worker spread and resting on two days only.

The dominant source of variability is therefore the operator, not the day, with worker 3 producing systematically light components.

6.7 Problem 6.7 — For the balanced data in Table 6.12, the analyses in Section 6.4.2 showed

Problem 6.7. For the balanced data in Table 6.12, the analyses in Section 6.4.2 showed that the hypothesis tests were independent. An alternative specification of the design matrix for the saturated Model (6.9) with the corner point constraints $\alpha_1 = \beta_1 = (\alpha\beta)_{11} = (\alpha\beta)_{12} = (\alpha\beta)_{21} = (\alpha\beta)_{31} = 0$ is

$$\beta = \begin{bmatrix} \mu \\ \alpha_2 \\ \alpha_3 \\ \beta_2 \\ (\alpha\beta)_{22} \\ (\alpha\beta)_{32} \end{bmatrix}, \qquad X = \begin{bmatrix} 1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & -1 & -1 \\ 1 & 1 & 0 & -1 & -1 & 0 \\ 1 & 1 & 0 & -1 & -1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & -1 & 0 & -1 \\ 1 & 0 & 1 & -1 & 0 & -1 \\ 1 & 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 \end{bmatrix},$$

where the columns of X corresponding to the terms $(\alpha\beta)_{jk}$ are the products of columns corresponding to terms α_j and β_k.

a. Show that $X^T X$ has the block diagonal form described in Section 6.2.5. Fit the Model (6.9) and also Models (6.10) to (6.12) and verify that the results in Table 6.11 are the same for this specification of X.

b. Show that the estimates for the mean of the subgroup with treatments A3 and B2 for two different models are the same as the values given at the end of Section 6.4.2.

Table 6.12 gives, for factor A at three levels and factor B at two levels with two replicates per subgroup: A1B1 6.8, 6.6; A1B2 5.3, 6.1; A2B1 7.5, 7.4; A2B2 7.2, 6.5; A3B1 7.8, 9.1; A3B2 8.8, 9.1. (difficulty: ⋆⋆⋆)

Solution. The printed X is not the corner-point design matrix (whose entries would be 0/1) but an effect coding: the A-columns take $(-1,-1)$, $(1,0)$, $(0,1)$ on A1, A2, A3 and the B-column -1 on B1, $+1$ on B2, with the symbols $\mu, \alpha_2, \ldots$ re-used as names for the six free parameters. What is preserved is the column space: X has rank 6 and is constant within each subgroup, so it spans the same six-dimensional space as the corner-point X of Section 6.4.2, and the fitted values, residual sums of squares and F tests are unchanged — which is what part (a) asks. Likewise the first four columns span the additive design, since the constant with $I_{A2} - I_{A1}$ and $I_{A3} - I_{A1}$ spans $\{1, I_{A2}, I_{A3}\}$ and the B-column is $2I_{B2} - 1$. (The cross-reference to Table 6.11 is a misprint: the results to reproduce are Tables 6.13 and 6.14.)

Part (a) — block diagonality.

```
y  <- c(6.8,6.6,5.3,6.1, 7.5,7.4,7.2,6.5, 7.8,9.1,8.8,9.1)
a2 <- rep(c(-1,1,0), each = 4)
a3 <- rep(c(-1,0,1), each = 4)
b2 <- rep(c(-1,-1,1,1), 3)
X  <- cbind(mu = 1, a2 = a2, a3 = a3, b2 = b2, ab22 = a2*b2, ab32 = a3*b2)
t(X) %*% X
```

```
      mu a2 a3 b2 ab22 ab32
mu    12  0  0  0    0    0
a2     0  8  4  0    0    0
a3     0  4  8  0    0    0
b2     0  0  0 12    0    0
ab22   0  0  0  0    8    4
ab32   0  0  0  0    4    8
```

X^TX is block diagonal with blocks

$$X_1^TX_1 = [12], \quad X_2^TX_2 = \begin{bmatrix} 8 & 4 \\ 4 & 8 \end{bmatrix}, \quad X_3^TX_3 = [12], \quad X_4^TX_4 = \begin{bmatrix} 8 & 4 \\ 4 & 8 \end{bmatrix},$$

corresponding to the partition $X = [X_1, X_2, X_3, X_4]$ into the constant, the two A-columns, the B-column and the two interaction columns. This is exactly the structure of Section 6.2.5: $X_j^TX_k = O$ for $j \neq k$.

The zeros come from balance: each level of A occurs four times, so the A-columns sum to 0 (giving $X_1^TX_2 = O$); within each level of A the B-column is -1 twice and $+1$ twice, so products cancel in pairs ($X_2^TX_3 = O$); and for the interaction columns a_jb_2, $\sum_i a_{ij}b_{i2} = 0$ and $\sum_i a_{ij}b_{i2}^2 = \sum_i a_{ij} = 0$. Hence, by Section 6.2.5, $b_j = (X_j^TX_j)^{-1}X_j^Ty$ is unchanged by other blocks and b^TX^Ty decomposes additively.

```r
Xty <- t(X) %*% y
b   <- solve(t(X) %*% X, Xty)
round(data.frame(Xty = Xty[,1], b = b[,1]), 4)
c(yty = sum(y^2), bXty = sum(b * Xty))
```

```
       Xty       b
mu   88.2  7.3500
a2    3.8 -0.2000
a3   10.0  1.3500
b2   -2.2 -0.1833
ab22  0.8 -0.1167
ab32  3.0  0.4333
   yty   bXty
664.10 662.62
```

$y^Ty = 664.10$ and $b^TX^Ty = 662.62$, matching the text exactly, so the saturated model has scaled deviance $\sigma^2D_S = 1.48$. Now the nested models: Model (6.10) drops the last two columns, Model (6.11) the last three, Model (6.12) keeps columns 1 and 4.

```r
idx <- list(saturated = 1:6, additive = 1:4, "mu+alpha" = 1:3,
            "mu+beta" = c(1,4), "mu only" = 1)
for (nm in names(idx)) {
  Xi <- X[, idx[[nm]], drop = FALSE]
  bi <- solve(t(Xi) %*% Xi, t(Xi) %*% y)
  cat(sprintf("%-10s df=%2d  bXty=%10.4f  scaled deviance=%8.4f\n",
      nm, 12 - ncol(Xi), sum(bi * (t(Xi) %*% y)),
      sum(y^2) - sum(bi * (t(Xi) %*% y))))
}
```

```
saturated  df= 6  bXty=  662.6200  scaled deviance=  1.4800
additive   df= 8  bXty=  661.4133  scaled deviance=  2.6867
mu+alpha   df= 9  bXty=  661.0100  scaled deviance=  3.0900
mu+beta    df=10  bXty=  648.6733  scaled deviance= 15.4267
mu only    df=11  bXty=  648.2700  scaled deviance= 15.8300
```

Every entry reproduces Table 6.13, so the F tests are identical: $F = 2.45$ on $(2, 6)$ for H_I, $F = 1.63$ on $(1, 6)$ for H_B, $F = 25.82$ on $(2, 6)$ for H_A. The orthogonal partition of Table 6.2 then gives Table 6.14 line by line, each from its own block:

```r
blocks <- list(Mean = 1, "Levels of A" = 2:3, "Levels of B" = 4, "Interactions" = 5:6)
ss <- sapply(blocks, function(j) {
  Xj <- X[, j, drop = FALSE]
  bj <- solve(t(Xj) %*% Xj, t(Xj) %*% y)
  sum(bj * (t(Xj) %*% y))
})
data.frame(df = sapply(blocks, length), SS = round(ss, 4))
c(residual = sum(y^2) - sum(ss), total = sum(y^2))
```

```
             df       SS
Mean          1 648.2700
Levels of A   2  12.7400
Levels of B   1   0.4033
Interactions  2   1.2067
residual    total
    1.48   664.10
```

These are Table 6.14 — 648.27, 12.74, 0.4033, 1.2067, residual 1.48, total 664.10 — obtained without fitting the other terms. That is the content of "the hypothesis tests are independent": with orthogonal X each block's contribution is fixed, whatever the order of entry.

Part (b) — the A3, B2 subgroup mean.

The A3B2 rows of X (rows 11 and 12) are $(1, 0, 1, 1, 0, 1)$, so the saturated-model estimate of that subgroup mean is $\hat{\mu} + \hat{\alpha}_3 + \hat{\beta}_2 + \widehat{(\alpha\beta)}_{32}$; for the additive model it is the first four entries only.

```
badd <- solve(t(X[,1:4]) %*% X[,1:4], t(X[,1:4]) %*% y)
round(t(badd), 4)
c(saturated = sum(X[11, ] * b), additive = sum(X[11, 1:4] * badd))
```

```
       mu   a2   a3      b2
[1,] 7.35 -0.2 1.35 -0.1833
saturated  additive
 8.950000  8.516667
```

The saturated model gives $7.35 + 1.35 - 0.1833 + 0.4333 = 8.95$ and the additive model $7.35 + 1.35 - 0.1833 = 8.5167$, precisely the values quoted at the end of Section 6.4.2 — although the estimates themselves differ from the corner-point ones $(6.7, 1.75, -1.0, 1.5$ there), since fitted values depend on the column space and not on its parametrisation. Orthogonality shows in the estimates too: $\hat{\mu}, \hat{\alpha}_2, \hat{\alpha}_3, \hat{\beta}_2$ are the same $7.35, -0.20, 1.35, -0.1833$ in both models, dropping the interaction block leaving the others untouched, as Section 6.2.5 predicts.

6.8 Problem 6.8 — Table 6.27 shows the data from a fictitious two-factor experiment.

Problem 6.8. Table 6.27 shows the data from a fictitious two-factor experiment.
a. Test the hypothesis that there are no interaction effects.
b. Test the hypothesis that there is no effect due to Factor A (i) by comparing the models

$$E(Y_{jkl}) = \mu + \alpha_j + \beta_k \quad \text{and} \quad E(Y_{jkl}) = \mu + \beta_k;$$

(ii) by comparing the models

$$E(Y_{jkl}) = \mu + \alpha_j \quad \text{and} \quad E(Y_{jkl}) = \mu.$$

Explain the results.
Table 6.27 Two-factor experiment with unbalanced data. Factor A has three levels and factor B two. Cell A1B1 contains the single value 5; A1B2 contains $3, 4$; A2B1 contains $6, 4$; A2B2 contains $4, 3$; A3B1 contains 7; A3B2 contains $6, 8$. (difficulty: ⋆⋆)

Solution. There is no interaction, and the two tests of H_A give different answers because this design is not orthogonal. It is the counterpart of Exercise 6.7: there the data were balanced and the tests independent, here the subgroup sizes are $1, 2, 2, 2, 1, 2$. The models are (6.9) to (6.12) again, with $N = 10$.

```
library(dobson)
data(unbalanced)
ub <- as.data.frame(unbalanced)
ub$factorA <- factor(ub$factorA); ub$factorB <- factor(ub$factorB)
table(ub$factorA, ub$factorB)
tapply(ub$data, list(ub$factorA, ub$factorB), mean)
```

```
    B1 B2
```

```
  A1  1  2
  A2  2  2
  A3  1  2
   B1  B2
A1  5 3.5
A2  5 3.5
A3  7 7.0
```

```r
sat <- lm(data ~ factorA * factorB, data = ub)   # Model (6.9)
add <- lm(data ~ factorA + factorB, data = ub)   # Model (6.10)
mA  <- lm(data ~ factorA, data = ub)             # Model (6.11)
mB  <- lm(data ~ factorB, data = ub)             # Model (6.12)
m0  <- lm(data ~ 1, data = ub)
round(t(sapply(list(saturated = sat, additive = add, A_only = mA,
                    B_only = mB, mean = m0),
                function(m) c(df = df.residual(m), RSS = deviance(m)))), 4)
```

```
          df     RSS
saturated  4  5.0000
additive   6  6.0714
A_only     7  8.7500
B_only     8 24.3333
mean       9 26.0000
```

Part (a) — no interaction.

```r
anova(add, sat)
```

```
Analysis of Variance Table

Model 1: data ~ factorA + factorB
Model 2: data ~ factorA * factorB
  Res.Df    RSS Df Sum of Sq      F Pr(>F)
1      6 6.0714
2      4 5.0000  2    1.0714 0.4286 0.6782
```

$F = (1.0714/2)/(5.0000/4) = 0.43$ on 2 and 4 degrees of freedom, $p = 0.68$: no evidence against H_I. (The cell means hint at one — the B1 minus B2 difference is 1.5 at A1 and A2 but 0 at A3 — which four residual degrees of freedom cannot resolve.) So we test the main effect of A.

Part (b)(i) — A adjusted for B.

```r
anova(mB, add)
```

```
Analysis of Variance Table

Model 1: data ~ factorB
Model 2: data ~ factorA + factorB
  Res.Df     RSS Df Sum of Sq      F  Pr(>F)
1      8 24.3333
2      6  6.0714  2    18.262 9.0235 0.01553 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

Improvement $24.3333 - 6.0714 = 18.262$ on 2 d.f., residual mean square $6.0714/6 = 1.0119$, so

$$F = \frac{18.262/2}{6.0714/6} = 9.02 \sim F(2, 6), \qquad p = 0.016.$$

Part (b)(ii) — A alone.

```r
anova(m0, mA)
```

```
Analysis of Variance Table

Model 1: data ~ 1
Model 2: data ~ factorA
  Res.Df   RSS Df Sum of Sq   F  Pr(>F)
1      9 26.00
2      7  8.75  2     17.25 6.9 0.02211 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

Improvement $26.00 - 8.75 = 17.25$ on 2 d.f., residual mean square $8.75/7 = 1.25$, so $F = 8.625/1.25 = 6.90$ on 2 and 7 degrees of freedom, $p = 0.022$.

Explaining the results.

The two tests of "no effect due to factor A" give different sums of squares, 18.262 with B fitted against 17.250 without, and different statistics, 9.02 against 6.90; in Exercise 6.7 the balanced counterpart gave 0.4033 both times. With unequal subgroup sizes the A-columns are not orthogonal to the B-column (A1 is observed once at B1 and twice at B2, A2 twice at each), so X^TX is not block diagonal, b^TX^Ty does not split additively, and the sum of squares for A depends on whether B was fitted first — the Type I versus Type III distinction at the end of Section 6.2.5. Two effects combine:

- Numerators. Test (i) measures what A explains after B has taken what it can; test (ii) what A explains alone, part of which is B acting through the unequal cell counts.
- Denominators. Test (ii) estimates $\hat{\sigma}^2$ from a model omitting B, so any real B effect inflates the error (1.25 against 1.0119) and pushes F down.

Both routes reject H_A at the 5% level here, so factor A does affect the response: the additive fit puts A3 about 3.0 units above A1 ($t = 3.65$, $p = 0.011$), A2 indistinguishable from A1 (0.07), and B a non-significant -1.07 ($p = 0.15$). But the reported sums of squares depend on the order of fitting, so an unbalanced ANOVA sum of squares must always be quoted with the terms already in the model.

6.9 Problem 6.9 — Examine if there is a non-linear association between age and cholesterol

Problem 6.9. Examine if there is a non-linear association between age and cholesterol using the fractional polynomial approach for the data in Table 6.24 (serum cholesterol, age and body mass index for thirty women, transcribed in Exercise 6.4). (difficulty: ⋆⋆)

Solution. There is no evidence of a non-linear association. The fractional polynomial approach of Section 6.8 fits

$$E(Y_i) = \beta_0 + \beta_1 x_i^p, \qquad i = 1, \ldots, N,$$

for the eight candidate powers $p \in \{-2, -1, -0.5, 0, 0.5, 1, 2, 3\}$, with x^0 meaning $\log_e x$. All eight have two parameters, so they rank directly on residual sum of squares with no penalty term. Scaling x as the text advises, ages 21 to 78 give $x = \text{age}/50$, near 1.

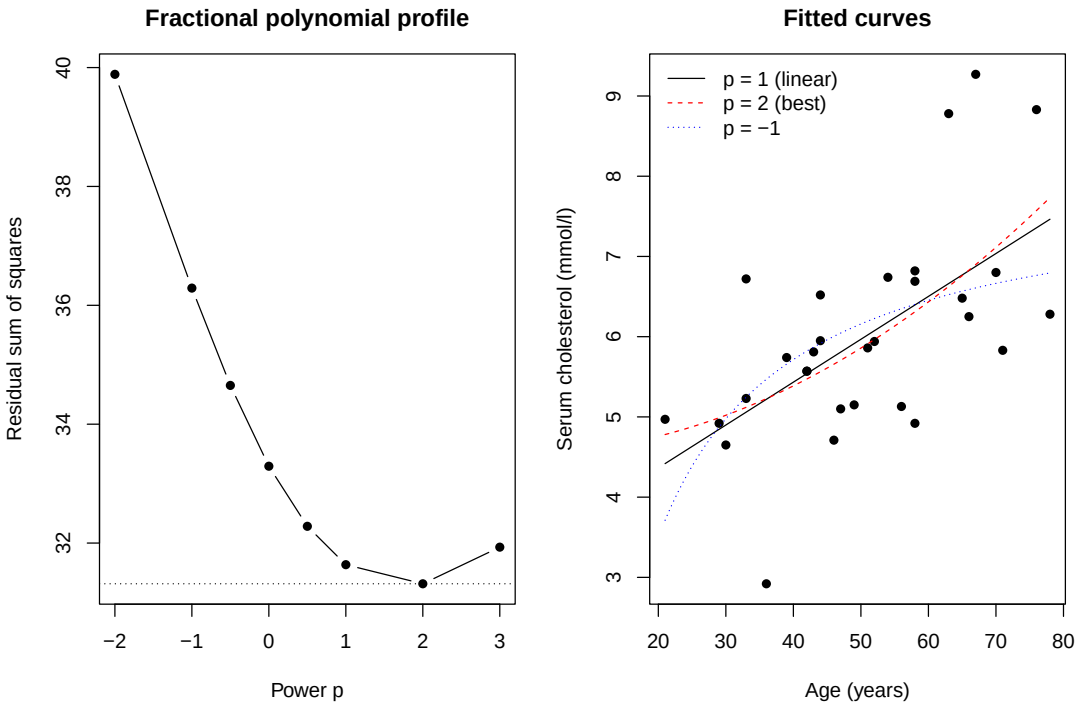
```
library(dobson)
data(cholesterol)
ch <- as.data.frame(cholesterol)
x  <- ch$age / 50
y  <- ch$chol
tf <- function(x, p) if (p == 0) log(x) else x^p
ps <- c(-2, -1, -0.5, 0, 0.5, 1, 2, 3)
res <- t(sapply(ps, function(p) {
  m <- lm(y ~ tf(x, p))
  c(p = p, RSS = deviance(m), AIC = AIC(m), R2 = summary(m)$r.squared)
}))
round(res, 4)
```

```
        p     RSS     AIC     R2
[1,] -2.0 39.8864 99.6815 0.1975
[2,] -1.0 36.2897 96.8464 0.2699
[3,] -0.5 34.6522 95.4613 0.3028
[4,]  0.0 33.2927 94.2605 0.3302
[5,]  0.5 32.2819 93.3356 0.3505
[6,]  1.0 31.6362 92.7294 0.3635
[7,]  2.0 31.3148 92.4231 0.3700
[8,]  3.0 31.9312 93.0079 0.3576
```

The profile is smooth and shallow, with a minimum at $p = 2$ (RSS 31.315) and the straight line $p = 1$ essentially tied behind it (RSS 31.636).

```
par(mfrow = c(1,2), mar = c(4.5,4.5,3,1))
plot(res[,"p"], res[,"RSS"], type = "b", pch = 16, xlab = "Power p",
```

```
     ylab = "Residual sum of squares", main = "Fractional polynomial profile")
abline(h = min(res[,"RSS"]), lty = 3)
plot(ch$age, y, pch = 16, xlab = "Age (years)",
     ylab = "Serum cholesterol (mmol/l)", main = "Fitted curves")
g <- seq(min(ch$age), max(ch$age), length = 200); gs <- g / 50
for (p in c(1, 2, -1)) {
  m <- lm(y ~ tf(x, p)); k <- which(c(1,2,-1) == p)
  lines(g, coef(m)[1] + coef(m)[2]*tf(gs, p), lty = k,
        col = c("black","red","blue")[k])
}
legend("topleft", c("p = 1 (linear)","p = 2 (best)","p = -1"),
       lty = 1:3, col = c("black","red","blue"), bty = "n")
```




```
summary(lm(y ~ tf(x, 2)))
```

```
Call:
lm(formula = y ~ tf(x, 2))

Residuals:
     Min       1Q   Median       3Q      Max
-2.30772 -0.59886  0.03643  0.39275  2.37140

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   4.5495     0.4076  11.162 8.05e-12 ***
tf(x, 2)      1.3082     0.3226   4.055 0.000363 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 1.058 on 28 degrees of freedom
Multiple R-squared:   0.37,        Adjusted R-squared:  0.3475
F-statistic: 16.44 on 1 and 28 DF,  p-value: 0.0003627
```

The gain from $p = 1$ to $p = 2$ is $31.636 - 31.315 = 0.32$ out of a total 49.7, about 0.6% of the residual variation, with R^2 moving from 0.364 to 0.370; in the fitted-curve panel the two coincide except at the extremes, where the data are thinnest. The eight-way comparison is a selection, not a test, so to test the curvature embed both in the quadratic $E(Y) = \beta_0 + \beta_1 x + \beta_2 x^2$, which contains the line as $\beta_2 = 0$.

```
anova(lm(y ~ x), lm(y ~ x + I(x^2)))
```

```
Analysis of Variance Table
```

```
Model 1: y ~ x
Model 2: y ~ x + I(x^2)
  Res.Df    RSS Df Sum of Sq      F Pr(>F)
1     28 31.636
2     27 31.307  1   0.32941 0.2841 0.5984
```

$F = 0.28$ on 1 and 27 degrees of freedom, $p = 0.60$: no evidence of curvature. The same holds after adjusting for body mass index, the covariate found relevant in Exercise 6.4.

```r
anova(lm(chol ~ age + bmi, data = ch), lm(chol ~ age + I(age^2) + bmi, data = ch))
```

```
Analysis of Variance Table

Model 1: chol ~ age + bmi
Model 2: chol ~ age + I(age^2) + bmi
  Res.Df    RSS Df Sum of Sq      F Pr(>F)
1     27 26.571
2     26 25.992  1   0.57809 0.5783 0.4538
```

So the search nominates $p = 2$, but the improvement on the line is negligible and no test finds curvature ($p = 0.60$ unadjusted, $p = 0.45$ adjusted for BMI): with $N = 30$ over ages 21 to 78 there is no evidence of a non-linear age–cholesterol association, and the linear term of Exercise 6.4, 0.053 mmol/l per year, remains the summary. The selection itself carries little weight — the RSS profile is nearly flat between $p = 0.5$ and $p = 3$, so the winner is decided well inside sampling noise, and the reported standard errors ignore that p was chosen from the same data.

7 Binary Variables and Logistic Regression

Contents

7.1 Problem 7.1 — The number of deaths from leukemia and other cancers among survivors

Problem 7.1. The number of deaths from leukemia and other cancers among survivors of the Hiroshima atom bomb are shown in Table 7.14, classified by the radiation dose received. The data refer to deaths during the period 1950–1959 among survivors who were aged 25 to 64 years in 1950 (from data set 13 of Cox and Snell, 1981, attributed to Otake, 1979).
a. Obtain a suitable model to describe the dose–response association between radiation and the proportional cancer mortality rates for leukemia. b. Examine how well the model describes the data. c. Interpret the results.
Table 7.14 (deaths from leukemia and other cancers classified by radiation dose received from the Hiroshima atomic bomb) has one column per radiation dose band, in rads: 0, 1–9, 10–49, 50–99, 100–199, 200+. The rows are
Leukemia deaths 13, 5, 5, 3, 4, 18
Other cancer deaths 378, 200, 151, 47, 31, 33
Total cancer deaths 391, 205, 156, 50, 35, 51
(difficulty: ⋆⋆)

Solution. A logistic dose–response model in dose, linear on the logit scale, fits these data well. A *proportional* mortality rate is the share of cancer deaths that are leukemia deaths, so

$$Y_i \sim \mathrm{Bin}(n_i, \pi_i), \qquad n_i = \text{total cancer deaths}, \qquad \pi_i = \Pr(\text{leukemia} \mid \text{cancer death}),$$

the setting of Section 7.4 with $N = 6$ covariate patterns. Conditioning on "died of cancer" removes the unknown number of survivors, at the price of reading the results relative to other cancer deaths rather than as absolute risks. The bands are intervals, so score them by midpoints 0, 5, 29.5, 74.5, 149.5 rads and, for the open-ended 200+ band, 300 rads, whose influence is checked below.

```
library(dobson)
data(hiroshima)
h <- hiroshima
names(h) <- c("dose", "leuk", "other", "total")
h$mid <- c(0, 5, 29.5, 74.5, 149.5, 300)
h$p <- h$leuk / h$total
data.frame(dose = as.character(h$dose), n = h$total, y = h$leuk,
           mid = h$mid, p = round(h$p, 4),
           logit = round(log(h$p / (1 - h$p)), 3))
```

```
       dose   n  y   mid      p  logit
1         0 391 13   0.0 0.0332 -3.370
2     1 to 9 205  5   5.0 0.0244 -3.689
3   10 to 49 156  5  29.5 0.0321 -3.408
4   50 to 99  50  3  74.5 0.0600 -2.752
5 100 to 199  35  4 149.5 0.1143 -2.048
6      200 +  51 18 300.0 0.3529 -0.606
```

The empirical logits are close to linear in dose, which is what the logistic dose–response model of Section 7.3 assumes.
(a) The model. Fit

$$\log\left(\frac{\pi_i}{1-\pi_i}\right) = \beta_1 + \beta_2 x_i,$$

by maximum likelihood, i.e. maximising the log-likelihood (7.4).

```
m1 <- glm(cbind(leuk, other) ~ mid, family = binomial, data = h)
summary(m1)
```

```
Call:
glm(formula = cbind(leuk, other) ~ mid, family = binomial, data = h)

Coefficients:
             Estimate Std. Error z value Pr(>|z|)
```

```
(Intercept) -3.523825   0.206908 -17.031  < 2e-16 ***
mid          0.009716   0.001228   7.912 2.53e-15 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 54.35089  on 5  degrees of freedom
Residual deviance:  0.67956  on 4  degrees of freedom
AIC: 26.345

Number of Fisher Scoring iterations: 4
```

So $b_1 = -3.524$ (0.207) and $b_2 = 0.009716$ (0.001228).

The dose effect is overwhelming: the drop in deviance from the minimal model to this one is $C = 54.351 - 0.680 = 53.67$ on 1 degree of freedom, which is the likelihood ratio chi-squared statistic of Section 7.5 (and Exercise 7.4), far beyond any tabulated $\chi^2(1)$ value.

(b) How well the model describes the data. The residual deviance (7.5) is $D = 0.680$ on $N - p = 6 - 2 = 4$ degrees of freedom, and the Pearson statistic (7.6) is $X^2 = 0.672$, also on 4 degrees of freedom.

```r
X2 <- sum(residuals(m1, type = "pearson")^2)
c(deviance = deviance(m1), pearson = X2, df = df.residual(m1),
  p_dev = pchisq(deviance(m1), 4, lower.tail = FALSE),
  p_X2 = pchisq(X2, 4, lower.tail = FALSE))
```

```
 deviance   pearson        df     p_dev      p_X2
0.6795634 0.6716142 4.0000000 0.9538250 0.9547828
```

Both fall far below their expected value of 4, $p \approx 0.95$ — the fit is if anything suspiciously good, common when a smooth monotone trend runs through six points. Cell by cell, the smallest expected leukemia count is 2.9, above the threshold flagged in Section 7.5, and no residual is large.

```r
data.frame(dose = as.character(h$dose), obs = h$leuk,
           fitted = round(fitted(m1) * h$total, 2),
           pearson = round(residuals(m1, "pearson"), 3),
           deviance = round(residuals(m1, "deviance"), 3))
```

```
        dose obs fitted pearson deviance
1          0  13  11.20   0.546    0.533
2      1 to 9   5   6.16  -0.473   -0.488
3    10 to 49   5   5.90  -0.376   -0.386
4    50 to 99   3   2.87   0.081    0.081
5 100 to 199   4   3.92   0.044    0.044
6       200 +  18  17.97   0.010    0.010
```

Three further checks. Adding a quadratic in dose buys nothing; the saturated (dose as a factor) model has a worse AIC than the two-parameter linear model; and the probit and complementary log-log links of Section 7.3 fit no better than the logit, so the data cannot discriminate between links here – which is expected, since all the fitted probabilities are below 0.4 where the three links are close.

```r
mq <- glm(cbind(leuk, other) ~ mid + I(mid^2), family = binomial, data = h)
mf <- glm(cbind(leuk, other) ~ factor(dose), family = binomial, data = h)
c(dev_quad = deviance(mq), p_quadratic_term = summary(mq)$coef[3, 4],
  AIC_linear = AIC(m1), AIC_saturated = AIC(mf),
  dev_probit = deviance(glm(cbind(leuk, other) ~ mid, binomial("probit"), data = h)),
  dev_cloglog = deviance(glm(cbind(leuk, other) ~ mid, binomial("cloglog"), data = h)))
```

```
  dev_quad p_quadratic_term       AIC_linear    AIC_saturated
 0.6687957        0.9176481       26.3445651       33.6650017
dev_probit      dev_cloglog
 0.8440787        0.6791914
```

The one genuinely soft assumption is the score of 300 rads for the open-ended top band. Refitting with 250 and 400 moves the slope but not the conclusion:

```r
sapply(c(250, 300, 400), function(top) {
  h$mid <- c(0, 5, 29.5, 74.5, 149.5, top)
  m <- glm(cbind(leuk, other) ~ mid, family = binomial, data = h)
  c(slope = coef(m)[2], deviance = deviance(m))
```

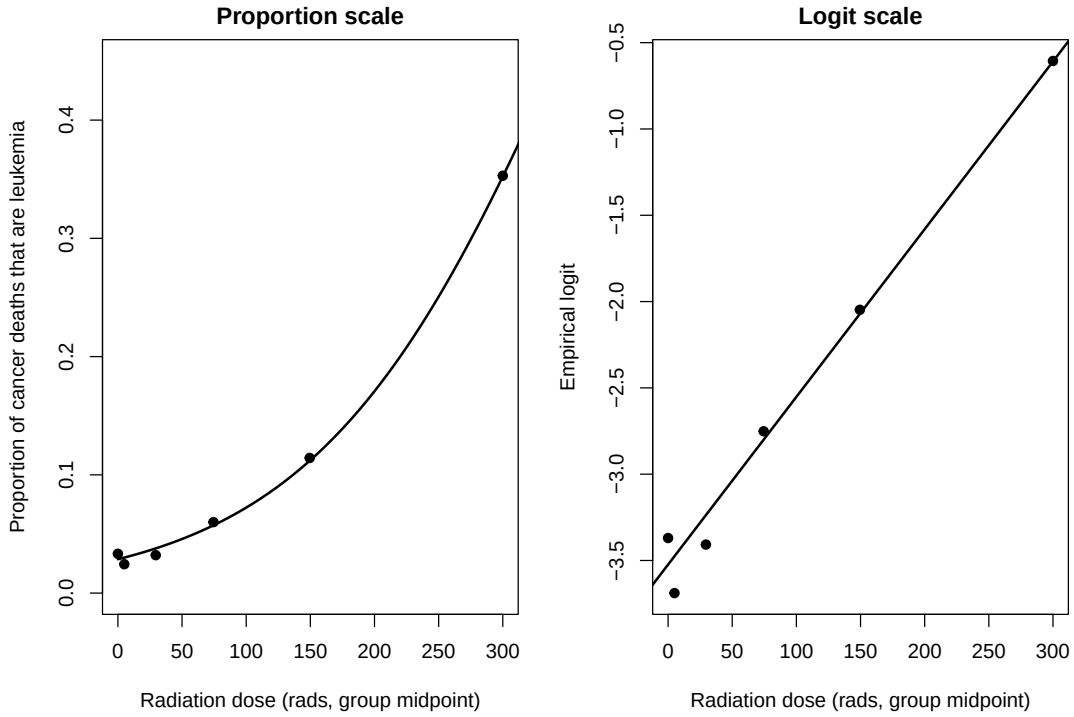
```
})
```

```
                [,1]        [,2]        [,3]
slope.mid 0.01160255 0.009716222 0.007232667
deviance  1.02076456 0.679563424 1.055412491
```

The slope is inversely proportional to the assumed midpoint, as it must be, and the fit is good under all three. So the **shape** of the dose–response relation is well established; the numerical value of "risk per rad" is only as good as the dose scoring.

The fitted curve against the data, on both the probability and the logit scale:

```
par(mfrow = c(1, 2), mar = c(4.5, 4.5, 2, 1))
plot(h$mid, h$p, pch = 19, ylim = c(0, 0.45), main = "Proportion scale",
     xlab = "Radiation dose (rads, group midpoint)",
     ylab = "Proportion of cancer deaths that are leukemia")
xx <- seq(0, 320, length = 200)
lines(xx, predict(m1, newdata = data.frame(mid = xx), type = "response"), lwd = 2)
plot(h$mid, log(h$p / (1 - h$p)), pch = 19, main = "Logit scale",
     xlab = "Radiation dose (rads, group midpoint)", ylab = "Empirical logit")
abline(coef(m1), lwd = 2)
```



(c) Interpretation. The estimated log-odds of a cancer death being a leukemia death rises linearly with dose at 0.00972 per rad. Exponentiating, each extra 100 rads multiplies the odds by

$$\exp(100 \times 0.009716) = 2.64,$$

with a Wald 95% interval $\exp(100 \times (0.009716 \pm 1.96 \times 0.001228)) = (2.08,\ 3.36)$.

```
exp(100 * c(est = coef(m1)[2], confint.default(m1)[2, ]))
```

```
 est.mid    2.5 %   97.5 %
2.642227 2.077027 3.361230
```

At zero dose $\hat{\pi} = e^{-3.524}/(1 + e^{-3.524}) = 0.0286$, the background share, rising to 0.352 at 300 rads — a twelve-fold increase. So radiation raises the leukemia death rate much more steeply than the rate from other cancers, dose-dependently across the whole observed range with no sign of a threshold. Two qualifications on the reading: the denominator being total cancer deaths, this is a *relative* statement, consistent with radiation raising both provided it raises leukemia faster; and by Section 7.9 an odds ratio of 2.64 per 100 rads is not a risk ratio — the two are close at low dose (fitted proportion ratio $0.0723/0.0286 = 2.53$ from 0 to 100 rads) but diverge by 200–300 rads.

7.2 Problem 7.2 — Odds ratios. Consider a 2×2 contingency table from a prospective study

Problem 7.2. *Odds ratios.* Consider a 2×2 contingency table from a prospective study in which people who were or were not exposed to some pollutant are followed up and, after several years, categorized according to the presence or absence of a disease. Table 7.15 shows the probabilities for each cell: the row "Exposed" has probability π_1 of being diseased and $1-\pi_1$ of not being diseased, and the row "Not exposed" has probability π_2 of being diseased and $1-\pi_2$ of not being diseased. The odds of disease for either exposure group is $O_i = \pi_i/(1-\pi_i)$, for $i = 1, 2$, and so the odds ratio

$$\phi = \frac{O_1}{O_2} = \frac{\pi_1(1-\pi_2)}{\pi_2(1-\pi_1)}$$

is a measure of the relative likelihood of disease for the exposed and not exposed groups.
a. For the simple logistic model $\pi_i = e^{\beta_i}/(1+e^{\beta_i})$, show that if there is no difference between the exposed and not exposed groups (i.e., $\beta_1 = \beta_2$), then $\phi = 1$. b. Consider J 2×2 tables like Table 7.15, one for each level x_j of a factor, such as age group, with $j = 1, \ldots, J$. For the logistic model

$$\pi_{ij} = \frac{\exp(\alpha_i + \beta_i x_j)}{1 + \exp(\alpha_i + \beta_i x_j)}, \qquad i = 1, 2, \quad j = 1, \ldots, J.$$

Show that $\log \phi$ is constant over all tables if $\beta_1 = \beta_2$ (McKinlay 1978).
(difficulty: ⋆)

Solution. (a) $\log \phi = \beta_1 - \beta_2$, so $\beta_1 = \beta_2$ gives $\phi = 1$. Under $\pi_i = e^{\beta_i}/(1+e^{\beta_i})$ we have $1-\pi_i = 1/(1+e^{\beta_i})$, whence

$$O_i = \frac{\pi_i}{1-\pi_i} = e^{\beta_i}, \qquad \phi = \frac{O_1}{O_2} = e^{\beta_1 - \beta_2},$$

which equals 1 exactly when $\beta_1 = \beta_2$.
(b) Within the j-th table the same step gives $O_{ij} = \exp(\alpha_i + \beta_i x_j)$, so

$$\log \phi_j = (\alpha_1 - \alpha_2) + (\beta_1 - \beta_2) x_j. \qquad (*)$$

If $\beta_1 = \beta_2$ the only j-dependent term vanishes and $\log \phi_j = \alpha_1 - \alpha_2$ for every j, a single odds ratio $\phi = \exp(\alpha_1 - \alpha_2)$ across all J tables. Conversely, provided the x_j are not all equal, $(*)$ is constant only if $\beta_1 = \beta_2$: equal slopes and a homogeneous odds ratio are the same no-interaction hypothesis, which is the difference between Models 1 and 2 of Section 7.4.
Numerically, with $\alpha_1 = -3.0$, $\alpha_2 = -3.8$ and common slope $\beta = 0.04$ over five age levels, $\log \phi_j$ should be $\alpha_1 - \alpha_2 = 0.8$ in every stratum.

```
x <- c(25, 35, 45, 55, 65)
a <- c(-3.0, -3.8)
b <- c(0.04, 0.04)
pi <- outer(1:2, x, function(i, xj) plogis(a[i] + b[i] * xj))
odds <- pi / (1 - pi)
round(rbind(pi1 = pi[1, ], pi2 = pi[2, ], logphi = log(odds[1, ] / odds[2, ])), 4)
```

```
          [,1]   [,2]   [,3]  [,4]   [,5]
pi1     0.1192 0.1680 0.2315 0.310 0.4013
pi2     0.0573 0.0832 0.1192 0.168 0.2315
logphi 0.8000 0.8000 0.8000 0.800 0.8000
```

The risks change greatly across strata while $\log \phi_j$ does not. With unequal slopes ($\beta_1 = 0.04$, $\beta_2 = 0.06$) it instead runs down linearly in x_j with slope $\beta_1 - \beta_2 = -0.02$:

```
b2 <- c(0.04, 0.06)
pi <- outer(1:2, x, function(i, xj) plogis(a[i] + b2[i] * xj))
odds <- pi / (1 - pi)
round(log(odds[1, ] / odds[2, ]), 4)
```

```
[1]  0.3  0.1 -0.1 -0.3 -0.5
```

7.3 Problem 7.3 — Tables 7.16 and 7.17 show the survival 50 years after graduation of men

Problem 7.3. Tables 7.16 and 7.17 show the survival 50 years after graduation of men and women who graduated each year from 1938 to 1947 from various faculties of the University of Adelaide (data compiled by J.A. Keats). The columns labelled S contain the number of graduates who survived and the columns labelled T contain the total number of graduates. There were insufficient women graduates from the faculties of Medicine and Engineering to warrant analysis.
a. Are the proportions of graduates who survived for 50 years after graduation the same all years of graduation? b. Are the proportions of male graduates who survived for 50 years after graduation the same for all Faculties? c. Are the proportions of female graduates who survived for 50 years after graduation the same for Arts and Science? d. Is the difference between men and women in the proportion of graduates who survived for 50 years after graduation the same for Arts and Science?
Table 7.16 (men) gives S and T by year of graduation for four faculties. Medicine: 1938 (18, 22), 1939 (16, 23), 1940 (7, 17), 1941 (12, 25), 1942 (24, 50), 1943 (16, 21), 1944 (22, 32), 1945 (12, 14), 1946 (22, 34), 1947 (28, 37); total (177, 275). Arts: 1938 (16, 30), 1939 (13, 22), 1940 (11, 25), 1941 (12, 14), 1942 (8, 12), 1943 (11, 20), 1944 (4, 10), 1945 (4, 12), 1946 no entry, 1947 (13, 23); total (92, 168). Science: 1938 (9, 14), 1939 (9, 12), 1940 (12, 19), 1941 (12, 15), 1942 (20, 28), 1943 (16, 21), 1944 (25, 31), 1945 (32, 38), 1946 (4, 5), 1947 (25, 31); total (164, 214). Engineering: 1938 (10, 16), 1939 (7, 11), 1940 (12, 15), 1941 (8, 9), 1942 (5, 7), 1943 (1, 2), 1944 (16, 22), 1945 (19, 25), 1946 no entry, 1947 (25, 35); total as printed (100, 139).
Table 7.17 (women) gives S and T for two faculties. Arts: 1938 (14, 19), 1939 (11, 16), 1940 (15, 18), 1941 (15, 21), 1942 (8, 9), 1943 (13, 13), 1944 (18, 22), 1945 (18, 22), 1946 (1, 1), 1947 (13, 16); total (126, 157). Science: 1938 (1, 1), 1939 (4, 4), 1940 (6, 7), 1941 (3, 3), 1942 (4, 4), 1943 (8, 9), 1944 (5, 5), 1945 (16, 17), 1946 (1, 1), 1947 (10, 10); total (58, 61).
(difficulty: ⋆⋆)

Solution. (a) No evidence of a year effect; (b) faculties differ; (c) Arts and Science differ; (d) no interaction. Each cell is a Binomial count $S_{fsy} \sim \text{Bin}(T_{fsy}, \pi_{fsy})$ for faculty f, sex s, year y, so all four questions are comparisons of nested logistic models tested by differences of deviance (7.5), as in Section 7.5.

```
library(dobson)
data(graduates)
g <- subset(as.data.frame(graduates), survive != "*")
g$survive <- as.numeric(g$survive)
g$total <- as.numeric(g$total)
g$died <- g$total - g$survive
g$faculty <- factor(g$faculty)
g$sex <- factor(g$sex)
tab <- aggregate(cbind(survive, total) ~ faculty + sex, data = g, FUN = sum)
tab$p <- round(tab$survive / tab$total, 3)
tab
```

```
      faculty   sex survive total     p
1        arts   men      92   168 0.548
2 engineering   men     103   142 0.725
3    medicine   men     177   275 0.644
4     science   men     164   214 0.766
5        arts women     126   157 0.803
6     science women      58    61 0.951
```

The two empty cells (Arts and Engineering men, 1946) are stored as $*$ and dropped. Table 7.16's printed Engineering totals $(100, 139)$ are three short of the yearly entries, which sum to $(103, 142)$; the models use the entries. Already women survive better than men, and Science better than Arts.
(a) Year of graduation. The groups are unbalanced across years, so year must be tested adjusted for faculty and sex; fit it both as a 9-degree-of-freedom factor and as a linear trend.

```
base <- glm(cbind(survive, died) ~ faculty * sex, family = binomial, data = g)
yr_f <- glm(cbind(survive, died) ~ faculty * sex + factor(year), family = binomial, data = g)
```

```r
anova(base, yr_f, test = "Chisq")
```

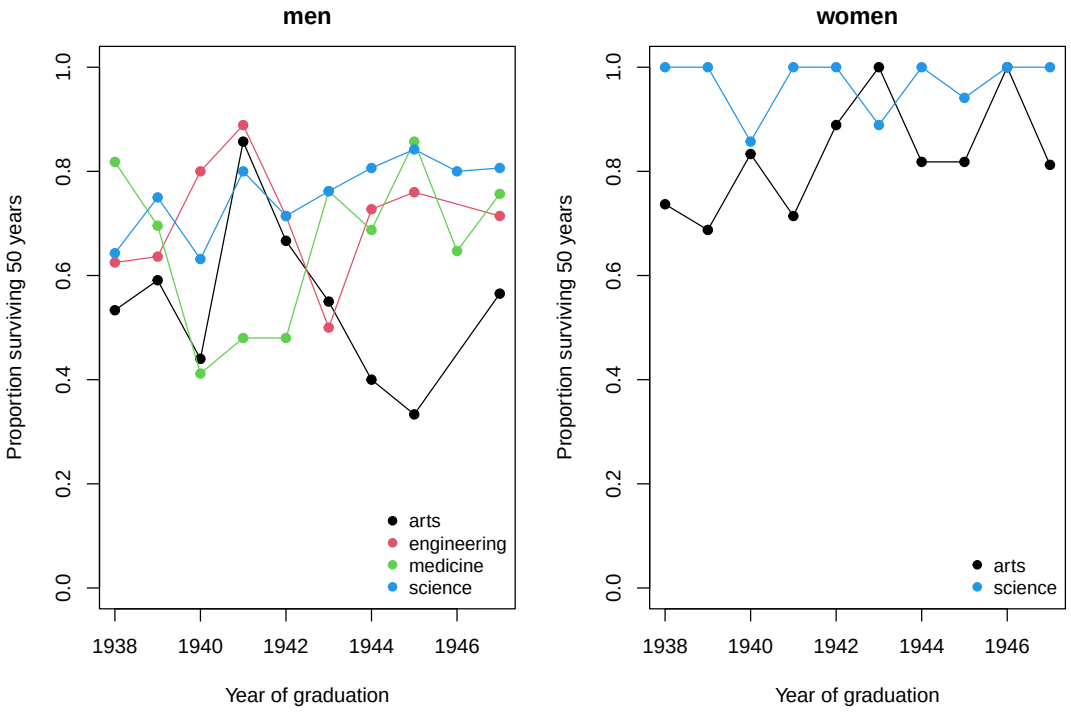
```
Analysis of Deviance Table

Model 1: cbind(survive, died) ~ faculty * sex
Model 2: cbind(survive, died) ~ faculty * sex + factor(year)
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
1        52     56.765
2        43     47.694  9    9.071   0.4307
```

```r
yr_l <- glm(cbind(survive, died) ~ faculty * sex + I(year - 1938), family = binomial, data =
↪  g)
anova(base, yr_l, test = "Chisq")
```

```
Analysis of Deviance Table

Model 1: cbind(survive, died) ~ faculty * sex
Model 2: cbind(survive, died) ~ faculty * sex + I(year - 1938)
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
1        52     56.765
2        51     53.314  1   3.4505  0.06323 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The unstructured year effect gives $\Delta D = 9.07$ on 9 df ($p = 0.43$), no evidence; the linear trend gives $\Delta D = 3.45$ on 1 df ($p = 0.063$), a hint of about 4.6% higher odds per year for later cohorts. Since every cell is followed exactly 50 years, age at follow-up is constant and a trend could not be an age artefact; falling background mortality over 1988–1997 and wartime service among the earliest men are the plausible sources. So there is no convincing evidence that survival differs by year of graduation, with a weak upward trend these data cannot resolve. The faculty-by-sex model is itself adequate, $D = 56.77$ on 52 df ($p = 0.30$), so the year-to-year scatter is Binomial noise.

```r
par(mfrow = c(1, 2), mar = c(4.5, 4.5, 2.5, 1))
cols <- c(arts = 1, engineering = 2, medicine = 3, science = 4)
for (s in c("men", "women")) {
  d <- subset(g, sex == s)
  plot(range(g$year), c(0, 1), type = "n", main = s,
       xlab = "Year of graduation", ylab = "Proportion surviving 50 years")
  for (f in levels(droplevels(d$faculty))) {
    dd <- subset(d, faculty == f)
    points(dd$year, dd$survive / dd$total, col = cols[f], pch = 19)
    lines(dd$year, dd$survive / dd$total, col = cols[f])
  }
  legend("bottomright", legend = levels(droplevels(d$faculty)),
         col = cols[levels(droplevels(d$faculty))], pch = 19, bty = "n", cex = 0.9)
}
```



The plot agrees: the year-to-year zig-zag is large but unsystematic, and the extreme points have tiny denominators (Engineering 1943 is 1 of 2; several women's Science cells have $T \leq 5$).

(b) Faculty, men. Test the four-level faculty factor against the minimal model on men alone.

```
men <- subset(g, sex == "men")
anova(glm(cbind(survive, died) ~ 1, binomial, data = men),
      glm(cbind(survive, died) ~ faculty, binomial, data = men), test = "Chisq")
```

```
Analysis of Deviance Table

Model 1: cbind(survive, died) ~ 1
Model 2: cbind(survive, died) ~ faculty
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
1        37     66.285
2        34     43.026  3   23.259 3.566e-05 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

$\Delta D = 23.26$ on 3 df, $p = 3.6 \times 10^{-5}$: the proportions are **not** the same across faculties. The odds ratios relative to Arts:

```
mb <- glm(cbind(survive, died) ~ faculty, binomial, data = men)
round(exp(cbind(OR = coef(mb), confint.default(mb))), 3)
```

```
                    OR 2.5 % 97.5 %
(Intercept)      1.211 0.893  1.640
facultyengineering 2.182 1.353  3.517
facultymedicine  1.492 1.009  2.207
facultyscience   2.710 1.747  4.202
```

Arts men fare worst (54.8%) and Science men best (76.6%, 2.7 times the odds), Engineering close behind at 2.2 and Medicine between (64.4%, odds ratio 1.49, interval barely excluding 1). The fit is acceptable, $D = 43.03$ on 34 df, and adding year changes nothing ($\Delta D = 10.01$ on 9 df, $p = 0.35$), so the ranking is not an artefact of cohort mix.

(c) Arts versus Science, women.

```
w <- subset(g, sex == "women")
anova(glm(cbind(survive, died) ~ 1, binomial, data = w),
      glm(cbind(survive, died) ~ faculty, binomial, data = w), test = "Chisq")
```

```
Analysis of Deviance Table

Model 1: cbind(survive, died) ~ 1
```

```
Model 2: cbind(survive, died) ~ faculty
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
1        19     22.555
2        18     13.739  1   8.8165 0.002985 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

$\Delta D = 8.82$ on 1 df, $p = 0.003$: the proportions differ. Science women survived at $58/61 = 95.1\%$ against $126/157 = 80.3\%$ in Arts, an odds ratio of $\exp(1.5595) = 4.76$. With only 3 deaths in 61 the estimate is imprecise — the Wald interval runs from about 1.4 to 16 — the small-expected-frequency case Section 7.5 warns of, so quote the deviance test rather than the Wald z.

(d) Sex difference in Arts versus Science. This is the faculty-by-sex interaction on the two faculties where both sexes appear.

```r
as2 <- droplevels(subset(g, faculty %in% c("arts", "science")))
anova(glm(cbind(survive, died) ~ faculty + sex, binomial, data = as2),
      glm(cbind(survive, died) ~ faculty * sex, binomial, data = as2), test = "Chisq")
```

```
Analysis of Deviance Table

Model 1: cbind(survive, died) ~ faculty + sex
Model 2: cbind(survive, died) ~ faculty * sex
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
1        36     31.153
2        35     30.358  1  0.79533   0.3725
```

$\Delta D = 0.80$ on 1 df, $p = 0.37$: no evidence of an interaction. By the algebra of Exercise 7.2(b), that means a single sex odds ratio describes both faculties. In the additive model

```r
add <- glm(cbind(survive, died) ~ faculty + sex, binomial, data = as2)
round(exp(cbind(OR = coef(add), confint.default(add))), 3)
```

```
                  OR 2.5 % 97.5 %
(Intercept)    1.168 0.872  1.565
facultyscience 2.920 1.945  4.382
sexwomen       3.697 2.357  5.798
```

women have 3.70 times the odds of surviving 50 years that men do (95% interval 2.36 to 5.80), in Arts and in Science alike, and Science graduates have 2.92 times the odds of Arts graduates in both sexes. The additive model fits well, $D = 31.15$ on 36 df ($p = 0.70$).

The separate estimates $\exp(0.9968) = 2.71$ (Science versus Arts among men) and $\exp(1.5595) = 4.76$ (among women) look different but differ by less than one standard error of the interaction term (0.563 ± 0.664). On the probability scale the sex gap is smaller in Science ($0.951 - 0.766 = 0.19$) than in Arts ($0.803 - 0.548 = 0.26$), but that is the logit squeeze near $\pi = 1$, which the constant-odds-ratio model reproduces. With 61 women in Science, only a very large interaction would have been detectable.

7.4 Problem 7.4 — Let l(bmin) denote the maximum value of the log-likelihood function for

Problem 7.4. Let $l(\mathbf{b}_{\min})$ denote the maximum value of the log-likelihood function for the minimal model with linear predictor $\mathbf{x}^T\boldsymbol{\beta} = \beta_1$, and let $l(\mathbf{b})$ be the corresponding value for a more general model $\mathbf{x}^T\boldsymbol{\beta} = \beta_1 + \beta_2 x_1 + \ldots + \beta_p x_{p-1}$.

a. Show that the likelihood ratio chi-squared statistic is

$$C = 2\left[l(\mathbf{b}) - l(\mathbf{b}_{\min})\right] = D_0 - D_1,$$

where D_0 is the deviance for the minimal model and D_1 is the deviance for the more general model.

b. Deduce that if $\beta_2 = \ldots = \beta_p = 0$, then C has the central chi-squared distribution with $(p-1)$ degrees of freedom.

(difficulty: ⋆⋆)

Solution. (a) Both deviances are measured from the same saturated model, so $l(\mathbf{b}_{\max})$ cancels. By Section 5.6.1, $D = 2[l(\mathbf{b}_{\max}) - l(\mathbf{b})]$, which for the Binomial is equation (7.5) upon substituting

$\widehat{\pi}_i^{\max} = y_i/n_i$ and $\widehat{\pi}_i = \widehat{y}_i/n_i$ into (7.4). Applying it to each model and subtracting,

$$\begin{aligned} D_0 - D_1 &= 2\left[l(\mathbf{b}_{\max}) - l(\mathbf{b}_{\min})\right] - 2\left[l(\mathbf{b}_{\max}) - l(\mathbf{b})\right] \\ &= 2\left[l(\mathbf{b}) - l(\mathbf{b}_{\min})\right] = C, \end{aligned}$$

the statistic of Section 7.5, with $\widetilde{\pi} = (\sum y_i)/(\sum n_i)$ the common probability under the minimal model. The cancellation needs only that both models are referred to the same saturated model; it is the distributional claim of (b) that needs nesting. Note also that D carries no nuisance parameter such as σ^2, so no scaling enters.

Numerically, on the Exercise 7.1 fit the two routes to C agree to machine precision:

```
library(dobson)
data(hiroshima)
h <- hiroshima
names(h) <- c("dose", "leuk", "other", "total")
h$mid <- c(0, 5, 29.5, 74.5, 149.5, 300)
m1 <- glm(cbind(leuk, other) ~ mid, family = binomial, data = h)
m0 <- glm(cbind(leuk, other) ~ 1, family = binomial, data = h)
c(D0 = deviance(m0), D1 = deviance(m1), D0_minus_D1 = deviance(m0) - deviance(m1),
  C_loglik = 2 * (as.numeric(logLik(m1)) - as.numeric(logLik(m0))))
```

```
        D0          D1 D0_minus_D1    C_loglik
54.3508862   0.6795634  53.6713228  53.6713228
```

(b) If $\beta_2 = \ldots = \beta_p = 0$ then both models are correct, so Section 5.6 applies to each, giving $D_0 \sim \chi^2(N-1)$ and $D_1 \sim \chi^2(N-p)$ asymptotically, with N covariate patterns. (The pointer beside C in Section 7.5 reads "Section 5.2"; the result invoked is in Section 5.6.) Decompose $D_0 = D_1 + C$. The Section 5.6 Taylor expansion writes each deviance as a quadratic form in asymptotically Normal quantities: D_0 is the squared residual projection onto the orthogonal complement of the one-dimensional model space, D_1 onto that of the p-dimensional space containing it. The spaces being nested, C is the squared projection onto their $(p-1)$-dimensional difference and is independent of D_1 — the independence condition Section 5.7 attaches to $\Delta D \sim \chi^2(p-q)$. By additivity of independent chi-squares,

$$C \sim \chi^2\left((N-1) - (N-p)\right) = \chi^2(p-1),$$

central because the minimal model is true, so the mean in the difference space is zero; equivalently, Wilks' theorem for the $(p-1)$ constraints. If the β_j are not all zero, D_1 is unaffected but C becomes non-central, with non-centrality growing in the information metric — which is what makes it a test statistic. All of this is asymptotic, and the chapter notes after (7.5) that it degrades when expected frequencies fall below about 1.

Simulating 5000 data sets under the minimal model ($\pi = 0.3$ at all 40 covariate patterns) with $p = 3$, C should be $\chi^2(2)$: mean 2, variance 4, upper 5% point 5.99.

```
set.seed(2026)
n <- rep(30, 40)
x1 <- rnorm(40)
x2 <- rnorm(40)
C <- replicate(5000, {
  y <- rbinom(40, n, 0.3)
  m0 <- glm(cbind(y, n - y) ~ 1, binomial)
  m1 <- glm(cbind(y, n - y) ~ x1 + x2, binomial)
  deviance(m0) - deviance(m1)
})
round(c(mean = mean(C), var = var(C), q95 = quantile(C, 0.95),
        chisq2_mean = 2, chisq2_var = 4, chisq2_q95 = qchisq(0.95, 2)), 3)
```

```
    mean         var     q95.95% chisq2_mean  chisq2_var  chisq2_q95
   2.027       4.227       6.089       2.000       4.000       5.991
```

Mean, variance and upper percentile all match $\chi^2(2)$ closely.

7.5 Problem 7.5 — Let Yi be the number of successes in ni trials with

Problem 7.5. Let Y_i be the number of successes in n_i trials with

$$Y_i \sim \text{Bin}(n_i, \pi_i),$$

where the probabilities π_i have a Beta distribution

$$\pi_i \sim \text{Be}(\alpha, \beta).$$

The probability density function for the Beta distribution is $f(x; \alpha, \beta) = x^{\alpha-1}(1-x)^{(\beta-1)}/B(\alpha, \beta)$ for x in $[0, 1]$, $\alpha > 0$, $\beta > 0$ and the beta function $B(\alpha, \beta)$ defining the normalizing constant required to ensure that $\int_0^1 f(x; \alpha, \beta)\, dx = 1$. It can be shown that $E(X) = \alpha/(\alpha + \beta)$ and $\text{var}(X) = \alpha\beta/[(\alpha + \beta)^2(\alpha + \beta + 1)]$. Let $\theta = \alpha/(\alpha + \beta)$, and hence, show that
a. $E(\pi_i) = \theta$ b. $\text{var}(\pi_i) = \theta(1-\theta)/(\alpha + \beta + 1) = \phi\theta(1-\theta)$ c. $E(Y_i) = n_i\theta$ d. $\text{var}(Y_i) = n_i\theta(1-\theta)[1+(n_i-1)\phi]$ so that $\text{var}(Y_i)$ is larger than the Binomial variance (unless $n_i = 1$ or $\phi = 0$). (difficulty: ⋆⋆)

Solution. This is the beta-binomial model for overdispersed Binomial data. Write $\phi = 1/(\alpha + \beta + 1)$, so $0 < \phi < 1$ for all admissible $\alpha, \beta > 0$.
(a) Immediate from the quoted Beta mean with $X = \pi_i$:

$$E(\pi_i) = \frac{\alpha}{\alpha + \beta} = \theta.$$

(b) Since $1 - \theta = \beta/(\alpha + \beta)$, we have $\theta(1-\theta) = \alpha\beta/(\alpha + \beta)^2$, so the quoted variance factorises as

$$\text{var}(\pi_i) = \frac{\alpha\beta}{(\alpha + \beta)^2(\alpha + \beta + 1)} = \frac{\theta(1-\theta)}{\alpha + \beta + 1} = \phi\,\theta(1-\theta).$$

Thus ϕ measures the spread of the π_i relative to the largest a mean-θ variable on $[0, 1]$ could have.
(c) By the tower property, with $E(Y_i \mid \pi_i) = n_i\pi_i$ from the Binomial mean and (a),

$$E(Y_i) = E\left[E(Y_i \mid \pi_i)\right] = n_i E(\pi_i) = n_i\theta,$$

so the mixing leaves the mean structure Binomial — this is a pure overdispersion model.
(d) Use the conditional variance decomposition

$$\text{var}(Y_i) = E\left[\text{var}(Y_i \mid \pi_i)\right] + \text{var}\left[E(Y_i \mid \pi_i)\right].$$

The two conditional Binomial moments are $\text{var}(Y_i \mid \pi_i) = n_i\pi_i(1-\pi_i)$ and $E(Y_i \mid \pi_i) = n_i\pi_i$, so

$$\text{var}(Y_i) = n_i E\left[\pi_i(1-\pi_i)\right] + n_i^2\,\text{var}(\pi_i).$$

For the first term, $E[\pi_i(1-\pi_i)] = E(\pi_i) - E(\pi_i^2)$ and $E(\pi_i^2) = \text{var}(\pi_i) + [E(\pi_i)]^2 = \phi\theta(1-\theta) + \theta^2$. Hence

$$E\left[\pi_i(1-\pi_i)\right] = \theta - \theta^2 - \phi\theta(1-\theta) = \theta(1-\theta)\left[1-\phi\right].$$

Substituting both terms,

$$\begin{aligned}\text{var}(Y_i) &= n_i\theta(1-\theta)(1-\phi) + n_i^2\phi\theta(1-\theta) \\ &= n_i\theta(1-\theta)\left[1 - \phi + n_i\phi\right] = n_i\theta(1-\theta)\left[1 + (n_i-1)\phi\right],\end{aligned}$$

which is the required result.
The Binomial variance with the same mean is $n_i\theta(1-\theta)$, so the factor is $1+(n_i-1)\phi \geq 1$, with equality exactly when $n_i = 1$ or $\phi = 0$:

- (i) $n_i = 1$: Y_i is Bernoulli with mean θ, hence determined by its mean, so ungrouped binary data cannot show this overdispersion however heterogeneous the π_i.

- (ii) $\phi = 0$: the π_i degenerate at θ and the model is exactly $\text{Bin}(n_i, \theta)$. This is unattainable for finite $\alpha, \beta > 0$, being the limit $\alpha+\beta \to \infty$, so for genuine Beta mixing with $n_i > 1$ the inequality is strict.

Since (c) leaves the mean model intact, fitting an ordinary Binomial GLM to such data keeps the estimates consistent but understates the variance by $1 + (n_i - 1)\phi$: standard errors are too small and D, X^2 are inflated against $\chi^2(N - p)$, most severely where the n_i are largest.

Numerically, with $\alpha = 2$, $\beta = 3$, $n = 20$: $\theta = 0.4$, $\phi = 1/6$, $\text{var}(\pi) = 0.04$, $E(Y) = 8$, and $\text{var}(Y) = 20 \times 0.24 \times (1 + 19/6) = 20$ against a Binomial 4.8.

```r
set.seed(7)
alpha <- 2; beta <- 3; n <- 20
theta <- alpha / (alpha + beta)
phi <- 1 / (alpha + beta + 1)
p <- rbeta(2e6, alpha, beta)
y <- rbinom(2e6, n, p)
round(c(theta = theta, mean_pi = mean(p),
        var_pi_theory = phi * theta * (1 - theta), var_pi_sim = var(p),
        EY_theory = n * theta, EY_sim = mean(y),
        varY_theory = n * theta * (1 - theta) * (1 + (n - 1) * phi), varY_sim = var(y),
        binomial_var = n * theta * (1 - theta)), 4)
```

```
    theta       mean_pi var_pi_theory    var_pi_sim     EY_theory
   0.4000        0.3998        0.0400        0.0400        8.0000
   EY_sim   varY_theory      varY_sim  binomial_var
   7.9972       20.0000       20.0048        4.8000
```

Every simulated moment matches its formula, and the realised variance of Y is more than four times the Binomial value – the overdispersion factor $1 + 19/6 = 4.17$.

8 Nominal and Ordinal Logistic Regression

Contents

8.1 Problem 8.1 — If there are only J = 2 response categories, show that models (8.4), (8.13),

Problem 8.1. If there are only $J = 2$ response categories, show that models (8.4), (8.13), (8.15) and (8.16) all reduce to the logistic regression model for binary data. (difficulty: ⋆)

Solution. All four reduce to the single equation $\text{logit}(\pi) = \mathbf{x}^T\boldsymbol{\beta}$, differing only in which category goes in the numerator. Section 8.2 settles the distributional half: for $J = 2$ the Multinomial (8.1) with $\pi_2 = 1-\pi_1$ and $y_2 = n-y_1$ is the Binomial $\text{B}(n, \pi_1)$ of (7.1). Only the systematic component remains, and each model gives exactly one equation, there being $J - 1 = 1$ non-redundant logit.

- (i) Nominal (8.4). The equations run over $j = 2, \ldots, J$, leaving $j = 2$ alone: $\log(\pi_2/\pi_1) = \log\{\pi_2/(1-\pi_2)\} = \mathbf{x}_2^T\boldsymbol{\beta}_2$, the Section 7.2 model with category 2 as "success"; equivalently $\text{logit}(\pi_1) = -\mathbf{x}_2^T\boldsymbol{\beta}_2$.
- (ii) Cumulative (8.13). One cutpoint, so $\log(\pi_1/\pi_2) = \text{logit}(\pi_1) = \mathbf{x}_1^T\boldsymbol{\beta}_1$, with category 1 as "success". The proportional odds specialisation (8.14) collapses β_{0j} to one intercept and is vacuous — there is nothing for the odds to be proportional across, which is why `MASS::polr` demands three or more levels.
- (iii) Adjacent category (8.15). The ratios $\pi_1/\pi_2, \ldots, \pi_{J-1}/\pi_J$ collapse to π_1/π_2, giving the same equation: with two categories the only adjacent pair is also the only split of the scale.
- (iv) Continuation ratio (8.16). The denominator $\pi_{j+1} + \ldots + \pi_J$ is π_2 at $j = 1$, and the conditioning event $z > C_{j-1}$ is empty there, so again $\text{logit}(\pi_1) = \mathbf{x}_1^T\boldsymbol{\beta}_1$.

Numerically, on the genuinely binary beetle mortality data of Section 7.3, with all four plus the ordinary binomial GLM:

```r
library(dobson)
library(nnet)
library(VGAM)
data(beetle)
Y <- cbind(killed = beetle$y, survived = beetle$n - beetle$y)
b <- data.frame(x = rep(beetle$x, 2),
                resp = factor(rep(c("killed", "survived"), each = nrow(beetle)),
                              levels = c("killed", "survived")),
                freq = c(beetle$y, beetle$n - beetle$y))
m.glm  <- glm(cbind(y, n - y) ~ x, family = binomial, data = beetle)
m.nom  <- multinom(resp ~ x, weights = freq, data = b, trace = FALSE,
                   maxit = 1000, reltol = 1e-14)
m.cum  <- vglm(Y ~ x, cumulative(parallel = TRUE), data = beetle)
# reverse = TRUE gives the book's log(pi_j / pi_{j+1}); sratio gives the book's (8.16)
m.acat <- vglm(Y ~ x, acat(reverse = TRUE, parallel = TRUE), data = beetle)
m.srat <- vglm(Y ~ x, sratio(reverse = FALSE, parallel = TRUE), data = beetle)
tab <- rbind("binomial glm: logit P(killed)" = coef(m.glm),
             "(8.4) nominal, log(pi2/pi1)"   = coef(m.nom),
             "(8.13) cumulative logit"       = coef(m.cum),
             "(8.15) adjacent category"      = coef(m.acat),
             "(8.16) continuation ratio"     = coef(m.srat))
colnames(tab) <- c("intercept", "slope")
round(tab, 4)
```

```
                              intercept    slope
binomial glm: logit P(killed)  -60.7175  34.2703
(8.4) nominal, log(pi2/pi1)     60.7175 -34.2703
(8.13) cumulative logit        -60.7175  34.2703
(8.15) adjacent category       -60.7175  34.2703
(8.16) continuation ratio      -60.7175  34.2703
```

Every fit reproduces $|\hat{\beta}_1| = 60.7175$ and $|\hat{\beta}_2| = 34.2703$ to all printed digits, and the signs agree once each model is written with the book's category on top; only (8.4), which by construction puts the non-reference category there, is reversed.

8.2 Problem 8.2 — The data in Table 8.5 are from an investigation into satisfaction with hous-

Problem 8.2. The data in Table 8.5 are from an investigation into satisfaction with housing conditions in Copenhagen (derived from Example W in Cox and Snell, 1981, from original data from Madsen, 1971). Residents in selected areas living in rented homes built between 1960 and 1968 were questioned about their satisfaction and the degree of contact with other residents. The data were tabulated by type of housing.
Table 8.5, satisfaction with housing conditions. The rows are the three types of housing and the columns are the six combinations of satisfaction (low, medium, high) with degree of contact with other residents (low, high), the counts being read across as (low satisfaction: low contact, high contact), (medium satisfaction: low contact, high contact), (high satisfaction: low contact, high contact). Tower block: 65, 34, 54, 47, 100, 100. Apartment: 130, 141, 76, 116, 111, 191. House: 67, 130, 48, 105, 62, 104.
a. Summarize the data using appropriate tables of percentages to show the associations between levels of satisfaction and contact with other residents, levels of satisfaction and type of housing, and contact and type of housing.
b. Use nominal logistic regression to model associations between level of satisfaction and the other two variables. Obtain a parsimonious model that summarizes the patterns in the data.
c. Do you think an ordinal model would be appropriate for associations between the levels of satisfaction and the other variables? Justify your answer. If you consider such a model to be appropriate, fit a suitable one and compare the results with those from (b).
d. From the best model you obtained in (c), calculate the standardized residuals and use them to find where the largest discrepancies are between the observed frequencies and expected frequencies estimated from the model. (difficulty: ⋆⋆⋆)

Solution. Satisfaction falls with housing type and rises with contact, and a proportional odds model in both is the parsimonious summary. (`MASS` also exports a `housing` data set — Copenhagen again, but 72 rows with an extra "influence" factor — and `MASS` is needed for `polr`, so every block below names `package = "dobson"` explicitly.)
Part (a). Three two-way marginal tables of row percentages.

```r
library(dobson)
data(housing, package = "dobson")
housing$satisfaction <- factor(housing$satisfaction, levels = c("low", "medium", "high"))
housing$contact      <- factor(housing$contact,      levels = c("low", "high"))
housing$type         <- factor(housing$type,         levels = c("tower block", "apartment", "house"))
tab <- xtabs(frequency ~ type + contact + satisfaction, data = housing)
round(100 * prop.table(margin.table(tab, c(2, 3)), 1), 1)   # satisfaction by contact
```

```
       satisfaction
contact  low medium high
   low  36.7   25.0 38.3
   high 31.5   27.7 40.8
```

```r
round(100 * prop.table(margin.table(tab, c(1, 3)), 1), 1)   # satisfaction by type of housing
```

```
             satisfaction
type           low medium high
  tower block 24.8   25.2 50.0
  apartment   35.4   25.1 39.5
  house       38.2   29.7 32.2
```

```r
round(100 * prop.table(margin.table(tab, c(1, 2)), 1), 1)   # contact by type of housing
```

```
             contact
type           low high
  tower block 54.8 45.2
  apartment   41.4 58.6
  house       34.3 65.7
```

```
round(100 * prop.table(ftable(tab, row.vars = c(1, 2)), 1), 1)
```

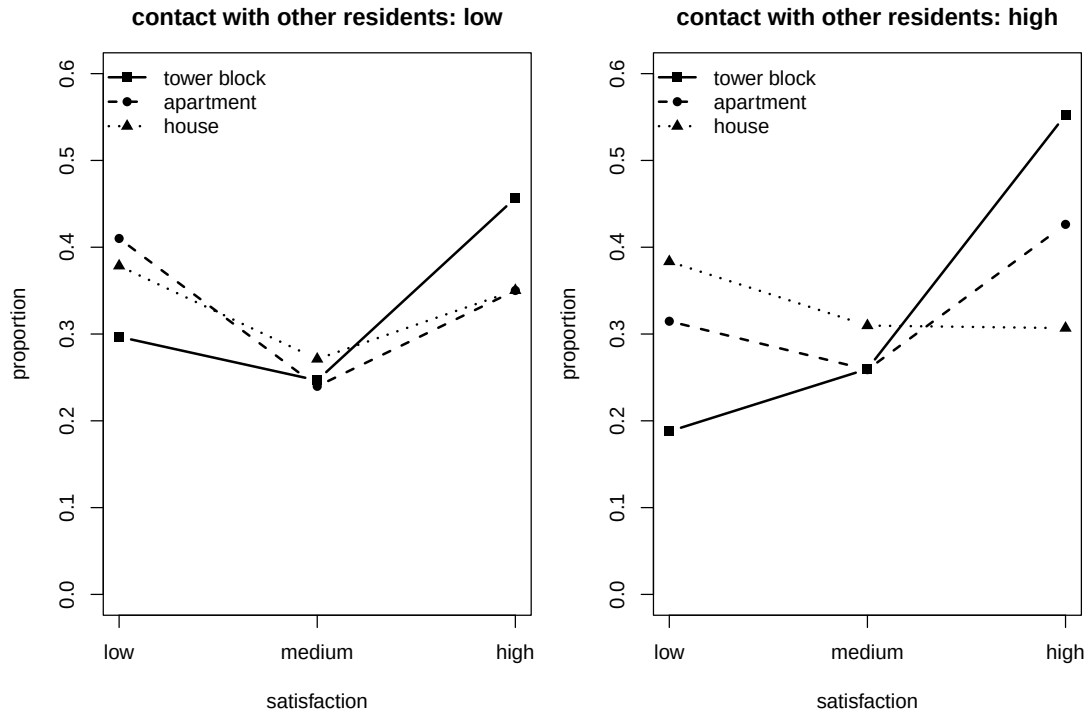
```
                    satisfaction  low medium high
type        contact
tower block low                   29.7   24.7 45.7
            high                  18.8   26.0 55.2
apartment   low                   41.0   24.0 35.0
            high                  31.5   25.9 42.6
house       low                   37.9   27.1 35.0
            high                  38.3   31.0 30.7
```

```
margin.table(tab, c(1, 2))
```

```
             contact
type          low high
  tower block 219  181
  apartment   317  448
  house       177  339
```

Satisfaction rises mildly with contact (high satisfaction 38.3% to 40.8%, low satisfaction 36.7% to 31.5%) and falls strongly across housing type (high satisfaction 50.0%, 39.5%, 32.2% for tower block, apartment, house; low satisfaction moving the other way). Contact also depends on type — 45.2%, 58.6%, 65.7% high contact — and that association runs against the first two, so the crude satisfaction-by-contact margin understates the contact effect: houses have the most contact and the least satisfaction, and the two partly cancel. The six-row table confirms it: high contact raises "highly satisfied" from 45.7% to 55.2% in tower blocks and 35.0% to 42.6% in apartments, but lowers it from 35.0% to 30.7% in houses — the only hint of an interaction.

```
pr <- prop.table(tab, c(1, 2))
par(mfrow = c(1, 2), mar = c(4, 4, 3, 1))
for (k in c("low", "high")) {
  plot(0, 0, type = "n", xlim = c(1, 3), ylim = c(0, 0.6), xaxt = "n",
       xlab = "satisfaction", ylab = "proportion",
       main = paste("contact with other residents:", k))
  axis(1, at = 1:3, labels = c("low", "medium", "high"))
  for (i in 1:3)
    lines(1:3, pr[i, k, ], type = "b", lty = i, pch = 14 + i, lwd = 2)
  legend("topleft", legend = dimnames(pr)$type, lty = 1:3, pch = 15:17, lwd = 2, bty = "n")
}
```



Part (b). Treat satisfaction as nominal with three categories, "low" as reference, and fit model (8.4)

with `multinom`. There are $3 \times 2 = 6$ covariate patterns, so the maximal model has 6 parameters for each of the $J - 1 = 2$ logits, 12 in all; deviances (8.7) are taken against that.

```
library(nnet)
f <- function(rhs) multinom(rhs, weights = frequency, data = housing, trace = FALSE,
                            maxit = 1000, reltol = 1e-14)
mods <- list(minimal = f(satisfaction ~ 1), contact = f(satisfaction ~ contact),
             type = f(satisfaction ~ type), `type+contact` = f(satisfaction ~ type +
             ↪  contact),
             `type*contact` = f(satisfaction ~ type * contact))
lsat <- as.numeric(logLik(mods[["type*contact"]]))
out <- t(sapply(mods, function(m) c(npar = length(coef(m)), logLik = as.numeric(logLik(m)),
                                    deviance = 2 * (lsat - as.numeric(logLik(m))),
                                    df = 12 - length(coef(m)), AIC = AIC(m))))
round(cbind(out, p = pchisq(out[, "deviance"], out[, "df"], lower.tail = FALSE)), 4)
```

```
             npar    logLik deviance df      AIC      p
minimal         2 -1824.439  50.2903 10 3652.878 0.0000
contact         4 -1821.876  45.1645  8 3651.752 0.0000
type            6 -1807.174  15.7608  6 3626.348 0.0151
type+contact    8 -1802.740   6.8930  4 3621.480 0.1417
type*contact   12 -1799.294   0.0000  0 3622.587 1.0000
```

The additive model has deviance $D = 6.89$ on 4 degrees of freedom ($p = 0.14$), so it describes the six covariate patterns adequately; adding the interaction buys 6.89 on 4 df and raises AIC (8.10) from 3621.5 to 3622.6. Dropping either main effect is not permissible: removing contact costs $15.76 - 6.89 = 8.87$ on 2 df ($p = 0.012$) and removing type costs $45.17 - 6.89 = 38.27$ on 4 df ($p < 10^{-7}$). The parsimonious nominal model is therefore

$$\log\left(\frac{\pi_j}{\pi_1}\right) = \beta_{0j} + \beta_{1j}x_1 + \beta_{2j}x_2 + \beta_{3j}x_3, \qquad j = 2, 3,$$

with $j = 1, 2, 3$ for low, medium and high satisfaction, $x_1 = 1$ for apartment, $x_2 = 1$ for house (tower block the reference) and $x_3 = 1$ for high contact.

```
mtc <- multinom(satisfaction ~ type + contact, weights = frequency, data = housing,
                trace = FALSE, maxit = 1000, reltol = 1e-14)
s <- summary(mtc)
res <- cbind(b = as.vector(t(s$coefficients)), se = as.vector(t(s$standard.errors)))
rownames(res) <- paste(rep(rownames(s$coefficients), each = ncol(s$coefficients)),
                       colnames(s$coefficients), sep = ": ")
round(cbind(res, z = res[, 1] / res[, 2], OR = exp(res[, 1]),
            lo = exp(res[, 1] - 1.96 * res[, 2]), hi = exp(res[, 1] + 1.96 * res[, 2])), 3)
```

```
                          b    se      z    OR    lo    hi
medium: (Intercept)   -0.107 0.152 -0.704 0.898 0.666 1.211
medium: typeapartment -0.407 0.171 -2.375 0.666 0.476 0.931
medium: typehouse     -0.337 0.180 -1.869 0.714 0.501 1.017
medium: contacthigh    0.296 0.130  2.275 1.344 1.042 1.735
high: (Intercept)      0.561 0.133  4.219 1.752 1.350 2.273
high: typeapartment   -0.642 0.150 -4.275 0.526 0.392 0.706
high: typehouse       -0.946 0.164 -5.749 0.388 0.281 0.536
high: contacthigh      0.328 0.118  2.777 1.389 1.101 1.750
```

Relative to a tower block, the odds of high rather than low satisfaction are multiplied by 0.53 (95% CI 0.39 to 0.71) in an apartment and 0.39 (0.28 to 0.54) in a house, with 0.67 and 0.71 for medium versus low; high contact multiplies the high-versus-low odds by 1.39 (1.10 to 1.75) and the medium-versus-low odds by 1.34 (1.04 to 1.74). Within each variable the two ratios line up in order — for type the high-versus-low ratio is further from 1 ($0.53 < 0.67$, $0.39 < 0.71$), for contact the two nearly coincide — which is the monotone ordering an ordinal model imposes.

Part (c). An ordinal model is appropriate: satisfaction low < medium < high orders a single underlying attitude, the latent-variable picture of Figure 8.2, and the estimates in (b) already behave accordingly. Fitting the proportional odds model (8.14),

$$\log\left(\frac{\pi_1 + \ldots + \pi_j}{\pi_{j+1} + \ldots + \pi_J}\right) = \beta_{0j} + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3, \qquad j = 1, 2,$$

costs three parameters instead of six and buys back three degrees of freedom.

```
library(MASS)
housing$satisfaction <- ordered(housing$satisfaction, levels = c("low", "medium", "high"))
p1 <- polr(satisfaction ~ type + contact, weights = frequency, data = housing, Hess = TRUE)
summary(p1)
```

```
Call:
polr(formula = satisfaction ~ type + contact, data = housing,
    weights = frequency, Hess = TRUE)

Coefficients:
                Value Std. Error t value
typeapartment -0.5009    0.11675  -4.291
typehouse     -0.7362    0.12610  -5.838
contacthigh    0.2524    0.09306   2.713

Intercepts:
            Value   Std. Error t value
low|medium  -0.9973  0.1075    -9.2794
medium|high  0.1152  0.1047     1.1004

Residual Deviance: 3610.286
AIC: 3620.286
```

```
c(polr = as.numeric(logLik(p1)), nominal = as.numeric(logLik(mtc)), saturated = lsat)
```

```
     polr   nominal saturated
-1805.143 -1802.740 -1799.294
```

```
anova(p1, polr(satisfaction ~ type * contact, weights = frequency, data = housing))
```

```
Likelihood ratio tests of ordinal regression models

Response: satisfaction
           Model Resid. df Resid. Dev   Test    Df LR stat.    Pr(Chi)
1 type + contact      1676   3610.286
2 type * contact      1674   3604.091 1 vs 2     2 6.195546 0.04514963
```

Note `polr` parameterises the cumulative logit as $\beta_{0j} - \boldsymbol{\beta}^T\mathbf{x}$, so a positive printed coefficient means more satisfaction. Against the maximal model, $D = 2(-1799.294 + 1805.143) = 11.70$ on $12 - 5 = 7$ df, $p = 0.11$, so the model fits; against the nominal model of (b), which tests proportional odds directly, $\Delta D = 4.81$ on 3 df, $p = 0.19$, no evidence against it, and AIC prefers the ordinal fit (3620.3 against 3621.5). As in the car preference example of Section 8.4.6, the two describe the data equally well and the ordinal one wins on parsimony.

Relative to a tower block, the odds of being at or below any given satisfaction level are multiplied by $e^{0.5009} = 1.65$ for an apartment and $e^{0.7362} = 2.09$ for a house, while high contact multiplies the odds of being above any given level by $e^{0.2524} = 1.29$ (95% CI 1.07 to 1.55). Each is a compromise between the two nominal odds ratios it replaces ($e^{-0.5009} = 0.61$ against 0.67 and 0.53), which is why the fits agree so closely. One qualification: within the proportional odds family the type-by-contact interaction is borderline, $\Delta D = 6.20$ on 2 df, $p = 0.045$, lowering AIC to 3618.1; in the nominal family it was not significant ($p = 0.14$), so the evidence is weak and family-dependent. Part (d) locates it.

Part (d). Expected frequencies are the additive proportional odds fitted probabilities times the covariate-pattern totals, and the standardized (Pearson) residuals are $r_i = (o_i - e_i)/\sqrt{e_i}$ from (8.5).

```
pat  <- unique(housing[, c("type", "contact")])
n    <- aggregate(frequency ~ type + contact, data = housing, sum)
prob <- predict(p1, newdata = pat, type = "probs")
tot  <- n$frequency[match(paste(pat$type, pat$contact), paste(n$type, n$contact))]
long <- reshape(data.frame(pat, tot * prob), direction = "long", varying = list(3:5),
                v.names = "expected", timevar = "satisfaction",
                times = c("low", "medium", "high"), idvar = c("type", "contact"))
res <- merge(housing, long, by = c("type", "contact", "satisfaction"))
res$satisfaction <- factor(res$satisfaction, levels = c("low", "medium", "high"))
res <- res[order(res$type, res$contact, res$satisfaction), ]
res$r <- (res$frequency - res$expected) / sqrt(res$expected)
```

```r
rownames(res) <- NULL
data.frame(res[, c("type", "contact", "satisfaction", "frequency")],
           expected = round(res$expected, 2), r = round(res$r, 3))
```

```
          type contact satisfaction frequency expected      r
1  tower block     low          low        65    59.01  0.779
2  tower block     low       medium        54    56.79 -0.370
3  tower block     low         high       100   103.20 -0.315
4  tower block    high          low        34    40.32 -0.995
5  tower block    high       medium        47    43.98  0.455
6  tower block    high         high       100    96.70  0.335
7    apartment     low          low       130   119.95  0.918
8    apartment     low       medium        76    85.89 -1.067
9    apartment     low         high       111   111.16 -0.015
10   apartment    high          low       141   143.84 -0.237
11   apartment    high       medium       116   120.45 -0.405
12   apartment    high         high       191   183.71  0.538
13       house     low          low        67    77.01 -1.141
14       house     low       medium        48    47.04  0.140
15       house     low         high        62    52.95  1.244
16       house    high          low       130   126.91  0.274
17       house    high       medium       105    91.89  1.368
18       house    high         high       104   120.20 -1.478
```

```r
sum(res$r^2)
```

```
[1] 11.64202
```

The chi-squared statistic (8.6) is $X^2 = 11.64$, close to the deviance $D = 11.70$ as it should be, and consistent with $\chi^2(7)$ ($p = 0.11$): no residual is anywhere near 2 in absolute value, so no cell is badly fitted.

The largest discrepancies are in the "house" rows and all concern contact. For houses with high contact the model predicts 120.2 highly satisfied residents against 104 observed ($r = -1.48$), the deficit reappearing as an excess at medium satisfaction (105 against 91.9, $r = 1.37$); for houses with low contact the reverse, 62 highly satisfied against 53.0 ($r = 1.24$) and a shortfall at low satisfaction (67 against 77.0, $r = -1.14$). The model imposes the same positive contact effect on every housing type, but among house dwellers contact goes with slightly *less* satisfaction (part (a): 35.0% against 30.7%) — the type-by-contact interaction flagged in (c). The apartment low-contact residuals (0.92, −1.07) are an ordinary medium-versus-low reshuffle. So the additive model is adequate, with any real departure living in the house-by-contact cells.

8.3 Problem 8.3 — The data in Table 8.6 show tumor responses of male and female patients

Problem 8.3. The data in Table 8.6 show tumor responses of male and female patients receiving treatment for small-cell lung cancer. There were two treatment regimes. For the sequential treatment, the same combination of chemotherapeutic agents was administered at each treatment cycle. For the alternating treatment, different combinations were alternated from cycle to cycle (data from Holtbrugger and Schumacher, 1991).

Table 8.6, tumor responses to two different treatments, numbers of patients in each category. The columns are progressive disease, no change, partial remission, complete remission. Sequential treatment, male: 28, 45, 29, 26; sequential, female: 4, 12, 5, 2. Alternating treatment, male: 41, 44, 20, 20; alternating, female: 12, 7, 3, 1.

a. Fit a proportional odds model to estimate the probabilities for each response category taking treatment and sex effects into account.

b. Examine the adequacy of the model fitted in (a) using residuals and goodness of fit statistics.

c. Use a Wald statistic to test the hypothesis that there is no difference in responses for the two treatment regimes.

d. Fit two proportional odds models to test the hypothesis of no treatment difference. Compare the results with those for (c) above.

e. Fit adjacent category models and continuation ratio models using logit, probit and complementary log-log link functions. How do the different models affect the interpretation of the results? (difficulty: ⋆⋆⋆)

Solution. Sequential treatment is the better regime ($W = 7.49$, $p = 0.006$), and every model family agrees. Order the response progressive disease < no change < partial remission < complete remission, so "large" means a good outcome, with sequential and male as reference levels: 16 cells from 4 covariate patterns and 299 patients.

Part (a). Model (8.14) with $J = 4$, so three cutpoints and two slopes:

$$\log\left(\frac{\pi_1 + \ldots + \pi_j}{\pi_{j+1} + \ldots + \pi_4}\right) = \beta_{0j} + \beta_1 x_1 + \beta_2 x_2, \qquad j = 1, 2, 3,$$

with $x_1 = 1$ for alternating treatment and $x_2 = 1$ for female.

```r
library(dobson)
library(MASS)
data(tumor, package = "dobson")
lev <- c("progressive", "no change", "partial remission", "complete remission")
tumor$response  <- ordered(tumor$response, levels = lev)
tumor$treatment <- factor(tumor$treatment, levels = c("sequential", "alternating"))
tumor$sex       <- factor(tumor$sex, levels = c("male", "female"))
m <- polr(response ~ treatment + sex, weights = frequency, data = tumor, Hess = TRUE)
summary(m)
```

```
Call:
polr(formula = response ~ treatment + sex, data = tumor, weights = frequency,
    Hess = TRUE)

Coefficients:
                     Value Std. Error t value
treatmentalternating -0.5807     0.2121  -2.737
sexfemale            -0.5414     0.2872  -1.885

Intercepts:
                                    Value   Std. Error t value
progressive|no change               -1.3180  0.1798    -7.3315
no change|partial remission          0.2492  0.1614     1.5443
partial remission|complete remission  1.3001  0.1850     7.0276

Residual Deviance: 789.0566
AIC: 799.0566
```

```r
pat <- unique(tumor[, c("treatment", "sex")])
cbind(pat, round(predict(m, newdata = pat, type = "probs"), 4))
```

```
     treatment    sex progressive no change partial remission
1   sequential   male      0.2111    0.3508            0.2239
5   sequential female      0.3150    0.3729            0.1752
9  alternating   male      0.3236    0.3728            0.1714
13 alternating female      0.4512    0.3464            0.1209
   complete remission
1              0.2142
5              0.1369
9              0.1323
13             0.0815
```

Here `polr` writes the cumulative logit as $\beta_{0j} - \boldsymbol{\beta}^T \mathbf{x}$, so a printed coefficient is the effect on the good end of the scale; both are negative, and in the book's parameterisation of (8.14) $\beta_1 = 0.5807$, $\beta_2 = 0.5414$. The odds of a response at or below any given category are multiplied by $e^{0.5807} = 1.79$ on the alternating regime and by $e^{0.5414} = 1.72$ for women. So the probability of complete remission falls from 0.214 to 0.132 for men and 0.137 to 0.082 for women on switching to alternating, while progressive disease rises from 0.211 to 0.324 and 0.315 to 0.451.

Part (b). Expected frequencies are the estimated probabilities times the group totals; residuals are the Pearson residuals (8.5), X^2 is (8.6), and the deviance (8.7) is taken against the maximal (nominal,

saturated) model, which has $4 \times 3 = 12$ parameters against the 5 of the proportional odds model.

```
library(nnet)
n    <- aggregate(frequency ~ treatment + sex, data = tumor, sum)
tot  <- n$frequency[match(paste(pat$treatment, pat$sex), paste(n$treatment, n$sex))]
long <- reshape(data.frame(pat, tot * predict(m, newdata = pat, type = "probs")),
                direction = "long", varying = list(3:6), v.names = "expected",
                timevar = "response", times = lev, idvar = c("treatment", "sex"))
res <- merge(tumor, long, by = c("treatment", "sex", "response"))
res$response <- factor(res$response, levels = lev)
res <- res[order(res$treatment, res$sex, res$response), ]
res$r <- (res$frequency - res$expected) / sqrt(res$expected)
rownames(res) <- NULL
data.frame(res[, c("treatment", "sex", "response", "frequency")],
           expected = round(res$expected, 2), r = round(res$r, 3))
```

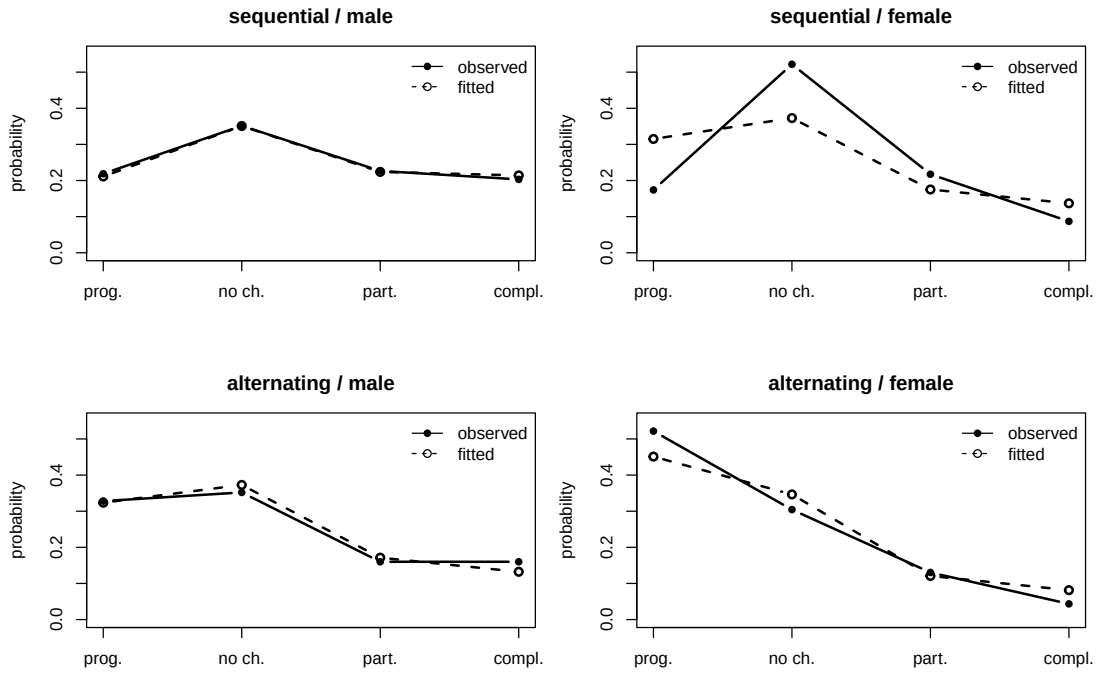
```
     treatment    sex            response frequency expected      r
1   sequential   male         progressive        28    27.03  0.187
2   sequential   male           no change        45    44.91  0.014
3   sequential   male   partial remission        29    28.65  0.065
4   sequential   male  complete remission        26    27.41 -0.270
5   sequential female         progressive         4     7.25 -1.206
6   sequential female           no change        12     8.58  1.169
7   sequential female   partial remission         5     4.03  0.484
8   sequential female  complete remission         2     3.15 -0.647
9  alternating   male         progressive        41    40.45  0.087
10 alternating   male           no change        44    46.59 -0.380
11 alternating   male   partial remission        20    21.42 -0.307
12 alternating   male  complete remission        20    16.54  0.851
13 alternating female         progressive        12    10.38  0.504
14 alternating female           no change         7     7.97 -0.343
15 alternating female   partial remission         3     2.78  0.131
16 alternating female  complete remission         1     1.87 -0.639
```

```
msat <- multinom(response ~ treatment * sex, weights = frequency, data = tumor,
                 trace = FALSE, maxit = 1000, reltol = 1e-14)
c(X2 = sum(res$r^2), D = 2 * (as.numeric(logLik(msat)) - as.numeric(logLik(m))))
```

```
      X2        D
5.352739 5.567678
```

Both have $12 - 5 = 7$ degrees of freedom: $X^2 = 5.35$ ($p = 0.62$) and $D = 5.57$ ($p = 0.59$), so the model describes the data well, with no residual above 1.21. The largest sit in the sequential/female row (4 and 12 observed against 7.3 and 8.6 expected), which has only 23 women and is where the asymptotics are weakest — all four expected frequencies below 9, two below 5. Two further checks: the treatment-by-sex interaction adds $\Delta D = 1.05$ on 1 df ($p = 0.31$), and the proportional odds assumption tested against the nominal model (8.4) gives $\Delta D = 3.02$ on 4 df ($p = 0.55$).

```
tab <- xtabs(frequency ~ treatment + sex + response, data = tumor)
obs <- prop.table(tab, c(1, 2))
fit <- predict(m, newdata = pat, type = "probs")
par(mfrow = c(2, 2), mar = c(4.5, 4, 3, 1))
for (i in 1:nrow(pat)) {
  tr <- as.character(pat$treatment[i]); sx <- as.character(pat$sex[i])
  plot(1:4, obs[tr, sx, ], type = "b", pch = 16, lwd = 2, ylim = c(0, 0.55),
       xaxt = "n", xlab = "", ylab = "probability", main = paste(tr, sx, sep = " / "))
  axis(1, at = 1:4, labels = c("prog.", "no ch.", "part.", "compl."))
  lines(1:4, fit[i, ], type = "b", pch = 1, lty = 2, lwd = 2)
  legend("topright", c("observed", "fitted"), pch = c(16, 1), lty = c(1, 2), bty = "n")
}
```



Part (c). The Wald statistic for $H_0 : \beta_1 = 0$ is $b_1/\text{s.e.}(b_1) = -0.5807/0.2121 = -2.737$, or $W = (b_1/\text{s.e.}(b_1))^2 = 7.49$ compared with $\chi^2(1)$.

```
z <- coef(summary(m))["treatmentalternating", "t value"]
c(z = z, W = z^2, p = pchisq(z^2, 1, lower.tail = FALSE))
```

```
         z          W          p
-2.7371661  7.4920782  0.0061971
```

So $p = 0.0062$: there is strong evidence of a treatment difference, sequential being better.

Part (d). Fit the proportional odds model with and without the treatment term and compare deviances, which is the likelihood ratio version of the same test.

```
m0 <- polr(response ~ sex, weights = frequency, data = tumor, Hess = TRUE)
anova(m0, m)
```

```
Likelihood ratio tests of ordinal regression models

Response: response
            Model Resid. df Resid. Dev   Test    Df LR stat.    Pr(Chi)
1             sex       295   796.6268
2 treatment + sex       294   789.0566 1 vs 2     1 7.570185 0.00593417
```

```
c(AIC.without = AIC(m0), AIC.with = AIC(m))
```

```
AIC.without    AIC.with
   804.6268    799.0566
```

The likelihood ratio statistic is $\Delta D = 796.63 - 789.06 = 7.57$ on 1 df, $p = 0.0059$, against the Wald $W = 7.49$, $p = 0.0062$, and AIC drops by 5.6 with treatment included. The two agree because the Wald statistic is the quadratic approximation to the likelihood ratio statistic (Section 5.2), and the log-likelihood is nearly quadratic near the maximum at this sample size. Where they disagree, the likelihood ratio statistic is to be preferred, being invariant to reparameterisation of β_1 as the Wald statistic is not.

Part (e). Two preliminaries on what can be fitted. Model (8.16) as written is $\log[\pi_j/(\pi_{j+1} + \ldots + \pi_J)]$, `VGAM`'s `sratio` family (`cratio` is the reciprocal and flips every sign). Its likelihood factorises — for each j the conditional distribution of "stop at j" given "reached j" is Binomial, so the four cell counts split into three independent Binomials — so it can be fitted by three stacked binomial GLMs with any link, even different links for different j. Model (8.15) instead models $\log(\pi_j/\pi_{j+1})$, an odds on $(0, \infty)$ rather than a probability on $(0, 1)$, so probit and complementary log-log are undefined for it and `VGAM` fails with `NaNs produced`. One can instead model the local conditional probability $\pi_j/(\pi_j + \pi_{j+1})$

with those links, which coincides with (8.15) at the logit; that is a pseudo-likelihood, since consecutive pairs share cell counts, so its standard errors are untrustworthy.

The exact maximum likelihood fits all carry 5 parameters on the same 16 counts and are comparable by AIC. The model of (a) is refitted through `VGAM` to land on the same log-likelihood scale: `polr` reports -394.53 and `vglm` -25.54, differing by the constant multinomial coefficient $\sum \log[n_i!/\prod_j y_{ij}!]$, which cancels in every comparison.

```
library(VGAM)
w <- reshape(tumor, direction = "wide", idvar = c("treatment", "sex"),
             timevar = "response", v.names = "frequency")
Y <- as.matrix(w[, 3:6]); colnames(Y) <- lev
fits <- list(
  po.logit   = vglm(Y ~ treatment + sex, cumulative(parallel = TRUE), data = w),
  cr.logit   = vglm(Y ~ treatment + sex, sratio(link = "logitlink",   parallel = TRUE), data
  ↪  = w),
  cr.probit  = vglm(Y ~ treatment + sex, sratio(link = "probitlink",  parallel = TRUE), data
  ↪  = w),
  cr.cloglog = vglm(Y ~ treatment + sex, sratio(link = "cloglog",  parallel = TRUE), data
  ↪  = w),
  acat.log   = vglm(Y ~ treatment + sex, acat(reverse = TRUE, parallel = TRUE), data = w))
est <- sapply(fits, coef)
se  <- sapply(fits, function(f) sqrt(diag(vcov(f))))
round(rbind(est, logLik = sapply(fits, logLik), AIC = sapply(fits, AIC)), 4)
```

```
                    po.logit cr.logit cr.probit cr.cloglog acat.log
(Intercept):1        -1.3180  -1.2184   -0.7507    -1.3097  -0.4577
(Intercept):2         0.2492  -0.2316   -0.1427    -0.5432   0.4558
(Intercept):3         1.3001  -0.0661   -0.0397    -0.4275  -0.0003
treatmentalternating  0.5807   0.3975    0.2457     0.2819   0.2889
sexfemale             0.5414   0.5355    0.3272     0.4153   0.3308
logLik              -25.5417 -25.9874  -25.9597   -26.1737 -25.7347
AIC                  61.0834  61.9748   61.9194    62.3474  61.4693
```

The first column is a useful check on part (a): `vglm` parameterises (8.14) exactly as the book does, with $\pi_1 + \ldots + \pi_j$ in the numerator and $+\mathbf{x}^T\boldsymbol{\beta}$ in the linear predictor, and it returns $\beta_1 = 0.5807$, $\beta_2 = 0.5414$ and $\beta_{0j} = (-1.3180, 0.2492, 1.3001)$, which are the `polr` numbers with the sign flip undone.

```
round(se, 4)
```

```
                    po.logit cr.logit cr.probit cr.cloglog acat.log
(Intercept):1         0.1801   0.1650    0.0982     0.1351   0.1649
(Intercept):2         0.1621   0.1625    0.1009     0.1221   0.1736
(Intercept):3         0.1852   0.2100    0.1308     0.1504   0.1988
treatmentalternating  0.2119   0.1710    0.1046     0.1292   0.1148
sexfemale             0.2953   0.2437    0.1499     0.1739   0.1684
```

```
round(est / se, 3)
```

```
                    po.logit cr.logit cr.probit cr.cloglog acat.log
(Intercept):1        -7.319   -7.384    -7.647     -9.694   -2.776
(Intercept):2         1.538   -1.425    -1.414     -4.448    2.625
(Intercept):3         7.021   -0.315    -0.303     -2.841   -0.002
treatmentalternating  2.741    2.325     2.348      2.182    2.515
sexfemale             1.834    2.197     2.182      2.388    1.964
```

(The proportional odds standard errors differ from `polr`'s in the fourth decimal, 0.2119 against 0.2121, because `vglm` uses the expected information and `polr` a numerical Hessian; the Wald statistic is 2.741 either way.)

The stated factorisation is worth verifying, since it is what licenses fitting (8.16) by ordinary binomial GLMs:

```
cr <- do.call(rbind, lapply(1:3, function(j)
  data.frame(w[, 1:2], cut = factor(j), y = Y[, j], n = rowSums(Y[, j:4, drop = FALSE]))))
g <- glm(cbind(y, n - y) ~ cut + treatment + sex, binomial("logit"), data = cr)
v <- vglm(Y ~ treatment + sex, sratio(link = "logitlink", parallel = TRUE), data = w)
rbind(stacked.glm = c(coef(g)[c("treatmentalternating", "sexfemale")],
                      logLik = as.numeric(logLik(g))),
      vglm.sratio = c(coef(v)[c("treatmentalternating", "sexfemale")],
```

```
                    logLik = as.numeric(logLik(v))))
```

```
            treatmentalternating sexfemale   logLik
stacked.glm            0.3975226 0.5355538 -25.9874
vglm.sratio            0.3975245 0.5355499 -25.9874
```

The same device applied to overlapping adjacent pairs gives the pseudo-likelihood adjacent-category fits under the three links:

```
ad <- do.call(rbind, lapply(1:3, function(j)
  data.frame(w[, 1:2], cut = factor(j), y = Y[, j], n = Y[, j] + Y[, j + 1])))
sapply(c("logit", "probit", "cloglog"), function(lk) {
  g <- glm(cbind(y, n - y) ~ cut + treatment + sex, binomial(link = lk), data = ad)
  round(coef(summary(g))[c("treatmentalternating", "sexfemale"), c(1, 2)], 4)
}, simplify = "array")
```

```
, , logit

                     Estimate Std. Error
treatmentalternating   0.3403     0.1926
sexfemale              0.2910     0.2654

, , probit

                     Estimate Std. Error
treatmentalternating   0.2105     0.1192
sexfemale              0.1801     0.1639

, , cloglog

                     Estimate Std. Error
treatmentalternating   0.2253     0.1315
sexfemale              0.2067     0.1750
```

The conclusion is unchanged across families: alternating treatment and female sex push the response towards the bad end, and the treatment effect is significant at 5% in every exact fit — proportional odds $|z| = 2.74$, continuation ratio 2.32 (logit), 2.35 (probit), 2.18 (cloglog), adjacent category 2.52. The AIC spread is only 1.26 over models with identical parameter counts on identical data, from 61.08 (proportional odds) to 62.35 (continuation ratio, cloglog), so the choice is not one of fit. Three things do change.

- (i) What the coefficient is an odds ratio for. Proportional odds: $e^{0.5807} = 1.79$ for the cumulative event "no better than category j", the same at every cutpoint. Continuation ratio: $e^{0.3975} = 1.49$ for stopping at j among those who reached j, a discrete hazard ratio. Adjacent category: $e^{0.2889} = 1.33$, between neighbouring categories only. These differ by more than a factor of two, so quoting one for another misstates the effect.
- (ii) The link rescales and little else. Within the continuation ratio family the probit coefficients are 0.62 times the logit ones (0.2457 against 0.3975) with near-identical fit (Δ logLik $= 0.03$) — the standard logistic has standard deviation $\pi/\sqrt{3} = 1.81$ against 1, and matching the two where the data sit rather than in the tails gives the familiar 0.59 to 0.62. The cloglog link fits marginally worse (Δ logLik $= 0.19$) and, being asymmetric, has no odds ratio reading at all: its covariate effect is a proportional hazards effect on the latent scale. Per Section 8.5, it earns its place only when the latent distribution is markedly skewed, which here it is not.
- (iii) The pseudo-likelihood adjacent-category fits should not be quoted. Their logit treatment coefficient is 0.3403 ± 0.1926 against the exact 0.2889 ± 0.1148, and the effect loses significance ($p = 0.077$) only because the overlapping-pairs construction reuses each count twice. The adjacent-category model is defined on an odds scale, so the logit is the only one of the three links that applies to it.

8.4 Problem 8.4 — Consider ordinal response categories which can be interpreted in terms of

Problem 8.4. Consider ordinal response categories which can be interpreted in terms of continuous latent variable as shown in Figure 8.2. Suppose the distribution of this underlying variable is Normal. Show that the probit is the natural link function in this situation (Hint: See Section 7.3).
Figure 8.2 shows the density of a continuous latent variable z cut by three cutpoints $C_1 < C_2 < C_3$ into four regions, whose areas are the category probabilities $\pi_1, \pi_2, \pi_3, \pi_4$: π_1 is the area to the left of C_1, π_2 the area between C_1 and C_2, π_3 the area between C_2 and C_3, and π_4 the area to the right of C_3. (difficulty: ⋆⋆)

Solution. With $z \sim \mathrm{N}(\mu, \sigma^2)$ and $\mu = \mathbf{x}^T\boldsymbol{\beta}^*$, the link that linearises the cumulative probabilities is Φ^{-1}. The cutpoints $C_1 < \ldots < C_{J-1}$ belong to the instrument, not the subject, and category j is observed when $C_{j-1} < z \leqslant C_j$ ($C_0 = -\infty$, $C_J = +\infty$), so with $\gamma_j = \pi_1 + \ldots + \pi_j$,

$$\gamma_j = P(z \leqslant C_j) = \Phi\left(\frac{C_j - \mathbf{x}^T\boldsymbol{\beta}^*}{\sigma}\right),$$

$$\Phi^{-1}(\gamma_j) = \frac{C_j}{\sigma} - \frac{\mathbf{x}^T\boldsymbol{\beta}^*}{\sigma} = \beta_{0j} - \mathbf{x}^T\boldsymbol{\beta},$$

exactly the structure of the proportional odds model (8.14) with Φ^{-1} for the logit: a cutpoint-specific intercept $\beta_{0j} = C_j/\sigma$ plus a linear predictor $\boldsymbol{\beta} = \boldsymbol{\beta}^*/\sigma$ free of j. (The minus sign is convention; the book writes +.) This is the argument of Section 7.3, where a Uniform tolerance distribution gives the identity link, a logistic one the logit and the Normal Φ^{-1}; at $J = 2$ it collapses to the binary probit exactly, consistent with Exercise 8.1.
The parallel structure is then a consequence, not an extra assumption: σ is common to all $J - 1$ equations, so a covariate shifts the latent distribution without changing its spread and moves every cutpoint on the probit scale equally. Were σ to depend on $\mathbf{x}$, the coefficient $\boldsymbol{\beta}^*/\sigma(\mathbf{x})$ would break it, for probit as for logit. Since C_j and $\boldsymbol{\beta}^*$ enter only as C_j/σ and $\boldsymbol{\beta}^*/\sigma$, the parameters are identified only up to the scale of z — $\sigma = 1$ is the usual normalisation — and shifting z with every C_j changes nothing, which is why there is no separate intercept. Note that "natural" here is the tolerance-distribution sense of Section 7.3, not canonical in the sense of Section 3.3: the canonical Binomial link is the logit.
Simulating a latent Normal with known σ, $\boldsymbol{\beta}^*$ and cutpoints:

```r
library(MASS)
set.seed(20260831)
n <- 200000
x <- rbinom(n, 1, 0.5)
beta.star <- 1.2; sigma <- 2; C <- c(-1, 0.5, 2.5)
z <- rnorm(n, mean = beta.star * x, sd = sigma)
y <- ordered(cut(z, breaks = c(-Inf, C, Inf), labels = 1:4))
fit <- polr(y ~ x, method = "probit")
round(rbind(fitted = c(fit$zeta, x = coef(fit)),
            theory = c(C / sigma, x = beta.star / sigma)), 4)
```

```
          1|2   2|3   3|4    x.x
fitted -0.4971 0.252 1.255 0.6008
theory -0.5000 0.250 1.250 0.6000
```

The estimates match $C_j/\sigma = (-0.5, 0.25, 1.25)$ and $\beta^*/\sigma = 0.6$ to Monte Carlo error, with neither σ nor the raw C_j separately recoverable.

9 Poisson Regression and Log-Linear Models

Contents

9.1 Problem 9.1 — Let Y1 , . . . ,YN be independent random variables with Yi ∼ Po(µi) and

Problem 9.1. Let $Y_1, \ldots, Y_N$ be independent random variables with $Y_i \sim \mathrm{Po}(\mu_i)$ and

$$\log \mu_i = \beta_1 + \sum_{j=2}^{J} x_{ij}\beta_j, \qquad i = 1, \ldots, N.$$

a. Show that the score statistic for β_1 is $U_1 = \sum_{i=1}^{N}(Y_i - \mu_i)$.
b. Hence, show that for maximum likelihood estimates $\widehat{\mu}_i$, $\sum \widehat{\mu}_i = \sum y_i$.
c. Deduce that the expression for the deviance in (9.6) simplifies to (9.7) in this case. (difficulty: ⋆)

Solution. Write $\eta_i = \mathbf{x}_i^T\boldsymbol{\beta}$ with $\mathbf{x}_i = (1, x_{i2}, \ldots, x_{iJ})^T$; the leading 1 making β_1 an intercept is the only feature of the model used below.
(a) From $f(y_i;\mu_i) = \mu_i^{y_i}e^{-\mu_i}/y_i!$ the log-likelihood is $\ell = \sum_i[y_i \log \mu_i - \mu_i - \log y_i!]$, and $\mu_i = \exp(\mathbf{x}_i^T\boldsymbol{\beta})$ gives $\partial\mu_i/\partial\beta_j = \mu_i x_{ij}$, so

$$U_j = \frac{\partial \ell}{\partial \beta_j} = \sum_{i=1}^{N}\left[\frac{y_i}{\mu_i} - 1\right]\mu_i x_{ij} = \sum_{i=1}^{N}(y_i - \mu_i)x_{ij}, \qquad j = 1, \ldots, J,$$

the Section 4.3 score specialised to the log link, which is canonical so the weights cancel. Taking $j = 1$ with $x_{i1} = 1$ gives $U_1 = \sum_{i=1}^{N}(Y_i - \mu_i)$, and $\mathrm{E}(U_1) = 0$ since $\mathrm{E}(Y_i) = \mu_i$.
(b) The estimates $\mathbf{b}$ solve $U_j = 0$ for every j; the $j = 1$ equation is $\sum_i(y_i - \widehat{\mu}_i) = 0$, so $\sum \widehat{\mu}_i = \sum y_i$ with $\widehat{\mu}_i = \exp(\mathbf{x}_i^T\mathbf{b})$ — in the notation of Section 9.2, $\sum e_i = \sum o_i$. Only the constant term was used, so this holds for every model in the chapter carrying an intercept (or indicators summing to a column of ones), including the log-linear models of Section 9.5.
(c) By (b) the correction term in (9.6) vanishes,

$$\sum_{i=1}^{N}(o_i - e_i) = \sum y_i - \sum \widehat{\mu}_i = 0, \qquad \text{so} \qquad D = 2\sum_{i=1}^{N} o_i \log\left(\frac{o_i}{e_i}\right),$$

which is (9.7), the likelihood ratio statistic G^2 of contingency tables. The two agree only because of the intercept: (9.6) is the deviance in general, and it is also the form guaranteeing $D \geqslant 0$ term by term, each summand being $2e_i h(o_i/e_i)$ with $h(t) = t\log t - t + 1 \geqslant 0$, whereas summands of (9.7) can be negative.
Numerically, on the British doctors data of Section 9.2.1 fitted with Model (9.9), plus a deliberately intercept-free model:

```r
library(dobson)
data(doctors)
d <- doctors
d$agecat <- rep(1:5, 2)
d$agesq  <- d$agecat^2
d$smoke  <- as.numeric(d$smoking == "smoker")
d$smkage <- d$smoke * d$agecat
# 'poisson' is a dobson data set, so the family function needs its namespace
fit <- glm(deaths ~ smoke + agecat + agesq + smkage +
             offset(log(`person-years`)), family = stats::poisson, data = d)
o <- d$deaths; e <- fitted(fit)
cat("sum(o) =", sum(o), "   sum(e) =", sum(e), "\n")
cat("score for beta1 = sum(o - e) =", sum(o - e), "\n")
cat("D from (9.6) =", 2 * sum(o * log(o / e)) - (o - e)),
    "  D from (9.7) =", 2 * sum(o * log(o / e)),
    "  deviance(fit) =", deviance(fit), "\n")
fit0 <- glm(deaths ~ 0 + agecat + offset(log(`person-years`)),
            family = stats::poisson, data = d)
e0 <- fitted(fit0)
```

```r
cat("no intercept: sum(o - e) =", sum(o - e0),
    "  (9.6) =", 2 * sum(o * log(o / e0) - (o - e0)),
    "  (9.7) =", 2 * sum(o * log(o / e0)), "\n")
```

```
sum(o) = 731    sum(e) = 731
score for beta1 = sum(o - e) = 9.361401e-13
D from (9.6) = 1.63537   D from (9.7) = 1.63537   deviance(fit) = 1.63537
no intercept: sum(o - e) = -1695.874   (9.6) = 13211   (9.7) = 9819.252
```

The intercept model reproduces the grand total 731 to numerical precision and the two deviance formulae agree at $D = 1.635$, the value quoted in Table 9.3. Removing the intercept breaks $\sum o_i = \sum e_i$, and (9.6) then exceeds (9.7) by exactly $-2\sum(o_i - e_i) = 3391.75$; only (9.6) equals `deviance()`.

9.2 Problem 9.2 — The data in Table 9.13 are numbers of insurance policies, n, and numbers

Problem 9.2. The data in Table 9.13 are numbers of insurance policies, n, and numbers of claims, y, for cars in various insurance categories, *CAR*, tabulated by age of policy holder, *AGE*, and district where the policy holder lived (*DIST* = 1, for London and other major cities, and *DIST* = 0, otherwise). The table is derived from the *CLAIMS* data set in Aitkin et al. (2005) obtained from a paper by Baxter et al. (1980).
a. Calculate the rate of claims y/n for each category and plot the rates by *AGE*, *CAR* and *DIST* to get an idea of the main effects of these factors.
b. Use Poisson regression to estimate the main effects (each treated as categorical and modelled using indicator variables) and interaction terms.
c. Based on the modelling in (b), Aitkin et al. (2005) determined that all the interactions were unimportant and decided that *AGE* and *CAR* could be treated as though they were continuous variables. Fit a model incorporating these features and compare it with the best model obtained in (b). What conclusions do you reach?
Table 9.13 (car insurance claims) gives, for each combination of $CAR = 1, 2, 3, 4$ and $AGE = 1, 2, 3, 4$, the pair (y, n) separately for *DIST* = 0 and *DIST* = 1. For *DIST* = 0 the sixteen pairs, in the order $CAR = 1$ with $AGE = 1, \ldots, 4$, then $CAR = 2$ with $AGE = 1, \ldots, 4$, and so on, are $(65, 317)$, $(65, 476)$, $(52, 486)$, $(310, 3259)$; $(98, 486)$, $(159, 1004)$, $(175, 1355)$, $(877, 7660)$; $(41, 223)$, $(117, 539)$, $(137, 697)$, $(477, 3442)$; $(11, 40)$, $(35, 148)$, $(39, 214)$, $(167, 1019)$. For *DIST* = 1, in the same order, they are $(2, 20)$, $(5, 33)$, $(4, 40)$, $(36, 316)$; $(7, 31)$, $(10, 81)$, $(22, 122)$, $(102, 724)$; $(5, 18)$, $(7, 39)$, $(16, 68)$, $(63, 344)$; $(0, 3)$, $(6, 16)$, $(8, 25)$, $(33, 114)$. (difficulty: ⋆⋆⋆)

Solution. Claim rates depend on all three factors, on none of their interactions, and linearly in the *CAR* and *AGE* scores. The response is a claim count out of a known number of policies, so this is the rate model of Section 9.2: $Y_i \sim \text{Po}(\mu_i)$ with $\mu_i = n_i\theta_i$ and, by equation (9.3),

$$\log \mu_i = \log n_i + \mathbf{x}_i^T \boldsymbol{\beta},$$

the offset $\log n_i$ carrying the exposure and the parameters read as rate ratios e^{β_j}.
(a) Observed rates.

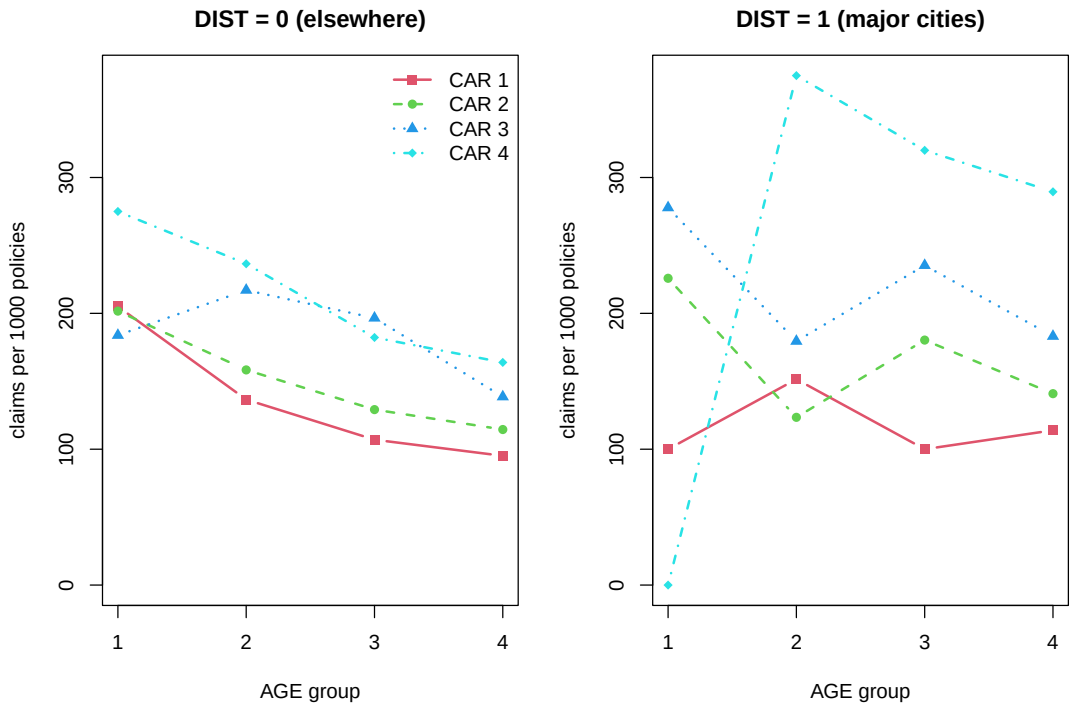
```r
library(dobson)
data(insurance)
ins <- insurance
ins$rate <- 1000 * ins$y / ins$n
print(round(xtabs(rate ~ car + age + district, data = ins), 1))
mg <- function(v) round(1000 * tapply(ins$y, ins[[v]], sum) / tapply(ins$n, ins[[v]], sum),
    1)
rbind(CAR = mg("car"), AGE = mg("age"))
mg("district")
```

```
, , district = 0

    age
car     1     2     3     4
```

```
  1 205.0 136.6 107.0  95.1
  2 201.6 158.4 129.2 114.5
  3 183.9 217.1 196.6 138.6
  4 275.0 236.5 182.2 163.9

, , district = 1

   age
car     1     2     3     4
  1 100.0 151.5 100.0 113.9
  2 225.8 123.5 180.3 140.9
  3 277.8 179.5 235.3 183.1
  4   0.0 375.0 320.0 289.5

        1     2     3     4
CAR 109.0 126.5 160.7 189.4
AGE 201.2 172.9 150.6 122.3

    0     1
132.2 163.5
```

Rates are claims per 1000 policies per year. The marginal patterns are monotone: the rate rises with *CAR* (109 to 189), falls with *AGE* (201 to 122), and runs about a quarter higher in the major cities (163.5 against 132.2).

```
op <- par(mfrow = c(1, 2), mar = c(4.5, 4.5, 3, 1))
for (dd in 0:1) {
  s <- ins[ins$district == dd, ]
  plot(range(s$age), range(ins$rate), type = "n", xlab = "AGE group",
       ylab = "claims per 1000 policies", xaxt = "n",
       main = paste0("DIST = ", dd, if (dd == 1) " (major cities)" else " (elsewhere)"))
  axis(1, at = 1:4)
  for (cc in 1:4) {
    z <- s[s$car == cc, ]
    lines(z$age, z$rate, type = "b", pch = 14 + cc, lty = cc, col = cc + 1, lwd = 2)
  }
  if (dd == 0) legend("topright", legend = paste("CAR", 1:4), pch = 15:18,
                      lty = 1:4, col = 2:5, bty = "n", lwd = 2)
}
par(op)
```



In the left panel ($DIST = 0$, holding nearly all the exposure) the four *CAR* curves stack in order and

fall with AGE at much the same rate — what an additive model on the log scale predicts. The only departure, $CAR = 3$ rising from $AGE = 1$ to 2, is within sampling error by part (b). The right panel is noisier because those cells hold very few policies: $CAR = 4$, $AGE = 1$ has $n = 3$, $y = 0$, so its jump from 0 to 375 per 1000 rests on three policies.

(b) Poisson regression with categorical effects.

```
ins$CAR <- factor(ins$car); ins$AGE <- factor(ins$age); ins$DIST <- factor(ins$district)
P <- function(f) glm(f, family = stats::poisson, data = ins, offset = log(n))
m0 <- P(y ~ 1);                    m1 <- P(y ~ CAR + AGE + DIST)
m2 <- P(y ~ CAR + AGE + DIST + CAR:AGE)
m3 <- P(y ~ CAR + AGE + DIST + CAR:DIST)
m4 <- P(y ~ CAR + AGE + DIST + AGE:DIST)
m5 <- P(y ~ (CAR + AGE + DIST)^2);  m6 <- P(y ~ CAR * AGE * DIST)
ms <- list(m0, m1, m2, m3, m4, m5, m6)
data.frame(model = c("minimal", "main effects", "+ CAR:AGE", "+ CAR:DIST",
                     "+ AGE:DIST", "all two-way", "saturated"),
           df = sapply(ms, df.residual),
           deviance = round(sapply(ms, deviance), 3),
           AIC = round(sapply(ms, AIC), 1))
```

```
         model df deviance   AIC
1      minimal 31  207.833 378.2
2 main effects 24   23.709 208.1
3    + CAR:AGE 15   13.192 215.6
4   + CAR:DIST 21   19.272 209.6
5   + AGE:DIST 21   19.920 210.3
6  all two-way  9    5.295 219.7
7    saturated  0    0.000 232.4
```

The three main effects drop the deviance from 207.8 on 31 d.f. to 23.7 on 24 d.f., and that already fits ($p = 0.48$ against $\chi^2(24)$). No interaction is needed:

```
rbind("CAR:AGE"  = unlist(anova(m1, m2, test = "Chisq")[2, c("Df", "Deviance", "Pr(>Chi)")]),
      "CAR:DIST" = unlist(anova(m1, m3, test = "Chisq")[2, c("Df", "Deviance", "Pr(>Chi)")]),
      "AGE:DIST" = unlist(anova(m1, m4, test = "Chisq")[2, c("Df", "Deviance", "Pr(>Chi)")]))
```

```
         Df  Deviance  Pr(>Chi)
CAR:AGE   9 10.517305 0.3102500
CAR:DIST  3  4.437058 0.2179738
AGE:DIST  3  3.789357 0.2851265
```

Each costs many parameters, buys almost nothing, and raises AIC, so the best model in (b) is the main-effects model:

```
summary(m1)
```

```
Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -1.81021    0.07532 -24.034  < 2e-16 ***
CAR2         0.16229    0.05052   3.213 0.001315 **
CAR3         0.39352    0.05498   7.157 8.25e-13 ***
CAR4         0.56540    0.07228   7.823 5.18e-15 ***
AGE2        -0.18902    0.08282  -2.282 0.022477 *
AGE3        -0.34211    0.08130  -4.208 2.58e-05 ***
AGE4        -0.53275    0.06979  -7.634 2.28e-14 ***
DIST1        0.21850    0.05853   3.733 0.000189 ***

    Null deviance: 207.833  on 31  degrees of freedom
Residual deviance:  23.709  on 24  degrees of freedom
AIC: 208.07
```

Relative to $CAR = 1$, $AGE = 1$, $DIST = 0$, the rate ratios are 1.18, 1.48, 1.76 across CAR and 0.83, 0.71, 0.59 across AGE, with 1.24 for city residence. Both sets are monotone and close to equally spaced on the log scale — CAR steps $0.162, 0.231, 0.172$, AGE steps $-0.189, -0.153, -0.191$ — which is the empirical fact behind part (c).

(c) AGE and CAR as continuous. Equal spacing of the log-scale contrasts is exactly what a linear term in the coded level $1, 2, 3, 4$ imposes, so replacing the factors by the scores should cost nothing.

```
mc <- glm(y ~ car + age + DIST, family = stats::poisson, data = ins, offset = log(n))
```

```r
summary(mc)
round(exp(cbind(estimate = coef(mc), confint.default(mc))), 3)
```

```
Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -1.85253    0.07990 -23.185  < 2e-16 ***
car          0.19777    0.02080   9.507  < 2e-16 ***
age         -0.17674    0.01849  -9.559  < 2e-16 ***
DIST1        0.21865    0.05853   3.736 0.000187 ***

    Null deviance: 207.833  on 31  degrees of freedom
Residual deviance:  24.685  on 28  degrees of freedom
AIC: 201.05

            estimate 2.5 % 97.5 %
(Intercept)    0.157 0.134  0.183
car            1.219 1.170  1.269
age            0.838 0.808  0.869
DIST1          1.244 1.110  1.396
```

```r
anova(mc, m1, test = "Chisq")
c(AIC.continuous = AIC(mc), AIC.categorical = AIC(m1))
X2 <- sum(residuals(mc, "pearson")^2)
c(X2 = X2, df = df.residual(mc), p = pchisq(X2, df.residual(mc), lower.tail = FALSE))
```

```
Analysis of Deviance Table

Model 1: y ~ car + age + DIST
Model 2: y ~ CAR + AGE + DIST
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
1        28     24.685
2        24     23.709  4  0.97633   0.9134

 AIC.continuous AIC.categorical
       201.0456        208.0693

       X2        df         p
23.497605 28.000000  0.707754
```

Collapsing six indicator parameters to two slopes costs only 0.98 of deviance on 4 d.f. ($p = 0.91$), so the linearity restriction is consistent with the data. The continuous model has $D = 24.69$ and $X^2 = 23.50$ on 28 d.f. ($p = 0.71$), fitting the 32 cells well in absolute terms, with AIC 7 points below the categorical model's.

```r
r <- rstandard(mc); o <- order(-abs(r))[1:4]
round(cbind(ins[o, c("car", "age", "district", "y", "n")],
            fitted = fitted(mc)[o], rstd = r[o]), 2)
```

```
   car age district   y   n fitted  rstd
1    1   1        0  65 317  50.77  2.07
11   3   3        0 137 697 116.44  1.92
9    3   1        0  41 223  53.05 -1.85
32   4   4        1  33 114  24.20  1.79
```

No standardised residual exceeds 2.1 over 32 cells, so no cell is badly missed — in particular the eye-catching $DIST = 1$ cells are not outliers once their small exposure is accounted for.

So the effects are multiplicative and act independently: each one-step rise in CAR multiplies the claim rate by 1.22 (95% CI 1.17 to 1.27), each one-step rise in AGE by 0.84 (0.81 to 0.87) so that the oldest band runs at $0.84^3 = 0.59$ of the youngest, and city residence by 1.24 (1.11 to 1.40). With no interaction, the city loading of about 24% applies uniformly to every CAR by AGE cell and the two gradients are the same inside and outside the cities. Reading the slopes literally does assume the four levels of each are equally spaced on some underlying scale; the justification is purely empirical, namely that the fitted categorical contrasts came out equally spaced.

9.3 Problem 9.3 — This question relates to the flu vaccine trial data in Table 9.6.

Problem 9.3. This question relates to the flu vaccine trial data in Table 9.6.
a. Using a conventional chi-squared test and an appropriate log-linear model, test the hypothesis that the distribution of responses is the same for the placebo and vaccine groups.
b. For the model corresponding to the hypothesis of homogeneity of response distributions, calculate the fitted values, the Pearson and deviance residuals, and the goodness of fit statistics X^2 and D. Which of the cells of the table contribute most to X^2 (or D)? Explain and interpret these results.
c. Re-analyze these data using ordinal logistic regression to estimate cutpoints for a latent continuous response variable and to estimate a location shift between the two treatment groups. Sketch a rough diagram to illustrate the model which forms the conceptual base for this analysis (see Exercise 8.4).
Table 9.6 (flu vaccine trial) is a 2×3 table of frequencies. The rows are the treatment groups and the columns are the response categories small, moderate and large. The placebo row is 25, 8, 5 with row total 38; the vaccine row is 6, 18, 11 with row total 35. (difficulty: ⋆⋆)

Solution. Homogeneity of the response distributions ($\theta_{jk} = \theta_{\cdot k}$) is the additive log-linear model $\mu + \alpha_j + \beta_k$, tested against the saturated $\mu + \alpha_j + \beta_k + (\alpha\beta)_{jk}$; the row totals 38 and 35 are fixed by design, so the sampling is product multinomial and by Section 9.5 every model must retain α_j.

(a) **Chi-squared test and log-linear model.**

```r
library(dobson)
data(vaccine)
v <- vaccine
v$response <- factor(v$response, levels = c("small", "moderate", "large"))
tab <- xtabs(frequency ~ treatment + response, data = v)
tab
chisq.test(tab)
```

```
          response
treatment small moderate large
  placebo    25        8     5
  vaccine     6       18    11

        Pearson's Chi-squared test

data:  tab
X-squared = 17.648, df = 2, p-value = 0.0001472
```

```r
sat <- glm(frequency ~ treatment * response, family = stats::poisson, data = v)
add <- glm(frequency ~ treatment + response, family = stats::poisson, data = v)
anova(add, sat, test = "Chisq")
```

```
Analysis of Deviance Table

Model 1: frequency ~ treatment + response
Model 2: frequency ~ treatment * response
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
1         2     18.642
2         0      0.000  2   18.642 8.95e-05 ***
```

By Section 9.7.1 the two are the Pearson and likelihood ratio versions of one test: $X^2 = 17.65$ and $\Delta D = 18.64$ on 2 d.f. ($p < 0.0002$). The interactions $(\alpha\beta)_{jk}$ are needed, so the response distribution is **not** the same in the two groups.

(b) **Fitted values and residuals under homogeneity.**

```r
data.frame(v[, c("treatment", "response")], observed = v$frequency,
           fitted = round(fitted(add), 3),
           pearson = round(residuals(add, "pearson"), 3),
           deviance = round(residuals(add, "deviance"), 3))
X2 <- sum(residuals(add, "pearson")^2); D <- deviance(add)
c(X2 = X2, D = D, df = df.residual(add),
  p.X2 = pchisq(X2, df.residual(add), lower.tail = FALSE),
  p.D  = pchisq(D,  df.residual(add), lower.tail = FALSE))
```

```
round(residuals(add, "pearson")^2, 3)
```

```
 treatment response observed fitted pearson deviance
   placebo    small       25 16.137   2.206    2.040
   placebo moderate        8 13.534  -1.504   -1.630
   placebo    large        5  8.329  -1.153   -1.247
   vaccine    small        6 14.863  -2.299   -2.615
   vaccine moderate       18 12.466   1.567    1.469
   vaccine    large       11  7.671   1.202    1.128

          X2            D           df         p.X2          p.D
1.764783e+01 1.864253e+01 2.000000e+00 1.471709e-04 8.950070e-05

    1     2     3     4     5     6
4.868 2.263 1.330 5.285 2.457 1.444
```

The fitted values are $e_{jk} = y_{j\cdot}y_{\cdot k}/n$ (e.g. $38 \times 31/73 = 16.14$) and reproduce the fixed row totals, as Exercise 9.1(b) requires of any model containing α_j; since the saturated alternative has zero deviance, $X^2 = 17.65$ and $D = 18.64$ on 2 d.f. are the same numbers as in (a).

The two "small" cells contribute $4.87 + 5.29 = 10.15$, 58% of X^2, and carry the two largest deviance residuals (2.04, −2.62): placebo gave 25 small responses against an expected 16, vaccine gave 6 against 15, and the signs reverse for moderate and large. The row percentages are 66/21/13 under placebo against 17/51/31 under vaccine, so the vaccine raises the antibody response. The discrepancies are monotone in an ordered response, so the 2 d.f. test wastes power – which (c) repairs.

(c) **Ordinal logistic regression.**

Take an unobserved latent antibody response z, recorded small/moderate/large as z falls below C_1, between C_1 and C_2, or above C_2, with treatment shifting the logistic latent distribution by β without changing shape (Exercise 8.4, Section 8.3.3); this is the proportional odds model

$$\log\left(\frac{\Pr(Y \leqslant j)}{1 - \Pr(Y \leqslant j)}\right) = C_j - \beta\, x, \qquad j = 1, 2,$$

with $x = 1$ for vaccine. Three parameters for 4 free cell probabilities leaves 1 d.f. to test fit.

```
suppressMessages(library(MASS))   # note: MASS masks the dobson 'housing' data set
v$response  <- factor(v$response, levels = c("small", "moderate", "large"), ordered = TRUE)
v$treatment <- factor(v$treatment, levels = c("placebo", "vaccine"))
po <- polr(response ~ treatment, weights = frequency, data = v, Hess = TRUE)
summary(po)
round(exp(c(OR = coef(po), confint.default(po))), 3)
```

```
Coefficients:
                 Value Std. Error t value
treatmentvaccine 1.838     0.4882   3.764

Intercepts:
                Value  Std. Error t value
small|moderate 0.5654 0.3434     1.6465
moderate|large 2.4414 0.4525     5.3948

Residual Deviance: 139.6736
AIC: 145.6736

OR.treatmentvaccine
              6.283               2.413              16.357
```

So $\widehat{C}_1 = 0.565$, $\widehat{C}_2 = 2.441$ and $\widehat{\beta} = 1.838$ (s.e. 0.488, 3.76 standard errors from zero): the vaccine multiplies the odds of a higher response category by $e^{1.838} = 6.3$ (95% CI 2.4 to 16.4), one ratio serving both cutpoints by the proportional odds assumption.

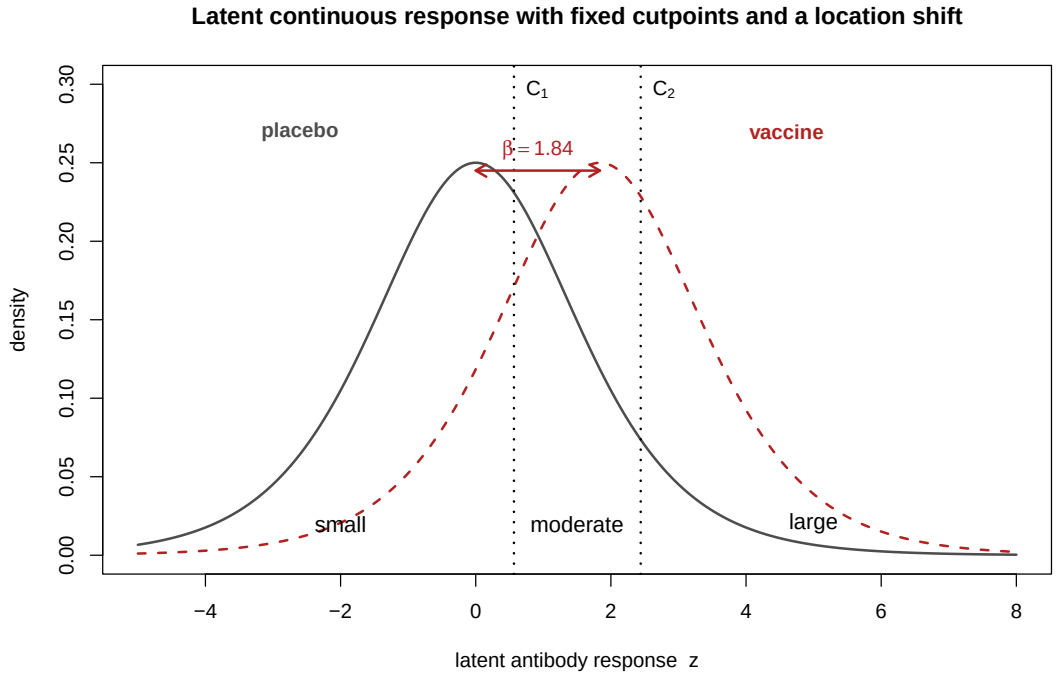
```
po0 <- polr(response ~ 1, weights = frequency, data = v, Hess = TRUE)
c(dev.diff = deviance(po0) - deviance(po),
  p = pchisq(deviance(po0) - deviance(po), 1, lower.tail = FALSE))
pr <- predict(po, newdata = data.frame(treatment = factor(c("placebo", "vaccine"))),
              type = "probs")
rownames(pr) <- c("placebo", "vaccine")
```

```r
round(pr, 3)
round(pr * c(38, 35), 2)
obs <- as.vector(t(tab)); ex <- as.vector(t(pr * c(38, 35)))
c(X2 = sum((obs - ex)^2 / ex), D = 2 * sum(obs * log(obs / ex)), df = 1)
```

```
    dev.diff            p
1.568242e+01 7.491725e-05

        small moderate large
placebo 0.638    0.282 0.080
vaccine 0.219    0.428 0.354

        small moderate large
placebo 24.23    10.72  3.04
vaccine  7.66    14.97 12.37

      X2        D       df
3.102269 2.960108 1.000000
```

The likelihood ratio test for the shift is 15.68 on **1** d.f. ($p = 7.5 \times 10^{-5}$) against 18.64 on 2 d.f., so the ordering recovers almost all the signal at half the cost. The restriction itself is acceptable: $X^2 = 3.10$, $D = 2.96$ on 1 d.f. ($p \approx 0.08$), the residual lack of fit sitting in the same "small" cells, whose fitted counts 24.2 and 7.7 understate the separation slightly.

```r
C1 <- 0.5654; C2 <- 2.4414; shift <- 1.838
z <- seq(-5, 8, length = 800)
plot(z, dlogis(z), type = "l", lwd = 2, col = "grey30", ylim = c(0, 0.30),
     xlab = "latent antibody response  z", ylab = "density",
     main = "Latent continuous response with fixed cutpoints and a location shift")
lines(z, dlogis(z, location = shift), lwd = 2, col = "firebrick", lty = 2)
abline(v = c(C1, C2), lty = 3, lwd = 2)
text(c(C1, C2), 0.295, c(expression(C[1]), expression(C[2])), pos = 4)
text(-2.6, 0.27, "placebo", col = "grey30", font = 2)
text(4.6, 0.27, "vaccine", col = "firebrick", font = 2)
arrows(0, 0.245, shift, 0.245, code = 3, length = 0.10, lwd = 2, col = "firebrick")
text(shift/2, 0.258, expression(beta == 1.84), col = "firebrick")
text(c(-2.0, 1.5, 5.0), 0.02, c("small", "moderate", "large"), cex = 1.05)
```



One latent density drawn twice – solid for placebo at 0, dashed for vaccine slid 1.84 to the right – with fixed cutpoints C_1, C_2 cutting off the response probabilities $0.638, 0.282, 0.080$ and $0.219, 0.428, 0.354$; the slide moves mass out of "small" into "large", the pattern the residuals in (b) showed.

9.4 Problem 9.4 — For a 2× 2 contingency table, the maximal log-linear model can be written

Problem 9.4. For a 2×2 contingency table, the maximal log-linear model can be written as

$$\eta_{11} = \mu + \alpha + \beta + (\alpha\beta), \qquad \eta_{12} = \mu + \alpha - \beta - (\alpha\beta),$$

$$\eta_{21} = \mu - \alpha + \beta - (\alpha\beta), \qquad \eta_{22} = \mu - \alpha - \beta + (\alpha\beta),$$

where $\eta_{jk} = \log \mathrm{E}(Y_{jk}) = \log(n\theta_{jk})$ and $n = \sum\sum Y_{jk}$.
Show that the interaction term $(\alpha\beta)$ is given by

$$(\alpha\beta) = \tfrac{1}{4} \log \phi,$$

where ϕ is the **odds ratio** $(\theta_{11}\theta_{22})/(\theta_{12}\theta_{21})$, and hence that $\phi = 1$ corresponds to no interaction. (difficulty: $\star$)

Solution. Take the contrast with signs $+, -, -, +$. In the four displayed expressions μ carries weights $+1, -1, -1, +1$, α carries $+1, -1, +1, -1$ and β carries $+1, +1, -1, -1$ – each summing to 0 – while $(\alpha\beta)$ carries $+1, +1, +1, +1$, so

$$\eta_{11} - \eta_{12} - \eta_{21} + \eta_{22} = 4(\alpha\beta).$$

Since $\eta_{jk} = \log n + \log \theta_{jk}$ and the weights sum to zero, $\log n$ cancels:

$$4(\alpha\beta) = \log \theta_{11} - \log \theta_{12} - \log \theta_{21} + \log \theta_{22} = \log \left(\frac{\theta_{11}\theta_{22}}{\theta_{12}\theta_{21}} \right) = \log \phi,$$

whence $(\alpha\beta) = \frac{1}{4} \log \phi$. As log is strictly increasing with $\log 1 = 0$,

$$(\alpha\beta) = 0 \iff \log \phi = 0 \iff \phi = 1,$$

and $\phi = 1$ reads $\theta_{11}\theta_{22} = \theta_{12}\theta_{21}$, which for probabilities summing to one is independence $\theta_{jk} = \theta_{j\cdot}\theta_{\cdot k}$ (Check!), that is, the additive model (9.10). So no interaction is exactly $\phi = 1$.
A numerical check on the gastric-ulcer half of Table 9.7, entries 62, 6 (controls) and 39, 25 (cases), with sum-to-zero contrasts:

```r
library(dobson)
data(ulcer)
g <- subset(ulcer, ulcer == "gastric")
g$CC <- factor(g$`case-control`, levels = c("control", "case"))
g$AP <- factor(g$aspirin,        levels = c("non-user", "user"))
sat <- glm(frequency ~ CC * AP, family = stats::poisson, data = g,
           contrasts = list(CC = "contr.sum", AP = "contr.sum"))
round(coef(sat), 6)
y <- xtabs(frequency ~ CC + AP, data = g)
phi <- (y[1, 1] * y[2, 2]) / (y[1, 2] * y[2, 1])
eta <- log(as.vector(t(y)))   # order (1,1) (1,2) (2,1) (2,2)
c(phi = phi, quarter.log.phi = log(phi) / 4,
  contrast = (eta[1] - eta[2] - eta[3] + eta[4]) / 4)
```

```
(Intercept)         CC1         AP1     CC1:AP1
   3.200333   -0.240886    0.695015    0.472672

            phi quarter.log.phi        contrast
      6.6239316       0.4726723       0.4726723
```

The fitted interaction, the contrast in the η_{jk} and $\frac{1}{4} \log \phi$ all equal 0.472672, with $\phi = 6.62$ far from 1 – the association of aspirin with gastric ulcer reported in Section 9.7.2.

9.5 Problem 9.5 — Use log-linear models to examine the housing satisfaction data in Ta-

Problem 9.5. Use log-linear models to examine the housing satisfaction data in Table 8.5. The numbers of people surveyed in each type of housing can be regarded as fixed.
a. First, analyze the associations between level of satisfaction (treated as a nominal categorical variable) and contact with other residents, separately for each type of housing.
b. Next, conduct the analyses in (a) simultaneously for all types of housing.
c. Compare the results from log-linear modelling with those obtained using nominal or ordinal logistic regression (see Exercise 8.2).
Table 8.5 (satisfaction with housing conditions, Copenhagen) cross-classifies residents by type of housing, level of satisfaction (low, medium, high) and degree of contact with other residents (low, high). The frequencies, given as (low contact, high contact) pairs for each satisfaction level, are: tower block – low satisfaction $(65, 34)$, medium $(54, 47)$, high $(100, 100)$; apartment – low $(130, 141)$, medium $(76, 116)$, high $(111, 191)$; house – low $(67, 130)$, medium $(48, 105)$, high $(62, 104)$. (difficulty: $\star\star\star$)

Solution. The model to report is the homogeneous association model $T:S + T:C + S:C$; it is the same fit as the nominal logistic regression $S \sim T + C$ of Exercise 8.2, and the ordinal version of the latter is the most parsimonious summary. Write T (type), S (satisfaction), C (contact). The numbers surveyed per housing type are fixed at 400, 765, 516, so by Section 9.5 every model must contain α_j^T. Note `MASS` carries a `housing` data set of its own, so the `dobson` one is named explicitly below.
(a) **Satisfaction against contact, one housing type at a time.**
Within a fixed type this is a 3×2 independence test, and by Section 9.7.1 fitting $S + C$ against $S * C$ is the conventional chi-squared test.

```r
library(dobson)
h <- dobson::housing
h$type <- factor(h$type, levels = c("tower block", "apartment", "house"))
h$satisfaction <- factor(h$satisfaction, levels = c("low", "medium", "high"))
h$contact <- factor(h$contact, levels = c("low", "high"))
for (tt in levels(h$type)) {
  s  <- subset(h, type == tt)
  tb <- xtabs(frequency ~ satisfaction + contact, data = s)
  add <- glm(frequency ~ satisfaction + contact, family = stats::poisson, data = s)
  cat("\n==", tt, "  n =", sum(tb), "\n")
  print(round(100 * prop.table(tb, 2), 1))
  cat("X2 =", round(chisq.test(tb)$statistic, 3),
      " D =", round(deviance(add), 3), " df =", df.residual(add),
      " p =", signif(pchisq(deviance(add), df.residual(add), lower.tail = FALSE), 4), "\n")
}
```

```
== tower block   n = 400
            contact
satisfaction  low high
      low    29.7 18.8
      medium 24.7 26.0
      high   45.7 55.2
X2 = 6.642  D = 6.742  df = 2  p = 0.03435

== apartment   n = 765
            contact
satisfaction  low high
      low    41.0 31.5
      medium 24.0 25.9
      high   35.0 42.6
X2 = 7.767  D = 7.745  df = 2  p = 0.02081

== house   n = 516
            contact
satisfaction  low high
```

```
       low    37.9 38.3
       medium 27.1 31.0
       high   35.0 30.7
X2 = 1.274  D = 1.274  df = 2  p = 0.529
```

Independence is rejected at 5% for tower blocks and apartments, in the same direction both times: high contact lowers the chance of low satisfaction (29.7% to 18.8%; 41.0% to 31.5%) and raises that of high satisfaction. For houses there is no association ($D = 1.27$ on 2 d.f.). Three subset analyses spend 6 d.f. on the association and cannot ask whether it differs by housing type, which is (b).

(b) **All housing types simultaneously.**

```
names(h)[1:3] <- c("T", "S", "C")
P <- function(f) glm(f, family = stats::poisson, data = h)
mods <- list("T" = P(frequency ~ T),
             "T + S + C" = P(frequency ~ T + S + C),
             "T + S + C + T:S" = P(frequency ~ T + S + C + T:S),
             "T + S + C + T:C" = P(frequency ~ T + S + C + T:C),
             "T:S + T:C" = P(frequency ~ T*S + T*C),
             "T:S + T:C + S:C" = P(frequency ~ (T + S + C)^2),
             "saturated" = P(frequency ~ T*S*C))
data.frame(terms = names(mods), df = sapply(mods, df.residual),
           deviance = round(sapply(mods, deviance), 3),
           X2 = round(sapply(mods, function(m) sum(residuals(m, "pearson")^2)), 3),
           AIC = round(sapply(mods, AIC), 1), row.names = NULL)
```

```
           terms df deviance      X2   AIC
1              T 15  172.837 172.831 291.9
2      T + S + C 12   89.348  85.347 214.5
3 T + S + C + T:S  8   54.819  54.751 187.9
4 T + S + C + T:C 10   50.290  49.055 179.4
5      T:S + T:C  6   15.761  15.683 152.9
6 T:S + T:C + S:C  4    6.893   6.932 148.0
7      saturated  0    0.000   0.000 149.1
```

```
anova(mods[["T:S + T:C"]], mods[["T:S + T:C + S:C"]], test = "Chisq")
anova(mods[["T:S + T:C + S:C"]], mods[["saturated"]], test = "Chisq")
```

```
Model 1: frequency ~ T * S + T * C
Model 2: frequency ~ (T + S + C)^2
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
1         6     15.761
2         4      6.893  2   8.8677  0.01187 *

Model 1: frequency ~ (T + S + C)^2
Model 2: frequency ~ T * S * C
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
1         4      6.893
2         0      0.000  4    6.893   0.1417
```

Both $T{:}S$ and $T{:}C$ are needed (adding $T{:}C$ to $T{:}S$ drops D by $54.82 - 15.76 = 39.06$ on 4 d.f.), and so is $S{:}C$ ($\Delta D = 8.87$ on 2 d.f., $p = 0.012$); the three-way term is not ($\Delta D = 6.89$ on 4 d.f., $p = 0.14$), and AIC is lowest for the all-two-way model. Hence

$$\log \mathrm{E}(Y_{jkl}) = \mu + \alpha_j^T + \alpha_k^S + \alpha_l^C + (\alpha^T\alpha^S)_{jk} + (\alpha^T\alpha^C)_{jl} + (\alpha^S\alpha^C)_{kl},$$

the **homogeneous association** model, with $D = 6.89$ and $X^2 = 6.93$ on 4 d.f.

```
round(summary(mods[["T:S + T:C + S:C"]])$coefficients, 4)
```

```
                  Estimate Std. Error z value Pr(>|z|)
(Intercept)         4.0943     0.1127 36.3376   0.0000
Tapartment          0.7402     0.1302  5.6867   0.0000
Thouse              0.2395     0.1417  1.6902   0.0910
Smedium            -0.1073     0.1524 -0.7037   0.4816
Shigh               0.5608     0.1329  4.2185   0.0000
Chigh              -0.4306     0.1293 -3.3306   0.0009
Tapartment:Smedium -0.4068     0.1713 -2.3745   0.0176
Thouse:Smedium     -0.3371     0.1804 -1.8690   0.0616
Tapartment:Shigh   -0.6416     0.1501 -4.2751   0.0000
```

```
Thouse:Shigh        -0.9456     0.1645 -5.7489   0.0000
Tapartment:Chigh     0.5744     0.1256  4.5749   0.0000
Thouse:Chigh         0.8906     0.1387  6.4193   0.0000
Smedium:Chigh        0.2960     0.1301  2.2750   0.0229
Shigh:Chigh          0.3282     0.1182  2.7772   0.0055
```

Interpretation, all on the odds scale relative to the corner categories (tower block, low satisfaction, low contact):

- $S:C$. High contact multiplies the odds of medium rather than low satisfaction by $e^{0.296} = 1.34$, of high rather than low by $e^{0.328} = 1.39$ – the association of (a), estimated once from all 1681 residents and, by the non-significance of the three-way term, common to all three housing types; the apparent absence among householders in (a) is sampling variation.
- $T:S$. The odds of high rather than low satisfaction are multiplied by $e^{-0.642} = 0.53$ for apartments and $e^{-0.946} = 0.39$ for houses.
- $T:C$. Contact rises in the same direction, $e^{0.574} = 1.78$ and $e^{0.891} = 2.44$, so T is associated with both other variables and must be conditioned on.
- μ and the T main effect are nuisance terms forced in by the fixed sample sizes.

(c) **Comparison with logistic regression.**

By Exercise 9.6 in three dimensions, the logistic model conditions on the $T \times C$ margin, so the log-linear model containing $T:C$ plus all terms linking S to the explanatory factors is the **same model** as the nominal logistic regression $S \sim T + C$ of Exercise 8.2, its S-involving coefficients being the logistic coefficients.

```r
suppressMessages({library(nnet); library(MASS)})
h2 <- dobson::housing
h2$type <- factor(h2$type, levels = c("tower block", "apartment", "house"))
h2$satisfaction <- factor(h2$satisfaction, levels = c("low", "medium", "high"))
h2$contact <- factor(h2$contact, levels = c("low", "high"))
ll <- glm(frequency ~ (type + satisfaction + contact)^2, family = stats::poisson, data = h2)
nm <- multinom(satisfaction ~ type + contact, weights = frequency, data = h2,
               trace = FALSE, maxit = 500, reltol = 1e-14)
round(coef(nm), 4)
round(coef(ll)[grep("satisfaction", names(coef(ll)))], 4)
```

```
       (Intercept) typeapartment typehouse contacthigh
medium     -0.1073       -0.4068   -0.3371      0.2960
high        0.5608       -0.6416   -0.9456      0.3282

              satisfactionmedium                satisfactionhigh
                         -0.1073                          0.5608
typeapartment:satisfactionmedium     typehouse:satisfactionmedium
                         -0.4068                         -0.3371
  typeapartment:satisfactionhigh       typehouse:satisfactionhigh
                         -0.6416                         -0.9456
  satisfactionmedium:contacthigh     satisfactionhigh:contacthigh
                          0.2960                          0.3282
```

The eight numbers agree to four decimals, and the nominal model's lack of fit against saturated $S \sim T * C$ is 6.893 on 4 d.f., the residual deviance of the all-two-way log-linear model: the same fit written twice. The log-linear version spends six extra nuisance parameters (μ, α^T, α^C, $(\alpha^T\alpha^C)$) reproducing the fixed margins that the logistic version conditions on.

Satisfaction is ordered, so the proportional odds model of Section 8.3.3 refines this:

```r
po <- polr(satisfaction ~ type + contact, weights = frequency, data = h2, Hess = TRUE)
round(summary(po)$coefficients, 4)
c(dev.nominal = deviance(nm), dev.ordinal = deviance(po),
  diff = deviance(po) - deviance(nm), df = 3,
  p = pchisq(deviance(po) - deviance(nm), 3, lower.tail = FALSE))
```

```
               Value Std. Error t value
typeapartment -0.5009     0.1168 -4.2906
typehouse     -0.7362     0.1261 -5.8383
contacthigh    0.2524     0.0931  2.7127
low|medium    -0.9973     0.1075 -9.2794
medium|high    0.1152     0.1047  1.1004
```

```
 dev.nominal  dev.ordinal         diff           df            p
3605.4803211 3610.2863798    4.8060587    3.0000000    0.1865619
```

The proportional odds restriction costs 4.81 in deviance for 3 saved parameters ($p = 0.19$), so it is acceptable and compresses the story to three numbers: high contact multiplies the odds of a higher satisfaction category by $e^{0.252} = 1.29$, apartments and houses by $e^{-0.501} = 0.61$ and $e^{-0.736} = 0.48$ relative to tower blocks. With 5 parameters against 8 and 14, it is what to report; the log-linear analysis earns its place by showing that $T:S$ and $T:C$ both exist and hence that T must be conditioned on. All three agree: satisfaction rises with contact, falls from tower blocks to houses, and the contact effect is common to all housing types.

9.6 Problem 9.6 — Consider a 2×K contingency table (Table 9.14) in which the column totals

Problem 9.6. Consider a $2 \times K$ contingency table (Table 9.14) in which the column totals $y_{\cdot k}$ are fixed for $k = 1, \ldots, K$. Table 9.14 has two rows, labelled Success and Failure, and K columns; the entries are y_{1k} in the Success row and y_{2k} in the Failure row, with column totals $y_{\cdot k}$, for $k = 1, \ldots, K$.
a. Show that the product multinomial distribution for this table reduces to

$$f(z_1, \ldots, z_K \mid n_1, \ldots, n_K) = \sum_{k=1}^{K} \binom{n_k}{z_k} \pi_k^{z_k} (1 - \pi_k)^{n_k - z_k},$$

where $n_k = y_{\cdot k}$, $z_k = y_{1k}$, $n_k - z_k = y_{2k}$, $\pi_k = \theta_{1k}$ and $1 - \pi_k = \theta_{2k}$ for $k = 1, \ldots, K$. This is the **product binomial distribution** and is the joint distribution for Table 7.1 (with appropriate changes in notation).
b. Show that the log-linear model with

$$\eta_{1k} = \log \mathrm{E}(Z_k) = \mathbf{x}_{1k}^T \boldsymbol{\beta}$$

and

$$\eta_{2k} = \log \mathrm{E}(n_k - Z_k) = \mathbf{x}_{2k}^T \boldsymbol{\beta}$$

is equivalent to the logistic model

$$\log \left(\frac{\pi_k}{1 - \pi_k} \right) = \mathbf{x}_k^T \boldsymbol{\beta},$$

where $\mathbf{x}_k = \mathbf{x}_{1k} - \mathbf{x}_{2k}$, $k = 1, \ldots, K$.
c. Based on (b), analyze the case-control study data on aspirin use and ulcers using logistic regression and compare the results with those obtained using log-linear models. (difficulty: ⋆⋆)

Solution. (a) **Product multinomial reduces to product binomial.**
The printed summation sign is a misprint for a product (a joint density of independent columns is a product, and the right side must sum to one); we prove the product form. With column totals fixed each column is an independent multinomial sample, so by Section 9.4.3 with $J = 2$ rows,

$$f(\mathbf{y} \mid y_{\cdot 1}, \ldots, y_{\cdot K}) = \prod_{k=1}^{K} y_{\cdot k}! \prod_{j=1}^{2} \frac{\theta_{jk}^{y_{jk}}}{y_{jk}!},$$

where $\sum_{j=1}^{2} \theta_{jk} = 1$ for each k; this last constraint eliminates θ_{2k}. The inner product has two factors, so substituting $n_k = y_{\cdot k}$, $z_k = y_{1k}$, $n_k - z_k = y_{2k}$, $\pi_k = \theta_{1k}$, $1 - \pi_k = \theta_{2k}$,

$$f(z_1, \ldots, z_K \mid n_1, \ldots, n_K) = \prod_{k=1}^{K} \frac{n_k!}{z_k!\,(n_k - z_k)!} \pi_k^{z_k} (1 - \pi_k)^{n_k - z_k} = \prod_{k=1}^{K} \binom{n_k}{z_k} \pi_k^{z_k} (1 - \pi_k)^{n_k - z_k}.$$

Each factor is the Binomial probability function (7.1) for $Z_k \sim \mathrm{Bin}(n_k, \pi_k)$ and the factorisation gives independence of the K columns: the joint distribution assumed for Table 7.1, with z_k the successes in the kth covariate pattern.

(b) **The log-linear model is the logistic model.**
Since $\mathrm{E}(Z_k) = n_k\pi_k$ and $\mathrm{E}(n_k - Z_k) = n_k(1-\pi_k)$,

$$\eta_{1k} = \log n_k + \log \pi_k, \qquad \eta_{2k} = \log n_k + \log(1-\pi_k).$$

Subtracting removes the nuisance term $\log n_k$:

$$\eta_{1k} - \eta_{2k} = \log\left(\frac{\pi_k}{1-\pi_k}\right) = \mathbf{x}_{1k}^T\boldsymbol{\beta} - \mathbf{x}_{2k}^T\boldsymbol{\beta} = (\mathbf{x}_{1k} - \mathbf{x}_{2k})^T\boldsymbol{\beta} = \mathbf{x}_k^T\boldsymbol{\beta},$$

the logistic model with $\mathbf{x}_k = \mathbf{x}_{1k} - \mathbf{x}_{2k}$ and the same $\boldsymbol{\beta}$. The converse holds provided the log-linear predictor is rich enough to absorb the K quantities $\log n_k$, i.e. provided the parameters corresponding to the fixed column totals are in the model – otherwise it constrains $\eta_{1k} + \eta_{2k}$, a statement about the fixed margins, not about π_k. That is precisely Birch's requirement quoted in Section 9.6, and with those terms present the two likelihoods differ by a factor free of $\boldsymbol{\beta}$, so estimates, standard errors and deviance differences coincide. The $\log n_k$ are the offset of equation (9.3), appearing on both rows and cancelling; the K parameters that reproduce the column totals are what the logistic model saves.
(c) **Aspirin and ulcers by logistic regression.**
The design of Section 9.7.2 fixes the four $CC \times GD$ group totals, so $K = 4$, "success" is aspirin use and n_k is the group size; by (b) the logistic response is aspirin use with case-control status CC and ulcer site GD explanatory.

```r
library(dobson)
data(ulcer)
u <- ulcer
u$CC <- factor(u$`case-control`, levels = c("control", "case"))
u$GD <- factor(u$ulcer,          levels = c("gastric", "duodenal"))
u$AP <- factor(u$aspirin,        levels = c("non-user", "user"))
w <- reshape(u[, c("GD", "CC", "AP", "frequency")], idvar = c("GD", "CC"),
             timevar = "AP", direction = "wide")
names(w)[3:4] <- c("nonuser", "user"); w$n <- w$nonuser + w$user
w
b0 <- glm(cbind(user, nonuser) ~ 1,       family = binomial, data = w)
b1 <- glm(cbind(user, nonuser) ~ CC,      family = binomial, data = w)
b2 <- glm(cbind(user, nonuser) ~ CC + GD, family = binomial, data = w)
b3 <- glm(cbind(user, nonuser) ~ CC * GD, family = binomial, data = w)
anova(b0, b1, b2, b3, test = "Chisq")
```

```
       GD      CC nonuser user  n
1  gastric control      62    6 68
3  gastric    case      39   25 64
5 duodenal control      53    8 61
7 duodenal    case      49    8 57

Analysis of Deviance Table

Model 1: cbind(user, nonuser) ~ 1
Model 2: cbind(user, nonuser) ~ CC
Model 3: cbind(user, nonuser) ~ CC + GD
Model 4: cbind(user, nonuser) ~ CC * GD
  Resid. Df Resid. Dev Df Deviance  Pr(>Chi)
1         3     21.789
2         2     10.538  1  11.2508 0.0007959 ***
3         1      6.283  1   4.2555 0.0391244 *
4         0      0.000  1   6.2830 0.0121903 *
```

The residual deviances 21.789, 10.538, 6.283 on $3, 2, 1$ d.f. are rows 2–4 of Table 9.11, with $\Delta D = 11.25$ for aspirin as a risk factor and 4.26 for ulcer site. Side by side the two families confirm (b):

```r
l1 <- glm(frequency ~ GD + CC + GD:CC,                    family = stats::poisson, data =
↪  u)
l2 <- glm(frequency ~ GD + CC + GD:CC + AP,               family = stats::poisson, data =
↪  u)
l3 <- glm(frequency ~ GD + CC + GD:CC + AP + AP:CC,       family = stats::poisson, data =
↪  u)
```

```r
l4 <- glm(frequency ~ GD + CC + GD:CC + AP + AP:CC + AP:GD, family = stats::poisson, data =
↪  u)
data.frame(loglinear = c("GD+CC+GD:CC", "+AP", "+AP:CC", "+AP:GD"),
           df = sapply(list(l1, l2, l3, l4), df.residual),
           deviance = round(sapply(list(l1, l2, l3, l4), deviance), 3),
           logistic = c("(not a logistic model)", "1", "CC", "CC + GD"))
round(coef(l4)[c("CCcase:APuser", "GDduodenal:APuser")], 5)
round(coef(b2)[-1], 5)
```

```
    loglinear df deviance               logistic
1 GD+CC+GD:CC  4  126.708 (not a logistic model)
2         +AP  3   21.789                      1
3      +AP:CC  2   10.538                     CC
4      +AP:GD  1    6.283                CC + GD

    CCcase:APuser GDduodenal:APuser
          1.14288          -0.70005

    CCcase GDduodenal
   1.14288   -0.70005
```

The log-linear $AP:CC$ and $AP:GD$ coefficients equal the logistic CC and GD coefficients to five decimals, as (b) requires. Row 1 of Table 9.11 has no logistic counterpart: dropping AP forces $\pi_k = \frac{1}{2}$, a constraint on the conditioned margin rather than a submodel.

```r
summary(b2)$coefficients
round(exp(cbind(OR = coef(b2), confint.default(b2))), 3)
```

```
              Estimate Std. Error   z value     Pr(>|z|)
(Intercept) -1.8219310  0.3079643 -5.916046 3.297722e-09
CCcase       1.1428772  0.3520746  3.246122 1.169886e-03
GDduodenal  -0.7000457  0.3460282 -2.023089 4.306401e-02

               OR 2.5 % 97.5 %
(Intercept) 0.162 0.088  0.296
CCcase      3.136 1.573  6.252
GDduodenal  0.497 0.252  0.978
```

Interpretation. Ulcer patients have $e^{1.143} = 3.14$ times the odds of aspirin use of their controls (95% CI 1.57 to 6.25); by symmetry of the odds ratio this is also the odds ratio for ulcer given aspirin use, which the case-control design cannot estimate as a risk. Aspirin use is less common among duodenal than gastric subjects ($e^{-0.700} = 0.50$), a feature of recruitment, not aetiology.

The additive model does not fit ($D = 6.28$ on 1 d.f., $p = 0.012$ – the lack of fit reported for Table 9.12): the missing term is the logistic $CC \times GD$ interaction, equivalently the three-way $AP \times CC \times GD$ log-linear term, so the case-control odds ratio for aspirin differs by site (question 3 of Section 9.3.3). The saturated fit gives $(62 \times 25)/(6 \times 39) = 6.62$ for gastric and $(53 \times 8)/(8 \times 49) = 1.08$ for duodenal ulcer, so the common odds ratio 3.14 averages two quite different things.

Both frameworks give identical estimates and tests; the logistic analysis uses 3 parameters where the log-linear uses 7, the four $GD + CC + GD:CC$ terms existing only to reproduce fixed margins. Log-linear modelling is what one would use had the group totals not been fixed by design.

9.7 Problem 9.7 — Mittlbock and Heinzl (2001) compare Poisson and logistic regression

Problem 9.7. Mittlbock and Heinzl (2001) compare Poisson and logistic regression models for data in which the event rate is small so that the Poisson distribution provides a reasonable approximation to the Binomial distribution. An example is the number of deaths from coronary heart disease among British doctors (Table 9.1). In Section 9.2.1 we fitted the model $Y_i \sim \text{Po}(deaths_i)$ with Equation (9.9)

$$\log(deaths_i) = \log(personyears_i) + \beta_1 + \beta_2\, smoke_i + \beta_3\, agecat_i + \beta_4\, agesq_i + \beta_5\, smkage_i.$$

An alternative is $Y_i \sim \text{Bin}(personyears_i, \pi_i)$ with

$$\text{logit}(\pi_i) = \beta_1 + \beta_2\, smoke_i + \beta_3\, agecat_i + \beta_4\, agesq_i + \beta_5\, smkage_i.$$

Another version is based on a Bernoulli distribution $Z_j \sim \text{B}(\pi_i)$ for each doctor in group i with

$$Z_j = \begin{cases} 1, & j = 1, \ldots, deaths_i \\ 0, & j = deaths_i + 1, \ldots, personyears_i \end{cases}$$

and

$$\text{logit}(\pi_i) = \beta_1 + \beta_2\, smoke_i + \beta_3\, agecat_i + \beta_4\, agesq_i + \beta_5\, smkage_i.$$

a. Fit all three models (in Stata the Bernoulli model cannot be fitted with `glm`; use `blogit` instead). Verify that the β estimates are very similar.
b. Calculate the statistics D, X^2 and pseudo R^2 for all three models. Notice that the pseudo R^2 is much smaller for the Bernoulli model. As Mittlbock and Heinzl (2001) point out this is because the Poisson and Binomial models are estimating the probability of death for each group (which is relatively easy) whereas the Bernoulli model is estimating the probability of death for an individual (which is much more difficult).
Table 9.1 gives deaths from coronary heart disease after 10 years among British male doctors by age group and 1951 smoking status, as (deaths, person-years): smokers – 35-44 $(32, 52407)$, 45-54 $(104, 43248)$, 55-64 $(206, 28612)$, 65-74 $(186, 12663)$, 75-84 $(102, 5317)$; non-smokers – 35-44 $(2, 18790)$, 45-54 $(12, 10673)$, 55-64 $(28, 5710)$, 65-74 $(28, 2585)$, 75-84 $(31, 1462)$. (difficulty: ⋆⋆)

Solution. All three agree on $\boldsymbol{\beta}$ and on C, and differ only in pseudo R^2. The largest observed rate is $186/12663 = 0.0147$, so every π_i is far below 0.05 and $\log(1-\pi_i) \approx -\pi_i \approx 0$, whence $\text{logit}(\pi_i) \approx \log \pi_i$: the Poisson linear predictor for $\log \pi_i$ and the Binomial one for $\text{logit}(\pi_i)$ describe nearly the same thing. Binomial and Bernoulli are identical, not merely close – by Exercise 9.6(a) in reverse, summing n_i Bernoulli variables with common π_i is a sufficiency reduction, so the likelihoods differ only by the $\binom{n_i}{y_i}$, free of $\boldsymbol{\beta}$.
(a) **Fitting the three models.**

```r
library(dobson)
data(doctors)
d <- doctors; names(d)[4] <- "personyears"
d$agecat <- rep(1:5, 2); d$agesq <- d$agecat^2
d$smoke  <- as.numeric(d$smoking == "smoker"); d$smkage <- d$smoke * d$agecat
mP <- glm(deaths ~ smoke + agecat + agesq + smkage + offset(log(personyears)),
          family = stats::poisson, data = d)
mB <- glm(cbind(deaths, personyears - deaths) ~ smoke + agecat + agesq + smkage,
          family = binomial, data = d)
# expand to one row per doctor-year for the Bernoulli version
idx <- rep(seq_len(nrow(d)), d$personyears)
be <- d[idx, c("smoke", "agecat", "agesq", "smkage")]
be$z <- unlist(lapply(seq_len(nrow(d)), function(i)
  c(rep(1, d$deaths[i]), rep(0, d$personyears[i] - d$deaths[i]))))
mZ <- glm(z ~ smoke + agecat + agesq + smkage, family = binomial, data = be)
cat("rows in the Bernoulli data frame:", nrow(be), "  events:", sum(be$z), "\n")
round(rbind(Poisson = coef(mP), Binomial = coef(mB), Bernoulli = coef(mZ)), 5)
round(rbind(Poisson   = summary(mP)$coefficients[, 2],
            Binomial  = summary(mB)$coefficients[, 2],
            Bernoulli = summary(mZ)$coefficients[, 2]), 5)
```

```
rows in the Bernoulli data frame: 181467   events: 731

          (Intercept)   smoke  agecat    agesq   smkage
Poisson     -10.79176 1.44097 2.37648 -0.19768 -0.30755
Binomial    -10.79888 1.44568 2.37889 -0.19705 -0.30849
Bernoulli   -10.79888 1.44568 2.37889 -0.19705 -0.30849
```

```
           (Intercept)   smoke  agecat   agesq  smkage
Poisson        0.45008 0.37220 0.20795 0.02737 0.09704
Binomial       0.45150 0.37347 0.20877 0.02749 0.09756
Bernoulli      0.45149 0.37347 0.20877 0.02749 0.09756
```

The Poisson estimates 2.376, −0.198, 1.441, −0.308 with standard errors 0.208, 0.027, 0.372, 0.097 are Table 9.2; the Binomial ones differ in the third decimal at most, two orders of magnitude below the standard errors. Binomial and Bernoulli agree to five decimals as the sufficiency argument requires, the intercept standard error discrepancy being numerical (summing 181467 terms rather than 10).

```
round(rbind(Poisson = exp(coef(mP))[-1], Binomial = exp(coef(mB))[-1],
            Bernoulli = exp(coef(mZ))[-1]), 4)
```

```
           smoke  agecat  agesq smkage
Poisson   4.2248 10.7669 0.8206 0.7352
Binomial  4.2447 10.7929 0.8211 0.7346
Bernoulli 4.2447 10.7929 0.8211 0.7346
```

On the interpretable scale all three say the same: smoking multiplies the coronary death rate by about 4.2 at the youngest age category, attenuated by 0.73 per category, so by *agecat* = 5 it is $4.22 \times 0.735^4 = 1.23$. The Poisson numbers are **rate ratios** and the logistic ones **odds ratios**, indistinguishable here only because π_i is small.

(b) D, X^2 **and pseudo** R^2**.**

By Section 9.2 the minimal model is $\log \mu_i = \log n_i + \beta_1$ for the Poisson version (the offset is retained) and intercept-only for the logistic ones, with pseudo $R^2 = [l(\mathbf{b}_{\min}) - l(\mathbf{b})]/l(\mathbf{b}_{\min})$ and $C = 2[l(\mathbf{b}) - l(\mathbf{b}_{\min})]$.

```
m0P <- glm(deaths ~ 1 + offset(log(personyears)), family = stats::poisson, data = d)
m0B <- glm(cbind(deaths, personyears - deaths) ~ 1, family = binomial, data = d)
m0Z <- glm(z ~ 1, family = binomial, data = be)
stat <- function(m, m0) c(D = deviance(m), X2 = sum(residuals(m, "pearson")^2),
  df = df.residual(m), l.b = as.numeric(logLik(m)), l.min = as.numeric(logLik(m0)),
  C = 2 * (as.numeric(logLik(m)) - as.numeric(logLik(m0))),
  pseudoR2 = (as.numeric(logLik(m0)) - as.numeric(logLik(m))) / as.numeric(logLik(m0)))
round(rbind(Poisson = stat(mP, m0P), Binomial = stat(mB, m0B),
            Bernoulli = stat(mZ, m0Z)), 4)
```

```
                 D          X2     df        l.b      l.min        C pseudoR2
Poisson     1.6354      1.5503      5   -28.3517  -495.0676 933.4320   0.9427
Binomial    1.6410      1.5578      5   -28.3130  -497.3464 938.0668   0.9431
Bernoulli 8583.0602 177765.6090 181462 -4291.5301 -4760.5635 938.0668   0.0985
```

The Poisson row reproduces Section 9.2.1: $X^2 = 1.550$, $D = 1.635$ on 5 d.f., $l(\mathbf{b}_{\min}) = -495.067$, $l(\mathbf{b}) = -28.352$, $C = 933.43$, pseudo $R^2 = 0.94$; the Binomial row matches to two decimals. Three separate points about the Bernoulli row:

(i) D and X^2. For the grouped models the saturated model has one parameter per group, so these measure the 5-parameter fit against 10 group rates and refer to $\chi^2(5)$: an excellent fit. For the Bernoulli model the saturated model has one parameter per **doctor-year**, its parameter count grows with n, and neither statistic has an asymptotic chi-squared distribution; $D = 8583$ and $X^2 = 177766$ on 181462 d.f. are uninterpretable rather than evidence of failure ($\widehat{\pi} \approx 0.004$ against $z \in \{0, 1\}$ predicts every observation badly).

(ii) C. The likelihood ratio statistic for $\beta_2 = \cdots = \beta_5 = 0$ is 938.07 for both logistic versions – identical because the binomial coefficients cancel in the difference of log-likelihoods – and 933.43 for the Poisson, the gap being the Poisson approximation alone. This is the statistic answering the scientific question, and it is invariant to the formulation.

(iii) Pseudo R^2: 0.94, 0.94, 0.10. Only the denominator $l(\mathbf{b}_{\min})$ changes (−495, −497, −4761); the numerator $l(\mathbf{b}_{\min}) - l(\mathbf{b}) = -C/2$ is −466.7, −469.0, −469.0, the same quantity thrice. The covariates buy the same likelihood; what differs is how much unexplained likelihood remains. The grouped target is ten group death rates, which age and smoking predict almost perfectly; the Bernoulli target is which individual doctor-year ends in death, and the best model still predicts $\widehat{\pi} \approx 0.004$ for everyone, so most of the log-likelihood is irreducible. That is Mittlbock and Heinzl's point: pseudo R^2 is not comparable across aggregation levels, and a small value for individual-level binary data is no criticism of the model.

10 Survival Analysis

Contents

10.1 Problem 10.1 — The data in Table 10.4 are survival times, in weeks, for leukemia patients.

Problem 10.1. The data in Table 10.4 are survival times, in weeks, for leukemia patients. There is no censoring. There are two covariates, white blood cell count (WBC) and the results of a test (AG positive and AG negative). The data set is from Feigl and Zelen (1965) and the data for the 17 patients with AG positive test results are described in Exercise 4.2.
Table 10.4 (leukemia survival times) lists, for the 17 AG positive patients, the pairs (survival time, white blood cell count): $(65, 2.30)$, $(156, 0.75)$, $(100, 4.30)$, $(134, 2.60)$, $(16, 6.00)$, $(108, 10.50)$, $(121, 10.00)$, $(4, 17.00)$, $(39, 5.40)$, $(143, 7.00)$, $(56, 9.40)$, $(26, 32.00)$, $(22, 35.00)$, $(1, 100.00)$, $(1, 100.00)$, $(5, 52.00)$, $(65, 100.00)$; and for the 16 AG negative patients: $(56, 4.40)$, $(65, 3.00)$, $(17, 4.00)$, $(7, 1.50)$, $(16, 9.00)$, $(22, 5.30)$, $(3, 10.00)$, $(4, 19.00)$, $(2, 27.00)$, $(3, 28.00)$, $(8, 31.00)$, $(4, 26.00)$, $(3, 21.00)$, $(30, 79.00)$, $(4, 100.00)$, $(43, 100.00)$.
(a) Obtain the empirical survivor functions $\widehat{S}(y)$ for each group (AG positive and AG negative), ignoring WBC.
(b) Use suitable plots of the estimates $\widehat{S}(y)$ to select an appropriate probability distribution to model the data.
(c) Use a parametric model to compare the survival times for the two groups, after adjustment for the covariate WBC, which is best transformed to log(WBC).
(d) Check the adequacy of the model using residuals and other diagnostic tests.
(e) Based on this analysis, is AG a useful prognostic indicator? (difficulty: ⋆⋆⋆)

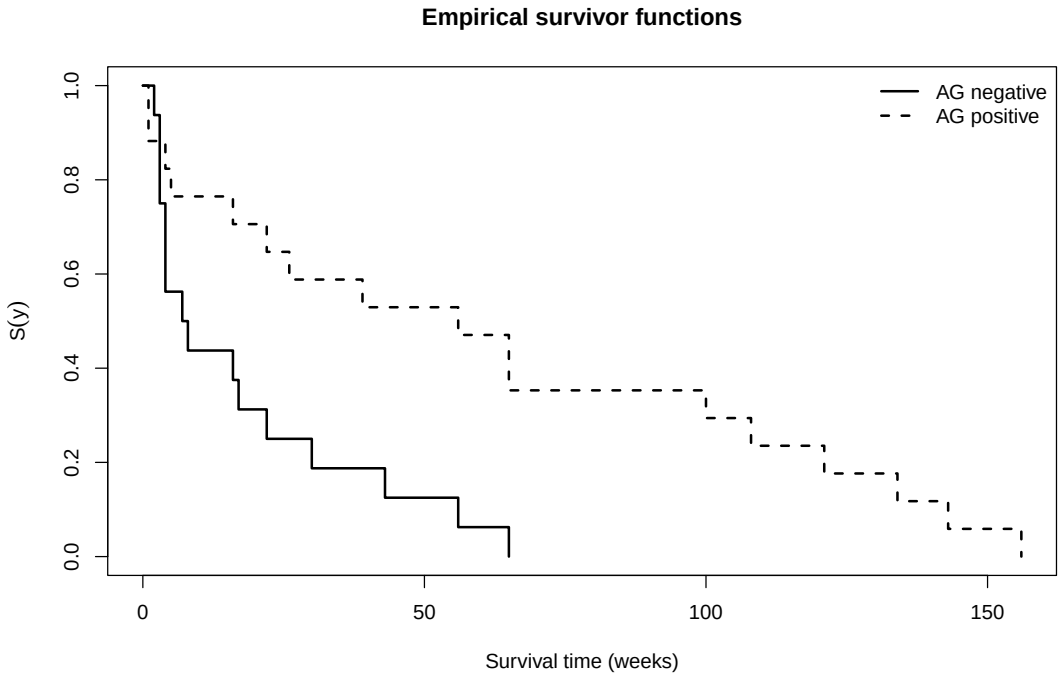
Solution. Yes: AG positivity carries a hazard ratio of 0.36 after adjusting for log(WBC), in an exponential proportional hazards model. The data are the `dobson` data frame `survival` (33 rows); there is no censoring, so $\delta_j = 1$ throughout and the likelihood (10.15) is $\prod_j f(y_j)$.
(a) With no censoring the Kaplan-Meier estimate of Section 10.3 is the proportion $\widetilde{S}(y) = \#\{y_j \geq y\}/n$, computed here with `survfit`.

```
library(dobson)
library(survival)
data(survival, package = "dobson")
leuk <- data.frame(time = survival[["survival time"]],
                   wbc  = survival$WBC,
                   ag   = factor(survival$AG, levels = c("-", "+")))
leuk$lwbc <- log(leuk$wbc)
km <- survfit(Surv(time, rep(1, nrow(leuk))) ~ ag, data = leuk)
summary(km)
```

```
Call: survfit(formula = Surv(time, rep(1, nrow(leuk))) ~ ag, data = leuk)

                ag=-
 time n.risk n.event survival std.err lower 95% CI upper 95% CI
    2     16       1   0.9375  0.0605      0.82609        1.000
    3     15       3   0.7500  0.1083      0.56520        0.995
    4     12       3   0.5625  0.1240      0.36513        0.867
    7      9       1   0.5000  0.1250      0.30632        0.816
    8      8       1   0.4375  0.1240      0.25101        0.763
   16      7       1   0.3750  0.1210      0.19921        0.706
   17      6       1   0.3125  0.1159      0.15108        0.646
   22      5       1   0.2500  0.1083      0.10699        0.584
   30      4       1   0.1875  0.0976      0.06761        0.520
   43      3       1   0.1250  0.0827      0.03419        0.457
   56      2       1   0.0625  0.0605      0.00937        0.417
   65      1       1   0.0000     NaN           NA           NA

                ag=+
 time n.risk n.event survival std.err lower 95% CI upper 95% CI
    1     17       2   0.8824  0.0781      0.74175        1.000
    4     15       1   0.8235  0.0925      0.66087        1.000
    5     14       1   0.7647  0.1029      0.58746        0.995
```

```
 16     13       1   0.7059  0.1105      0.51936       0.959
 22     12       1   0.6471  0.1159      0.45548       0.919
 26     11       1   0.5882  0.1194      0.39521       0.876
 39     10       1   0.5294  0.1211      0.33818       0.829
 56      9       1   0.4706  0.1211      0.28423       0.779
 65      8       2   0.3529  0.1159      0.18543       0.672
100      6       1   0.2941  0.1105      0.14083       0.614
108      5       1   0.2353  0.1029      0.09987       0.554
121      4       1   0.1765  0.0925      0.06320       0.493
134      3       1   0.1176  0.0781      0.03200       0.432
143      2       1   0.0588  0.0571      0.00879       0.394
156      1       1   0.0000     NaN           NA          NA
```

```r
plot(km, lty = c(1, 2), lwd = 2, xlab = "Survival time (weeks)",
     ylab = expression(hat(S)(y)), main = "Empirical survivor functions")
legend("topright", c("AG negative", "AG positive"), lty = c(1, 2), lwd = 2, bty = "n")
```



The AG negative curve falls to 0.5 by week 7 and the AG positive one not until week 56; `survfit` reports medians 7.5 and 56 weeks, roughly a sevenfold difference.

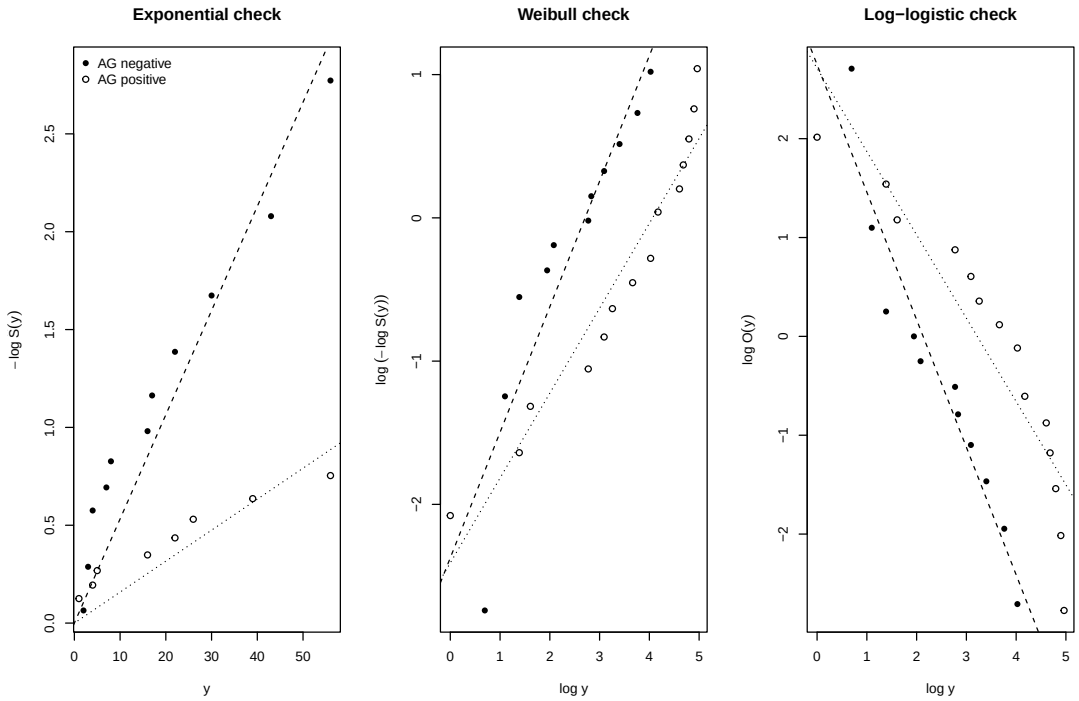
(b) Three linearising plots, from Section 10.6 and Exercise 10.5(c):

- exponential, from (10.6): $H(y) = -\log S(y) = \theta y$, so $-\log \widehat{S}(y)$ against y should be a straight line through the origin;
- Weibull, from (10.13): $\log[-\log \widehat{S}(y)]$ against $\log y$ should be straight with slope λ;
- log-logistic, from Exercise 10.5(c): $\log \widehat{O}(y) = \log[\widehat{S}/(1-\widehat{S})]$ against $\log y$ should be straight with slope $-\lambda$.

The final point of each survivor function has $\widehat{S} = 0$ and is dropped.

```r
tab <- function(g) {
  sub <- subset(leuk, ag == g)
  s <- survfit(Surv(time, rep(1, nrow(sub))) ~ 1, data = sub)
  d <- data.frame(y = s$time, S = s$surv)
  d[d$S > 0 & d$S < 1, ]
}
neg <- tab("-"); pos <- tab("+")
par(mfrow = c(1, 3))
plot(neg$y, -log(neg$S), pch = 16, xlab = "y", ylab = expression(-log~hat(S)(y)),
     main = "Exponential check", ylim = range(-log(c(neg$S, pos$S))))
points(pos$y, -log(pos$S), pch = 1)
abline(lm(-log(neg$S) ~ neg$y + 0), lty = 2); abline(lm(-log(pos$S) ~ pos$y + 0), lty = 3)
legend("topleft", c("AG negative", "AG positive"), pch = c(16, 1), bty = "n")
```

```
plot(log(neg$y), log(-log(neg$S)), pch = 16, xlab = "log y",
     ylab = expression(log~(-log~hat(S)(y))), main = "Weibull check",
     xlim = range(log(c(neg$y, pos$y))), ylim = range(log(-log(c(neg$S, pos$S)))))
points(log(pos$y), log(-log(pos$S)), pch = 1)
abline(lm(log(-log(neg$S)) ~ log(neg$y)), lty = 2)
abline(lm(log(-log(pos$S)) ~ log(pos$y)), lty = 3)
plot(log(neg$y), log(neg$S/(1 - neg$S)), pch = 16, xlab = "log y",
     ylab = expression(log~hat(O)(y)), main = "Log-logistic check",
     xlim = range(log(c(neg$y, pos$y))),
     ylim = range(log(c(neg$S, pos$S)/(1 - c(neg$S, pos$S)))))
points(log(pos$y), log(pos$S/(1 - pos$S)), pch = 1)
abline(lm(log(neg$S/(1 - neg$S)) ~ log(neg$y)), lty = 2)
abline(lm(log(pos$S/(1 - pos$S)) ~ log(pos$y)), lty = 3)
```




```
rbind(negative = coef(lm(log(-log(neg$S)) ~ log(neg$y))),
      positive = coef(lm(log(-log(pos$S)) ~ log(pos$y))))
```

```
         (Intercept) log(neg$y)
negative   -2.372757  0.8760273
positive   -2.408514  0.5925132
```

The left panel is nearly linear through the origin in both groups, arguing for the exponential; the middle panel is roughly linear with a constant vertical gap, supporting the Weibull family with proportional hazards (10.9). Its slopes 0.88 and 0.59 are unweighted least squares fits to Kaplan-Meier points, which overweight the unreliable tail, so the difference should not be over-read – the maximum likelihood fit in (c) gives $\widehat{\lambda} = 0.96$ for both groups, consistent with the exponential special case $\lambda = 1$ of (10.10). The right panel is no straighter, so the log-logistic gains nothing. Take the exponential, checked against the Weibull in (c).

(c) Fit the proportional hazards models of Section 10.2.2, $h_j(y) = \exp(\beta_0 + \beta_1 x_{1j} + \beta_2 x_{2j})$ with $x_1 = 1$ for AG positive and $x_2 = \log(\text{WBC})$; `survreg` writes these as accelerated failure time models $\log Y = \mathbf{x}^T\boldsymbol{\alpha} + \sigma W$, so its exponential coefficients are $-\beta$.

```
S <- Surv(leuk$time, rep(1, nrow(leuk)))
m.exp <- survreg(S ~ ag + lwbc, data = leuk, dist = "exponential")
m.wei <- survreg(S ~ ag + lwbc, data = leuk, dist = "weibull")
m.llg <- survreg(S ~ ag + lwbc, data = leuk, dist = "loglogistic")
summary(m.exp)
```

```
Call:
survreg(formula = S ~ ag + lwbc, data = leuk, dist = "exponential")
```

```
             Value Std. Error     z      p
(Intercept)  3.713      0.454  8.17  3e-16
ag+          1.018      0.364  2.80 0.0051
lwbc        -0.304      0.124 -2.45 0.0144

Scale fixed at 1

Exponential distribution
Loglik(model)= -146.5   Loglik(intercept only)= -155.5
        Chisq= 17.82 on 2 degrees of freedom, p= 0.00014
Number of Newton-Raphson Iterations: 5
n= 33
```

```r
c(exponential = AIC(m.exp), weibull = AIC(m.wei), loglogistic = AIC(m.llg),
  weibull.scale = m.wei$scale)
```

```
exponential       weibull   loglogistic weibull.scale
 299.081049    300.997595    301.164852      1.040689
```

The Weibull scale $\widehat{\sigma} = 1.041$ gives shape $\widehat{\lambda} = 0.96$, indistinguishable from $\lambda = 1$, and the extra parameter costs two AIC units; the exponential has the smallest AIC and is chosen, as in Section 10.7. The same fit follows from the Poisson device of Section 10.4, the log-likelihood (10.17) being proportional to that of independent $D_j \sim \text{Po}(\theta_j y_j)$ with $\log y_j$ as offset.

```r
g <- glm(rep(1, nrow(leuk)) ~ ag + lwbc + offset(log(time)),
         family = stats::poisson(), data = leuk)
round(summary(g)$coefficients, 4)
```

```
             Estimate Std. Error z value Pr(>|z|)
(Intercept)  -3.7127     0.4542 -8.1748   0.0000
ag+          -1.0176     0.3637 -2.7983   0.0051
lwbc          0.3044     0.1244  2.4479   0.0144
```

The estimates match `survreg` with reversed sign, so the Poisson coefficients are the proportional hazards parameters $\boldsymbol{\beta}$ of (10.8). Tests of the terms use $D = 2(\widehat{l}_1 - \widehat{l}_0)$ of Section 10.5:

```r
anova(survreg(S ~ lwbc, data = leuk, dist = "exponential"), m.exp)
anova(m.exp, survreg(S ~ ag * lwbc, data = leuk, dist = "exponential"))
```

```
      Terms Resid. Df    -2*LL Test Df Deviance    Pr(>Chi)
1      lwbc        31 300.5704      NA       NA          NA
2 ag + lwbc        30 293.0810  +ag  1 7.489309 0.006206637
      Terms Resid. Df    -2*LL     Test Df Deviance  Pr(>Chi)
1 ag + lwbc        30 293.0810          NA       NA        NA
2 ag * lwbc        29 291.3166 +ag:lwbc  1 1.764485 0.1840661
```

Adding AG to a model containing log(WBC) reduces $-2l$ by 7.49 on 1 d.f. ($p = 0.006$), and the interaction is not needed ($D = 1.76$, $p = 0.18$), so one hazard ratio applies at every white cell count. The fitted hazard is

$$\widehat{h}(y) = \exp\{-3.713 - 1.018\, x_1 + 0.304\, x_2\},$$

constant in y. By (10.7) the AG positive versus negative hazard ratio is $e^{-1.018} = 0.36$ (95% CI $e^{-1.018 \pm 1.96 \times 0.364} = (0.18, 0.74)$): at equal white cell count an AG positive patient dies at a third the rate, equivalently survives $e^{1.018} = 2.77$ times as long. Each unit of log(WBC) multiplies the hazard by $e^{0.304} = 1.36$, so a doubling of WBC multiplies it by $2^{0.304} = 1.23$ – higher counts are bad, as Exercise 4.2(a) suggested. Mean survival at WBC $= 10$ is $\exp(3.713 + 1.018 - 0.304 \log 10) = 56$ weeks if AG positive against 20 weeks if negative.

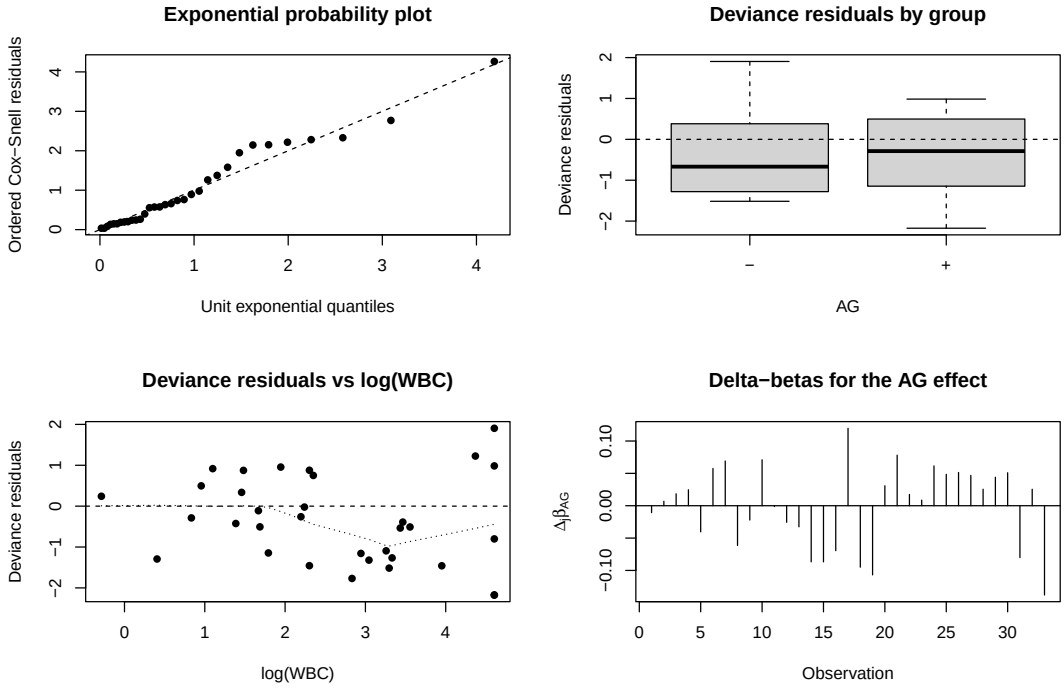
(d) The Cox-Snell residuals (10.19) are $r_{Cj} = \widehat{H}_j(y_j) = y_j \widehat{\theta}_j$ here; under the model they are a sample from the unit exponential, so mean and variance should be near 1 and the probability plot should follow $y = x$. No censoring, so the Δ correction of Section 10.6 is not needed.

```r
rc <- leuk$time / exp(predict(m.exp, type = "lp"))
rd <- residuals(m.exp, type = "deviance")
c(mean = mean(rc), variance = var(rc))
```

```
    mean variance
1.000000 1.019736
```

```r
par(mfrow = c(2, 2))
```

```
plot(qexp(ppoints(nrow(leuk))), sort(rc), pch = 16,
     xlab = "Unit exponential quantiles", ylab = "Ordered Cox-Snell residuals",
     main = "Exponential probability plot"); abline(0, 1, lty = 2)
boxplot(rd ~ leuk$ag, xlab = "AG", ylab = "Deviance residuals",
        main = "Deviance residuals by group"); abline(h = 0, lty = 2)
plot(leuk$lwbc, rd, pch = 16, xlab = "log(WBC)", ylab = "Deviance residuals",
     main = "Deviance residuals vs log(WBC)")
abline(h = 0, lty = 2); lines(lowess(leuk$lwbc, rd), lty = 3)
db <- residuals(m.exp, type = "dfbeta")
plot(seq_len(nrow(leuk)), db[, 2], type = "h", xlab = "Observation",
     ylab = expression(Delta[j]*beta[AG]), main = "Delta-betas for the AG effect")
abline(h = 0)
```




```
round(rbind(CoxSnell = quantile(rc), deviance = quantile(rd)), 3)
```

```
             0%    25%    50%   75%  100%
CoxSnell  0.036  0.202  0.633 1.581 4.265
deviance -2.175 -1.266 -0.425 0.496 1.905
```

The Cox-Snell mean 1.000 and variance 1.020 are as the unit exponential requires, and the probability plot tracks the reference line with mild sagging in the upper tail. The deviance residuals have similar distributions in the two groups (means -0.39, -0.34), so the AG term has absorbed the group difference; the slight downward lowess drift against log(WBC) at high counts is weak evidence at $n = 33$, and agrees with the non-significant interaction in (c). The most influential observation for $\widehat{\beta}_{\mathrm{AG}}$ is subject 33 (AG negative, 43 weeks at WBC = 100), whose removal moves the estimate by 0.14, under half a standard error; the largest deviance residual -2.17 is subject 14 (AG positive, WBC = 100, died week 1). Neither is troubling. The exponential itself assumes constant hazard, hence no memory (Section 10.2.1); the checks in (b) and $\widehat{\lambda} = 0.96$ do not contradict it, though 33 observations give little power.

(e) Yes. Adjusted for log(WBC), AG positivity carries a hazard ratio 0.36 (95% CI 0.18 to 0.74; $D = 7.49$ on 1 d.f., $p = 0.006$), roughly a tripling of expected survival, not confounded with WBC (which is in the model, with negligible interaction) nor driven by any one patient. Against the small observational sample and the constant-hazard assumption, AG still separates a median survival of about two months from one of over a year.

10.2 Problem 10.2 — The log-logistic distribution with the probability density function

Problem 10.2. The log-logistic distribution with the probability density function

$$f(y) = \frac{e^{\theta}\lambda y^{\lambda-1}}{(1+e^{\theta}y^{\lambda})^2}$$

is sometimes used for modelling survival times.
(a) Find the survivor function $S(y)$, the hazard function $h(y)$ and the cumulative hazard function $H(y)$.
(b) Show that the median survival time is $\exp(-\theta/\lambda)$.
(c) Plot the hazard function for $\lambda = 1$ and $\lambda = 5$ with $\theta = -5$, $\theta = -2$ and $\theta = \frac{1}{2}$. (difficulty: ⋆⋆)

Solution. $S(y) = (1+e^{\theta}y^{\lambda})^{-1}$, $h(y) = e^{\theta}\lambda y^{\lambda-1}/(1+e^{\theta}y^{\lambda})$ and $H(y) = \log(1+e^{\theta}y^{\lambda})$, with median $e^{-\theta/\lambda}$. Throughout $y \geq 0$, $\lambda > 0$, θ unrestricted.
(a) Substituting $u = e^{\theta}t^{\lambda}$, whose differential $du = e^{\theta}\lambda t^{\lambda-1}dt$ is the numerator of f,

$$F(y) = \int_0^y \frac{e^{\theta}\lambda t^{\lambda-1}}{(1+e^{\theta}t^{\lambda})^2}\,dt = \int_0^{e^{\theta}y^{\lambda}} \frac{du}{(1+u)^2} = \left[-\frac{1}{1+u}\right]_0^{e^{\theta}y^{\lambda}} = 1 - \frac{1}{1+e^{\theta}y^{\lambda}}.$$

Hence, from (10.1),

$$S(y) = 1 - F(y) = \frac{1}{1+e^{\theta}y^{\lambda}}.$$

Then (10.2) gives the hazard:

$$h(y) = \frac{f(y)}{S(y)} = \frac{e^{\theta}\lambda y^{\lambda-1}}{(1+e^{\theta}y^{\lambda})^2}\left(1+e^{\theta}y^{\lambda}\right) = \frac{e^{\theta}\lambda y^{\lambda-1}}{1+e^{\theta}y^{\lambda}},$$

the baseline hazard h_0 of Exercise 10.4(c), and (10.4) gives

$$H(y) = -\log S(y) = \log\left(1+e^{\theta}y^{\lambda}\right).$$

(Check! $-\frac{d}{dy}\log S(y) = h(y)$, as (10.3) requires.) The name comes from writing $Z = \log Y$:

$$\Pr(Z \leq z) = F(e^z) = \frac{e^{\theta+\lambda z}}{1+e^{\theta+\lambda z}},$$

$\log Y$ is logistic with location $-\theta/\lambda$ and scale $1/\lambda$, equivalently $\operatorname{logit}[F(y)] = \theta + \lambda\log y$, the source of the log-odds plot of Exercise 10.5(c).
(b) The median solves $S(y) = \frac{1}{2}$:

$$\frac{1}{1+e^{\theta}y^{\lambda}} = \frac{1}{2} \quad\Longleftrightarrow\quad e^{\theta}y^{\lambda} = 1 \quad\Longleftrightarrow\quad y^{\lambda} = e^{-\theta} \quad\Longleftrightarrow\quad y(50) = e^{-\theta/\lambda}.$$

The median is quoted rather than the mean because $\mathrm{E}(Y) = (\pi/\lambda)e^{-\theta/\lambda}/\sin(\pi/\lambda)$ exists only for $\lambda > 1$.
(c) Taking logarithms,

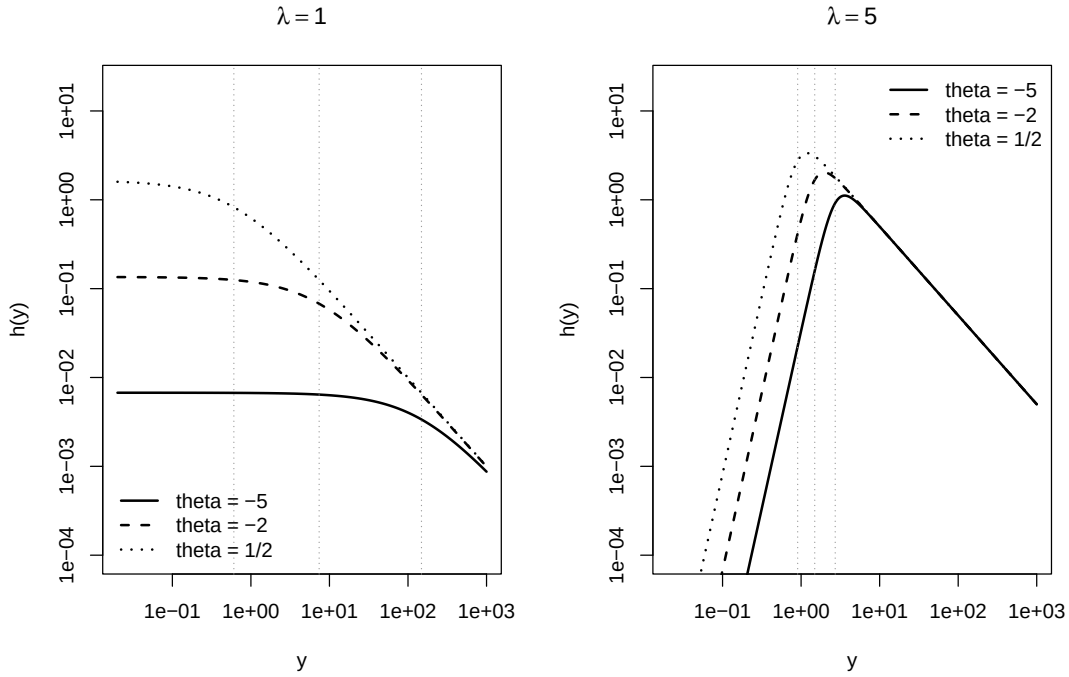
$$\log h(y) = \log\lambda + \theta + (\lambda-1)\log y - \log\left(1+e^{\theta}y^{\lambda}\right),$$

so

$$\frac{d}{dy}\log h(y) = \frac{\lambda-1}{y} - \frac{\lambda e^{\theta}y^{\lambda-1}}{1+e^{\theta}y^{\lambda}} = \frac{(\lambda-1) - e^{\theta}y^{\lambda}}{y\,(1+e^{\theta}y^{\lambda})}.$$

so: (i) for $\lambda \leq 1$ the numerator is negative for all $y > 0$ and the hazard decreases monotonically from $h(0^+) = e^{\theta}$ (from $+\infty$ if $\lambda < 1$); (ii) for $\lambda > 1$ it rises from 0, peaks at $y = \{(\lambda-1)e^{-\theta}\}^{1/\lambda}$ and decays like λ/y. The eventual decrease distinguishes the log-logistic from the Weibull (10.12), whose hazard is monotone for every λ.

```r
h <- function(y, th, lam) lam * exp(th) * y^(lam - 1) / (1 + exp(th) * y^lam)
ths <- c(-5, -2, 0.5)
labs <- c("theta = -5", "theta = -2", "theta = 1/2")
par(mfrow = c(1, 2))
y <- exp(seq(log(0.02), log(1000), length = 600))
for (lam in c(1, 5)) {
  plot(NA, xlim = range(y), ylim = c(1e-4, 20), log = "xy", xlab = "y", ylab = "h(y)",
       main = bquote(lambda == .(lam)))
  for (k in 1:3) lines(y, h(y, ths[k], lam), lty = k, lwd = 2)
  for (k in 1:3) abline(v = exp(-ths[k]/lam), col = "grey60", lty = 3)
  legend(if (lam == 1) "bottomleft" else "topright", labs, lty = 1:3, lwd = 2, bty = "n")
}
```



Both axes are logarithmic; the vertical grey lines mark the medians $e^{-\theta/\lambda}$ from (b).

```r
mode5 <- function(th) ((5 - 1) * exp(-th))^(1/5)
rbind(theta = ths, median.lam1 = exp(-ths), h0.lam1 = exp(ths),
      median.lam5 = exp(-ths/5), mode.lam5 = mode5(ths),
      peak.h.lam5 = mapply(function(t) h(mode5(t), t, 5), ths))
```

```
                   [,1]       [,2]      [,3]
theta        -5.000000000 -2.0000000 0.5000000
median.lam1 148.413159103  7.3890561 0.6065307
h0.lam1       0.006737947  0.1353353 1.6487213
median.lam5   2.718281828  1.4918247 0.9048374
mode.lam5     3.586794376  1.9684745 1.1939401
peak.h.lam5   1.115201927  2.0320304 3.3502517
```

Left panel ($\lambda = 1$): the hazard $e^{\theta}/(1 + e^{\theta}y)$ starts at e^{θ} and decreases to $1/y$ whatever θ, so the curves are ordered by θ at small y and merge at large y, the median moving from 0.61 at $\theta = \frac{1}{2}$ to 148 at $\theta = -5$. Right panel ($\lambda = 5$): each curve rises as y^4, peaks at $y = \{4e^{-\theta}\}^{1/5}$ (3.59, 1.97, 1.19) and falls as $5/y$. So θ is a scale shift on the time axis and λ sets the shape, monotone decreasing or hump-shaped.

10.3 Problem 10.3 — For accelerated failure time models the explanatory variables for subject

Problem 10.3. For accelerated failure time models the explanatory variables for subject i, η_i, act multiplicatively on the time variable so that the hazard function for subject i is

$$h_i(y) = \eta_i h_0(\eta_i y),$$

where $h_0(y)$ is the baseline hazard function. Show that the Weibull and log-logistic distributions both have this property but the exponential distribution does not. (Hint: Obtain the hazard function for the random variable $T = \eta_i Y$.) (difficulty: ⋆⋆)

Solution. The Weibull and log-logistic families are closed under $h_0(y) \mapsto \eta h_0(\eta y)$, with $\phi_i = \eta_i^\lambda \phi$ and $\theta_i = \theta + \lambda \log \eta_i$; the exponential is not, in the sense that the map degenerates to a rescaling of the hazard level. For $T_i = Y/\eta_i$ with baseline S_0,

$$S_i(y) = \Pr(Y \geq \eta_i y) = S_0(\eta_i y), \qquad h_i(y) = -\frac{d}{dy} \log S_0(\eta_i y) = \eta_i h_0(\eta_i y)$$

by (10.3) and the chain rule, so the displayed equation is what a multiplicative change of the time scale does to any hazard. (In the hint's direction, $T = \eta_i Y$ gives $h_T(t) = \eta_i^{-1} h_0(\eta_i^{-1} t)$.) What must be shown is therefore closure of the family, so that the accelerated model is the same distribution with a covariate-dependent parameter; since $\log T_i = \log Y - \log \eta_i$, that is a location model for $\log Y$, the `survreg` parameterisation of Exercise 10.1.

(i) **Weibull.** From (10.12), $h_0(y) = \lambda \phi y^{\lambda-1}$, so

$$\eta h_0(\eta y) = \eta\, \lambda \phi (\eta y)^{\lambda-1} = \lambda \left(\eta^\lambda \phi\right) y^{\lambda-1},$$

again a Weibull hazard with the same shape λ and $\phi_i = \eta_i^\lambda \phi$. Taking $\eta_i = e^{\mathbf{x}_i^T \boldsymbol{\gamma}}$ gives $\phi_i = \phi e^{\mathbf{x}_i^T (\lambda \boldsymbol{\gamma})}$, the multiplicative form $\phi = \alpha e^{\mathbf{x}^T \boldsymbol{\beta}}$ of page 230 with $\boldsymbol{\beta} = \lambda \boldsymbol{\gamma}$ – which is why the Weibull is both an accelerated failure time and a proportional hazards model (Exercise 10.4(b)), the two parameterisations differing by the factor λ.

(ii) **Log-logistic.** From Exercise 10.2(a), $h_0(y) = e^\theta \lambda y^{\lambda-1}/(1 + e^\theta y^\lambda)$, so

$$\eta h_0(\eta y) = \frac{\eta\, e^\theta \lambda (\eta y)^{\lambda-1}}{1 + e^\theta (\eta y)^\lambda} = \frac{\left(e^\theta \eta^\lambda\right) \lambda y^{\lambda-1}}{1 + \left(e^\theta \eta^\lambda\right) y^\lambda},$$

absorbing $\eta \cdot \eta^{\lambda-1} = \eta^\lambda$ into the constant: again log-logistic with the same λ and $\theta_i = \theta + \lambda \log \eta_i$, so $\eta_i = e^{\mathbf{x}_i^T \boldsymbol{\gamma}}$ gives $\theta_i = \theta + \mathbf{x}_i^T (\lambda \boldsymbol{\gamma})$. (Equivalently, by Exercise 10.2(a) $\log Y$ is logistic with location $-\theta/\lambda$ and scale $1/\lambda$, and subtracting $\log \eta_i$ shifts the location only.)

(iii) **Exponential.** Here $h_0(y) = \theta$ is constant, so $\eta h_0(\eta y) = \eta \theta$: the acceleration inside the argument does nothing and only the leading factor survives. Read as bare closure the exponential does satisfy the equation; what it lacks is an accelerated structure **distinct** from a rescaling of the hazard, since $h_i(y) = \eta_i h_0(\eta_i y) = \eta_i h_0(y)$ is simultaneously the proportional hazards model (10.20), so η_i is not identifiable as an acceleration factor. Acceleration must act on the shape of the hazard, and a constant hazard has no shape to act on; in the Weibull case the two operations differ by the factor λ, and the exponential is the case $\lambda = 1$ where the distinction collapses. This is the sense of the remark on page 230.

A simulation, using $Y = \{e^{-\theta}(1/U - 1)\}^{1/\lambda}$ and $Y = \{-\log(U)/\phi\}^{1/\lambda}$ with U uniform:

```r
set.seed(2026)
qs <- c(.1, .25, .5, .75, .9)
n <- 2e5; eta <- 2.5
rllog <- function(n, th, lam) { u <- runif(n); (exp(-th) * (1/u - 1))^(1/lam) }
qllog <- function(p, th, lam) (exp(-th) * (1/(1 - p) - 1))^(1/lam)
th <- -2; lam <- 3
Tt <- rllog(n, th, lam) / eta
```

```
round(rbind(simulated = quantile(Tt, qs),
            theoretical = qllog(qs, th + lam * log(eta), lam)), 4)
```

```
                10%    25%    50%    75%    90%
simulated    0.3740 0.5390 0.7771 1.1237 1.6166
theoretical  0.3745 0.5402 0.7791 1.1236 1.6206
```

```
lam <- 1.7; phi <- 0.4
Tt <- (-log(runif(n))/phi)^(1/lam) / eta
qwei <- function(p, lam, phi) (-log(1 - p)/phi)^(1/lam)
round(rbind(simulated = quantile(Tt, qs),
            theoretical = qwei(qs, lam, eta^lam * phi)), 4)
```

```
                10%    25%    50%    75%    90%
simulated    0.1828 0.3306 0.5538 0.8322 1.1192
theoretical  0.1825 0.3295 0.5527 0.8310 1.1200
```

Dividing by η shifts θ by $\lambda \log \eta$ in the log-logistic case and multiplies ϕ by η^λ in the Weibull case, as derived.

10.4 Problem 10.4 — For proportional hazards models the explanatory variables for subject

Problem 10.4. For proportional hazards models the explanatory variables for subject i, η_i, act multiplicatively on the hazard function. If $\eta_i = e^{\mathbf{x}_i^T \boldsymbol{\beta}}$, then the hazard function for subject i is

$$h_i(y) = e^{\mathbf{x}_i^T \boldsymbol{\beta}} h_0(y), \tag{10.20}$$

where $h_0(y)$ is the baseline hazard function.
(a) For the exponential distribution if $h_0 = \theta$, show that if $\theta_i = e^{\mathbf{x}_i^T \boldsymbol{\beta}} \theta$ for the ith subject, then (10.20) is satisfied.
(b) For the Weibull distribution if $h_0 = \lambda \phi y^{\lambda - 1}$, show that if $\phi_i = e^{\mathbf{x}_i^T \boldsymbol{\beta}} \phi$ for the ith subject, then (10.20) is satisfied.
(c) For the log-logistic distribution if $h_0 = e^\theta \lambda y^{\lambda-1}/(1 + e^\theta y^\lambda)$, show that if $e^{\theta_i} = e^{\theta + \mathbf{x}_i^T \boldsymbol{\beta}}$ for the ith subject, then (10.20) is not satisfied. Hence, or otherwise, deduce that the log-logistic distribution does not have the proportional hazards property. (difficulty: ⋆⋆)

Solution. Write $\eta_i = e^{\mathbf{x}_i^T \boldsymbol{\beta}}$; in each part substitute the subject's parameter into the hazard and compare with h_0.
(a) The exponential hazard (10.5) is the constant θ, so with $\theta_i = \eta_i \theta$,

$$h_i(y) = \theta_i = \eta_i \theta = e^{\mathbf{x}_i^T \boldsymbol{\beta}} h_0(y),$$

identically in y, with $h_0(y) = \theta$ the hazard at $\mathbf{x}_i = \mathbf{0}$. Absorbing θ into $\beta_0 = \log \theta$ gives the model $h(y; \boldsymbol{\beta}) = e^{\mathbf{x}^T \boldsymbol{\beta}}$ of Section 10.2.2, fitted in Exercise 10.1(c), whose hazard ratio (10.7) for a binary x_k is e^{β_k}.
(b) From (10.12), $h(y; \lambda, \phi) = \lambda \phi y^{\lambda - 1}$ with λ fixed and $\phi_i = \eta_i \phi$, so

$$h_i(y) = \lambda \phi_i y^{\lambda-1} = \lambda\, \eta_i \phi\, y^{\lambda-1} = e^{\mathbf{x}_i^T \boldsymbol{\beta}} \lambda \phi y^{\lambda-1} = e^{\mathbf{x}_i^T \boldsymbol{\beta}} h_0(y),$$

for every y: this is (10.14) with $\phi = \alpha e^{\mathbf{x}^T \boldsymbol{\beta}}$. Constancy of λ across subjects is essential, since a varying λ_i would leave a factor $y^{\lambda_i - \lambda}$ in the ratio. With Exercise 10.3 this makes the Weibull both an accelerated failure time and a proportional hazards family, linked by $\boldsymbol{\beta} = \lambda \boldsymbol{\gamma}$.
(c) Substituting $e^{\theta_i} = \eta_i e^\theta$ into the hazard of Exercise 10.2(a),

$$h_i(y) = \frac{e^{\theta_i} \lambda y^{\lambda-1}}{1 + e^{\theta_i} y^\lambda} = \frac{\eta_i e^\theta \lambda y^{\lambda-1}}{1 + \eta_i e^\theta y^\lambda},$$

so the hazard ratio is

$$\frac{h_i(y)}{h_0(y)} = \eta_i \frac{1 + e^\theta y^\lambda}{1 + \eta_i e^\theta y^\lambda}.$$

Since η_i appears in the denominator too, the ratio is a genuine function of y unless $\eta_i = 1$:

$$\lim_{y\to 0}\frac{h_i(y)}{h_0(y)} = \eta_i, \qquad \lim_{y\to\infty}\frac{h_i(y)}{h_0(y)} = \eta_i \cdot \frac{e^{\theta}y^{\lambda}}{\eta_i e^{\theta}y^{\lambda}} = 1.$$

The ratio starts at η_i and decays to 1, so the hazards converge and (10.20) fails; equivalently $H_i(y) = \log(1+\eta_i e^{\theta}y^{\lambda})$ do not differ by a constant, so the log-cumulative-hazard curves of Section 10.6 are not parallel. Numerically, with $\theta = -2$, $\lambda = 3$, $\eta_i = 3$, against the Weibull:

```
h <- function(y, th, lam) lam * exp(th) * y^(lam - 1) / (1 + exp(th) * y^lam)
th <- -2; lam <- 3; xb <- log(3); y <- c(0.01, 0.1, 0.5, 1, 2, 5, 20)
round(rbind(y = y,
            ratio.loglogistic = h(y, th + xb, lam) / h(y, th, lam),
            ratio.weibull = (lam * exp(xb) * 0.4 * y^(lam - 1)) /
                            (lam * 0.4 * y^(lam - 1))), 4)
```

```
                  [,1]   [,2]   [,3]   [,4]   [,5]   [,6]    [,7]
y                 0.01 0.1000 0.5000 1.0000 2.0000 5.0000 20.0000
ratio.loglogistic 3.00 2.9992 2.9034 2.4225 1.4708 1.0386  1.0006
ratio.weibull     3.00 3.0000 3.0000 3.0000 3.0000 3.0000  3.0000
```

The Weibull ratio is $e^{\mathbf{x}^T\boldsymbol{\beta}} = 3$ at every time; the log-logistic ratio falls from 3 to 1.
Hence the family has no proportional hazards parameterisation at all. Suppose two log-logistic distributions with parameters (θ_1, λ_1) and (θ_0, λ_0) had proportional hazards, so that for some $c > 0$

$$\frac{h(y;\theta_1,\lambda_1)}{h(y;\theta_0,\lambda_0)} = \frac{\lambda_1}{\lambda_0}\, e^{\theta_1-\theta_0}\, y^{\lambda_1-\lambda_0}\, \frac{1+e^{\theta_0}y^{\lambda_0}}{1+e^{\theta_1}y^{\lambda_1}} = c \quad \text{for all } y > 0.$$

Let $y \to 0$. The last fraction tends to 1, so the left side behaves like $(\lambda_1/\lambda_0)e^{\theta_1-\theta_0}y^{\lambda_1-\lambda_0}$, which has a finite non-zero limit only if $\lambda_1 = \lambda_0 = \lambda$. With the shapes equal the condition becomes

$$e^{\theta_1-\theta_0}\,\frac{1+e^{\theta_0}y^{\lambda}}{1+e^{\theta_1}y^{\lambda}} = c,$$

whose value is $e^{\theta_1-\theta_0}$ as $y \to 0$ and 1 as $y \to \infty$; a constant equal to both forces $\theta_1 = \theta_0$, $c = 1$ and the two distributions coincide. The reason is structural: by Exercise 10.2(a) the log-logistic hazard eventually decreases like λ/y whatever the parameters, so any two members' hazards merge at large y.

10.5 Problem 10.5 — As the survivor function S(y) is the probability of surviving beyond time

Problem 10.5. As the survivor function $S(y)$ is the probability of surviving beyond time y, the odds of survival past time y are

$$O(y) = \frac{S(y)}{1-S(y)}.$$

For proportional odds models the explanatory variables for subject i, η_i, act multiplicatively on the odds of survival beyond time y,

$$O_i = \eta_i O_0,$$

where O_0 is the baseline odds.
(a) Find the odds of survival beyond time y for the exponential, Weibull and log-logistic distributions.
(b) Show that only the log-logistic distribution has the proportional odds property.
(c) For the log-logistic distribution show that the log odds of survival beyond time y are

$$\log O(y) = \log\left[\frac{S(y)}{1-S(y)}\right] = -\theta - \lambda\log y.$$

Therefore, if $\log \widehat{O}_i$ (estimated from the empirical survivor function) plotted against $\log y$ is approximately linear, then the log-logistic distribution may provide a suitable model.

(d) From (b) and (c) deduce that for two groups of subjects with explanatory variables η_1 and η_2 plots of $\log \widehat{O}_1$ and $\log \widehat{O}_2$ against $\log y$ should produce approximately parallel straight lines. (difficulty: $\star\star$)

Solution. (a) Substitute each survivor function into $O = S/(1-S)$. Exponential, from (10.6) $S(y) = e^{-\theta y}$:

$$O(y) = \frac{e^{-\theta y}}{1 - e^{-\theta y}} = \frac{1}{e^{\theta y} - 1}.$$

Weibull, from (10.11) $S(y) = \exp(-\phi y^{\lambda})$:

$$O(y) = \frac{\exp(-\phi y^{\lambda})}{1 - \exp(-\phi y^{\lambda})} = \frac{1}{\exp(\phi y^{\lambda}) - 1}.$$

(the exponential is the case $\lambda = 1$, $\phi = \theta$). Log-logistic, from Exercise 10.2(a) $S(y) = 1/(1 + e^{\theta} y^{\lambda})$, whence $1 - S(y) = e^{\theta} y^{\lambda}/(1 + e^{\theta} y^{\lambda})$ and

$$O(y) = \frac{1/(1 + e^{\theta} y^{\lambda})}{e^{\theta} y^{\lambda}/(1 + e^{\theta} y^{\lambda})} = \frac{1}{e^{\theta} y^{\lambda}} = e^{-\theta} y^{-\lambda}.$$

Only the log-logistic odds are a pure power of y.
(b) Proportional odds requires $O_i(y)/O_0(y)$ constant in y. (i) **Log-logistic.** For two members with common shape λ,

$$\frac{O_i(y)}{O_0(y)} = \frac{e^{-\theta_i} y^{-\lambda}}{e^{-\theta} y^{-\lambda}} = e^{\theta - \theta_i},$$

free of y, so $\theta_i = \theta - \log \eta_i$ (in a regression, $\theta_i = \theta - \mathbf{x}_i^T \boldsymbol{\beta}$) gives $O_i(y) = \eta_i O_0(y)$ exactly: the log-logistic is a proportional odds family with the covariates entering θ linearly. The same reparameterisation destroys proportional hazards (Exercise 10.4(c)).
(ii) **Weibull, and exponential as the case $\lambda = 1$.** Suppose $O_i(y)/O_0(y) = c$ for all y, with parameters (λ_i, ϕ_i) and (λ, ϕ). As $y \to 0$, $\exp(\phi y^{\lambda}) - 1 = \phi y^{\lambda}\{1 + O(y^{\lambda})\}$, so $O(y) \sim 1/(\phi y^{\lambda})$ and

$$\frac{O_i(y)}{O_0(y)} \sim \frac{\phi}{\phi_i} y^{\lambda - \lambda_i}.$$

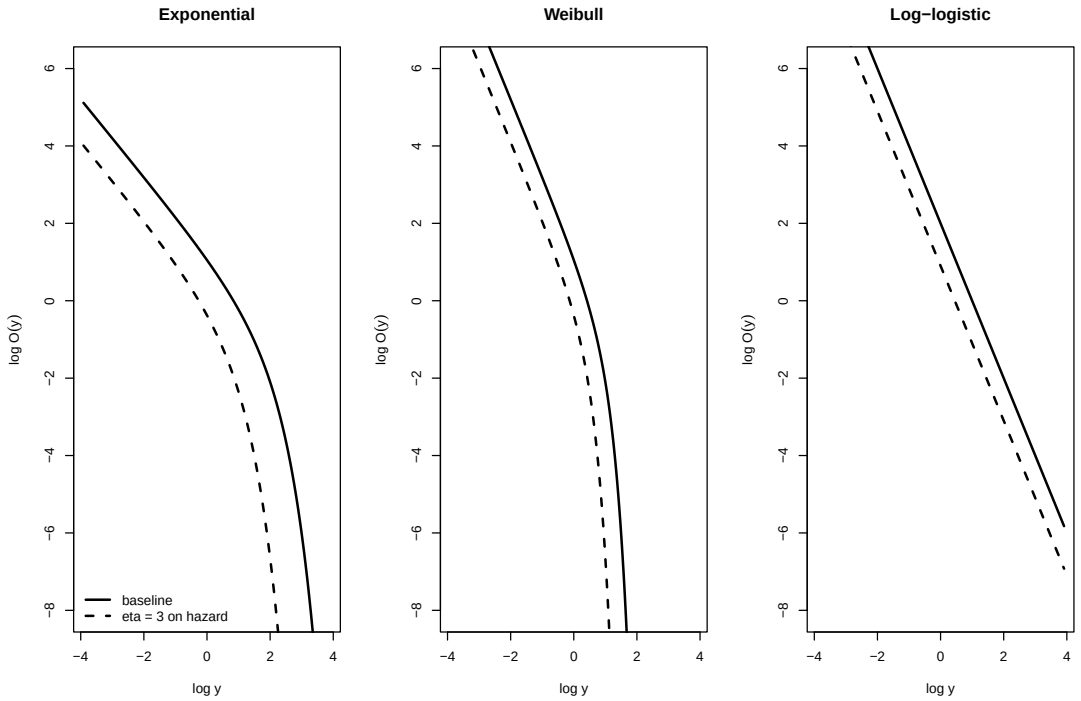
A finite non-zero limit forces $\lambda_i = \lambda$, the limit then being ϕ/ϕ_i. As $y \to \infty$, $O(y) \sim \exp(-\phi y^{\lambda})$, so with $\lambda_i = \lambda$,

$$\frac{O_i(y)}{O_0(y)} \sim \exp\left\{(\phi - \phi_i) y^{\lambda}\right\},$$

which tends to 0 if $\phi_i > \phi$ and to ∞ if $\phi_i < \phi$; a constant ratio forces $\phi_i = \phi$, hence $c = 1$ and identical distributions. So no non-trivial proportional odds model exists in the Weibull family, nor in the exponential ($\lambda = 1$) – their survivor functions decay exponentially, so their log-odds fall like $-\phi y^{\lambda}$ and cannot be vertical translates of one another.
On the $\log O$ against $\log y$ scale of (c), each panel comparing a baseline with a parameter multiplied by 3:

```r
y <- exp(seq(log(0.02), log(50), length = 500))
lo <- function(S) log(S/(1 - S))
par(mfrow = c(1, 3))
th <- 0.3
plot(log(y), lo(exp(-th*y)), type = "l", lwd = 2, ylim = c(-8, 6),
     xlab = "log y", ylab = expression(log~O(y)), main = "Exponential")
lines(log(y), lo(exp(-3*th*y)), lwd = 2, lty = 2)
legend("bottomleft", c("baseline", "eta = 3 on hazard"), lty = 1:2, lwd = 2, bty = "n")
lam <- 2; phi <- 0.3
plot(log(y), lo(exp(-phi*y^lam)), type = "l", lwd = 2, ylim = c(-8, 6),
     xlab = "log y", ylab = expression(log~O(y)), main = "Weibull")
lines(log(y), lo(exp(-3*phi*y^lam)), lwd = 2, lty = 2)
Sll <- function(y, th, lam) 1/(1 + exp(th)*y^lam)
```

```
th <- -2; lam <- 2
plot(log(y), lo(Sll(y, th, lam)), type = "l", lwd = 2, ylim = c(-8, 6),
     xlab = "log y", ylab = expression(log~O(y)), main = "Log-logistic")
lines(log(y), lo(Sll(y, th + log(3), lam)), lwd = 2, lty = 2)
```



Only the third panel gives two straight lines a constant distance apart; in the first two the curves bend and the gap widens without limit.

(c) Taking logarithms of the odds found in (a),

$$\log O(y) = \log\left(e^{-\theta}y^{-\lambda}\right) = -\theta - \lambda \log y,$$

a straight line in $\log y$ with intercept $-\theta$ and slope $-\lambda$; equivalently $\operatorname{logit}[1 - S(y)] = \theta + \lambda \log y$, so the log-logistic is the distribution whose cumulative distribution function is logistic in $\log y$. The diagnostic is therefore to plot $\log \widehat{O}(y) = \log[\widehat{S}(y)/\{1 - \widehat{S}(y)\}]$ against $\log y$ for the empirical survivor function of Section 10.3, dropping the points with $\widehat{S} \in \{0, 1\}$: linearity supports the log-logistic, the intercept estimating $-\theta$ and minus the slope λ. This is the third panel of Exercise 10.1(b), counterpart to the exponential and Weibull plots of Section 10.6.

(d) Let the groups be log-logistic with common shape λ and odds multipliers η_1, η_2, so by (b) $\theta_g = \theta - \log \eta_g$. Taking logarithms of $O_g = \eta_g O_0$ and using (c),

$$\log O_g(y) = \log \eta_g + \log O_0(y) = (\log \eta_g - \theta) - \lambda \log y, \qquad g = 1, 2.$$

Both are straight lines in $\log y$ with the same slope $-\lambda$, and their vertical separation is

$$\log O_1(y) - \log O_2(y) = \log\left(\frac{\eta_1}{\eta_2}\right) = \theta_2 - \theta_1,$$

constant in y. So the two plots of $\log \widehat{O}_g$ against $\log y$ should be roughly parallel straight lines whose vertical gap estimates $\log(\eta_1/\eta_2)$, in analogy with the parallel log-cumulative-hazard lines of (10.9). Curvature of either line refutes the log-logistic; straight but non-parallel lines refute proportional odds, the groups differing in λ as well as location.

10.6 Problem 10.6 — The data in Table 10.5 are survival times, in months, of 44 patients with

Problem 10.6. The data in Table 10.5 are survival times, in months, of 44 patients with chronic active hepatitis. They participated in a randomized controlled trial of prednisolone compared with no treatment. There were 22 patients in each group. One patient was lost to follow-up and several in each group were still alive at the end of the trial. The data are from Altman and Bland (1998). Table 10.5 gives the survival times in months, where an asterisk marks a censored time and a double asterisk marks the patient lost to follow-up. Prednisolone group: 2, 6, 12, 54, 56**, 68, 89, 96, 96, 125*, 128*, 131*, 140*, 141*, 143, 145*, 146, 148*, 162*, 168, 173*, 181*. No treatment group: 2, 3, 4, 7, 10, 22, 28, 29, 32, 37, 40, 41, 54, 61, 63, 71, 127*, 140*, 146*, 158*, 167*, 182*.
(a) Calculate the empirical survivor functions for each group.
(b) Use suitable plots to investigate the properties of accelerated failure times, proportional hazards and proportional odds, using the results from Exercises 10.3, 10.4 and 10.5, respectively.
(c) Based on the results from (b) fit an appropriate model to the data in Table 10.5 to estimate the relative effect of prednisolone. (difficulty: ⋆⋆⋆)

Solution. All three structures fit these data about equally well, and each puts prednisolone's effect at a hazard ratio near 0.44. The data are the `dobson hepatitis` frame; the patient lost to follow-up at 56 months carries the same information as a censored observation and is coded so, assuming loss to follow-up is unrelated to prognosis.
(a) With censoring the Kaplan-Meier product limit estimate of Section 10.3 is required; only death times contribute a step.

```
library(dobson)
library(survival)
data(hepatitis, package = "dobson")
hep <- data.frame(time = hepatitis[["survival time"]],
                  dead = as.integer(hepatitis$censor == "died"),
                  grp  = factor(hepatitis$group,
                                levels = c("no treatment", "prednisolone")))
table(hep$grp, hep$dead)
km <- survfit(Surv(time, dead) ~ grp, data = hep)
km
```

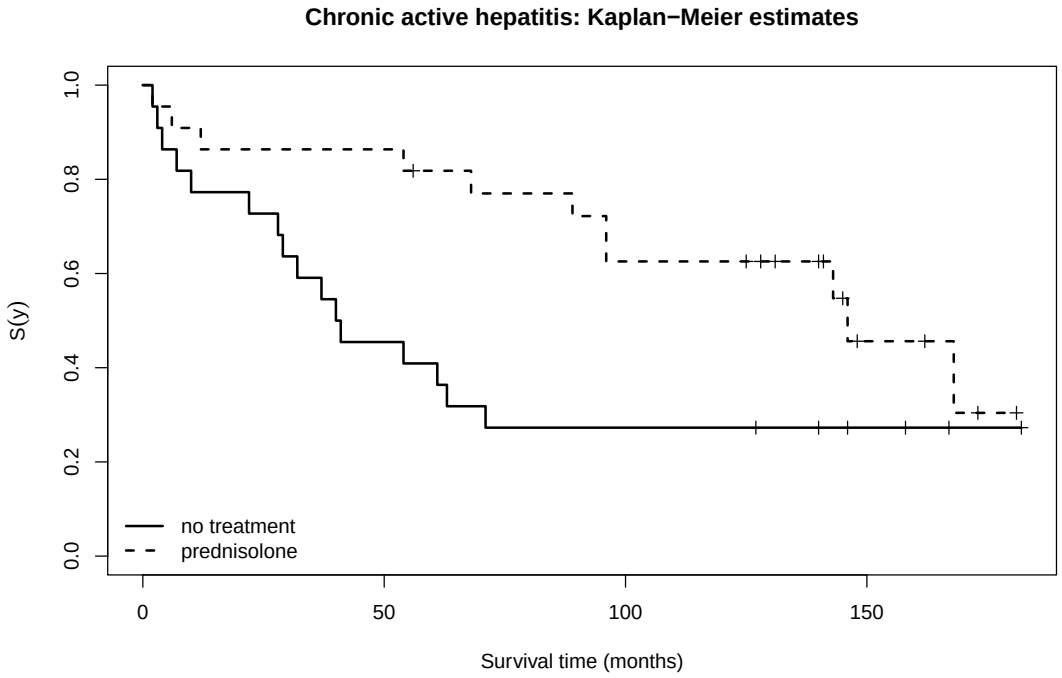
```
               0  1
 no treatment  6 16
 prednisolone 11 11
Call: survfit(formula = Surv(time, dead) ~ grp, data = hep)
                 n events median 0.95LCL 0.95UCL
grp=no treatment 22     16   40.5      29      NA
grp=prednisolone 22     11  146.0      96      NA
```

```
summary(km)
```

```
Call: survfit(formula = Surv(time, dead) ~ grp, data = hep)

                grp=no treatment
 time n.risk n.event survival std.err lower 95% CI upper 95% CI
    2     22       1    0.955  0.0444        0.871        1.000
    3     21       1    0.909  0.0613        0.797        1.000
    4     20       1    0.864  0.0732        0.732        1.000
    7     19       1    0.818  0.0822        0.672        0.996
   10     18       1    0.773  0.0893        0.616        0.969
   22     17       1    0.727  0.0950        0.563        0.939
   28     16       1    0.682  0.0993        0.513        0.907
   29     15       1    0.636  0.1026        0.464        0.873
   32     14       1    0.591  0.1048        0.417        0.837
   37     13       1    0.545  0.1062        0.372        0.799
   40     12       1    0.500  0.1066        0.329        0.759
   41     11       1    0.455  0.1062        0.288        0.718
   54     10       1    0.409  0.1048        0.248        0.676
```

```
    61      9       1    0.364  0.1026        0.209        0.632
    63      8       1    0.318  0.0993        0.173        0.587
    71      7       1    0.273  0.0950        0.138        0.540

                grp=prednisolone
  time n.risk n.event survival std.err lower 95% CI upper 95% CI
     2     22       1    0.955  0.0444        0.871        1.000
     6     21       1    0.909  0.0613        0.797        1.000
    12     20       1    0.864  0.0732        0.732        1.000
    54     19       1    0.818  0.0822        0.672        0.996
    68     17       1    0.770  0.0904        0.612        0.969
    89     16       1    0.722  0.0967        0.555        0.939
    96     15       2    0.626  0.1051        0.450        0.870
   143      8       1    0.547  0.1175        0.359        0.834
   146      6       1    0.456  0.1285        0.263        0.793
   168      3       1    0.304  0.1509        0.115        0.804
```

```r
plot(km, lty = c(1, 2), lwd = 2, xlab = "Survival time (months)",
     ylab = expression(hat(S)(y)), mark.time = TRUE,
     main = "Chronic active hepatitis: Kaplan–Meier estimates")
legend("bottomleft", c("no treatment", "prednisolone"), lty = c(1, 2), lwd = 2, bty = "n")
```

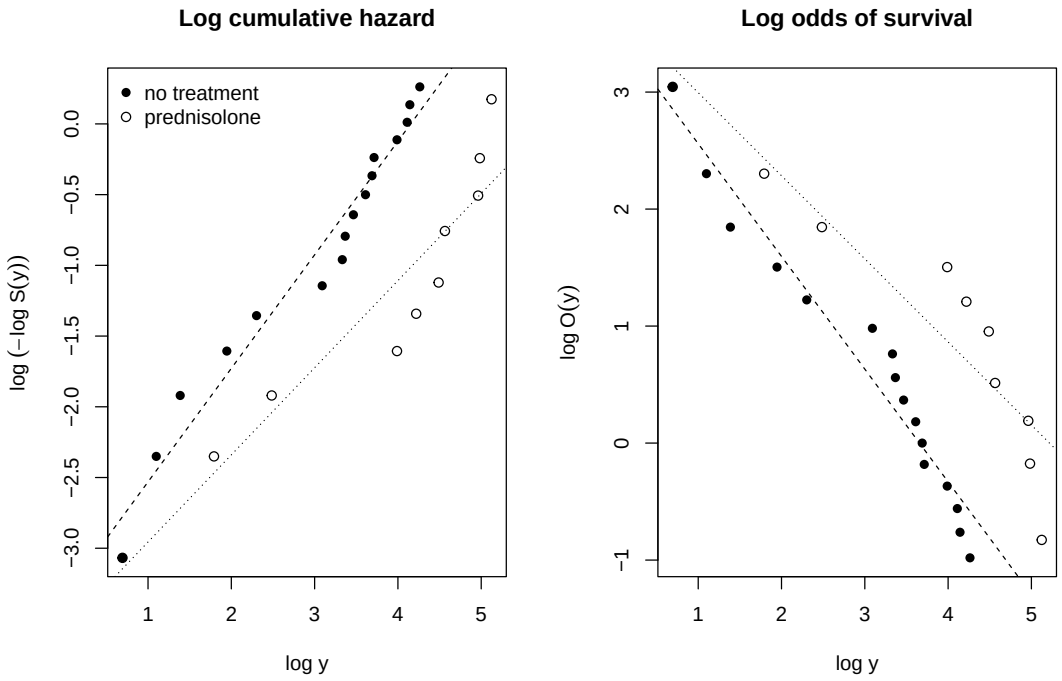


Median survival is 40.5 months untreated against 146 months treated. The censoring differs between arms – 16 of 22 untreated died against 11 of 22 treated, the treated censored times concentrated after 125 months – so the right end of the treated curve rests on three patients at risk and its band is wide. (b) Two linearising plots, both from the same Kaplan-Meier estimates, dropping $\widehat{S} \in \{0, 1\}$:

- Accelerated failure times (Exercise 10.3): under a Weibull accelerated failure time model (10.13) gives $\log[-\log \widehat{S}(y)] = \log \phi + \lambda \log y$, straight in each group; under a log-logistic one the log-odds plot is straight instead. Straightness diagnoses the distribution, the acceleration being a horizontal shift.
- Proportional hazards (Exercise 10.4): by (10.9) the two log cumulative hazard curves are parallel, separated by β_k. The same plot thus serves twice, its slope estimating λ.
- Proportional odds (Exercise 10.5(c),(d)): $\log \widehat{O}(y) = \log[\widehat{S}/(1 - \widehat{S})]$ against $\log y$ gives two parallel straight lines of slope $-\lambda$.

```r
get <- function(g) {
  s <- survfit(Surv(time, dead) ~ 1, data = subset(hep, grp == g))
  d <- data.frame(y = s$time, S = s$surv, n = s$n.event)
  d[d$n > 0 & d$S > 0 & d$S < 1, ]
```

```
}
nt <- get("no treatment"); pr <- get("prednisolone")
par(mfrow = c(1, 2))
plot(log(nt$y), log(-log(nt$S)), pch = 16, xlab = "log y",
     ylab = expression(log~(-log~hat(S)(y))), main = "Log cumulative hazard",
     xlim = range(log(c(nt$y, pr$y))), ylim = range(log(-log(c(nt$S, pr$S)))))
points(log(pr$y), log(-log(pr$S)), pch = 1)
abline(lm(log(-log(nt$S)) ~ log(nt$y)), lty = 2)
abline(lm(log(-log(pr$S)) ~ log(pr$y)), lty = 3)
legend("topleft", c("no treatment", "prednisolone"), pch = c(16, 1), bty = "n")
plot(log(nt$y), log(nt$S/(1 - nt$S)), pch = 16, xlab = "log y",
     ylab = expression(log~hat(O)(y)), main = "Log odds of survival",
     xlim = range(log(c(nt$y, pr$y))),
     ylim = range(log(c(nt$S, pr$S)/(1 - c(nt$S, pr$S)))))
points(log(pr$y), log(pr$S/(1 - pr$S)), pch = 1)
abline(lm(log(nt$S/(1 - nt$S)) ~ log(nt$y)), lty = 2)
abline(lm(log(pr$S/(1 - pr$S)) ~ log(pr$y)), lty = 3)
```




```
round(rbind(
  cumhaz.no.treatment  = coef(lm(log(-log(nt$S)) ~ log(nt$y))),
  cumhaz.prednisolone  = coef(lm(log(-log(pr$S)) ~ log(pr$y))),
  logodds.no.treatment = coef(lm(log(nt$S/(1 - nt$S)) ~ log(nt$y))),
  logodds.prednisolone = coef(lm(log(pr$S/(1 - pr$S)) ~ log(pr$y)))), 3)
```

```
                     (Intercept) log(nt$y)
cumhaz.no.treatment       -3.333     0.803
cumhaz.prednisolone       -3.572     0.616
logodds.no.treatment       3.522    -0.963
logodds.prednisolone       3.705    -0.710
```

Both plots are acceptably straight and acceptably parallel, so the Weibull and log-logistic are both plausible and both proportional hazards and proportional odds are tenable. The slopes are 0.80, 0.62 (log cumulative hazard) and -0.96, -0.71 (log odds), the treated line flatter each time; with 16 and 11 death times and the treated points confined to the right of the range, that difference is within sampling variation. Log-cumulative-hazard slopes around 0.7 point to a Weibull with $\lambda < 1$, a hazard falling with time, which makes the exponential suspect here in a way it was not in Exercise 10.1. That both plots work equally well is expected at $n = 44$ with heavy censoring, so the choice falls to likelihood in (c).

(c) Fit the four candidates by maximum likelihood from the censored likelihood (10.15) and compare by AIC as in Section 10.7.

```
S <- Surv(hep$time, hep$dead)
fits <- list(exponential = survreg(S ~ grp, data = hep, dist = "exponential"),
             weibull     = survreg(S ~ grp, data = hep, dist = "weibull"),
             loglogistic = survreg(S ~ grp, data = hep, dist = "loglogistic"),
             lognormal   = survreg(S ~ grp, data = hep, dist = "lognormal"))
round(sapply(fits, function(f) c(coef(f), scale = f$scale,
                                 logLik = as.numeric(logLik(f)), AIC = AIC(f))), 4)
```

```
                exponential   weibull loglogistic lognormal
(Intercept)          4.4886    4.4811      3.8182    3.8522
grpprednisolone      0.9009    1.0544      1.3272    1.2496
scale                1.0000    1.2673      0.9831    1.7752
logLik            -158.1025 -157.0170   -156.3152 -156.7166
AIC                320.2051  320.0339    318.6303  319.4332
```

The log-logistic has the smallest AIC over a spread of only 1.6 units, so the evidence between families is weak, as the plots showed. The Weibull scale 1.267 gives $\widehat{\lambda} = 0.79$, matching the empirical slopes and a decreasing hazard, though $\lambda = 1$ is not rejected ($\log \widehat{\sigma} = 0.237$, s.e. 0.169); the log-logistic scale 0.983 gives $\widehat{\lambda} = 1.02$. Take the log-logistic as primary and report the Weibull proportional hazards fit alongside.

```
summary(fits$loglogistic)
```

```
Call:
survreg(formula = S ~ grp, data = hep, dist = "loglogistic")
                  Value Std. Error     z      p
(Intercept)      3.8182     0.3671 10.40 <2e-16
grpprednisolone  1.3272     0.5349  2.48  0.013
Log(scale)      -0.0171     0.1678 -0.10  0.919

Scale= 0.983

Log logistic distribution
Loglik(model)= -156.3   Loglik(intercept only)= -159.2
        Chisq= 5.85 on 1 degrees of freedom, p= 0.016
Number of Newton-Raphson Iterations: 4
n= 44
```

`survreg` writes the model as $\log Y = \mu_g + \sigma W$ with W standard logistic, so in the notation of Exercise 10.2, $\lambda = 1/\sigma$ and $\theta_g = -\mu_g/\sigma$.

```
m <- fits$loglogistic; b <- coef(m); sg <- m$scale
se <- sqrt(vcov(m)[2, 2]); ci <- b[2] + c(-1, 1) * 1.96 * se
round(c(lambda = 1/sg, median.no.treatment = exp(b[1]),
        median.prednisolone = exp(b[1] + b[2]),
        time.ratio = exp(b[2]), tr.lo = exp(ci[1]), tr.hi = exp(ci[2]),
        odds.ratio = exp(b[2]/sg), or.lo = exp(ci[1]/sg), or.hi = exp(ci[2]/sg)), 3)
```

```
                        lambda median.no.treatment.(Intercept)
                         1.017                           45.523
median.prednisolone.(Intercept)      time.ratio.grpprednisolone
                       171.636                            3.770
                         tr.lo                            tr.hi
                         1.321                           10.758
     odds.ratio.grpprednisolone                            or.lo
                         3.857                            1.328
                         or.hi
                        11.207
```

Interpretation. By Exercise 10.2(b) the fitted median $e^{-\theta/\lambda} = e^{\mu}$ is 45.5 months untreated and 171.6 treated, bracketing the Kaplan-Meier medians 40.5 and 146. On the accelerated failure time scale of Exercise 10.3 prednisolone multiplies survival time by $\widehat{\eta} = e^{1.327} = 3.77$ (95% CI 1.32 to 10.76); on the proportional odds scale of Exercise 10.5 it multiplies the odds of surviving beyond any time by $\exp(1.327/0.983) = 3.86$ (95% CI 1.33 to 11.21). Wald gives $z = 2.48$, $p = 0.013$; the likelihood ratio statistic of Section 10.5 is $D = 5.85$ on 1 d.f., $p = 0.016$. In the hazard metric of (10.20), since $\phi_g = \exp(-\mu_g/\sigma)$ the Weibull hazard ratio is $\exp(-\widehat{\beta}_{\mathrm{AFT}}/\widehat{\sigma})$:

```
mw <- fits$weibull; me <- fits$exponential
```

```
round(c(weibull.lambda = 1/mw$scale,
        weibull.HR = exp(-coef(mw)[2]/mw$scale),
        exponential.HR = exp(-coef(me)[2]),
        exp.HR.lo = exp(-(coef(me)[2] + 1.96*sqrt(vcov(me)[2,2]))),
        exp.HR.hi = exp(-(coef(me)[2] - 1.96*sqrt(vcov(me)[2,2])))), 3)
```

```
                 weibull.lambda      weibull.HR.grpprednisolone
                          0.789                           0.435
exponential.HR.grpprednisolone       exp.HR.lo.grpprednisolone
                          0.406                           0.189
     exp.HR.hi.grpprednisolone
                          0.875
```

Prednisolone roughly halves the death rate: $\widehat{HR} = 0.44$ (Weibull), 0.41 (exponential). The log-rank test and the semi-parametric Cox model agree.

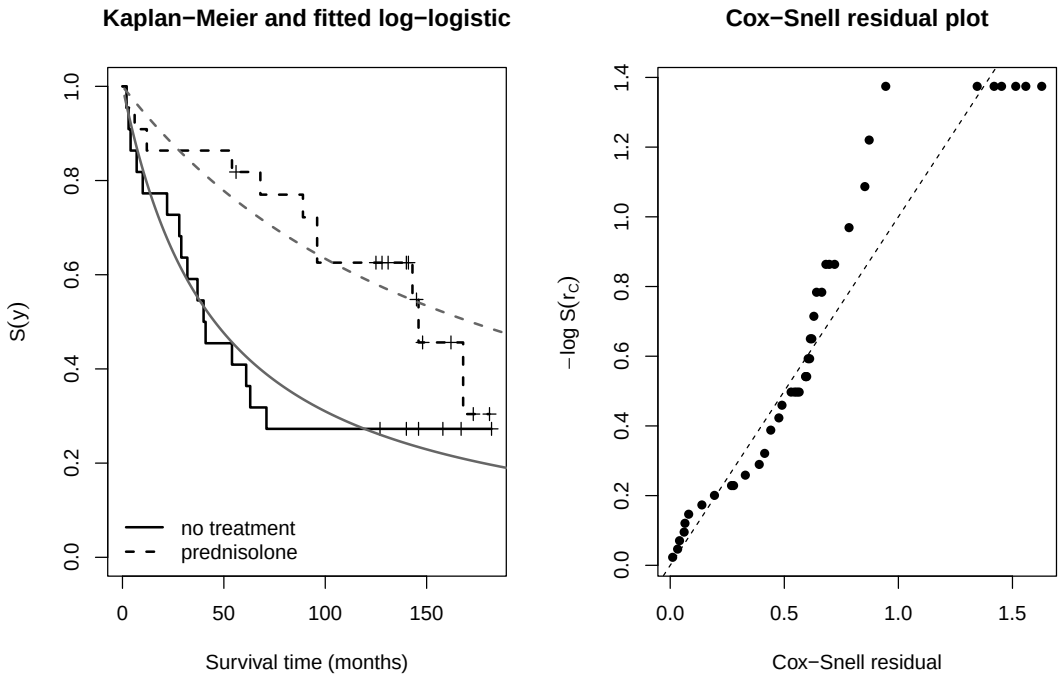
```
survdiff(S ~ grp, data = hep)
summary(coxph(S ~ grp, data = hep))$conf.int
```

```
Call:
survdiff(formula = S ~ grp, data = hep)

                  N Observed Expected (O-E)^2/E (O-E)^2/V
grp=no treatment 22       16     10.6      2.73      4.66
grp=prednisolone 22       11     16.4      1.77      4.66

 Chisq= 4.7  on 1 degrees of freedom, p= 0.03
                exp(coef) exp(-coef) lower .95 upper .95
grpprednisolone 0.4357837   2.294716 0.2000254 0.9494164
```

The Cox estimate $\widehat{HR} = 0.436$ (95% CI 0.20 to 0.95) matches the Weibull 0.435, so the parametric assumption buys precision without distorting the point estimate.

For checking, overlay the fitted log-logistic survivor curves on the Kaplan-Meier estimates and plot $-\log \widehat{S}(r_C)$ against the Cox-Snell residuals (10.19) $r_{Cj} = \widehat{H}_j(y_j) = \log(1 + e^{\widehat{\theta}_g} y_j^{\widehat{\lambda}})$, their survivor function estimated with the original censoring indicators retained; under the model they are a censored unit-exponential sample, so the points should lie on the line of slope one through the origin.

```
par(mfrow = c(1, 2))
plot(km, lty = c(1, 2), lwd = 2, xlab = "Survival time (months)",
     ylab = expression(hat(S)(y)), mark.time = TRUE,
     main = "Kaplan-Meier and fitted log-logistic")
lam <- 1/m$scale; th <- -b[1]/m$scale; th2 <- -(b[1] + b[2])/m$scale
yy <- seq(1, 200, length = 400)
lines(yy, 1/(1 + exp(th)*yy^lam), col = "grey40", lwd = 2)
lines(yy, 1/(1 + exp(th2)*yy^lam), col = "grey40", lwd = 2, lty = 2)
legend("bottomleft", c("no treatment", "prednisolone"), lty = c(1, 2), lwd = 2, bty = "n")
rc <- log(1 + exp(ifelse(hep$grp == "no treatment", th, th2)) * hep$time^lam)
sr <- survfit(Surv(rc, hep$dead) ~ 1)
plot(sr$time, -log(sr$surv), pch = 16, xlab = "Cox-Snell residual",
     ylab = expression(-log~hat(S)(r[C])), main = "Cox-Snell residual plot")
abline(0, 1, lty = 2)
```



The fitted curves track both Kaplan-Meier estimates. The clearest discrepancy is early in the treated arm, flat between 12 and 54 months while the log-logistic curve is already falling; a Weibull with $\lambda > 1$ would fit that stretch better and the untreated arm worse. The Cox-Snell points sit slightly above the reference line mid-range and flatten at the top, where the last residuals are censored and $\widehat{S}(r_C)$ rests on a handful of patients – the usual artefact of a Kaplan-Meier estimate ending in censored observations. Prednisolone materially improves survival: hazard ratio about 0.44, equivalently an odds-of-survival ratio about 3.9 or a time stretch about 3.8, median survival rising from roughly 46 to 172 months, significant at 5% by every test applied (p between 0.01 and 0.04). The intervals are wide (the time ratio's lower limit is 1.3) on 44 patients and 27 deaths, and the three structures cannot be told apart here – but they give the same conclusion.

11 Clustered and Longitudinal Data

Contents

11.1 Problem 11.1 — The measurement of left ventricular volume of the heart is important for

Problem 11.1. The measurement of left ventricular volume of the heart is important for studies of cardiac physiology and clinical management of patients with heart disease. An indirect way of measuring the volume, y, involves a measurement called *parallel conductance volume*, x. Boltwood et al. (1989) found an approximately linear association between y and x in a study of dogs under various "load" conditions. The results, reported by Glantz and Slinker (1990), are shown in Table 11.9: measurements of left ventricular volume y and parallel conductance volume x on five dogs under eight different load conditions.
Dog 1: y = 81.7, 84.3, 72.8, 71.7, 76.7, 75.8, 77.3, 86.3; x = 54.3, 62.0, 62.3, 47.3, 53.6, 38.0, 54.2, 54.0. Dog 2: y = 105.0, 113.6, 108.7, 83.9, 89.0, 86.1, 88.7, 117.6; x = 81.5, 80.8, 74.5, 71.9, 79.5, 73.0, 74.7, 88.6. Dog 3: y = 95.5, 95.7, 84.0, 85.8, 98.8, 106.2, 106.4, 115.0; x = 65.0, 68.3, 67.9, 61.0, 66.0, 81.8, 71.4, 96.0. Dog 4: y = 113.1, 116.5, 100.8, 101.5, 120.8, 95.0, 91.9, 94.0; x = 87.5, 93.6, 70.4, 66.1, 101.4, 57.0, 82.5, 80.9. Dog 5: y = 99.5, 99.2, 106.1, 85.2, 106.3, 84.6, 92.1, 101.2; x = 79.4, 82.5, 87.9, 66.4, 68.4, 59.5, 58.5, 69.2.

(a) Conduct an exploratory analysis of these data.

(b) Let (Y_{jk}, x_{jk}) denote the kth measurement on dog j, $(j = 1, \ldots, 5;\ k = 1, \ldots, 8)$. Fit the linear model

$$\mathrm{E}(Y_{jk}) = \mu = \alpha + \beta x_{jk}, \qquad Y \sim \mathrm{N}(\mu, \sigma^2),$$

assuming the random variables Y_{jk} are independent (i.e., ignoring the repeated measures on the same dogs). Compare the estimates of the intercept α and slope β and their standard errors from this pooled analysis with the results you obtain using a data reduction approach.

(c) Fit a suitable random effects model.

(d) Fit a clustered model using a GEE.

(e) Compare the results you obtain from each approach. Which method(s) do you think are most appropriate? Why?

(difficulty: ⋆⋆⋆)

Solution. Every method puts $\widehat{\beta}$ between 0.63 and 0.83 and they differ only in the standard error, by a factor of five. The design is clustered, not longitudinal: the conditions $k = 1, \ldots, 8$ are imposed load states with no ordering, so the exchangeable structure (11.7) is the natural first choice. Each dog is a cluster of size $K = 8$ and there are $J = 5$ clusters – few enough that every method here works at the edge of its asymptotics.

(a) Exploratory analysis.

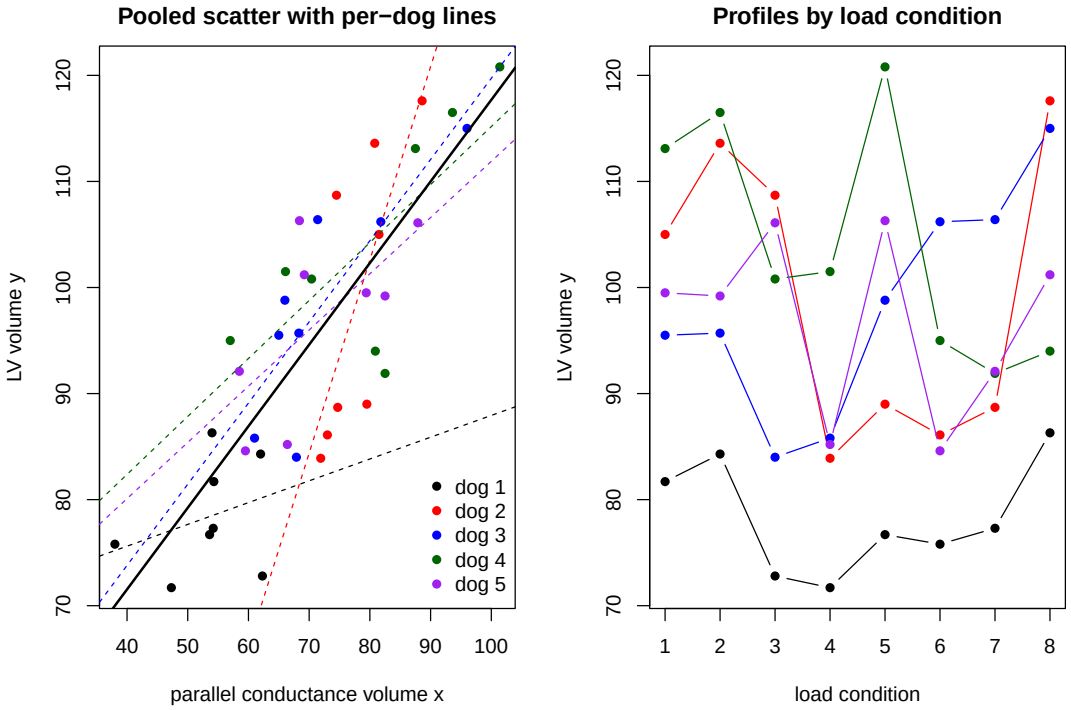
```r
library(dobson)
data(dogs)
dogs <- as.data.frame(dogs)
dogs$dog <- factor(dogs$dog)
aggregate(cbind(y, x) ~ dog, data = dogs,
          FUN = function(v) c(mean = mean(v), sd = sd(v)))
round(cor(dogs$y, dogs$x), 3)
sapply(split(dogs, dogs$dog), function(d) round(cor(d$y, d$x), 3))
```

```
  dog     y.mean       y.sd    x.mean      x.sd
1   1  78.325000   5.280354 53.212500  7.829511
2   2  99.075000  13.573477 78.062500  5.606358
3   3  98.425000  10.572032 72.175000 11.393325
4   4 104.200000  11.115498 79.925000 14.738458
5   5  96.775000   8.574339 71.475000 10.732294
[1] 0.806
    1     2     3     4     5
0.305 0.752 0.825 0.725 0.663
```

Dog 1 sits below the others on both variables (mean $y = 78.3$ against 97–104, mean $x = 53.2$ against 71–80): a small heart gives eight small y's and eight small x's. The pooled correlation 0.806 is thus inflated by between-dog contrast, the within-dog correlations running from 0.31 (dog 1) to 0.83 (dog

3).

```
par(mfrow = c(1, 2), mar = c(4.5, 4.5, 2.5, 1))
cols <- c("black", "red", "blue", "darkgreen", "purple")
plot(dogs$x, dogs$y, col = cols[dogs$dog], pch = 16,
     xlab = "parallel conductance volume x", ylab = "LV volume y",
     main = "Pooled scatter with per-dog lines")
for (j in levels(dogs$dog)) {
  d <- dogs[dogs$dog == j, ]
  abline(lm(y ~ x, data = d), col = cols[as.integer(j)], lty = 2)
}
abline(lm(y ~ x, data = dogs), lwd = 2)
legend("bottomright", legend = paste("dog", 1:5), col = cols, pch = 16, bty = "n")
matplot(1:8, matrix(dogs$y, nrow = 8), type = "b", pch = 16, lty = 1, col = cols,
        xlab = "load condition", ylab = "LV volume y",
        main = "Profiles by load condition")
dev.off()
```



The five per-dog lines fan out rather than lying parallel: dogs 3, 4, 5 have slopes near the pooled line, dog 1 is flatter, and dog 2 is near vertical, its x spanning only 71.9 to 88.6 against y from 83.9 to 117.6. The profiles share a shape across conditions (dips at 4 and 6, a rise at 8) with no monotone trend in k, as expected for load states; dog 1's profile lies clear below the rest, the signature of a dog effect. Decomposing x into $\bar{x}_{j\cdot}$ and $x_{jk} - \bar{x}_{j\cdot}$ makes the between/within split explicit:

```
xbar <- tapply(dogs$x, dogs$dog, mean); ybar <- tapply(dogs$y, dogs$dog, mean)
round(coef(lm(ybar ~ xbar)), 3)
dogs$xb <- xbar[dogs$dog]; dogs$xw <- dogs$x - dogs$xb
round(summary(lm(y ~ xw + xb, data = dogs))$coef, 4)
```

```
(Intercept)        xbar
     29.958       0.922

            Estimate Std. Error t value Pr(>|t|)
(Intercept)  29.9584     9.2653  3.2334   0.0026
xw            0.6288     0.1242  5.0617   0.0000
xb            0.9215     0.1294  7.1212   0.0000
```

The between-dog slope is 0.92 and the within-dog slope 0.63. These answer different questions: 0.63 is how y moves when the load on a given dog changes, 0.92 how much larger y is for a dog with larger conductance volume. Boltwood's calibration question is the within-dog one.

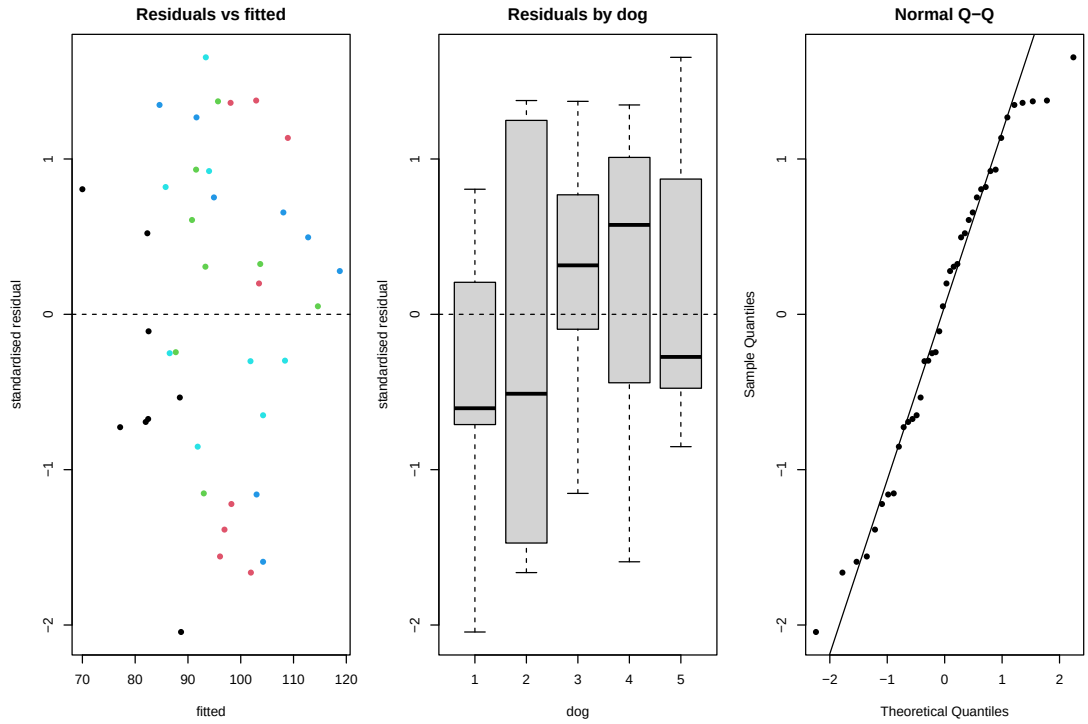
(b) Pooled analysis versus data reduction.

```r
pooled <- lm(y ~ x, data = dogs)
summary(pooled)
```

```
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 40.76808    6.61726   6.161 3.43e-07 ***
x            0.76923    0.09156   8.401 3.42e-10 ***

Residual standard error: 7.911 on 38 degrees of freedom
Multiple R-squared:   0.65,        Adjusted R-squared:  0.6408
F-statistic: 70.58 on 1 and 38 DF,  p-value: 3.416e-10
```

So $\hat{\alpha} = 40.77$ (s.e. 6.62) and $\hat{\beta} = 0.769$ (s.e. 0.0916) on 38 residual degrees of freedom – a fiction unless the within-dog correlation is zero, since 40 observations come from 5 independent dogs. Check the fit first.

```r
par(mfrow = c(1, 3), mar = c(4.5, 4.5, 2.5, 1))
plot(fitted(pooled), rstandard(pooled), pch = 16, col = dogs$dog,
     xlab = "fitted", ylab = "standardised residual", main = "Residuals vs fitted")
abline(h = 0, lty = 2)
boxplot(rstandard(pooled) ~ dogs$dog, xlab = "dog", ylab = "standardised residual",
        main = "Residuals by dog")
abline(h = 0, lty = 2)
qqnorm(rstandard(pooled), pch = 16, main = "Normal Q-Q")
qqline(rstandard(pooled))
dev.off()
```



No curvature, constant spread and a straight Q-Q plot, so the marginal Normal assumptions hold. The middle panel is the one that matters: a strong dog effect would displace the five boxes from zero and narrow each, whereas all five straddle zero and all five are wide, foreshadowing the zero variance component in (c). Spread is largest for dog 2, whose fitted line is the outlier. Data reduction (Section 11.2) fits a line per dog and treats the five intercepts and slopes as the data:

```r
co <- t(sapply(split(dogs, dogs$dog), function(d) coef(lm(y ~ x, data = d))))
round(co, 3)
round(rbind(mean = colMeans(co), se = apply(co, 2, sd) / sqrt(5)), 3)
t.test(co[, 2])
```

```
  (Intercept)     x
1      67.389 0.206
2     -43.076 1.821
```

```
3      43.178 0.765
4      60.514 0.547
5      58.892 0.530

     (Intercept)     x
mean       37.38 0.774
se         20.50 0.277

        One Sample t-test

data:  co[, 2]
t = 2.7967, df = 4, p-value = 0.04897
alternative hypothesis: true mean is not equal to 0
95 percent confidence interval:
 0.005610799 1.541811613
sample estimates:
mean of x
0.7737112
```

The slopes agree (0.769 against 0.774) and the intercepts tolerably (40.8 against 37.4), but the standard errors differ by a factor of 3.0 (0.277 against 0.0916; 20.5 against 6.6) – the phenomenon of Tables 11.3 and 11.5–11.6. The pooled analysis counts 40 independent observations, data reduction counts 5, and on 4 d.f. the slope only just reaches significance ($p = 0.049$). The inflation is driven by dog 2, whose fitted slope is 1.82 against 0.21–0.77, and whose narrow x range makes it the least well determined; data reduction weights all five equally and ignores "the random error in the estimates" (Section 11.2). So 0.277 is honest about the number of independent units but inefficient.

(c) Random effects model. Put a random intercept on dog:

$$Y_{jk} = \alpha + \beta x_{jk} + b_j + e_{jk}, \qquad b_j \sim \mathrm{N}(0, \sigma_b^2), \quad e_{jk} \sim \mathrm{N}(0, \sigma^2),$$

independently. This induces exactly the equicorrelation matrix (11.7) with $\rho = \sigma_b^2/(\sigma_b^2 + \sigma^2)$, i.e. compound symmetry.

```r
library(lme4)
m1 <- lmer(y ~ x + (1 | dog), data = dogs, REML = TRUE)
summary(m1)
```

```
boundary (singular) fit: see help('isSingular')
Linear mixed model fit by REML ['lmerMod']
Formula: y ~ x + (1 | dog)

Random effects:
 Groups   Name        Variance Std.Dev.
 dog      (Intercept)  0.00    0.000
 Residual             62.58    7.911
Number of obs: 40, groups:  dog, 5

Fixed effects:
            Estimate Std. Error t value
(Intercept) 40.76808    6.61726   6.161
x            0.76923    0.09156   8.401
```

The between-dog variance is estimated at the boundary, $\hat{\sigma}_b^2 = 0$, so the mixed model collapses onto the pooled fit of (b), estimates and standard errors identical. That is a finding, not a software failure: once x is in the model nothing is left for a dog effect, because the dog means of y and x move together (the between-dog slope 0.92 of (a)). Fitting dog as a fixed factor says the same:

```r
round(summary(lm(y ~ x + dog, data = dogs))$coef, 4)
a <- anova(lm(resid(lm(y ~ x, data = dogs)) ~ dogs$dog))
MSB <- a[1, 3]; MSW <- a[2, 3]
round(c(MSB = MSB, MSW = MSW, rho = (MSB - MSW) / (MSB + 7 * MSW)), 3)
```

```
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  44.8626     7.2807  6.1619   0.0000
x             0.6288     0.1264  4.9746   0.0000
dog2          5.1232     5.0386  1.0168   0.3164
dog3          8.1755     4.6114  1.7729   0.0852
```

```
dog4          9.0770     5.1886  1.7494   0.0892
dog5          6.9657     4.5660  1.5256   0.1364

   MSB    MSW    rho
47.716 62.490 -0.030
```

None of the four dog contrasts is significant at 5%. The second calculation is the one-way moment estimator of the intra-class correlation applied to the pooled residuals,

$$\widehat{\rho} = \frac{\mathrm{MS}_{\text{between}} - \mathrm{MS}_{\text{within}}}{\mathrm{MS}_{\text{between}} + (K-1)\mathrm{MS}_{\text{within}}},$$

with $K = 8$. The between-dog mean square, 47.7, is *smaller* than the within-dog mean square, 62.5, so $\widehat{\rho} = -0.030$. A variance component cannot be negative, so the likelihood is maximised on the boundary and $\widehat{\sigma}^2_b$ is pinned at zero.

Allowing the slope to vary as well does not help:

```r
m2 <- lmer(y ~ x + (x | dog), data = dogs, REML = TRUE)
anova(update(m1, REML = FALSE), update(m2, REML = FALSE))
```

```
Data: dogs
Models:
update(m1, REML = FALSE): y ~ x + (1 | dog)
update(m2, REML = FALSE): y ~ x + (x | dog)
                         npar    AIC    BIC  logLik -2*log(L) Chisq Df Pr(>Chisq)
update(m1, REML = FALSE)    4 284.92 291.68 -138.46    276.92
update(m2, REML = FALSE)    6 288.94 299.08 -138.47    276.94     0  2          1
```

The random slope model is singular too (intercept-slope correlation exactly -1), the deviance does not drop and AIC rises by 4: five dogs carry no information about a slope variance. Report the random intercept model, with $\hat{\sigma}^2_b = 0$ and $\hat{\beta} = 0.769$ (s.e. 0.092).

(d) GEE. Model the correlation directly, solving (11.12) with identity link and Gaussian variance function and the sandwich estimator of Section 11.3.

```r
library(geepack)
gi <- geeglm(y ~ x, id = dog, data = dogs, family = gaussian, corstr = "independence")
ge <- geeglm(y ~ x, id = dog, data = dogs, family = gaussian, corstr = "exchangeable")
ga <- geeglm(y ~ x, id = dog, waves = condition, data = dogs,
             family = gaussian, corstr = "ar1")
for (g in list(gi, ge, ga)) {
  cat("corstr =", g$corstr, "\n")
  print(round(summary(g)$coefficients, 4))
  if (nrow(summary(g)$corr) > 0) print(round(summary(g)$corr, 4))
  cat("\n")
}
```

```
corstr = independence
            Estimate Std.err     Wald Pr(>|W|)
(Intercept)  40.7681  4.5237  81.2165        0
x             0.7692  0.0518 220.6030        0

corstr = exchangeable
            Estimate Std.err     Wald Pr(>|W|)
(Intercept)  36.5514  3.9915  83.8541        0
x             0.8286  0.0481 296.5865        0
      Estimate Std.err
alpha  -0.0769  0.0342

corstr = ar1
            Estimate Std.err     Wald Pr(>|W|)
(Intercept)  46.3112  5.2577  77.5852        0
x             0.6941  0.0626 122.8725        0
      Estimate Std.err
alpha   0.2858  0.1021
```

The three working structures give $\hat{\beta} = 0.769$, 0.829, 0.694, a spread inside one data-reduction standard error, illustrating the Liang-Zeger robustness result of Section 11.4. The exchangeable fit gives $\hat{\alpha}_{\text{corr}} = -0.077$, small and negative like the moment estimate -0.030 of (c): no positive clustering survives

adjustment for x. Discount the AR(1) fit, since $\rho^{|j-k|}$ is meaningless for unordered load states and its $\hat{\alpha} = 0.286$ is an artefact of the listing order.

The sandwich standard error for the slope under independence is 0.052 against 0.092 by least squares – **smaller**, not larger. With $J = 5$ the sandwich matrix $C = \sum_j \mathbf{x}_j^T \hat{\mathbf{V}}_j^{-1}(\mathbf{y}_j - \mathbf{x}_j\hat{\beta})(\mathbf{y}_j - \mathbf{x}_j\hat{\beta})^T \hat{\mathbf{V}}_j^{-1}\mathbf{x}_j$ is a sum of five rank-one terms and badly downward biased; consistency holds as $J \to \infty$. These standard errors should not be believed.

(e) Comparison.

Method	$\hat{\alpha}$	s.e.	$\hat{\beta}$	s.e.
Pooled OLS (ignores clusters)	40.77	6.62	0.769	0.0916
Data reduction (5 dog lines)	37.38	20.50	0.774	0.2770
Random intercept (lmer)	40.77	6.62	0.769	0.0916
GEE, independence, sandwich	40.77	4.52	0.769	0.0518
GEE, exchangeable, sandwich	36.55	3.99	0.829	0.0481
Dog as fixed factor (within)	44.86	7.28	0.629	0.1264

Left ventricular volume rises by roughly 0.7–0.8 units per unit of parallel conductance volume on every method; the disagreement is about precision, and hence about how many independent units the study has.

The random effects model of (c) is the right description, being the only one that asks whether a dog effect exists rather than assuming one; its answer of no is what licenses the otherwise indefensible pooled analysis of (b). The data reduction interval is the most defensible, using only the five independent units and assuming nothing about the within-dog covariance, but inefficient in discarding their unequal precisions. The GEE analysis is the least trustworthy: Section 11.7's recommendation of Wald statistics with the sandwich estimator rests on the Liang-Zeger (1986) asymptotics in the number of clusters, absent at $J = 5$, and the standard errors here are visibly anticonservative.

All the marginal fits estimate a blend of the within-dog slope 0.63 and the between-dog slope 0.92. For the calibration question – how y responds when the load on a given animal changes – quote 0.63 from the fixed-dog fit, or equivalently the centred-x coefficient of (a); the pooled 0.769 is biased upward by the between-dog contrast.

11.2 Problem 11.2 — Suppose that (Y jk , x jk) are observations on the kth subject in cluster k (with

Problem 11.2. Suppose that (Y_{jk}, x_{jk}) are observations on the kth subject in cluster j (with $j = 1, \ldots, J$; $k = 1, \ldots, K$) and the goal is to fit a "regression through the origin" model

$$\mathrm{E}(Y_{jk}) = \beta x_{jk},$$

where the variance-covariance matrix for Y's in the same cluster is the $K \times K$ equicorrelation matrix

$$\mathbf{V}_j = \sigma^2 \begin{bmatrix} 1 & \rho & \cdots & \rho \\ \rho & 1 & & \rho \\ \vdots & & \ddots & \vdots \\ \rho & \rho & \cdots & 1 \end{bmatrix},$$

that is, every diagonal element is σ^2 and every off-diagonal element is $\sigma^2\rho$, and Y's in different clusters are independent.

(a) From Section 11.3, if the Y's are Normally distributed, then

$$\widehat{\boldsymbol{\beta}} = \Big(\sum_{j=1}^{J} \mathbf{x}_j^T \mathbf{V}_j^{-1} \mathbf{x}_j\Big)^{-1} \Big(\sum_{j=1}^{J} \mathbf{x}_j^T \mathbf{V}_j^{-1} \mathbf{y}_j\Big) \quad \text{with} \quad \mathrm{var}(\widehat{\boldsymbol{\beta}}) = \Big(\sum_{j=1}^{J} \mathbf{x}_j^T \mathbf{V}_j^{-1} \mathbf{x}_j\Big)^{-1},$$

where $\mathbf{x}_j^T = [x_{j1}, \ldots, x_{jK}]$. Deduce that the estimate b of β is unbiased.

(b) As

$$\mathbf{V}_j^{-1} = c\begin{bmatrix} 1 & \phi & \cdots & \phi \\ \phi & 1 & & \phi \\ \vdots & & \ddots & \vdots \\ \phi & \phi & \cdots & 1 \end{bmatrix}, \quad \text{where} \quad c = \frac{1}{\sigma^2[1+(K-1)\phi\rho]} \quad \text{and} \quad \phi = \frac{-\rho}{1+(K-2)\rho},$$

show that

$$\text{var}(b) = \frac{\sigma^2[1+(K-1)\phi\rho]}{\sum_j\{\sum_k x_{jk}^2 + \phi[(\sum_k x_{jk})^2 - \sum_k x_{jk}^2]\}}.$$

(c) If the clustering is ignored, show that the estimate b^* of β has $\text{var}(b^*) = \sigma^2/\sum_j\sum_k x_{jk}^2$.

(d) If $\rho = 0$, show that $\text{var}(b) = \text{var}(b^*)$ as expected if there is no correlation within clusters.

(e) If $\rho = 1$, $\mathbf{V}_j/\sigma^2$ is a matrix of ones, so the inverse does not exist. But the case of maximum correlation is equivalent to having just one element per cluster. If $K = 1$, show that $\text{var}(b) = \text{var}(b^*)$, in this situation.

(f) If the study is designed so that $\sum_k x_{jk} = 0$ and $\sum_k x_{jk}^2$ is the same for all clusters, let $W = \sum_j\sum_k x_{jk}^2$ and show that

$$\text{var}(b) = \frac{\sigma^2[1+(K-1)\phi\rho]}{W(1-\phi)}.$$

(g) With this notation $\text{var}(b^*) = \sigma^2/W$; hence, show that

$$\frac{\text{var}(b)}{\text{var}(b^*)} = \frac{[1+(K-1)\phi\rho]}{1-\phi} = 1-\rho.$$

Deduce the effect on the estimated standard error of the slope estimate for this model if the clustering is ignored.
(difficulty: ⋆⋆)

Solution. With $\mathbf{1}$ the $K \times 1$ vector of ones and $\mathbf{J}_K = \mathbf{1}\mathbf{1}^T$, the equicorrelation matrix (11.7) is

$$\mathbf{V}_j = \sigma^2[(1-\rho)\mathbf{I}_K + \rho\mathbf{J}_K] \equiv \mathbf{V},$$

the same for every cluster; $\mathbf{x}_j$ is $K \times 1$, every quadratic form below is a scalar, and b is the estimate written $\widehat{\beta}$ in the statement. (The printed statement says "the kth subject in cluster k" where cluster j is meant.) Used repeatedly:

$$\mathbf{x}^T\mathbf{I}_K\mathbf{x} = \sum_k x_k^2, \qquad \mathbf{x}^T\mathbf{J}_K\mathbf{x} = (\mathbf{1}^T\mathbf{x})^2 = \Big(\sum_k x_k\Big)^2.$$

(a) Under the model $\text{E}(\mathbf{y}_j) = \beta\mathbf{x}_j$, and with $\mathbf{V}_j$ a known constant matrix b is linear in $\mathbf{y}$, so

$$\text{E}(b) = \Big(\sum_j \mathbf{x}_j^T\mathbf{V}_j^{-1}\mathbf{x}_j\Big)^{-1}\sum_j \mathbf{x}_j^T\mathbf{V}_j^{-1}\text{E}(\mathbf{y}_j) = \Big(\sum_j \mathbf{x}_j^T\mathbf{V}_j^{-1}\mathbf{x}_j\Big)^{-1}\Big(\sum_j \mathbf{x}_j^T\mathbf{V}_j^{-1}\mathbf{x}_j\Big)\beta = \beta.$$

unbiased whatever ρ: the correlation affects precision, not centring. Two hypotheses do work here. The scalar $\sum_j \mathbf{x}_j^T\mathbf{V}_j^{-1}\mathbf{x}_j$ must be non-zero, which holds since $\mathbf{V}_j$ is positive definite for $-1/(K-1) < \rho < 1$; and $\mathbf{V}_j$ must be fixed rather than estimated from the same $\mathbf{y}$ – with $\mathbf{V}$ estimated by the iterative scheme after (11.6), b is only consistent and asymptotically unbiased.
(b) Write the claimed inverse as $\mathbf{V}^{-1} = c[(1-\phi)\mathbf{I}_K + \phi\mathbf{J}_K]$. Sherman-Morrison applied to $\mathbf{I} + \frac{\rho}{1-\rho}\mathbf{1}\mathbf{1}^T$ gives

$$\mathbf{V}^{-1} = \frac{1}{\sigma^2(1-\rho)}\Big[\mathbf{I}_K - \frac{\rho}{1+(K-1)\rho}\mathbf{J}_K\Big],$$

and with $\phi = -\rho/[1+(K-2)\rho]$,

$$1-\phi = \frac{1+(K-1)\rho}{1+(K-2)\rho}, \qquad 1+(K-1)\phi\rho = \frac{1+(K-2)\rho-(K-1)\rho^2}{1+(K-2)\rho} = \frac{(1-\rho)[1+(K-1)\rho]}{1+(K-2)\rho},$$

using $1+(K-2)\rho-(K-1)\rho^2=(1-\rho)[1+(K-1)\rho]$. Hence

$$c=\frac{1+(K-2)\rho}{\sigma^2(1-\rho)[1+(K-1)\rho]},\qquad c(1-\phi)=\frac{1}{\sigma^2(1-\rho)},\qquad c\phi=\frac{-\rho}{\sigma^2(1-\rho)[1+(K-1)\rho]},$$

the coefficients of $\mathbf{I}_K$ and $\mathbf{J}_K$ in the standard inverse, with diagonal entry $c(1-\phi)+c\phi=c$ and off-diagonal $c\phi$ as printed. The quadratic form is then

$$\mathbf{x}_j^T\mathbf{V}^{-1}\mathbf{x}_j=c\big[(1-\phi)\mathbf{x}_j^T\mathbf{I}\mathbf{x}_j+\phi\,\mathbf{x}_j^T\mathbf{J}_K\mathbf{x}_j\big]=c\Big[\sum_k x_{jk}^2+\phi\Big\{\Big(\sum_k x_{jk}\Big)^2-\sum_k x_{jk}^2\Big\}\Big].$$

and summing over clusters and inverting, as in (11.6),

$$\begin{aligned}\operatorname{var}(b)&=\Big(\sum_j \mathbf{x}_j^T\mathbf{V}^{-1}\mathbf{x}_j\Big)^{-1}=\frac{1}{c\sum_j\{\sum_k x_{jk}^2+\phi[(\sum_k x_{jk})^2-\sum_k x_{jk}^2]\}}\\&=\frac{\sigma^2[1+(K-1)\phi\rho]}{\sum_j\{\sum_k x_{jk}^2+\phi[(\sum_k x_{jk})^2-\sum_k x_{jk}^2]\}},\end{aligned}$$

since $1/c=\sigma^2[1+(K-1)\phi\rho]$, as required. Written as

$$\operatorname{var}(b)^{-1}=c\sum_j\Big[(1-\phi)\sum_k x_{jk}^2+\phi\Big(\sum_k x_{jk}\Big)^2\Big],$$

cluster j's information splits into a within-cluster part weighted by $c(1-\phi)=1/[\sigma^2(1-\rho)]$ and a cluster-total part weighted by $c\phi$, negative when $\rho>0$: positive intra-class correlation discounts the totals and leaves the within-cluster contrasts untouched.

(c) Ignoring clustering sets $\rho=0$, so $\mathbf{V}_j^{-1}=\sigma^{-2}\mathbf{I}_K$ and the estimator is ordinary least squares through the origin,

$$b^*=\frac{\sum_j\sum_k x_{jk}y_{jk}}{\sum_j\sum_k x_{jk}^2},\qquad \operatorname{var}(b^*)=\Big(\sum_j\frac{1}{\sigma^2}\mathbf{x}_j^T\mathbf{x}_j\Big)^{-1}=\frac{\sigma^2}{\sum_j\sum_k x_{jk}^2}.$$

the nominal variance; whether it is the true variance of b^* is part (g).

(d) If $\rho=0$ then $\phi=0$, so $c=1/\sigma^2$, the bracketed denominator term reduces to $\sum_k x_{jk}^2$ and the leading factor is σ^2, whence

$$\operatorname{var}(b)=\frac{\sigma^2}{\sum_j\sum_k x_{jk}^2}=\operatorname{var}(b^*).$$

(e) At $K=1$, $\phi=-\rho/(1-\rho)$ but the coefficient it multiplies vanishes: the leading factor is $1+(K-1)\phi\rho=1$ and $(\sum_k x_{jk})^2-\sum_k x_{jk}^2=0$, so

$$\operatorname{var}(b)=\frac{\sigma^2}{\sum_j x_{j1}^2}=\operatorname{var}(b^*).$$

which is the statement's remark: with one observation per cluster there are no within-cluster pairs for ρ to describe. The limiting case $\rho\to1$ is equivalent, every observation in a cluster then being the same random variable so the cluster carries one observation's information rather than K.

(f) With $\sum_k x_{jk}=0$ and $\sum_k x_{jk}^2=W/J$ for each j, where $W=\sum_j\sum_k x_{jk}^2$, each cluster contributes

$$\sum_k x_{jk}^2+\phi\Big[\Big(\sum_k x_{jk}\Big)^2-\sum_k x_{jk}^2\Big]=\sum_k x_{jk}^2+\phi[0-\textstyle\sum_k x_{jk}^2]=(1-\phi)\sum_k x_{jk}^2,$$

so summing over j gives $(1-\phi)W$ and

$$\operatorname{var}(b)=\frac{\sigma^2[1+(K-1)\phi\rho]}{W(1-\phi)}.$$

(Only $\sum_k x_{jk} = 0$ is used; constancy of $\sum_k x_{jk}^2$ merely makes W/J a per-cluster quantity.)
(g) Dividing (f) by $\mathrm{var}(b^*) = \sigma^2/W$,

$$\frac{\mathrm{var}(b)}{\mathrm{var}(b^*)} = \frac{1 + (K-1)\phi\rho}{1-\phi}.$$

and the two expressions computed in (b) give

$$\frac{1 + (K-1)\phi\rho}{1-\phi} = \frac{(1-\rho)[1 + (K-1)\rho]}{1 + (K-2)\rho} \cdot \frac{1 + (K-2)\rho}{1 + (K-1)\rho} = 1 - \rho.$$

So $\mathrm{var}(b) = (1-\rho)\,\mathrm{var}(b^*)$, i.e. $\mathrm{se}(b^*)/\mathrm{se}(b) = (1-\rho)^{-1/2}$: ignoring the clustering reports a standard error too **large** by that factor, so the naive analysis is conservative – 41% wider at $\rho = 0.5$, 100% at $\rho = 0.75$. The reason is the design: $\sum_k x_{jk} = 0$ makes the slope a purely within-cluster contrast, out of which the shared cluster-level disturbance represented by an exchangeable $\rho > 0$ cancels.
The familiar inflation appears when the covariate varies between clusters. If $x_{jk} = x_j$ then $\sum_k x_{jk}^2 = Kx_j^2$ and $(\sum_k x_{jk})^2 = K^2 x_j^2$, so cluster j contributes $cKx_j^2[1 + (K-1)\phi]$; with $1 + (K-1)\phi = (1-\rho)/[1 + (K-2)\rho]$ the same algebra gives

$$\frac{\mathrm{var}(b)}{\mathrm{var}(b^*)} = 1 + (K-1)\rho,$$

the classical design effect: now the naive standard error is too **small** by $[1 + (K-1)\rho]^{1/2}$, the case Section 11.1 warns about. The direction of the bias is set by whether the covariate is a within- or between-cluster contrast.
A check against direct matrix computation with $K = 5$, $J = 4$, $\sigma^2 = 2.3$, $\rho = 0.4$:

```r
K <- 5; J <- 4; sig2 <- 2.3; rho <- 0.4
Vj  <- sig2 * ((1 - rho) * diag(K) + rho)
phi <- -rho / (1 + (K - 2) * rho)
cc  <- 1 / (sig2 * (1 + (K - 1) * phi * rho))
cat("max |V^-1 (book) - solve(V)| =", max(abs(cc * ((1 - phi) * diag(K) + phi) -
↪  solve(Vj))), "\n")

set.seed(11)
X <- matrix(rnorm(J * K), nrow = K)          # columns are clusters
varb.direct  <- 1 / sum(sapply(1:J, function(j) t(X[, j]) %*% solve(Vj) %*% X[, j]))
varb.formula <- sig2 * (1 + (K - 1) * phi * rho) /
  sum(apply(X, 2, function(x) sum(x^2) + phi * (sum(x)^2 - sum(x^2))))
cat("(b) var(b) direct =", varb.direct, " formula =", varb.formula, "\n")

Xc <- apply(X, 2, function(x) { x <- x - mean(x); x / sqrt(sum(x^2)) })   # design of (f)
W  <- sum(Xc^2)
vb <- 1 / sum(sapply(1:J, function(j) t(Xc[, j]) %*% solve(Vj) %*% Xc[, j]))
cat("(f) var(b) =", vb, " formula =", sig2 * (1 + (K - 1) * phi * rho) / (W * (1 - phi)),
↪  "\n")
cat("(g) ratio =", vb / (sig2 / W), "  1 - rho =", 1 - rho, "\n")

Xk <- matrix(rep(rnorm(J), each = K), nrow = K)                          # cluster-level x
vk <- 1 / sum(sapply(1:J, function(j) t(Xk[, j]) %*% solve(Vj) %*% Xk[, j]))
cat("cluster-level x: ratio =", vk / (sig2 / sum(Xk^2)), "  1 + (K-1)rho =", 1 + (K - 1) *
↪  rho, "\n")
```

```
max |V^-1 (book) - solve(V)| = 1.110223e-16
(b) var(b) direct = 0.1090953  formula = 0.1090953
(f) var(b) = 0.345  formula = 0.345
(g) ratio = 0.6   1 - rho = 0.6
cluster-level x: ratio = 2.6   1 + (K-1)rho = 2.6
```

Every identity checks to machine precision, both ratios included: $0.345/0.575 = 0.6 = 1 - \rho$ for the within-cluster design and $2.6 = 1 + (K-1)\rho$ for the cluster-level covariate.

11.3 Problem 11.3 — Data on the ears or eyes of subjects are a classical example of clustering—

Problem 11.3. Data on the ears or eyes of subjects are a classical example of clustering — the ears or eyes of the same subject are unlikely to be independent. The data in Table 11.10 are the responses to two treatments coded CEF and AMO of children who had acute otitis media in both ears (data from Rosner, 1989). Table 11.10 gives the numbers of ears clear of acute otitis media at 14 days, cross-classified by antibiotic treatment and age of the child; each entry is a number of children, classified by how many of their two ears were clear (0, 1 or 2).
Treatment CEF: age < 2: 8 children with 0 clear, 2 with 1 clear, 8 with 2 clear (total 18); age 2–5: 6, 6, 10 (total 22); age ≥ 6: 0, 1, 3 (total 4); column totals 14, 9, 21 (total 44). Treatment AMO: age < 2: 11, 2, 2 (total 15); age 2–5: 3, 1, 5 (total 9); age ≥ 6: 1, 0, 6 (total 7); column totals 15, 3, 13 (total 31).

(a) Conduct an exploratory analysis to compare the effects of treatment and age of the child on the success of the treatments, ignoring the clustering within each child.

(b) Let Y_{ijkl} denote the response of the lth ear of the kth child in the treatment group j and age group i. The Y_{ijkl}'s are binary variables with possible values of 1 denoting cured and 0 denoting not cured. A possible model is

$$\text{logit}\left(\frac{\pi_{ijkl}}{1-\pi_{ijkl}}\right) = \beta_0 + \beta_1\,\text{age} + \beta_2\,\text{treatment} + b_k,$$

where b_k denotes the random effect for the kth child and β_0, β_1 and β_2 are fixed parameters. Fit this model (and possibly other related models) to compare the two treatments. How well do the models fit? What do you conclude about the treatments?

(c) An alternative approach, similar to the one proposed by Rosner, is to use nominal logistic regression with response categories 0, 1 or 2 cured ears for each child. Fit a model of this type and compare the results with those obtained in (b). Which approach is preferable considering the assumptions made, ease of computation and ease of interpretation?

(difficulty: ⋆⋆⋆)

Solution. Once clustering is accounted for the treatment difference is not established (p between 0.15 and 0.23 on all three approaches, against a misleading 0.08 naive); age dominates. There are 75 children and 150 ears, each child a cluster of size $K = 2$. The statement writes b_k with one subscript, but the random effect belongs to the child: the model is one random intercept per child.

(a) Exploratory analysis, clustering ignored.

```r
library(dobson)
data(ear)
ear <- as.data.frame(ear)
names(ear)[3] <- "nclear"
ear$age <- factor(ear$age, levels = c("< 2", "2 to 5", ">= 6"))
ear$treatment <- factor(ear$treatment, levels = c("AMO", "CEF"))
agg <- aggregate(cbind(children = frequency, cured = nclear * frequency,
                       ears = 2 * frequency) ~ age + treatment, data = ear, FUN = sum)
agg$prop <- round(agg$cured / agg$ears, 3)
agg
```

```
     age treatment children cured ears  prop
1    < 2       AMO       15     6   30 0.200
2 2 to 5       AMO        9    11   18 0.611
3   >= 6       AMO        7    12   14 0.857
4    < 2       CEF       18    18   36 0.500
5 2 to 5       CEF       22    26   44 0.591
6   >= 6       CEF        4     7    8 0.875
```

Overall $51/88 = 58\%$ of CEF ears cleared against $29/62 = 47\%$ of AMO ears, and the cure rate climbs with age: 36% under 2, 60% at 2–5, 86% at 6 or over. The apparent treatment advantage sits in the youngest group (50% against 20%) and has vanished by age 6. Treating the 150 ears as independent binomial observations:

```r
m <- glm(cbind(cured, ears - cured) ~ age + treatment, family = binomial, data = agg)
summary(m)$coef
anova(m, test = "Chisq")
mi <- glm(cbind(cured, ears - cured) ~ age * treatment, family = binomial, data = agg)
anova(m, mi, test = "Chisq")
```

```
              Estimate Std. Error   z value     Pr(>|z|)
(Intercept)  -0.9244678  0.3397914 -2.720692 0.0065145406
age2 to 5     0.8670782  0.3699752  2.343611 0.0190980579
age>= 6       2.5703802  0.6868940  3.742033 0.0001825374
treatmentCEF  0.6424520  0.3723252  1.725513 0.0844350227

          Df Deviance Resid. Df Resid. Dev  Pr(>Chi)
NULL                         5    26.2434
age        2  19.6149         3     6.6285 5.504e-05 ***
treatment  1   3.0294         2     3.5991   0.08177 .

Model 1: cbind(cured, ears - cured) ~ age + treatment
Model 2: cbind(cured, ears - cured) ~ age * treatment
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
1         2     3.5991
2         0     0.0000  2   3.5991   0.1654
```

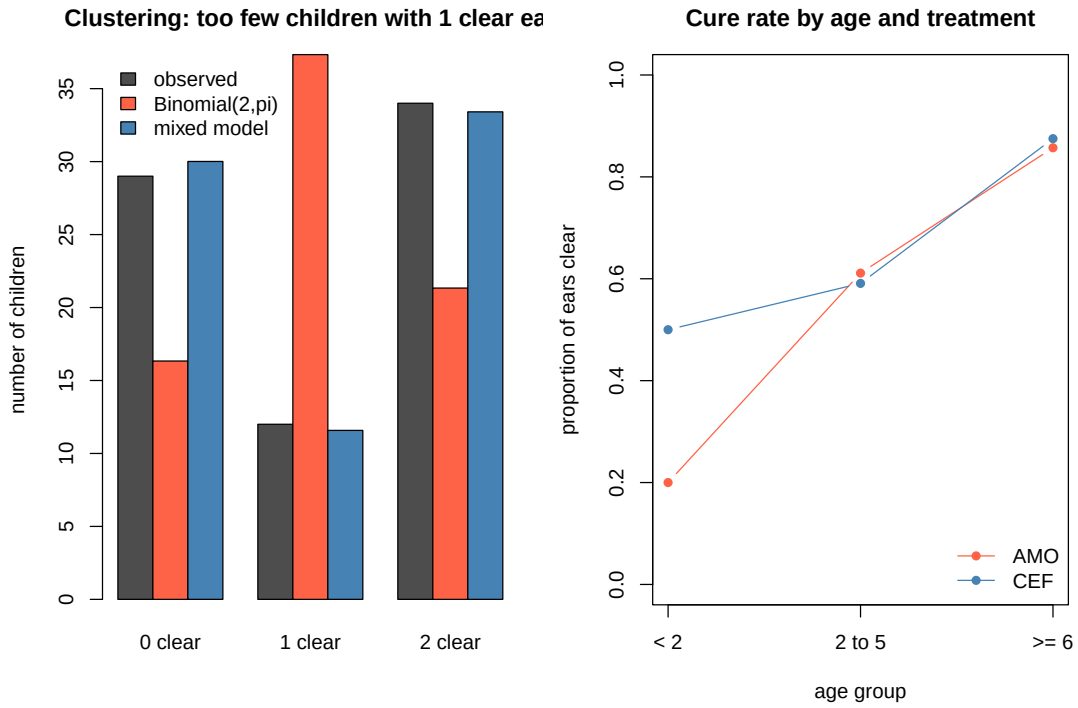
The additive model has residual deviance 3.60 on 2 d.f., an acceptable fit; the age effect is strong ($\Delta D = 19.6$ on 2 d.f.), the treatment effect is marginal ($\Delta D = 3.03$ on 1 d.f., $p = 0.082$, odds ratio $e^{0.643} = 1.90$), and the age by treatment interaction is not significant ($\Delta D = 3.60$ on 2 d.f., $p = 0.165$). All of this is untrustworthy: independent ears is grossly violated, as comparing the observed distribution of clear ears per child with $\mathrm{Bi}(2, \pi)$ shows.

```r
f <- tapply(ear$frequency, ear$nclear, sum)
n <- sum(f); p <- sum(f * (0:2)) / (2 * n)
rbind(observed = as.numeric(f), expected = n * c((1 - p)^2, 2 * p * (1 - p), p^2))
o <- as.numeric(f); e <- n * c((1 - p)^2, 2 * p * (1 - p), p^2)
c(X2 = sum((o - e)^2 / e), df = 1, p = 1 - pchisq(sum((o - e)^2 / e), 1))
```

```
             [,1]     [,2]     [,3]
observed 29.00000 12.00000 34.00000
expected 16.33333 37.33333 21.33333

          X2           df            p
3.453444e+01 1.000000e+00 4.187761e-09
```

Only 12 children had exactly one clear ear where 37 are expected: a child's two ears respond alike. The chi-square statistic is 34.5 on $3 - 1 - 1 = 1$ d.f. (three categories, less one for the total and one for the estimated π), $p = 4 \times 10^{-9}$ – severe positive intra-class correlation, so the naive standard errors are too small.

```r
par(mfrow = c(1, 2), mar = c(4.5, 4.5, 3, 1))
M <- rbind(observed = o, `Binomial(2,pi)` = e, `mixed model` = c(30.01, 11.58, 33.41))
barplot(M, beside = TRUE, names.arg = c("0 clear", "1 clear", "2 clear"),
        col = c("grey30", "tomato", "steelblue"), ylab = "number of children",
        main = "Clustering: too few children with 1 clear ear")
legend("topleft", rownames(M), fill = c("grey30", "tomato", "steelblue"), bty = "n")
pr <- matrix(agg$cured / agg$ears, nrow = 3,
             dimnames = list(levels(ear$age), levels(ear$treatment)))
matplot(1:3, pr, type = "b", pch = 16, lty = 1, col = c("tomato", "steelblue"),
        xaxt = "n", ylim = c(0, 1), xlab = "age group",
        ylab = "proportion of ears clear", main = "Cure rate by age and treatment")
axis(1, at = 1:3, labels = levels(ear$age))
legend("bottomright", colnames(pr), col = c("tomato", "steelblue"),
       lty = 1, pch = 16, bty = "n")
dev.off()
```



(The third bar in the left panel is the mixed model of (b).)

(b) Random effects logistic regression. Expand to one binary row per ear. Which ear of a one-clear child is labelled clear is arbitrary, and since no ear-level covariate enters the model the two ears are exchangeable and the likelihood is unaffected; the labelling does matter for a raw ear-by-ear correlation, so that is computed over both orderings.

```
library(lme4)
kids <- ear[rep(seq_len(nrow(ear)), ear$frequency), c("age", "treatment", "nclear")]
kids$child <- factor(seq_len(nrow(kids)))
ears <- kids[rep(seq_len(nrow(kids)), each = 2), ]
ears$ear <- rep(1:2, nrow(kids))
ears$y <- ifelse(ears$nclear == 2, 1, ifelse(ears$nclear == 0, 0, ears$ear - 1))
c(children = nrow(kids), ears = nrow(ears), cured = sum(ears$y))
E <- matrix(ears$y, nrow = 2)
round(cor(c(E[1, ], E[2, ]), c(E[2, ], E[1, ])), 3)
g1 <- glmer(y ~ age + treatment + (1 | child), data = ears, family = binomial,
            control = glmerControl(optimizer = "bobyqa"))
summary(g1)
```

```
children     ears    cured
      75      150       80

[1] 0.679

Random effects:
 Groups Name        Variance Std.Dev.
 child  (Intercept) 16.24    4.03
Number of obs: 150, groups:  child, 75

Fixed effects:
             Estimate Std. Error z value Pr(>|z|)
(Intercept)    -3.112      1.803  -1.726   0.0843
age2 to 5       3.118      2.074   1.503   0.1328
age>= 6         7.466      3.120   2.393   0.0167
treatmentCEF    1.872      1.476   1.268   0.2049

     AIC       BIC    logLik  df.resid
   169.8     184.8     -79.9       145
```

The between-child variance is $\hat{\sigma}_b^2 = 16.24$, a latent-scale intra-class correlation $16.24/(16.24 + \pi^2/3) = 0.83$ against a raw ear-to-ear correlation 0.68. All coefficients are roughly tripled relative to the naive

glm ($0.643 \to 1.872$ for treatment, $2.570 \to 7.466$ for age ≥ 6), as are the standard errors: the *subject-specific* against *population-averaged* distinction, the marginal coefficients being attenuated by about $(1 + 0.346\hat{\sigma}_b^2)^{-1/2} = 0.39$, and $0.643/0.39 = 1.65$ agrees fairly with 1.872.

```
g0 <- glm(y ~ age + treatment, data = ears, family = binomial)
c(logLik.glmer = as.numeric(logLik(g1)), logLik.glm = as.numeric(logLik(g0)),
  LR = 2 * as.numeric(logLik(g1) - logLik(g0)))
ears$agesc <- as.numeric(ears$age)
ctl <- glmerControl(optimizer = "bobyqa")
g2 <- glmer(y ~ agesc + treatment + (1 | child), ears, binomial, control = ctl)
g3 <- glmer(y ~ age * treatment + (1 | child), ears, binomial, control = ctl)
g4 <- glmer(y ~ age + (1 | child), ears, binomial, control = ctl)
g5 <- glmer(y ~ treatment + (1 | child), ears, binomial, control = ctl)
round(AIC(g1, g2, g3, g4, g5), 2)
anova(g4, g1)
anova(g1, g3)
round(summary(g2)$coef, 4)
```

```
logLik.glmer   logLik.glm           LR
   -79.87736    -92.31631     24.87790

   df    AIC
g1  5 169.75
g2  4 167.93
g3  7 170.42
g4  4 169.81
g5  3 182.62

g4: y ~ age + (1 | child)
g1: y ~ age + treatment + (1 | child)
   npar    AIC    BIC  logLik -2*log(L)  Chisq Df Pr(>Chisq)
g4    4 169.81 181.86 -80.907    161.81
g1    5 169.75 184.81 -79.877    159.75 2.0587  1     0.1513

g1: y ~ age + treatment + (1 | child)
g3: y ~ age * treatment + (1 | child)
   npar    AIC    BIC  logLik -2*log(L)  Chisq Df Pr(>Chisq)
g1    5 169.75 184.81 -79.877    159.75
g3    7 170.42 191.49 -78.208    156.42 3.3385  2     0.1884

             Estimate Std. Error z value Pr(>|z|)
(Intercept)   -7.2518     3.5524 -2.0414   0.0412
agesc          3.8529     1.7641  2.1840   0.0290
treatmentCEF   1.8137     1.5220  1.1916   0.2334
```

The random effect is needed: LR $= 24.9$ against the boundary null $\frac{1}{2}\chi^2_0 + \frac{1}{2}\chi^2_1$, $p < 10^{-6}$. Dropping treatment costs $\Delta(-2\log L) = 2.06$ on 1 d.f. ($p = 0.15$) and the interaction 3.34 on 2 d.f. ($p = 0.19$); age as a linear score $1, 2, 3$ loses nothing and has the lowest AIC (167.93 against 169.75), with $\hat{\beta}_1 = 3.85$ per band. With binary responses the residual deviance is no goodness-of-fit statistic, so simulate the fitted distribution of clear ears per child:

```
set.seed(9418)
sim <- simulate(g1, nsim = 2000)
cnt <- sapply(sim, function(s) table(factor(colSums(matrix(s, nrow = 2)), levels = 0:2)))
rbind(observed = o, fitted.mean = round(rowMeans(cnt), 2))
round(apply(cnt, 1, quantile, c(0.025, 0.975)), 1)
```

```
                0     1     2
observed    29.00 12.00 34.00
fitted.mean 30.01 11.58 33.41

       0  1  2
2.5%  22  6 26
97.5% 38 18 41
```

The mixed model reproduces the observed $(29, 12, 34)$ almost exactly, all three counts inside the simulated 95% intervals: against 12 children with one clear ear the independence model predicts 37 and the mixed model 11.6. For a population-averaged comparison, the GEE of Section 11.4 with exchangeable

working correlation:

```
library(geepack)
gee <- geeglm(y ~ age + treatment, id = child, data = ears[order(ears$child), ],
              family = binomial, corstr = "exchangeable")
summary(gee)$coefficients
summary(gee)$corr
```

```
               Estimate   Std.err     Wald    Pr(>|W|)
(Intercept)  -0.9244678 0.4070739 5.157474 0.023146540
age2 to 5     0.8670782 0.4772004 3.301527 0.069215505
age>= 6       2.5703802 0.8652488 8.824960 0.002971379
treatmentCEF  0.6424520 0.4711431 1.859412 0.172692648

       Estimate   Std.err
alpha 0.6005782 0.1756817
```

The estimates equal the naive glm's, as they must with a common cluster size and no ear-level covariate, but the sandwich standard errors are inflated about 25% and the treatment p-value moves from 0.084 to 0.173; with $J = 75$ clusters this sandwich estimator is trustworthy, unlike Exercise 11.1's. The working correlation $\hat{\alpha} = 0.60$ agrees with the raw 0.68.

Age is the dominant determinant: subject-specific odds multiply by $e^{3.85} = 47$ per age band, the observed cure rate rising from 36% to 86%. CEF beats AMO on every point estimate (subject-specific odds ratio $e^{1.87} = 6.5$, population-averaged $e^{0.64} = 1.90$) but the evidence is weak once clustering is accounted for ($p = 0.15$ mixed, 0.17 GEE, against a misleading 0.08 naive). These data do not establish a difference.

(c) Nominal logistic regression on the child-level response. Rosner's alternative makes each child one observation with an unordered three-category response $0, 1, 2$ clear ears, fitted by the nominal model (8.4) with category 0 as reference.

```
library(nnet)
ear$resp <- factor(ear$nclear, levels = 0:2)
nm <- multinom(resp ~ age + treatment, weights = frequency, data = ear, trace = FALSE)
summary(nm)$coefficients
summary(nm)$standard.errors
round(2 * (1 - pnorm(abs(summary(nm)$coefficients / summary(nm)$standard.errors))), 4)
nm0 <- multinom(resp ~ age, weights = frequency, data = ear, trace = FALSE)
anova(nm0, nm)
sat <- multinom(resp ~ age * treatment, weights = frequency, data = ear, trace = FALSE)
c(dev.model = deviance(nm), dev.saturated = deviance(sat),
  GOF = deviance(nm) - deviance(sat), df = 4,
  p = 1 - pchisq(deviance(nm) - deviance(sat), 4))
```

```
  (Intercept) age2 to 5  age>= 6 treatmentCEF
1   -2.235765  1.186796 1.864286    1.1417153
2   -1.077013  1.065243 3.048775    0.7880926

  (Intercept) age2 to 5  age>= 6 treatmentCEF
1   0.7753158 0.7599566 1.548088    0.7953606
2   0.5195994 0.5846200 1.148851    0.5775238

  (Intercept) age2 to 5 age>= 6 treatmentCEF
1      0.0039    0.1184  0.2285       0.1512
2      0.0382    0.0684  0.0080       0.1724

Likelihood ratio tests of Multinomial Models
            Model Resid. df Resid. Dev   Test    Df LR stat.   Pr(Chi)
1             age        30   139.8153
2 age + treatment        28   136.8639 1 vs 2     2 2.951444 0.2286136

dev.model dev.saturated       GOF            df             p
136.86390     131.73832   5.12558       4.00000       0.27470
```

The nominal model fits: against the saturated model (a free trinomial in each of the six age by treatment cells) the deviance difference is 5.13 on 4 d.f., $p = 0.27$. Treatment costs LR $= 2.95$ on 2 d.f., $p = 0.23$, the same verdict as the mixed model and GEE. Its two treatment coefficients 1.14 ("1 versus 0") and

0.79 (“2 versus 0”) both favour CEF and are of similar size, suggesting the logits can be constrained by a proportional odds model (8.14):

```
library(MASS)
po <- polr(resp ~ age + treatment, weights = frequency, data = ear, Hess = TRUE)
summary(po)$coefficients
c(AIC.nominal = AIC(nm), AIC.propodds = AIC(po))
```

```
                 Value Std. Error  t value
age2 to 5    0.8896723  0.4915286 1.810011
age>= 6      2.5941220  0.8709245 2.978584
treatmentCEF 0.5715353  0.4901230 1.166106
0|1          0.5387183  0.4435641 1.214522
1|2          1.2945423  0.4655489 2.780680

 AIC.nominal AIC.propodds
    152.8639     149.5351
```

The proportional odds model has the lower AIC (149.5 against 152.9) and its treatment log odds ratio 0.572 (s.e. 0.490) is close to the GEE’s 0.643 (s.e. 0.471), both being marginal summaries.

Which approach is preferable? Four comparisons.

Assumptions. (c) assumes only independent children and a log-linear form for the trinomial cell probabilities, saying nothing about *how* the ears correlate since that is absorbed into the free category probabilities. (b) assumes a Normal child-level random intercept and needs it to be right for the standard errors to be right – verified here by simulation. The GEE assumes least about the correlation but needs many clusters, satisfied at 75.

Computation. (c) is a one-line `multinom` call on the printed 18-row table; (b) needs expansion to 150 rows and numerical integration over the random effect.

Interpretation. (b) wins: β_2 is a log odds ratio for a single ear, and it separates the treatment effect from the child-to-child heterogeneity $\hat{\sigma}_b^2 = 16.2$, itself informative. The nominal model’s coefficients are contrasts between child-level categories with no per-ear reading, and give only a 2 d.f. test.

Scaling. (c) works only because $K = 2$ yields three categories; with more units per cluster the categories explode, while (b) and the GEE are unaffected.

Report the mixed model of (b), with the GEE as population-averaged cross-check and (c) as a robustness check that assumes nothing about the correlation structure.

12 Bayesian Analysis

Contents

12.1 Problem 12.1 — Reconsider Example 12.1.4 on Schistosoma japonicum.

Problem 12.1. Reconsider Example 12.1.4 on *Schistosoma japonicum*. In that example the parameter θ is the proportion of a village's population infected, the two hypotheses are H_0: infection is not endemic ($\theta \le 0.5$) and H_1: infection is endemic ($\theta > 0.5$), the discrete parameter space is $\theta = 0.0, 0.1, \ldots, 1.0$, and the prior mass $P(H_0)$ is spread uniformly over the six values $0.0, \ldots, 0.5$ while $P(H_1)$ is spread uniformly over the five values $0.6, \ldots, 1.0$. The likelihood is binomial, $y \sim \text{Bin}(10, \theta)$.
a. Using Table 12.1 calculate the posterior probability for H_1 for the following priors and observed data. The table to be completed has two rows, one for the prior $P(H_1) = 0.5$ and one for the prior $P(H_1) = 0.99$, and two columns of observed data, "5 out of 10 positive" and "1 out of 10 positive".
b. Recalculate the above probabilities using the finer parameter space of $\theta = 0.00, 0.01, 0.02, \ldots, 0.99, 1.00$. Explain the differences in your results. (difficulty: ⋆⋆)

Solution. The four posterior probabilities are 0.408, 0.986 ($y = 5$) and 0.0025, 0.198 ($y = 1$) on the coarse grid, and all rise on the fine one because $\Delta\theta = 0.1$ has no point just above $\theta = 0.5$. Everything is Equation (12.3),

$$P(\theta \mid y) = \frac{P(y \mid \theta)P(\theta)}{\sum_\theta P(y \mid \theta)P(\theta)}, \qquad P(H_1 \mid y) = \sum_{\theta > 0.5} P(\theta \mid y),$$

with $P(y \mid \theta) = \binom{10}{y}\theta^y(1-\theta)^{10-y}$ and a prior placing mass $P(H_1)$ uniformly above 0.5 and $1 - P(H_1)$ uniformly at or below it. Only the prior mass and the grid change, so one function serves.

```
postH1 <- function(theta, y, n, pH1) {
  H1    <- theta > 0.5
  prior <- ifelse(H1, pH1 / sum(H1), (1 - pH1) / sum(!H1))
  lik   <- dbinom(y, n, theta)
  post  <- lik * prior / sum(lik * prior)
  sum(post[H1])
}
theta <- seq(0, 1, by = 0.1)
postH1(theta, 7, 10, 0.8)   # reproduces the last column of Table 12.1
```

```
[1] 0.954498
```

That is the 0.9545 at the foot of Table 12.1, so the arithmetic is the book's.
(a) The eleven-point grid. For the first new cell ($P(H_1) = 0.5$, $y = 5$):

```
theta <- seq(0, 1, by = 0.1)
H1    <- theta > 0.5
prior <- ifelse(H1, 0.5 / 5, 0.5 / 6)
lik   <- dbinom(5, 10, theta)
data.frame(theta,
           hypothesis = ifelse(H1, "H1", "H0"),
           prior      = round(prior, 4),
           likelihood = round(lik, 4),
           lik.prior  = round(lik * prior, 4),
           posterior  = round(lik * prior / sum(lik * prior), 4))
```

```
   theta hypothesis  prior likelihood lik.prior posterior
1    0.0         H0 0.0833     0.0000    0.0000    0.0000
2    0.1         H0 0.0833     0.0015    0.0001    0.0015
3    0.2         H0 0.0833     0.0264    0.0022    0.0271
4    0.3         H0 0.0833     0.1029    0.0086    0.1055
5    0.4         H0 0.0833     0.2007    0.0167    0.2057
6    0.5         H0 0.0833     0.2461    0.0205    0.2523
7    0.6         H1 0.1000     0.2007    0.0201    0.2469
8    0.7         H1 0.1000     0.1029    0.0103    0.1266
9    0.8         H1 0.1000     0.0264    0.0026    0.0325
10   0.9         H1 0.1000     0.0015    0.0001    0.0018
11   1.0         H1 0.1000     0.0000    0.0000    0.0000
```

The normalising constant is 0.0813 and the H_1 rows sum to 0.4078. All four cells:

```r
theta <- seq(0, 1, by = 0.1)
tab <- sapply(c(5, 1), function(y)
         sapply(c(0.5, 0.99), function(p) postH1(theta, y, 10, p)))
dimnames(tab) <- list(c("P(H1)=0.50", "P(H1)=0.99"), c("5 of 10", "1 of 10"))
round(tab, 4)
```

```
          5 of 10 1 of 10
P(H1)=0.50  0.4078  0.0025
P(H1)=0.99  0.9855  0.1976
```

Under an even-handed prior, $y = 5$ sits on the boundary between the hypotheses, so $P(H_1 \mid y) = 0.408$ stays near the prior 0.5, tilted to H_0 because $\theta = 0.5$ itself belongs to H_0 and carries the largest likelihood; $y = 1$ is strong evidence against endemicity and gives 0.0025. Under $P(H_1) = 0.99$, borderline data leave the investigator at 0.986 and even $y = 1$ pulls her only to 0.198: prior odds of $99 : 1$ take a great deal of evidence to overturn, the point of Section 12.2.

(b) The 101-point grid. Now H_0 has 51 points and H_1 has 50; the mass per point changes, the total mass on each hypothesis does not.

```r
fine <- seq(0, 1, by = 0.01)
tab2 <- sapply(c(5, 1), function(y)
          sapply(c(0.5, 0.99), function(p) postH1(fine, y, 10, p)))
dimnames(tab2) <- list(c("P(H1)=0.50", "P(H1)=0.99"), c("5 of 10", "1 of 10"))
round(tab2, 4)
```

```
          5 of 10 1 of 10
P(H1)=0.50  0.4914  0.0054
P(H1)=0.99  0.9897  0.3516
```

Every entry rises, because (12.3) on a grid is a Riemann sum for the integral in the continuous Bayes theorem and $\Delta\theta = 0.1$ is coarse quadrature. Two explanations compete. (i) The coarse grid mislocates mass near the boundary: for $y = 5$ the likelihood peaks at $\theta = 0.5$, assigned wholly to H_0, while the interval $(0.5, 0.6)$ belongs to H_1 and has no grid point of its own; for $y = 1$ the H_1 likelihood is largest just above the boundary ($P(y \mid 0.51) = 0.0083$ against $P(y \mid 0.6) = 0.0016$), so the leftmost H_1 point understates by a factor of five. (ii) The coarse grid wastes prior mass on impossible values: at $y = 1$ both $\theta = 0$ and $\theta = 1$ have zero likelihood, yet hold a sixth of the H_0 and a fifth of the H_1 prior. Since the prior is uniform within each hypothesis the calculation collapses to one ratio,

$$P(H_1 \mid y) = \frac{P(H_1)\, B}{P(H_1)\, B + 1 - P(H_1)}, \qquad B = \frac{\overline{P(y \mid \theta)}_{H_1}}{\overline{P(y \mid \theta)}_{H_0}},$$

each average over that hypothesis's grid points, so the grid enters only through B and the two explanations separate cleanly.

```r
gridBF <- function(theta, y, n) {
  H1 <- theta > 0.5
  mean(dbinom(y, n, theta[H1])) / mean(dbinom(y, n, theta[!H1]))
}
co <- seq(0, 1, by = 0.1)
fi <- seq(0, 1, by = 0.01)
bf <- rbind("11-point grid"      = sapply(c(5, 1), function(y) gridBF(co, y, 10)),
            "11-point, ends cut" = sapply(c(5, 1), function(y) gridBF(co[co > 0 & co < 1],
            ↪  y, 10)),
            "101-point grid"     = sapply(c(5, 1), function(y) gridBF(fi, y, 10)))
colnames(bf) <- c("y = 5", "y = 1")
signif(bf, 4)
```

```
                    y = 5    y = 1
11-point grid      0.6887 0.002488
11-point, ends cut 0.7174 0.002592
101-point grid     0.9662 0.005478
```

Deleting the two dead end points barely moves B ($0.00249 \to 0.00259$ at $y = 1$, $0.689 \to 0.717$ at $y = 5$), so (ii) explains almost none of the change, whereas refining the grid moves B to 0.00548 and 0.966: the effect is (i). The same identity explains why the $P(H_1) = 0.99$ row moves further at $y = 1$. Posterior odds are prior odds times B, and B roughly doubles under refinement in both rows; at prior

odds $1:1$ that takes 0.0025 to 0.0054 as a probability, at $99:1$ it takes 0.198 to 0.352. The quadrature error is identical, only the leverage differs.

Driving the grid to the continuum confirms this. Under a uniform prior on $[0,1]$ – the $P(H_1) = 0.5$ row in the limit, the hypotheses then having equal length – Equation (12.6) gives the posterior $\mathrm{Be}(y+1, n-y+1)$, so $P(H_1 \mid y) = 1 - F_{\mathrm{Be}}(0.5)$ exactly.

```r
c(exact_y5 = 1 - pbeta(0.5, 5 + 1, 10 - 5 + 1),
  exact_y1 = 1 - pbeta(0.5, 1 + 1, 10 - 1 + 1))
for (k in c(10, 100, 1000, 10000))
  cat(sprintf("step %8.5f   y=5: %.4f   y=1: %.4f\n", 1 / k,
      postH1(seq(0, 1, length = k + 1), 5, 10, 0.5),
      postH1(seq(0, 1, length = k + 1), 1, 10, 0.5)))
```

```
   exact_y5    exact_y1
0.500000000 0.005859375
step  0.10000   y=5: 0.4078   y=1: 0.0025
step  0.01000   y=5: 0.4914   y=1: 0.0054
step  0.00100   y=5: 0.4991   y=1: 0.0058
step  0.00010   y=5: 0.4999   y=1: 0.0059
```

The grid answers converge to 0.5 and 0.005859, the 101-point values already within 0.01 and 0.0005. So the fine grid gives less biased answers to the same question, at the price flagged in Section 12.1.4: 11 rows become 101, and with m parameters the work multiplies by 10^m.

12.2 Problem 12.2 — Show that the posterior distribution using a Normally distributed prior

Problem 12.2. Show that the posterior distribution using a Normally distributed prior $\mathrm{N}(\mu_0, \sigma_0^2)$ and Normally distributed likelihood $\mathrm{N}(\mu_l, \sigma_l^2)$ is also Normally distributed with mean

$$\frac{\mu_0\sigma_l^2 + \mu_l\sigma_0^2}{\sigma_0^2 + \sigma_l^2}$$

and variance

$$\frac{\sigma_l^2\sigma_0^2}{\sigma_0^2 + \sigma_l^2}.$$

(difficulty: ⋆⋆)

Solution. Complete the square; by (12.2), $P(\theta \mid \mathbf{y}) \propto P(\mathbf{y} \mid \theta)P(\theta)$, so the normalising constant never enters. With θ the parameter (the log hazard ratio), the prior is

$$P(\theta) = \frac{1}{\sigma_0\sqrt{2\pi}} \exp\!\left(-\frac{(\theta-\mu_0)^2}{2\sigma_0^2}\right),$$

and the likelihood, regarded as a function of θ, is

$$P(\mathbf{y} \mid \theta) = \frac{1}{\sigma_l\sqrt{2\pi}} \exp\!\left(-\frac{(\mu_l-\theta)^2}{2\sigma_l^2}\right),$$

with μ_l the maximum likelihood estimate and σ_l^2 its sampling variance, both known. Since $(\mu_l-\theta)^2 = (\theta-\mu_l)^2$ this is a Normal kernel in θ centred at μ_l, so the exponents combine: multiplying and discarding factors free of θ,

$$P(\theta \mid \mathbf{y}) \;\propto\; \exp\!\left(-\tfrac{1}{2}Q(\theta)\right), \qquad Q(\theta) = \frac{(\theta-\mu_0)^2}{\sigma_0^2} + \frac{(\theta-\mu_l)^2}{\sigma_l^2}.$$

Expanding Q and collecting powers of θ,

$$Q(\theta) = \theta^2\left(\frac{1}{\sigma_0^2} + \frac{1}{\sigma_l^2}\right) - 2\theta\left(\frac{\mu_0}{\sigma_0^2} + \frac{\mu_l}{\sigma_l^2}\right) + \left(\frac{\mu_0^2}{\sigma_0^2} + \frac{\mu_l^2}{\sigma_l^2}\right).$$

The quadratic coefficient is the sum of the two precisions, so define

$$\frac{1}{\sigma_p^2} = \frac{1}{\sigma_0^2} + \frac{1}{\sigma_l^2} = \frac{\sigma_0^2 + \sigma_l^2}{\sigma_0^2 \sigma_l^2}, \qquad \text{so} \qquad \sigma_p^2 = \frac{\sigma_l^2 \sigma_0^2}{\sigma_0^2 + \sigma_l^2},$$

the required variance, and

$$\mu_p = \sigma_p^2 \left(\frac{\mu_0}{\sigma_0^2} + \frac{\mu_l}{\sigma_l^2} \right) = \frac{\sigma_0^2 \sigma_l^2}{\sigma_0^2 + \sigma_l^2} \cdot \frac{\mu_0 \sigma_l^2 + \mu_l \sigma_0^2}{\sigma_0^2 \sigma_l^2} = \frac{\mu_0 \sigma_l^2 + \mu_l \sigma_0^2}{\sigma_0^2 + \sigma_l^2},$$

the required mean. Then

$$Q(\theta) = \frac{\theta^2 - 2\theta\mu_p}{\sigma_p^2} + c_1 = \frac{(\theta - \mu_p)^2}{\sigma_p^2} + c_2,$$

with c_1, c_2 free of θ ($c_2 = c_1 - \mu_p^2/\sigma_p^2$), and $\exp(-c_2/2)$ is absorbed into the proportionality:

$$P(\theta \mid \mathbf{y}) \;\propto\; \exp\!\left(-\frac{(\theta - \mu_p)^2}{2\sigma_p^2} \right).$$

The kernel integrates to $\sigma_p\sqrt{2\pi}$ and $\int P(\theta \mid \mathbf{y})\, d\theta = 1$ fixes the constant, so a density proportional to it is the $\mathrm{N}(\mu_p, \sigma_p^2)$ density:

$$\theta \mid \mathbf{y} \;\sim\; \mathrm{N}\!\left(\frac{\mu_0 \sigma_l^2 + \mu_l \sigma_0^2}{\sigma_0^2 + \sigma_l^2},\; \frac{\sigma_l^2 \sigma_0^2}{\sigma_0^2 + \sigma_l^2} \right),$$

as required, so the Normal family is conjugate to a Normal likelihood with known variance (Section 12.2.2). Precisions add, so $\sigma_p^2 < \min(\sigma_0^2, \sigma_l^2)$, and

$$\mu_p = \frac{\sigma_0^{-2}}{\sigma_0^{-2} + \sigma_l^{-2}}\, \mu_0 + \frac{\sigma_l^{-2}}{\sigma_0^{-2} + \sigma_l^{-2}}\, \mu_l$$

lies between μ_0 and μ_l, weighted towards the more precise source – which is why the sceptical posterior of Figure 12.1 sits between prior and likelihood. A flat prior is the limit $\sigma_0^2 \to \infty$, giving $\mu_p \to \mu_l$ and $\sigma_p^2 \to \sigma_l^2$.

Feeding in the sceptical prior $\mathrm{N}(0, 0.1907^2)$ and trial likelihood $\mathrm{N}(0.580, 0.2266^2)$ of Section 12.2.2, which reports posterior mean 0.240 and $P(\mathrm{LHR} > 0.3137) = 0.31$:

```
mu0 <- 0;     s0 <- 0.1907     # sceptical prior, Section 12.2.2
mul <- 0.580; sl <- 0.2266     # observed LHR and its standard error
mup <- (mu0 * sl^2 + mul * s0^2) / (s0^2 + sl^2)
sp  <- sqrt(sl^2 * s0^2 / (s0^2 + sl^2))
c(post_mean = mup, post_sd = sp, P_improvement_over_10pct = 1 - pnorm(0.3137, mup, sp))
```

```
post_mean                  post_sd P_improvement_over_10pct
0.2404696                0.1459070                 0.3078697
```

Both printed values are recovered, without ever needing the normalising constant c of Section 12.2.2.

12.3 Problem 12.3 — Reconsider Example 12.2.2 about the cancer clinical trial. The 11 special-

Problem 12.3. Reconsider Example 12.2.2 about the cancer clinical trial. The 11 specialists taking part in the trial had an enthusiastic prior opinion that the median expected improvement in survival was 10%, which corresponds to an LHR of 0.3137. Assume that their prior opinion can be represented as a Normal distribution with a mean of 0.3137 and a standard deviation of 0.1907 (as per the sceptics' prior).

a. What is their prior probability that the new treatment is effective?

b. What is their posterior probability that the new treatment is effective? (difficulty: ⋆)

Solution. The prior probability of effectiveness is 0.950 and the posterior is 0.998. Work on the log-hazard-ratio scale of Equation (12.4),

$$\mathrm{LHR} = \log\left(\frac{H_1}{H_2}\right) = \log\left(\frac{-\log P_1}{-\log P_2}\right),$$

with $P_1 = 0.15$ two-year survival on conventional therapy and P_2 that on the new treatment. Effectiveness is $H_2 < H_1$, i.e. $\theta = \mathrm{LHR} > 0$, so both parts ask for $P(\theta > 0)$. The enthusiastic prior is $\theta \sim \mathrm{N}(0.3137,\, 0.1907^2)$, and the trial of Section 12.2.2 (78 deaths among 256 patients) gives the likelihood $\mathrm{N}(0.580,\, 0.2266^2)$, its standard deviation from the interval 0.580 ± 0.444.
(a) Prior probability of effectiveness.

$$P(\theta > 0) = 1 - \Phi\left(\frac{0 - 0.3137}{0.1907}\right) = \Phi(1.6449) = 0.950.$$

```
mu0 <- 0.3137; s0 <- 0.1907    # enthusiastic prior
1 - pnorm(0, mu0, s0)          # prior P(LHR > 0)
```

```
[1] 0.9500143
```

The 0.95 is by construction: 0.1907 was chosen in Section 12.2.2 so that $1.645\sigma = 0.3137$, so centring at 0.3137 puts zero exactly 1.645 standard deviations below the mean. The two priors are mirror images about $\mathrm{LHR} = 0.157$ – sceptics give probability 0.05 to an improvement over 10%, enthusiasts 0.05 to no improvement at all, i.e. 19 : 1 odds before any patient is seen.
(b) By Exercise 12.2 the posterior is Normal with

$$\mu_p = \frac{\mu_0\sigma_l^2 + \mu_l\sigma_0^2}{\sigma_0^2 + \sigma_l^2}, \qquad \sigma_p^2 = \frac{\sigma_l^2\sigma_0^2}{\sigma_0^2 + \sigma_l^2},$$

so no numerical integration is needed:

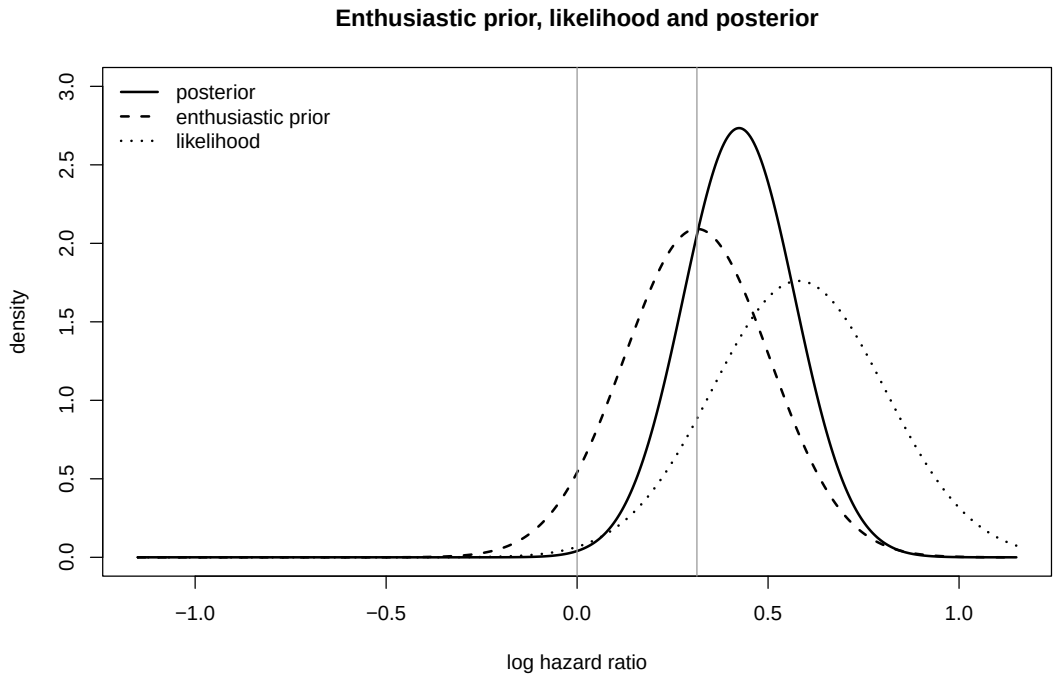
```
mul <- 0.580; sl <- 0.2266     # likelihood: observed LHR and its standard error
mup <- (mu0 * sl^2 + mul * s0^2) / (s0^2 + sl^2)
sp  <- sqrt(sl^2 * s0^2 / (s0^2 + sl^2))
c(post_mean = mup, post_sd = sp,
  P_effective = 1 - pnorm(0, mup, sp),
  P_over_10pct = 1 - pnorm(0.3137, mup, sp),
  abs_improvement = 0.15^exp(-mup) - 0.15)
```

```
post_mean         post_sd     P_effective    P_over_10pct abs_improvement
0.4241087       0.1459070       0.9981737       0.7753871       0.1389835
```

The posterior is $\mathrm{N}(0.424,\, 0.146^2)$, so

$$P(\theta > 0 \mid \mathbf{y}) = 1 - \Phi\left(\frac{-0.4241}{0.1459}\right) = \Phi(2.907) = 0.998.$$

```
th <- seq(-1.15, 1.15, length = 500)
plot(th, dnorm(th, mup, sp), type = "l", lwd = 2, ylim = c(0, 3), xlab = "log hazard ratio",
     ylab = "density", main = "Enthusiastic prior, likelihood and posterior")
lines(th, dnorm(th, mu0, s0), lty = 2, lwd = 2)
lines(th, dnorm(th, mul, sl), lty = 3, lwd = 2)
abline(v = c(0, 0.3137), col = "grey60")
legend("topleft", c("posterior", "enthusiastic prior", "likelihood"), lty = 1:3, lwd = 2,
  bty = "n")
```



The posterior mean 0.424 lies between 0.3137 and 0.580, as Exercise 12.2 guarantees, nearer the prior because the prior is the more precise ($0.1907 < 0.2266$). On the survival scale it gives $P_2 = 0.15^{\exp(-0.424)} = 0.289$, an absolute improvement of about 14 percentage points.
The same data through the sceptical prior $\mathrm{N}(0, 0.1907^2)$ give posterior mean 0.240, probability 0.31 of an improvement over 10% and 0.95 of effectiveness; through the enthusiastic prior, 0.775 and 0.998. The trial moves the enthusiasts from 0.95 to 0.998 – small in probability, but from 19 : 1 to 546 : 1 in odds. Under a flat prior the posterior is the likelihood, giving $P(\theta > 0 \mid \mathbf{y}) = 1 - \Phi(-0.580/0.2266) = 0.9948$ and $P(\theta > 0.3137 \mid \mathbf{y}) = 0.880$, the figures quoted at the end of Section 12.2.2 – which is why Section 12.2.1 asks for the uninformative-prior result alongside.

12.4 Problem 12.4 — Reconsider Example 12.2.3 on overdoses among released prisoners. You

Problem 12.4. Reconsider Example 12.2.3 on overdoses among released prisoners, in which none of the $n = 91$ contactable released prisoners had overdosed in the four weeks after release. You may find the First Bayes software useful for answering these questions.
a. Use an argument based on $\alpha - 1$ previous successes and $\beta - 1$ previous failures to calculate a heuristic Beta prior. Combine this prior with the data to give a Beta posterior.
b. Calculate the mean of the posterior. Compare this mean to the investigator's prior opinion of 1 overdose in 200 subjects (0.005). Considering that there were no overdoses in the data, what is wrong with this posterior? (difficulty: ⋆⋆)

Solution. (a) The heuristic prior is $\mathrm{Be}(2, 200)$ and the posterior $\mathrm{Be}(2, 291)$, whose mean 0.0068 exceeds the prior opinion 0.005 – the defect diagnosed in (b). By Section 12.2.3 a $\mathrm{Be}(\alpha, \beta)$ prior behaves as $\alpha - 1$ prior successes and $\beta - 1$ failures, and one overdose per 200 prisoners gives 1 and 199, so

$$\alpha - 1 = 1 \;\Rightarrow\; \alpha = 2, \qquad \beta - 1 = 199 \;\Rightarrow\; \beta = 200,$$

and Equation (12.6), $P(\theta \mid \mathbf{y}) \sim \mathrm{Be}(y + \alpha,\, n - y + \beta)$ with $n = 91$, $y = 0$, gives

$$\theta \mid \mathbf{y} \;\sim\; \mathrm{Be}(0 + 2,\; 91 - 0 + 200) = \mathrm{Be}(2, 291).$$

```
a0 <- 2; b0 <- 200          # 1 prior overdose, 199 prior non-overdoses
n  <- 91; y <- 0            # 91 contactable prisoners, no overdoses
```

```r
a1 <- y + a0; b1 <- n - y + b0
c(prior_mean = a0/(a0 + b0), prior_mode = (a0 - 1)/(a0 + b0 - 2),
  post_alpha = a1, post_beta = b1)
```

```
 prior_mean  prior_mode  post_alpha   post_beta
9.90099e-03 5.00000e-03 2.00000e+00 2.91000e+02
```

The prior *mode* is exactly $1/200 = 0.005$ but the prior *mean* is $2/202 = 0.0099$, nearly twice the stated opinion.

(b) By Exercise 7.5, $\mathrm{E}(\theta) = \alpha/(\alpha+\beta)$, so the posterior mean is $2/293$.

```r
c(post_mean = a1/(a1 + b1), post_mode = (a1 - 1)/(a1 + b1 - 2),
  lower = qbeta(0.025, a1, b1), upper = qbeta(0.975, a1, b1),
  investigator_prior_mean = 0.005)
```

```
   post_mean              post_mode                  lower
0.0068259386           0.0034364261           0.0008305628
       upper investigator_prior_mean
0.0189322698           0.0050000000
```

So $\widehat{\theta} = 2/293 = 0.00683$, about 1 in 147, with 95% interval $(0.00083, 0.0189)$. What is wrong: 91 prisoners with *no overdoses* is evidence the rate is at or below the prior guess, yet the posterior mean 0.0068 exceeds the prior opinion 0.005 by more than a third. No coherent updating rule does that, so the fault is in the prior. The culprit is the heuristic, which Section 12.2.3 flags as "only true for relatively large values of α and β": the pseudo-count reading matches the *mode*,

$$\text{mode} = \frac{\alpha - 1}{\alpha + \beta - 2} = \frac{1}{200} = 0.005,$$

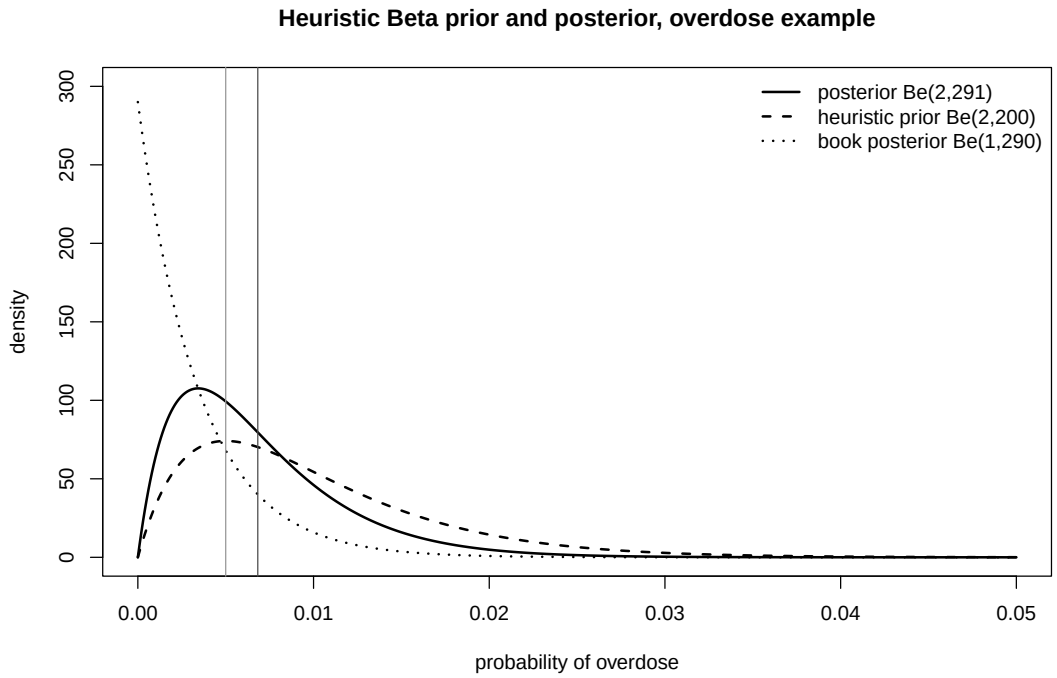
not the mean, and for a density this skewed the two are far apart. The prior elicited has mean $2/202 = 0.0099$, so the analysis encoded "1 in 101" as the expected rate and merely made 1 in 200 the most likely value; Bayes' theorem then moved the mean down from 0.0099 to 0.0068, faithfully. The comparison with 0.005 is against a number the prior never represented. Matching the moment actually stated, $\alpha/(\alpha+\beta) = 1/200$ with $\alpha = 1$, gives the $\mathrm{Be}(1, 199)$ of Table 12.2 and posterior $\mathrm{Be}(1, 290)$ with mean $1/291 = 0.00344$, below 0.005 as the zero count demands.

```r
rbind("Be(2,200) heuristic"        = c(prior = 2/202,  posterior = 2/293),
      "Be(1,199) book, Table 12.2" = c(prior = 1/200, posterior = 1/291))
```

```
                              prior   posterior
Be(2,200) heuristic        0.00990099 0.006825939
Be(1,199) book, Table 12.2 0.00500000 0.003436426
```

The *mode* of $\mathrm{Be}(2, 291)$ is $1/291 = 0.003436$, the mean of $\mathrm{Be}(1, 290)$, and not by accident: the heuristic route gives $\mathrm{Be}(y+2,\, n-y+200)$ with mode $(y+1)/(n+200)$, the book's gives $\mathrm{Be}(y+1,\, n-y+199)$ with mean $(y+1)/(n+200)$. The extra unit of α converts a mean into a mode.

```r
p <- seq(0, 0.05, length = 500)
plot(p, dbeta(p, a1, b1), type = "l", lwd = 2, ylim = c(0, 300),
     xlab = "probability of overdose", ylab = "density",
     main = "Heuristic Beta prior and posterior, overdose example")
lines(p, dbeta(p, a0, b0), lty = 2, lwd = 2)
lines(p, dbeta(p, 1, 290), lty = 3, lwd = 2)
abline(v = c(0.005, a1/(a1 + b1)), col = c("grey60", "grey30"))
legend("topright", c("posterior Be(2,291)", "heuristic prior Be(2,200)",
                     "book posterior Be(1,290)"), lty = 1:3, lwd = 2, bty = "n")
```



The heuristic posterior $\mathrm{Be}(2, 291)$ (solid) rises from zero to an interior mode at 0.0034 and decays with a long right tail, and that tail alone drags the mean out to 0.0068 past the investigator's 0.005. The book's $\mathrm{Be}(1, 290)$ (dotted) has $\alpha = 1$, so it is monotone decreasing with density largest at $\theta = 0$ – yet its mean is the solid curve's mode. One unit of α separates a density saying "zero is the most likely rate" from one saying "0.0034 is".

13 Markov Chain Monte Carlo Methods

Contents

13.1 Problem 13.1 — Reconsider the example on Schistosoma japonicum from the previous

Problem 13.1. Reconsider the example on *Schistosoma japonicum* from the previous chapter (Section 12.1.4). In Table 12.1 the posterior probability for H_0 was calculated using an equally spaced set of values for θ. Recalculate the values in Table 12.1 using 11 values for θ generated from the Uniform distribution U[0, 1]. Compare the results obtained using the fixed and random values for θ. Should any restrictions be placed on the samples generated from the Uniform distribution?
For reference, the setting is: θ is the prevalence of infection in a village, $H_0 : \theta \le 0.5$ (not endemic) and $H_1 : \theta > 0.5$ (endemic); the investigator's prior gives $\Pr(H_0) = 0.2$ and $\Pr(H_1) = 0.8$, spread uniformly over the parameter values in each region; and the data are $y = 7$ positive stool samples out of $n = 10$, so the likelihood is $P(y \mid \theta) = \binom{10}{7}\theta^7(1-\theta)^3$. In Table 12.1 the eleven values $\theta = 0.0, 0.1, \ldots, 1.0$ are used, giving prior $0.2/6 = 0.0333$ to each of the six values with $\theta \le 0.5$ and $0.8/5 = 0.1600$ to each of the five values with $\theta > 0.5$; the resulting posterior is $P(H_0 \mid y) = 0.0455$, $P(H_1 \mid y) = 0.9545$. (difficulty: $\star$)

Solution. Eleven random draws gave $P(H_1 \mid y) = 0.933$ against the grid's 0.9545; the random estimator is unbiased for the continuous answer 0.9691 but its standard deviation 0.035 is too large to decide the 0.95 threshold, so restrictions are needed. First, Equation (12.3) on the grid,

$$P(\theta_k \mid y) = \frac{P(y \mid \theta_k)P(\theta_k)}{\sum_j P(y \mid \theta_j)P(\theta_j)},$$

and $P(H_0 \mid y)$ is the sum of the posterior column over the rows with $\theta \le 0.5$.

```r
lik <- function(th) dbinom(7, 10, th)
th  <- seq(0, 1, by = 0.1)
H0  <- th <= 0.5
pri <- ifelse(H0, 0.2 / sum(H0), 0.8 / sum(!H0))
lp   <- lik(th) * pri
post <- lp / sum(lp)
data.frame(theta = th, hyp = ifelse(H0, "H0", "H1"), prior = round(pri, 4),
           lik = round(lik(th), 4), lik.x.prior = round(lp, 4),
           posterior = round(post, 4))
c(P.H0 = sum(post[H0]), P.H1 = sum(post[!H0]))
```

```
   theta hyp  prior    lik lik.x.prior posterior
1    0.0  H0 0.0333 0.0000      0.0000    0.0000
2    0.1  H0 0.0333 0.0000      0.0000    0.0000
3    0.2  H0 0.0333 0.0008      0.0000    0.0002
4    0.3  H0 0.0333 0.0090      0.0003    0.0024
5    0.4  H0 0.0333 0.0425      0.0014    0.0114
6    0.5  H0 0.0333 0.1172      0.0039    0.0315
7    0.6  H1 0.1600 0.2150      0.0344    0.2771
8    0.7  H1 0.1600 0.2668      0.0427    0.3439
9    0.8  H1 0.1600 0.2013      0.0322    0.2595
10   0.9  H1 0.1600 0.0574      0.0092    0.0740
11   1.0  H1 0.1600 0.0000      0.0000    0.0000
      P.H0       P.H1
0.04550201 0.95449799
```

This is Table 12.1, fixing the arithmetic the random version must imitate. The grid is crude quadrature for the continuous problem whose prior is the step density

$$p(\theta) = \begin{cases} 0.2/0.5 = 0.4, & 0 \le \theta \le 0.5, \\ 0.8/0.5 = 1.6, & 0.5 < \theta \le 1, \end{cases}$$

so that

$$P(H_1 \mid y) = \frac{1.6 \int_{0.5}^{1} \theta^7(1-\theta)^3 \, d\theta}{0.4 \int_{0}^{0.5} \theta^7(1-\theta)^3 \, d\theta + 1.6 \int_{0.5}^{1} \theta^7(1-\theta)^3 \, d\theta}.$$

Both integrals are incomplete beta functions, so the exact answer is closed form.

```
I0 <- pbeta(0.5, 8, 4) * beta(8, 4)
I1 <- (1 - pbeta(0.5, 8, 4)) * beta(8, 4)
exact <- 1.6 * I1 / (0.4 * I0 + 1.6 * I1)
exact
```

```
0.9690502
```

The grid answer 0.9545 is 0.015 below the truth, because the eleven equally spaced points include $\theta = 0$ and $\theta = 1$, where the likelihood vanishes: two evaluations are wasted, both in the tails, so the grid understates $P(H_1 \mid y)$.

Now replace the grid by $\theta_1, \ldots, \theta_{11} \sim \mathrm{U}[0,1]$, keeping the prior structure: whichever m draws land in $[0, 0.5]$ share the mass 0.2, the other $11 - m$ share 0.8. This is stratified Monte Carlo integration and preserves the stated prior probabilities exactly.

```
set.seed(13001)
th  <- sort(runif(11))
H0  <- th <= 0.5
pri <- ifelse(H0, 0.2 / sum(H0), 0.8 / sum(!H0))
lp   <- lik(th) * pri
post <- lp / sum(lp)
data.frame(theta = round(th, 4), hyp = ifelse(H0, "H0", "H1"),
           prior = round(pri, 4), lik = round(lik(th), 4),
           lik.x.prior = round(lp, 4), posterior = round(post, 4))
c(P.H0 = sum(post[H0]), P.H1 = sum(post[!H0]))
```

```
    theta hyp  prior    lik lik.x.prior posterior
1  0.0550  H0 0.0333 0.0000      0.0000    0.0000
2  0.1874  H0 0.0333 0.0005      0.0000    0.0001
3  0.3533  H0 0.0333 0.0223      0.0007    0.0058
4  0.4269  H0 0.0333 0.0584      0.0019    0.0151
5  0.4473  H0 0.0333 0.0726      0.0024    0.0188
6  0.4867  H0 0.0333 0.1050      0.0035    0.0272
7  0.7255  H1 0.1600 0.2626      0.0420    0.3266
8  0.7736  H1 0.1600 0.2309      0.0369    0.2871
9  0.8055  H1 0.1600 0.1943      0.0311    0.2416
10 0.8968  H1 0.1600 0.0615      0.0098    0.0765
11 0.9794  H1 0.1600 0.0009      0.0001    0.0011
      P.H0       P.H1
0.06704378 0.93295622
```

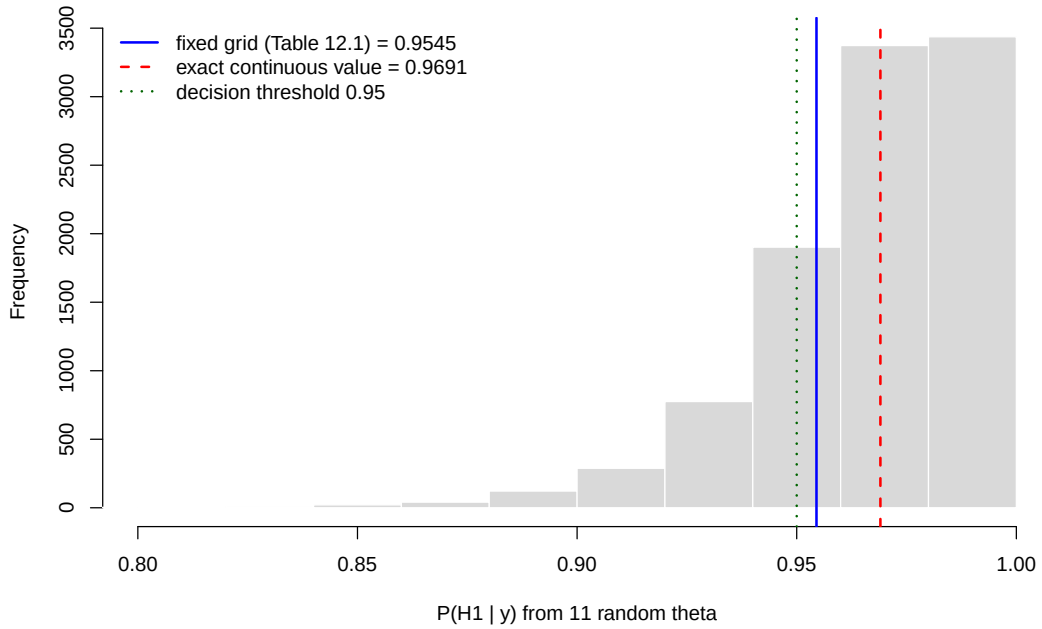
This sample split 6/5, so the prior column matches Table 12.1, but $P(H_1 \mid y) = 0.933$ rather than 0.9545: the same qualitative conclusion, yet no longer clearing the investigator's 0.95 stopping threshold. The random answer is itself random, so compare the fixed 0.9545 with the whole sampling distribution over 10,000 replicates:

```
set.seed(13002)
sim <- replicate(10000, {
  th <- runif(11); H0 <- th <= 0.5; m <- sum(H0)
  if (m == 0 || m == 11) return(NA_real_)
  pri <- ifelse(H0, 0.2 / m, 0.8 / (11 - m))
  lp <- lik(th) * pri
  sum(lp[!H0]) / sum(lp)
})
c(failures = sum(is.na(sim)), mean = mean(sim, na.rm = TRUE),
  sd = sd(sim, na.rm = TRUE), quantile(sim, c(0.025, 0.975), na.rm = TRUE))
mean(sim < 0.95, na.rm = TRUE)
```

```
  failures       mean         sd       2.5%      97.5%
4.00000000 0.96615023 0.03463462 0.90303777 0.99936818
[1] 0.2031813
```

```
hist(sim, breaks = 60, col = 'grey85', border = 'white',
     xlab = 'P(H1 | y) from 11 random theta', main = '', xlim = c(0.80, 1.0))
abline(v = 0.954498,  col = 'blue',      lwd = 2)
abline(v = 0.9690502, col = 'red',       lwd = 2, lty = 2)
abline(v = 0.95,      col = 'darkgreen', lwd = 2, lty = 3)
legend('topleft', bty = 'n', lwd = 2, lty = c(1, 2, 3),
```

```
       col = c('blue', 'red', 'darkgreen'),
       legend = c('fixed grid (Table 12.1) = 0.9545',
                  'exact continuous value = 0.9691',
                  'decision threshold 0.95'))
```



- The random estimator is roughly unbiased for the **continuous** answer 0.9691 (mean 0.9662) where the grid is systematically low at 0.9545, since random points never land on $\theta = 0$ or 1.
- The price is variance: standard deviation 0.035, central 95% from 0.903 to 0.999, where the grid gives the same number every time.
- That variance decides the question: about 20% of the time the eleven points give $P(H_1 \mid y) < 0.95$, so the investigator keeps testing on the luck of the draw.

Restrictions are therefore needed, of two kinds. (i) *Logical.* At least one draw must fall in $[0, 0.5]$ and one in $(0.5, 1]$; if all eleven land on one side the other hypothesis's prior mass has no θ to sit on, its numerator is 0 by construction and its posterior probability is forced to 0 whatever the data. At $M = 11$ this has probability $2 \times 2^{-11} = 0.00098$ and occurred 4 times in the 10,000 replicates. Reject and redraw, or better stratify by design: 6 points from U$[0, 0.5]$ and 5 from U$[0.5, 1]$. (ii) *Accuracy.* Eleven is far too few, Monte Carlo error falling only as $M^{-1/2}$:

```
set.seed(13003)
for (M in c(11, 50, 200, 1000)) {
  s <- replicate(2000, {
    th <- runif(M); H0 <- th <= 0.5
    w <- lik(th) * ifelse(H0, 0.4, 1.6)
    sum(w[!H0]) / sum(w) })
  cat("M =", M, " sd =", round(sd(s), 4),
      " RMSE from exact =", round(sqrt(mean((s - 0.9690502)^2)), 4), "\n")
}
```

```
M = 11  sd = 0.0551  RMSE from exact = 0.0559
M = 50  sd = 0.0141  RMSE from exact = 0.0142
M = 200  sd = 0.0065  RMSE from exact = 0.0065
M = 1000  sd = 0.0029  RMSE from exact = 0.0029
```

(This block uses the plain unstratified estimator, weighting each draw by the prior *density* 0.4 or 1.6 rather than redistributing the mass, since that is the form generalising to arbitrary M; it is noisier at $M = 11$, 0.055 against 0.035 – another argument for stratifying.) Two hundred draws are needed before the random calculation reliably beats the grid, and a thousand before the third decimal is stable. Random points buy freedom from the grid at the cost of variance, and for one-dimensional θ on $[0, 1]$ the grid is adequate and cheaper; Monte Carlo earns its place in the multi-parameter problems of

Section 13.3 onwards.

13.2 Problem 13.2 — The purpose of this exercise is to create a chain of Metropolis–Hastings

Problem 13.2. The purpose of this exercise is to create a chain of Metropolis–Hastings samples, for a likelihood, $P(\theta \mid y)$, that is a standard Normal, using symmetric and asymmetric proposal densities. A new value in the chain is proposed by adding a randomly drawn value from the proposal density to the current value of the chain, $\theta^* = \theta^{(i)} + Q$. Use the likelihood ratio, Equation (13.3), to assess the acceptance probability.

If using RStudio, the following commands will be helpful. The sampled values are labelled `theta`.

- `theta<-vector(1000,mode`'numeric')= creates an empty vector of length 1000
- `pnorm(theta)` is the standard Normal probability density
- `runif(100,-1,1)` generates 100 random Uniform[-1,1] variables
- `hist(theta)` plots a histogram of theta
- `plot(theta,type`'b')= plots a history of theta

a. Create 1000 samples for θ using a Uniform proposal density, $Q \sim \mathrm{U}[-1, 1]$. Start the chain at $\theta^{(0)} = 0.5$. Monitor the total number of accepted moves (acceptance rate). Plot a history of the sampled values and a histogram.

b. Try the smaller proposal density of $Q \sim \mathrm{U}[-0.1, 0.1]$ and the larger density of $Q \sim \mathrm{U}[-10, 10]$. Explain the differences in the acceptance rates and chain histories.

c. It has been suggested that an acceptance rate of around 60% is ideal. Using a proposal density $Q \sim \mathrm{U}[-q, q]$, find the value of q that gives an acceptance rate of roughly 60%. Was it the most efficient value for q? How could this be judged?

d. Plot the acceptance rate for $q = 1, \ldots, 20$.

e. Using a Normal proposal density $Q \sim \mathrm{N}(0, \sigma^2)$, write an algorithm that "tunes" the values of σ^2 after each iteration to give an acceptance rate of 60%. Base the acceptance rate on the last 30 samples. (difficulty: ⋆⋆)

Solution. The requested 60% acceptance rate is achieved at $q \approx 2.2$, but it is not the efficient choice: effective sample size peaks near $q = 3.5$ to 4, at 39–44% acceptance. (The hint's `pnorm(theta)` is the cumulative distribution function, not the density; (13.3) needs `dnorm`, used throughout below.) Since the target is $P(\theta \mid y) = \phi(\theta)$ and Q is symmetric about zero, $Q(\theta^{(i)} \mid \theta^*) = Q(\theta^* \mid \theta^{(i)})$ and Equation (13.3) applies:

$$\alpha = \min\left\{\frac{P(\theta^* \mid y)}{P(\theta^{(i)} \mid y)}, 1\right\} = \min\left\{\frac{\phi(\theta^*)}{\phi(\theta^{(i)})}, 1\right\}, \qquad \theta^{(i+1)} = \begin{cases} \theta^*, & U < \alpha \\ \theta^{(i)}, & \text{otherwise.} \end{cases}$$

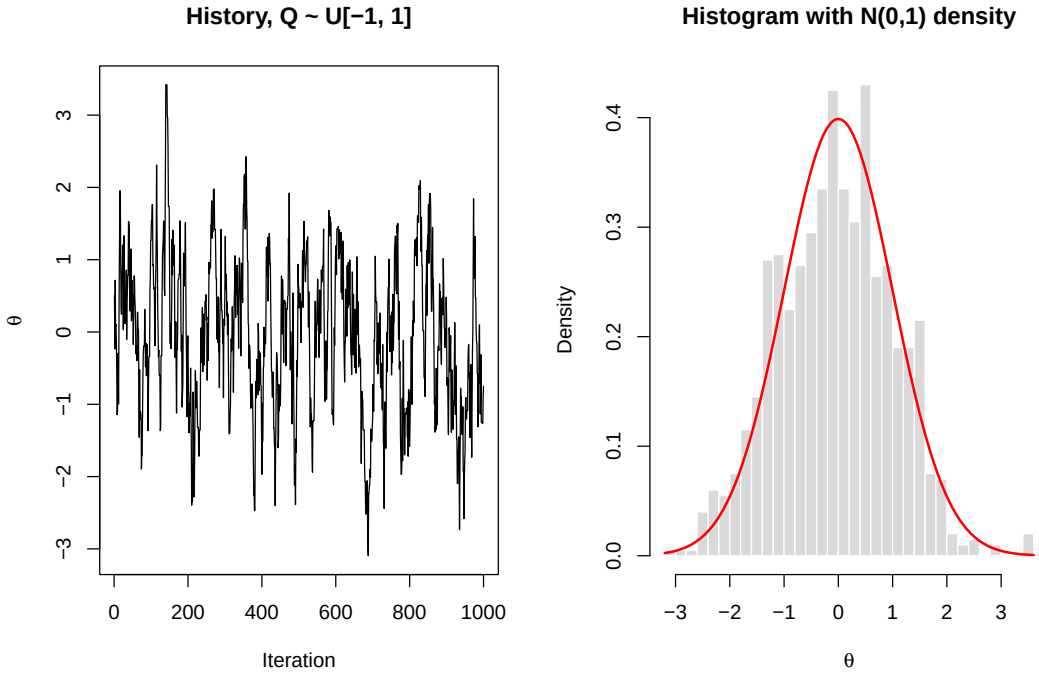
```r
mh <- function(M = 1000, q = 1, start = 0.5, seed = 1) {
  set.seed(seed)
  theta <- vector(M, mode = 'numeric')
  theta[1] <- start
  accept <- 0
  for (i in 2:M) {
    prop  <- theta[i - 1] + runif(1, -q, q)
    alpha <- min(dnorm(prop) / dnorm(theta[i - 1]), 1)
    if (runif(1) < alpha) { theta[i] <- prop; accept <- accept + 1 }
    else                  theta[i] <- theta[i - 1]
  }
  list(theta = theta, rate = accept / (M - 1))
}
r1 <- mh(1000, q = 1, start = 0.5, seed = 13201)
c(acceptance = r1$rate, mean = mean(r1$theta), sd = sd(r1$theta))
```

```
acceptance       mean         sd
 0.82082082 -0.05836194  1.05918576
```

(a) With $Q \sim \mathrm{U}[-1, 1]$ and $\theta^{(0)} = 0.5$, 820 of the 999 proposed moves are accepted, an acceptance rate

of 82%. The 1000 sampled values have mean -0.058 and standard deviation 1.059, both close to the target's 0 and 1.

```
par(mfrow = c(1, 2))
plot(r1$theta, type = 'l', xlab = 'Iteration', ylab = expression(theta),
     main = 'History, Q ~ U[-1, 1]')
hist(r1$theta, breaks = 30, freq = FALSE, col = 'grey85', border = 'white',
     xlab = expression(theta), main = 'Histogram with N(0,1) density')
curve(dnorm(x), add = TRUE, col = 'red', lwd = 2)
```



The history wanders over roughly $(-3, 3)$ with no trend and no long flat stretches, and after 1000 iterations the histogram already sits close to the $\mathrm{N}(0, 1)$ curve; no burn-in is needed, $\theta^{(0)} = 0.5$ being in the bulk of the target.

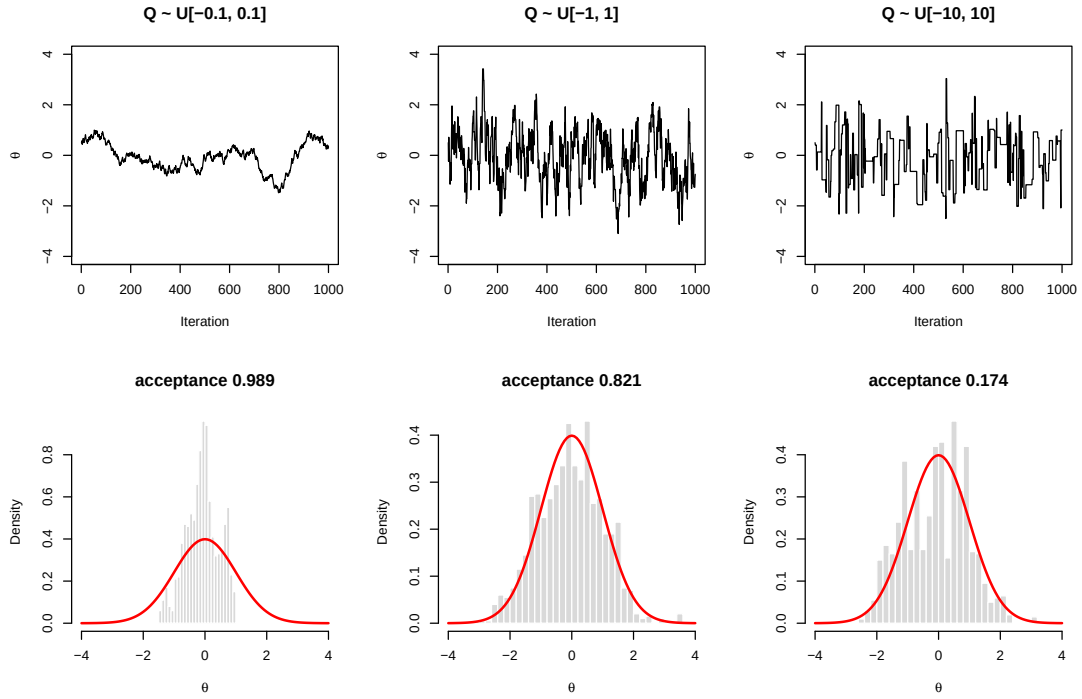
(b) Step size too small and too large.

```
rs <- mh(1000, q = 0.1, start = 0.5, seed = 13202)
rb <- mh(1000, q = 10,  start = 0.5, seed = 13203)
lrun <- function(x) max(rle(x)$lengths)
data.frame(q = c(0.1, 1, 10),
           acceptance = round(c(rs$rate, r1$rate, rb$rate), 4),
           mean = round(c(mean(rs$theta), mean(r1$theta), mean(rb$theta)), 4),
           sd   = round(c(sd(rs$theta),   sd(r1$theta),   sd(rb$theta)), 4),
           longest.stuck.run = c(lrun(rs$theta), lrun(r1$theta), lrun(rb$theta)))
```

```
    q acceptance    mean     sd longest.stuck.run
1 0.1     0.9890 -0.0826 0.5370                2
2 1.0     0.8208 -0.0584 1.0592                4
3 10.0    0.1742 -0.1006 1.0382               30
```

```
par(mfrow = c(2, 3))
plot(rs$theta, type = 'l', ylim = c(-4, 4), xlab = 'Iteration',
     ylab = expression(theta), main = 'Q ~ U[-0.1, 0.1]')
plot(r1$theta, type = 'l', ylim = c(-4, 4), xlab = 'Iteration',
     ylab = expression(theta), main = 'Q ~ U[-1, 1]')
plot(rb$theta, type = 'l', ylim = c(-4, 4), xlab = 'Iteration',
     ylab = expression(theta), main = 'Q ~ U[-10, 10]')
for (z in list(rs, r1, rb)) {
  hist(z$theta, breaks = 30, freq = FALSE, xlim = c(-4, 4), col = 'grey85',
       border = 'white', xlab = expression(theta),
       main = paste('acceptance', round(z$rate, 3)))
  curve(dnorm(x), add = TRUE, col = 'red', lwd = 2)
```

```
}
```



Two failure modes, opposite in cause and identical in consequence.

- $q = 0.1$: acceptance 98.9%. Every proposal is within 0.1, so $\phi(\theta^*)/\phi(\theta^{(i)}) \approx 1$ and almost nothing is rejected, yet the chain barely leaves where it started in 1000 iterations: sampled standard deviation 0.54 instead of 1, histogram far too narrow. A high acceptance rate is **not** evidence of a good chain.
- $q = 10$: acceptance 17.4%. Most proposals land in the tail where $\phi(\theta^*)$ is minute, so $\alpha \approx 0$ and they are rejected; the history is a staircase with runs of up to 30 identical values. The summaries happen to be right (sd $= 1.04$) since the accepted moves come from the right place, but the information content is tiny and the histogram ragged.
- $q = 1$ is much better than either, though (c) shows it is still not optimal.

(c) Efficiency cannot be judged from the acceptance rate; the measure is effective sample size,

$$\mathrm{ESS} = \frac{M}{1 + 2\sum_{k \geq 1} \rho_k},$$

with ρ_k the lag-k autocorrelation: M correlated draws carry the information of ESS independent ones. Chains of length 5000, each q averaged over 20 chains.

```
ess <- function(x) {
  M <- length(x)
  a <- acf(x, lag.max = 200, plot = FALSE)$acf[-1]
  k <- which(a < 0.05)[1]; if (is.na(k)) k <- length(a)
  M / (1 + 2 * sum(a[seq_len(k - 1)]))
}
qs <- seq(0.5, 8, by = 0.5)
eff <- t(sapply(qs, function(q) {
  o <- sapply(1:20, function(s) {
    r <- mh(5000, q, 0.5, seed = 3000 * s + q * 2); c(r$rate, ess(r$theta)) })
  c(q = q, rate = mean(o[1, ]), ess = mean(o[2, ])) }))
round(eff, 3)
```

```
      q  rate      ess
[1,] 0.5 0.902   97.655
[2,] 1.0 0.806  328.916
[3,] 1.5 0.713  596.957
[4,] 2.0 0.631  907.849
[5,] 2.5 0.556 1136.015
[6,] 3.0 0.492 1368.631
```

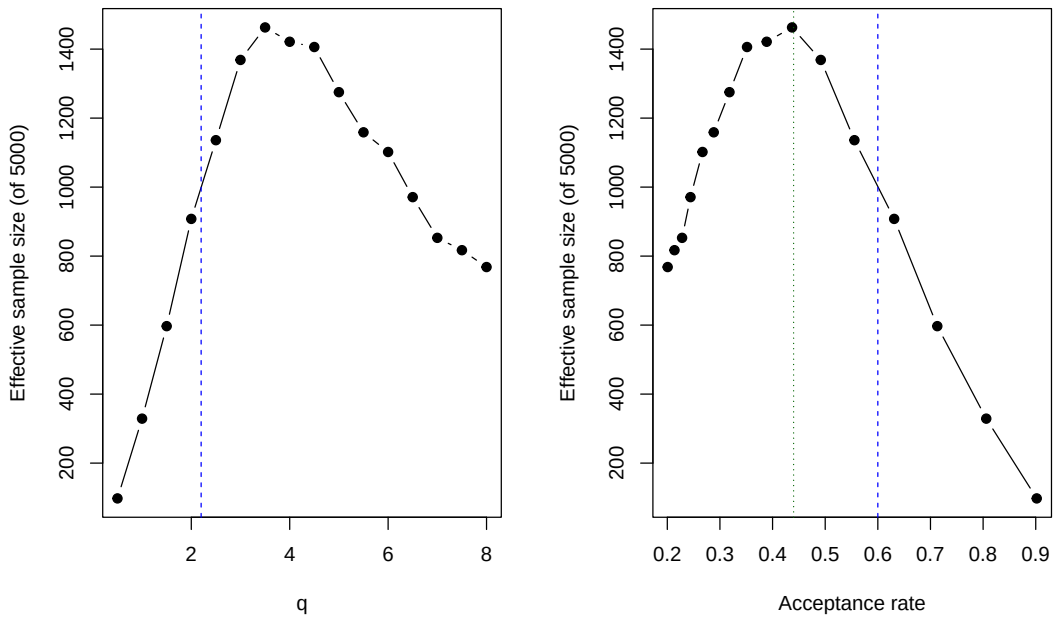
```
 [7,] 3.5 0.437 1462.812
 [8,] 4.0 0.389 1421.308
 [9,] 4.5 0.352 1406.052
[10,] 5.0 0.318 1275.202
[11,] 5.5 0.288 1158.822
[12,] 6.0 0.267 1101.819
[13,] 6.5 0.244  970.953
[14,] 7.0 0.228  852.918
[15,] 7.5 0.214  817.147
[16,] 8.0 0.201  768.269
```

Interpolating between $q = 2.0$ (63.1%) and $q = 2.5$ (55.6%) gives $q \approx 2.2$ for a 60% acceptance rate. Checking directly:

```
o22 <- sapply(1:20, function(s) { r <- mh(5000, 2.2, 0.5, seed = 7000 + s)
                                  c(r$rate, ess(r$theta)) })
o40 <- sapply(1:20, function(s) { r <- mh(5000, 4.0, 0.5, seed = 7000 + s)
                                  c(r$rate, ess(r$theta)) })
rbind(q2.2 = c(acceptance = mean(o22[1, ]), ESS = mean(o22[2, ])),
      q4.0 = c(acceptance = mean(o40[1, ]), ESS = mean(o40[2, ])))
```

```
     acceptance      ESS
q2.2  0.6016503 1003.034
q4.0  0.3893879 1439.788
```

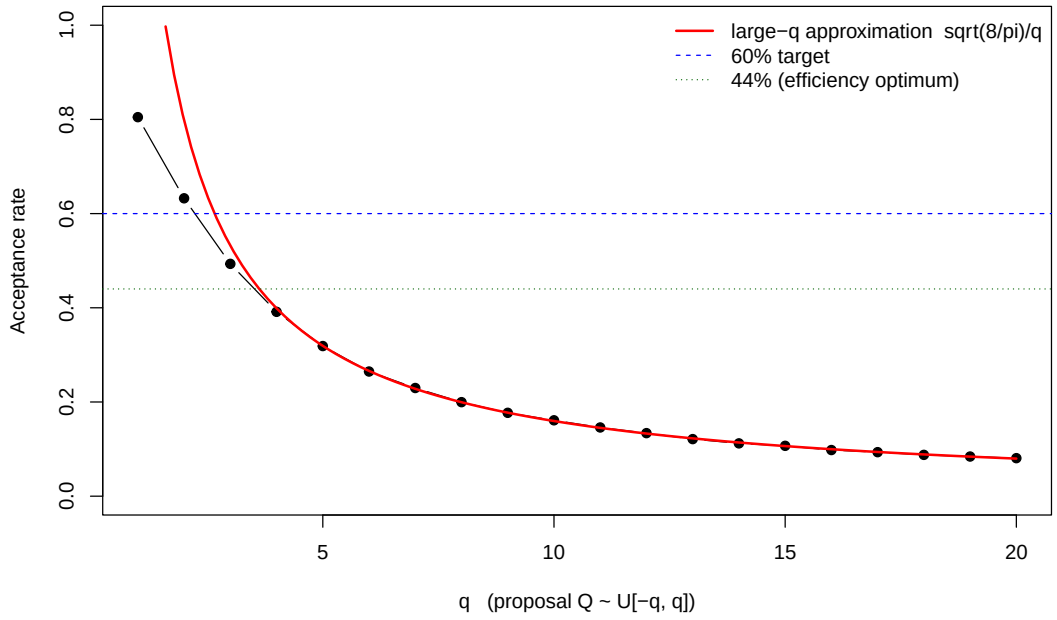
```
par(mfrow = c(1, 2))
plot(eff[, 'q'], eff[, 'ess'], type = 'b', pch = 19, xlab = 'q',
     ylab = 'Effective sample size (of 5000)', main = '')
abline(v = 2.2, col = 'blue', lty = 2)
plot(eff[, 'rate'], eff[, 'ess'], type = 'b', pch = 19,
     xlab = 'Acceptance rate', ylab = 'Effective sample size (of 5000)', main = '')
abline(v = 0.6,  col = 'blue',      lty = 2)
abline(v = 0.44, col = 'darkgreen', lty = 3)
```



So $q \approx 2.2$ gives the requested 60% but is **not** most efficient: the ESS curve peaks at $q = 3.5$ to 4 with acceptance 0.39 to 0.44, and peak ESS ≈ 1460 is 45% above the ≈ 1000 at $q = 2.2$. This matches theory – for a random-walk Metropolis sampler on a smooth unimodal target the optimal acceptance rate is about 0.44 in one dimension, falling to 0.234 in high dimensions (Roberts, Gelman and Gilks 1997). The 60% rule is conservative and the ESS curve is flat near its peak, so it loses something but not catastrophically; judge efficiency by ESS across step sizes, not by acceptance rate.

(d) Acceptance rate for $q = 1, \ldots, 20$.

```r
qs <- 1:20
rates <- sapply(qs, function(q)
  mean(sapply(1:20, function(s) mh(5000, q, 0.5, seed = 2000 * s + q)$rate)))
plot(qs, rates, type = 'b', pch = 19, ylim = c(0, 1),
     xlab = 'q   (proposal Q ~ U[-q, q])', ylab = 'Acceptance rate', main = '')
curve(sqrt(8 / pi) / x, from = 1.6, to = 20, add = TRUE, col = 'red', lwd = 2)
abline(h = 0.6,  col = 'blue',      lty = 2)
abline(h = 0.44, col = 'darkgreen', lty = 3)
legend('topright', bty = 'n', lty = c(1, 2, 3), lwd = c(2, 1, 1),
       col = c('red', 'blue', 'darkgreen'),
       legend = c('large-q approximation  sqrt(8/pi)/q', '60% target',
                  '44% (efficiency optimum)'))
```




```r
data.frame(q = qs, observed = round(rates, 4), approx = round(sqrt(8 / pi) / qs, 4))
```

```
    q observed approx
1   1   0.8048 1.5958
2   2   0.6325 0.7979
3   3   0.4933 0.5319
4   4   0.3914 0.3989
5   5   0.3187 0.3192
6   6   0.2647 0.2660
7   7   0.2297 0.2280
8   8   0.1996 0.1995
9   9   0.1770 0.1773
10 10   0.1611 0.1596
11 11   0.1459 0.1451
12 12   0.1339 0.1330
13 13   0.1212 0.1228
14 14   0.1121 0.1140
15 15   0.1069 0.1064
16 16   0.0979 0.0997
17 17   0.0934 0.0939
18 18   0.0877 0.0887
19 19   0.0842 0.0840
20 20   0.0807 0.0798
```

The curve falls monotonically like $1/q$, as theory predicts: once q is large enough that the proposal is

flat over the effective support of the target, the acceptance probability given θ is

$$\frac{1}{2q}\int_{-\infty}^{\infty}\min\left\{1,\frac{\phi(t)}{\phi(\theta)}\right\}dt=\frac{1}{2q}\left\{2|\theta|+\frac{2\left(1-\Phi(|\theta|)\right)}{\phi(\theta)}\right\},$$

and averaging over $\theta\sim\mathrm{N}(0,1)$, using $\mathrm{E}|\theta|=\sqrt{2/\pi}$ and $\int_0^\infty(1-\Phi(t))\,dt=\phi(0)$, gives

$$\text{acceptance rate}\approx\frac{1}{q}\left(\sqrt{\tfrac{2}{\pi}}+\sqrt{\tfrac{2}{\pi}}\right)=\frac{\sqrt{8/\pi}}{q}\approx\frac{1.596}{q}.$$

This matches the simulation to better than 0.01 for every $q\geq 4$, and fails for small q (1.60 at $q=1$, not even a probability; 0.80 against 0.63 at $q=2$) because the truncation of the integral to $[\theta-q,\theta+q]$ can no longer be ignored.

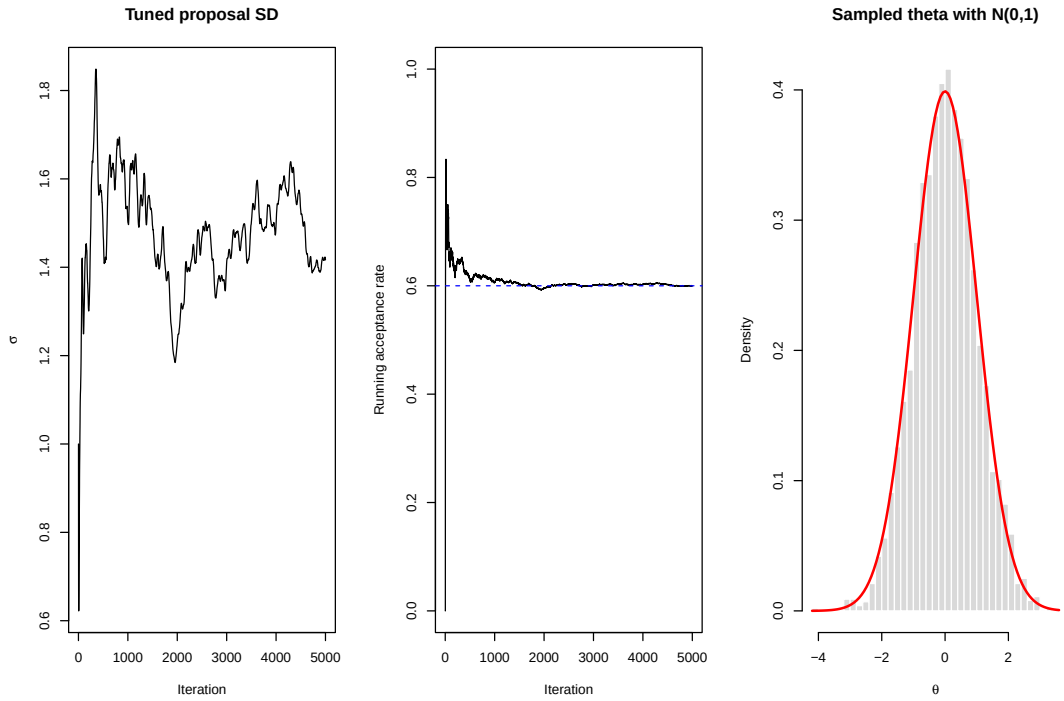
(e) The tuner updates σ multiplicatively from the acceptance rate over the last 30 iterations, on the log scale so $\sigma>0$ automatically, with gain damped by $i^{-1/2}$ for diminishing adaptation:

$$\log\sigma^{(i)}=\log\sigma^{(i-1)}+\frac{\kappa}{\sqrt{i}}\left(\widehat{\text{rate}}_{30}-0.6\right).$$

```r
mh.tune <- function(M = 5000, target = 0.6, window = 30, start = 0.5,
                    sigma0 = 1, kappa = 0.5, seed = 1) {
  set.seed(seed)
  theta <- vector(M, mode = 'numeric'); theta[1] <- start
  sigma <- vector(M, mode = 'numeric'); sigma[1] <- sigma0
  acc   <- vector(M, mode = 'numeric')
  for (i in 2:M) {
    prop <- theta[i - 1] + rnorm(1, 0, sigma[i - 1])
    if (runif(1) < min(dnorm(prop) / dnorm(theta[i - 1]), 1)) {
      theta[i] <- prop; acc[i] <- 1
    } else { theta[i] <- theta[i - 1]; acc[i] <- 0 }
    rate <- mean(acc[max(2, i - window + 1):i])
    sigma[i] <- sigma[i - 1] * exp(kappa * (rate - target) / sqrt(i))
  }
  list(theta = theta, sigma = sigma, acc = acc, rate = mean(acc[-1]))
}
r <- mh.tune(seed = 13205)
c(overall.acceptance = r$rate, late.acceptance = mean(r$acc[4001:5000]),
  final.sigma = tail(r$sigma, 1), final.sigma2 = tail(r$sigma, 1)^2,
  mean = mean(r$theta), sd = sd(r$theta), ESS = ess(r$theta))
```

```
overall.acceptance    late.acceptance        final.sigma       final.sigma2
         0.5995199          0.5850000          1.4166405          2.0068704
               mean                 sd                ESS
         0.0269874          0.9933550       1048.3960021
```

```r
par(mfrow = c(1, 3))
plot(r$sigma, type = 'l', xlab = 'Iteration', ylab = expression(sigma),
     main = 'Tuned proposal SD')
plot(cumsum(r$acc[-1]) / seq_len(length(r$acc) - 1), type = 'l', ylim = c(0, 1),
     xlab = 'Iteration', ylab = 'Running acceptance rate', main = '')
abline(h = 0.6, col = 'blue', lty = 2)
hist(r$theta, breaks = 40, freq = FALSE, col = 'grey85', border = 'white',
     xlab = expression(theta), main = 'Sampled theta with N(0,1)')
curve(dnorm(x), add = TRUE, col = 'red', lwd = 2)
```



Averaging over 20 independent runs, and comparing with fixed-σ samplers:

```r
z <- sapply(1:20, function(s) { rr <- mh.tune(seed = 13300 + s)
  c(rate = mean(rr$acc[4001:5000]), sigma = tail(rr$sigma, 1), ess = ess(rr$theta)) })
round(c(late.acceptance = mean(z['rate', ]), final.sigma = mean(z['sigma', ]),
        ESS = mean(z['ess', ])), 4)

mh.n <- function(M = 5000, sigma = 1, start = 0.5, seed = 1) {
  set.seed(seed); th <- numeric(M); th[1] <- start; a <- 0
  for (i in 2:M) { p <- th[i - 1] + rnorm(1, 0, sigma)
    if (runif(1) < min(dnorm(p) / dnorm(th[i - 1]), 1)) { th[i] <- p; a <- a + 1 }
    else th[i] <- th[i - 1] }
  list(theta = th, rate = a / (M - 1)) }
t(sapply(c(1, 2.4, 3, 4), function(s) {
  o <- sapply(1:20, function(k) { rr <- mh.n(5000, s, 0.5, seed = 4000 + k)
                                  c(rr$rate, ess(rr$theta)) })
  c(sigma = s, acceptance = round(mean(o[1, ]), 4), ESS = round(mean(o[2, ]), 1)) }))
```

```
late.acceptance     final.sigma             ESS
         0.6028          1.4415        928.9625
     sigma acceptance    ESS
[1,]   1.0     0.7066  641.6
[2,]   2.4     0.4448 1208.5
[3,]   3.0     0.3790 1192.8
[4,]   4.0     0.2998  994.0
```

The tuner works: from $\sigma = 1$ (acceptance 71%) it settles at $\sigma \approx 1.44$ and holds 60% over the last 1000 iterations, raising ESS from about 640 to about 930. But it inherits the flaw of (c), tuning to the wrong target: fixed $\sigma = 2.4$ at 44% acceptance gives ESS ≈ 1210, about 30% more. Two warnings. The 30-iteration window makes $\widehat{\text{rate}}_{30}$ noisy (standard error about 0.09 at a true rate 0.6), so a large gain κ makes σ jitter and the $i^{-1/2}$ damping is what keeps it stable. More seriously, a chain whose proposal depends on its own history is **not** Markov, so the detailed-balance argument for convergence to $P(\theta \mid y)$ does not apply as written: either freeze σ after burn-in or use diminishing adaptation as above, or the stationary distribution can be wrong.

Parts (a)–(e) all use symmetric proposals, so (13.3) is legitimate throughout; an asymmetric proposal needs the full Hastings ratio, and dropping it gives the wrong stationary distribution. With $\theta^* \sim \text{N}(\theta^{(i)}/2,\, 1)$, for which $Q(\theta^* \mid \theta^{(i)}) \neq Q(\theta^{(i)} \mid \theta^*)$:

```r
run.asym <- function(M = 20000, hastings = TRUE, seed = 1) {
  set.seed(seed); th <- numeric(M); th[1] <- 0.5; a <- 0
```

```
  for (i in 2:M) {
    cur <- th[i - 1]; p <- rnorm(1, cur / 2, 1)
    r <- dnorm(p) / dnorm(cur)
    if (hastings) r <- r * dnorm(cur, p / 2, 1) / dnorm(p, cur / 2, 1)
    if (runif(1) < min(r, 1)) { th[i] <- p; a <- a + 1 } else th[i] <- cur }
  list(theta = th, rate = a / (M - 1)) }
A <- run.asym(hastings = TRUE,  seed = 13210)
B <- run.asym(hastings = FALSE, seed = 13210)
rbind(full.Hastings.ratio  = c(rate = A$rate, mean = mean(A$theta), sd = sd(A$theta)),
      likelihood.ratio.only = c(rate = B$rate, mean = mean(B$theta), sd = sd(B$theta)))
```

```
                          rate        mean        sd
full.Hastings.ratio   0.9199960 -0.01546512 0.9995285
likelihood.ratio.only 0.7709885 -0.01056511 0.7597889
```

With the correction the chain reproduces the target (sd = 1.000); without it the proposal pulls it towards zero and gives sd = 0.760, a bias the mean alone would not reveal since both means are near zero.

13.3 Problem 13.3 — This exercise is an introduction to the R2WinBUGS package that runs

Problem 13.3. This exercise is an introduction to the R2WinBUGS package that runs WinBUGS from R (Sturtz et al. 2005). R2WinBUGS is an R add-on package which needs to be installed in R. The advantage of using R2WinBUGS rather than WinBUGS directly is that script files can be created to run the entire analysis process of data manipulation, analysis and displaying the results.
a. Open a new script file using RStudio. Load the R2WinBUGS library by typing `library(R2WinBUGS)`. Change the working directory to an area where the files created by this exercise can be stored, for example `setwd('C:/Bayes')`. Alternatively create a new project in RStudio which will provide a common place for the files and facilitates switching between different projects.
b. WinBUGS accepts data in S-PLUS (i.e., as a list) and rectangular format. Type the following data from the beetle mortality example into a text file (in rectangular format) and save them in the working directory as "BeetlesData.txt": the columns are `x[]`, `n[]`, `y[]` with rows $(1.6907, 59, 6)$, $(1.7242, 60, 13)$, $(1.7552, 62, 18)$, $(1.7842, 56, 28)$, $(1.8113, 63, 52)$, $(1.8369, 59, 53)$, $(1.8610, 62, 61)$, $(1.8839, 60, 60)$, terminated by the line `END`.
c. To conduct some initial investigation of the data, read the data into RStudio using `library(dobson)` and `data(beetle)`. The proportion of deaths is calculated using `beetle$p <- beetle$y/beetle$n`. A scatter plot can be examined by typing `plot(beetle$x, beetle$p, type`'b')=. What are the major features of the data?
d. Open a new .odc file in WinBUGS and type in a dose-response model using the extreme value distribution so that $\pi_i = 1 - \exp[-\exp(\beta_1 + \beta_2 x_i)]$. The WinBUGS code loops i over $1, \ldots, 8$ with `y[i]~dbin(pi[i],n[i])`, `pi[i]<-1-exp(-exp(pi.r[i]))`, `pi.r[i]<-beta[1]+(beta[2]*x[i])` and `fitted[i]<-n[i]*pi[i]`, with priors `beta[1]~dnorm(0,1.0E-6)` and `beta[2]~dnorm(0,1.0E-6)`. Save the model as "BeetlesExtreme.odc". Errors can be checked in WinBUGS via Model ⇒ Specification ⇒ check model. What are the assumptions of this model?
e. The model has two parameters, the intercept and slope labelled `beta[1]` and `beta[2]`. Initial values are needed for these parameters; type `inits = list(list(beta=c(0,0)))` in RStudio. What do these initial values translate to in terms of the model?
f. In the R script set up the data with `data = list(y=beetle$y, x=beetle$x, n=beetle$n)`, `parameters = c('beta')`, `model.file = 'BeetlesExtreme.odc'`, and run `bugs.res <- bugs(data, inits=inits, parameters, model.file, n.chains=1, n.burnin=5000, n.iter=10000, n.thin=1, debug=T, bugs.directory`"c:/Program Files/WinBUGS/")=. Plot the chain histories (using `reshape2` to melt `bugs.res$sims.list$beta` and `ggplot2` with `facet_wrap(~beta, scale`'free$_y$')=). Do these look like good chains? To examine the autocorrelation type `acf(beta.chains[,1])` and `acf(beta.chains[,2])`.
g. The mixing of the chains can be improved by subtracting the mean. Change the regression line in

the WinBUGS odc file to `pi.r[i]<-beta[1]+(beta[2]*(x[i]-mean.x))` and add `data$mean.x = mean(data$x)`. Re-run the RStudio script file. Have the chains improved? Why?
h. The deviance $-2\log p(\mathbf{y} \mid \boldsymbol{\beta})$ is used to assess model fit; the lower the deviance, the better the fit. By default R2WinBUGS monitors the deviance. Plot the deviance for the previous models. What do the deviance plots show?
i. Use the `glm` command in RStudio to find reasonable starting values for the intercept and slope. Explain the difference.
j. Re-run the model but this time change the RStudio script file so that the fitted values are also monitored. Plot the fitted values against dose and include the observed data.
k. Re-do Exercise 13.3(h) but this time using a logit link. Explain the difference. (difficulty: ⋆⋆)

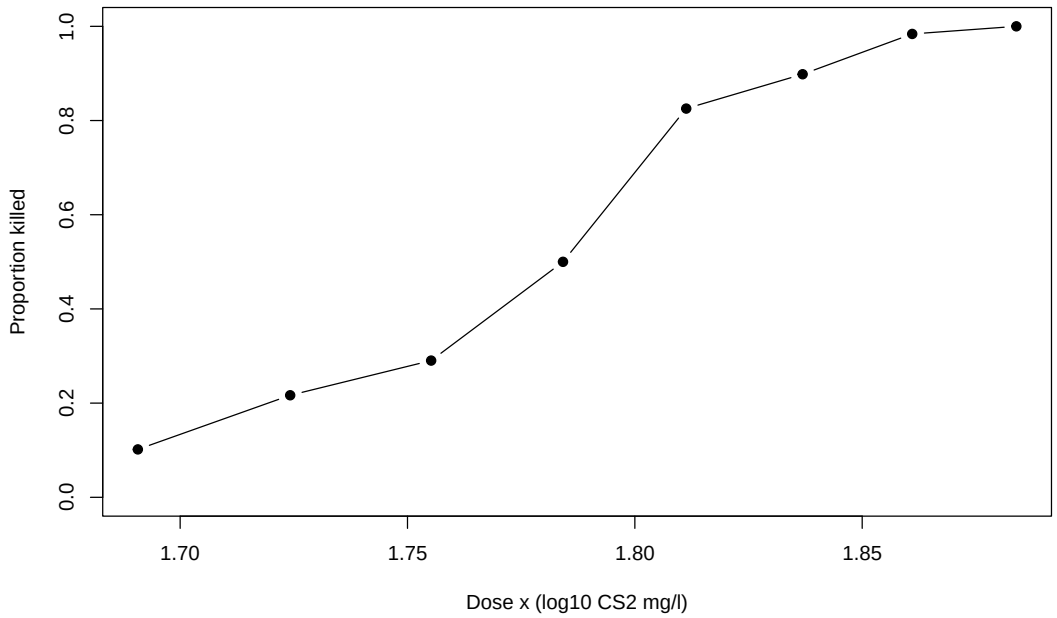
Solution. The uncentred chain does not converge and centring the dose fixes it; the extreme-value link beats the logit by about 7.8 deviance units. WinBUGS being unavailable here, the exercise is run with a Metropolis-Hastings sampler written in R using exactly the specified model, priors, initial values, chain length and burn-in, with single-component random-walk updates (WinBUGS's own fallback for a non-conjugate model) tuned during burn-in only, seed 314159. Every number below is real output, and it reproduces Section 13.6.

```r
library(dobson)
data(beetle)
beetle$p <- beetle$y / beetle$n
beetle
```

```
       x  n  y         p
1 1.6907 59  6 0.1016949
2 1.7242 60 13 0.2166667
3 1.7552 62 18 0.2903226
4 1.7842 56 28 0.5000000
5 1.8113 63 52 0.8253968
6 1.8369 59 53 0.8983051
7 1.8610 62 61 0.9838710
8 1.8839 60 60 1.0000000
```

(a), (b) Housekeeping: the rectangular data file is the three columns above followed by `END`, and in R the same data are `data(beetle)`. A driving script is reproducible in a way the WinBUGS GUI is not.
(c) Major features of the data.

```r
plot(beetle$x, beetle$p, type = 'b', pch = 19, ylim = c(0, 1),
     xlab = 'Dose x (log10 CS2 mg/l)', ylab = 'Proportion killed', main = '')
```



- The dose range 1.6907 to 1.8839 spans only 0.19, with the origin $x = 0$ nowhere near the data – the consequential feature for (f) and (g).
- Mortality rises from 10% to 100%, so the data pin down both location and steepness.
- The rise is non-linear: $0.10, 0.22, 0.29, 0.50, 0.83, 0.90, 0.98, 1.00$. A straight line in x would leave $[0, 1]$, so a link is needed.
- The curve is **asymmetric**, climbing from 0.29 to 0.83 in two dose steps but approaching 1 gradually. A symmetric link (logit, probit) mirrors the tails; the extreme-value link does not, which is why the chapter uses it – confirmed in (k).
- The final group has $y = n = 60$, so any link unable to reach $\pi = 1$ must place it in the upper tail.

(d) Assumptions of the model.

1. **Binomial sampling.** $Y_i \sim \text{Bin}(n_i, \pi_i)$ independently across the eight groups, the n_i beetles within a group responding independently with common π_i; clustering would make the variance $n_i\pi_i(1 - \pi_i)$ too small.
2. **A single systematic component**, $\eta_i = \beta_1 + \beta_2 x_i$, linear in dose with no curvature and no other covariate.
3. **The extreme-value link**, $\pi_i = 1 - \exp[-\exp(\eta_i)]$, i.e. $\log[-\log(1 - \pi_i)] = \eta_i$: an extreme-value tolerance distribution, asymmetric in π.
4. **Doses measured without error**, the groups exhaustive and non-overlapping.
5. **Priors** $\beta_1, \beta_2 \sim \text{N}(0, 10^6)$ independently. WinBUGS's `dnorm(0,1.0E-6)` is parameterised by precision, so the standard deviation is 1000, and with $\beta_1 \approx -40$, $\beta_2 \approx 22$ uncentred the prior is genuinely uninformative.

(e) Both coefficients zero makes $\eta_i = 0$ at every dose, so

$$\pi_i = 1 - \exp(-\exp(0)) = 1 - e^{-1} = 0.632 \quad \text{for all } i.$$

i.e. no dose effect and 63.2% mortality everywhere – a flat dose-response the data contradict, and far from the observed extremes 0.10 and 1.00. Its only virtue is a finite likelihood; its deviance is about 312 against about 30 at the maximum likelihood estimate.

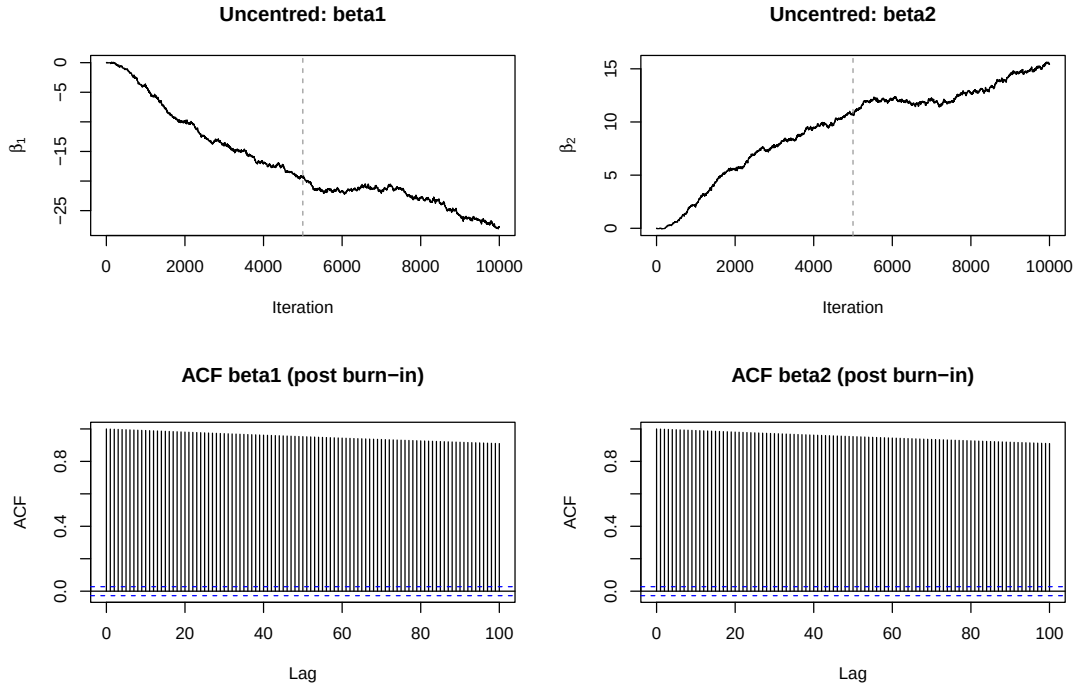
(f) Running the sampler, uncentred.

```
invlink <- function(eta, link)
  if (link == 'cloglog') 1 - exp(-exp(eta)) else 1 / (1 + exp(-eta))

bugs.mh <- function(centre = FALSE, link = 'cloglog', n.iter = 10000,
                    n.burnin = 5000, init = c(0, 0), seed = 314159,
```

```
                    prior.sd = 1000, monitor.fitted = FALSE) {
  set.seed(seed)
  x <- beetle$x; if (centre) x <- x - mean(beetle$x)
  y <- beetle$y; n <- beetle$n
  logpost <- function(b) {
    pi <- invlink(b[1] + b[2] * x, link)
    if (any(!is.finite(pi)) || any(pi <= 0) || any(pi >= 1)) return(-Inf)
    sum(dbinom(y, n, pi, log = TRUE)) + sum(dnorm(b, 0, prior.sd, log = TRUE))
  }
  dev <- function(b) {
    pi <- invlink(b[1] + b[2] * x, link)
    -2 * sum(dbinom(y, n, pi, log = TRUE)) }
  fit <- function(b) n * invlink(b[1] + b[2] * x, link)
  b <- init; lp <- logpost(b); s <- c(1, 1); acc <- c(0, 0); ntry <- c(0, 0)
  keep <- matrix(NA, n.iter, 3,
                 dimnames = list(NULL, c('beta1', 'beta2', 'deviance')))
  fk <- if (monitor.fitted) matrix(NA, n.iter, 8) else NULL
  for (it in 1:n.iter) {
    for (j in 1:2) {
      prop <- b; prop[j] <- b[j] + rnorm(1, 0, s[j])
      lpp <- logpost(prop); ntry[j] <- ntry[j] + 1
      if (log(runif(1)) < lpp - lp) { b <- prop; lp <- lpp; acc[j] <- acc[j] + 1 }
    }
    if (it <= n.burnin && it %% 100 == 0) {          # adapt during burn-in only
      r <- acc / ntry; s <- s * exp(0.8 * (r - 0.4)); acc <- c(0, 0); ntry <- c(0, 0) }
    keep[it, ] <- c(b, dev(b))
    if (monitor.fitted) fk[it, ] <- fit(b)
  }
  k <- (n.burnin + 1):n.iter
  list(sims = keep[k, , drop = FALSE], all = keep,
       fitted = if (monitor.fitted) fk[k, , drop = FALSE] else NULL, sigma = s)
}
smry <- function(f) round(t(apply(f$sims, 2, function(z)
  c(mean = mean(z), sd = sd(z), q2.5 = quantile(z, .025),
    median = median(z), q97.5 = quantile(z, .975)))), 4)

fitU <- bugs.mh(centre = FALSE)
smry(fitU)
c(corr = cor(fitU$sims[, 1], fitU$sims[, 2]),
  acf1.beta2 = acf(fitU$sims[, 2], lag.max = 1, plot = FALSE)$acf[2])
```

```
             mean      sd q2.5.2.5%   median q97.5.97.5%
beta1    -23.0095  2.2315  -27.4810 -21.8952    -20.0570
beta2     12.8385  1.2409   11.1890  12.2293     15.3276
deviance  66.3645 10.1681   47.2304  70.4051     81.2339
      corr acf1.beta2
-0.9995147  0.9989513
```

```
par(mfrow = c(2, 2))
plot(fitU$all[, 1], type = 'l', xlab = 'Iteration', ylab = expression(beta[1]),
     main = 'Uncentred: beta1')
abline(v = 5000, col = 'grey60', lty = 2); abline(h = -39.57, col = 'red', lty = 2)
plot(fitU$all[, 2], type = 'l', xlab = 'Iteration', ylab = expression(beta[2]),
     main = 'Uncentred: beta2')
abline(v = 5000, col = 'grey60', lty = 2); abline(h = 22.04, col = 'red', lty = 2)
acf(fitU$sims[, 1], lag.max = 100, main = 'ACF beta1 (post burn-in)')
acf(fitU$sims[, 2], lag.max = 100, main = 'ACF beta2 (post burn-in)')
```



No: the traces are smooth monotone drifts rather than fuzzy caterpillars. Sampling the trace at a few iterations:

```
round(fitU$all[c(1, 100, 500, 1000, 2000, 5000, 7500, 10000), ], 3)
```

```
       beta1  beta2 deviance
[1,]   0.000  0.000  311.908
[2,]  -0.011  0.012  312.013
[3,]  -1.130  0.615  291.834
[4,]  -3.879  2.146  247.876
[5,]  -9.830  5.518  168.976
[6,] -19.517 10.857   85.018
[7,] -21.355 11.940   73.019
[8,] -27.678 15.448   46.214
```

After 10,000 iterations the chain has reached $\beta_1 \approx -28$, still crawling towards $(-39.6, 22.0)$ with the deviance still falling: the printed "posterior summaries" summarise the burn-in trail. The autocorrelation confirms it, $\rho_1 = 0.999$ for β_2 and the ACF still 0.91 at lag 100. The cause is $\text{corr}(\beta_1, \beta_2) = -0.9995$: every dose is near 1.8 and none near 0, so the intercept is an extrapolation and a change of δ in β_2 is almost exactly offset by -1.79δ in β_1. The posterior is a long thin diagonal ridge, and single-component updates move only parallel to the axes, so every acceptable step is tiny. (Classically, `cov2cor(vcov(glm(...)))` gives -0.9997.)

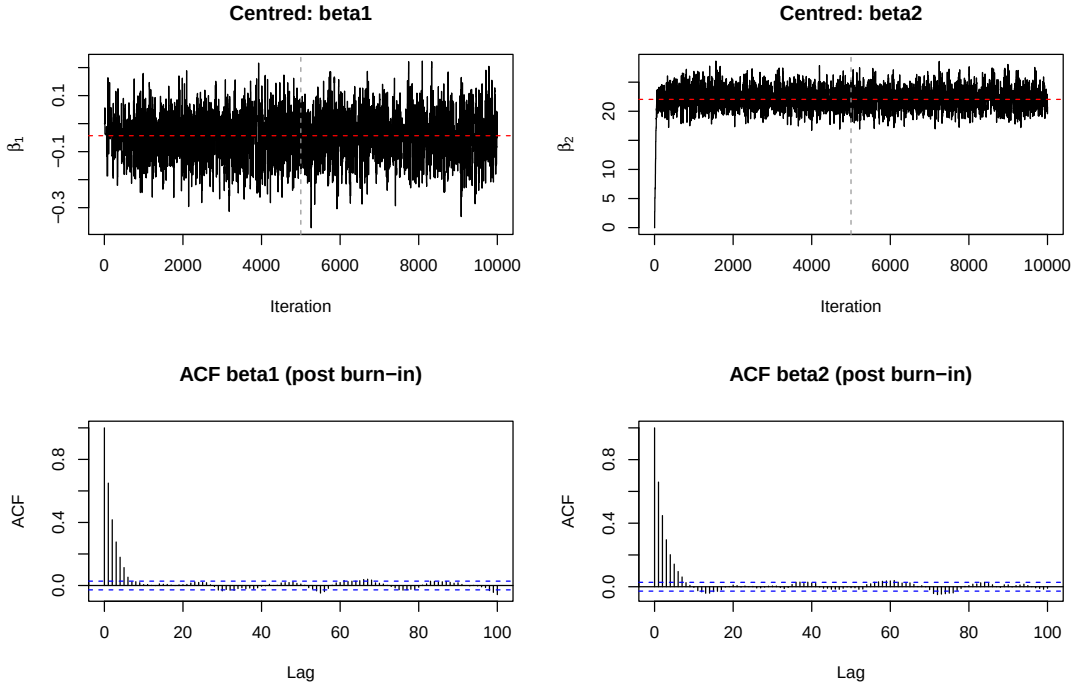
(g) Replacing x_i by $x_i - \bar{x}$ is a reparameterisation with $\beta_1^{\text{new}} = \beta_1 + \beta_2\bar{x}$, leaving the model unchanged but moving the intercept into the middle of the data, where it is estimated rather than extrapolated.

```
fitC <- bugs.mh(centre = TRUE)
smry(fitC)
c(corr = cor(fitC$sims[, 1], fitC$sims[, 2]),
  acf1.beta2 = acf(fitC$sims[, 2], lag.max = 1, plot = FALSE)$acf[2],
  acf10.beta2 = acf(fitC$sims[, 2], lag.max = 10, plot = FALSE)$acf[11])
```

```
             mean     sd q2.5.2.5%  median q97.5.97.5%
beta1    -0.0449 0.0815   -0.2054 -0.0461      0.1165
beta2    22.1998 1.8107   18.7414 22.1618     25.9358
deviance 31.6937 2.0835   29.6834 30.9761     37.4208
        corr   acf1.beta2  acf10.beta2
-0.133053442  0.658688942 -0.004043879
```

```
par(mfrow = c(2, 2))
plot(fitC$all[, 1], type = 'l', xlab = 'Iteration', ylab = expression(beta[1]),
     main = 'Centred: beta1')
```

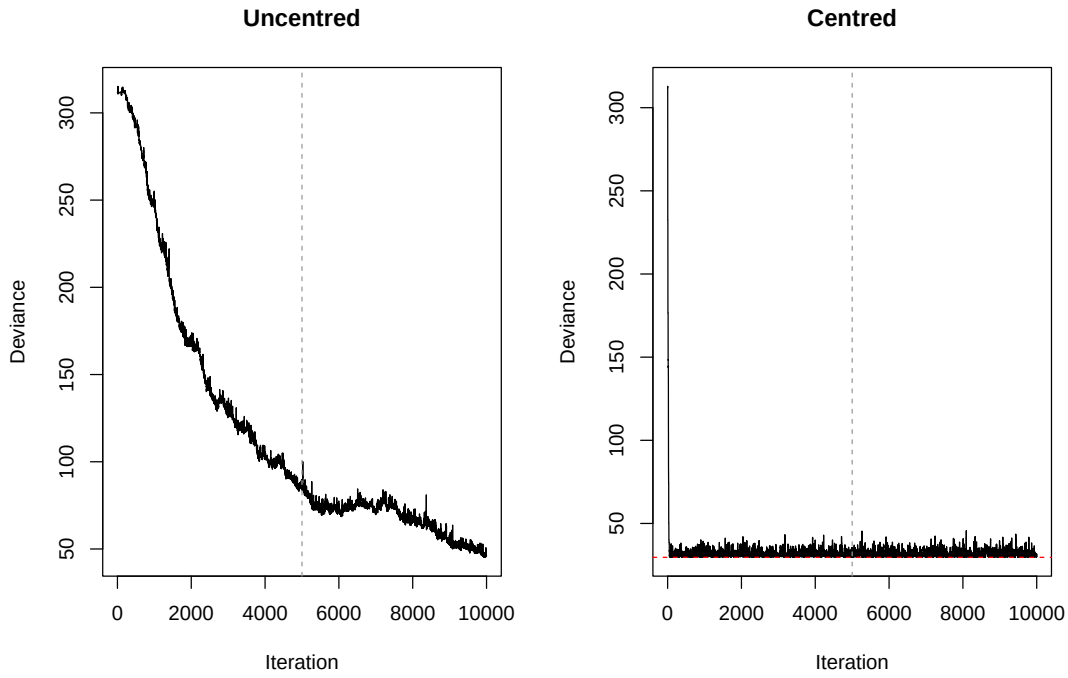
```r
abline(v = 5000, col = 'grey60', lty = 2); abline(h = -0.0431, col = 'red', lty = 2)
plot(fitC$all[, 2], type = 'l', xlab = 'Iteration', ylab = expression(beta[2]),
     main = 'Centred: beta2')
abline(v = 5000, col = 'grey60', lty = 2); abline(h = 22.04, col = 'red', lty = 2)
acf(fitC$sims[, 1], lag.max = 100, main = 'ACF beta1 (post burn-in)')
acf(fitC$sims[, 2], lag.max = 100, main = 'ACF beta2 (post burn-in)')
```



Enormously improved: the traces are stationary fuzz within a few hundred iterations, lag-1 autocorrelation falls from 0.999 to 0.66 with the ACF indistinguishable from zero by lag 10, and the posterior correlation falls from -0.9995 to -0.13. Centring makes β_1 the value of $\log[-\log(1-\pi)]$ at the **mean** dose, which the data determine almost independently of the slope; geometrically the ridge is rotated onto the coordinate axes, so single-component updates move along the directions in which the posterior varies. It costs nothing – the original intercept is $\beta_1 - 22.20 \times 1.793425 = -39.86$ against the classical -39.57. The posterior mean $(-0.045, 22.20)$ and mean deviance 31.69 match the $(-0.046, 22.1)$ and 31.7 of Section 13.6.

(h) Deviance plots.

```r
par(mfrow = c(1, 2))
plot(fitU$all[, 3], type = 'l', xlab = 'Iteration', ylab = 'Deviance',
     main = 'Uncentred')
abline(v = 5000, col = 'grey60', lty = 2); abline(h = 29.64, col = 'red', lty = 2)
plot(fitC$all[, 3], type = 'l', xlab = 'Iteration', ylab = 'Deviance',
     main = 'Centred')
abline(v = 5000, col = 'grey60', lty = 2); abline(h = 29.64, col = 'red', lty = 2)
```




```
rbind(uncentred = c(min = min(fitU$sims[, 3]), mean = mean(fitU$sims[, 3])),
      centred   = c(min = min(fitC$sims[, 3]), mean = mean(fitC$sims[, 3])))
```

```
              min     mean
uncentred 45.21887 66.36451
centred   29.64473 31.69374
```

The deviance trace is the most useful diagnostic here, one number summarising the whole parameter vector.

- **Uncentred**: it falls monotonically for all 10,000 iterations, 312 down to about 46, never levelling off and never nearing the attainable 29.6. A deviance still falling at the end proves the chain is in transient burn-in and the retained sample worthless.
- **Centred**: it drops from 312 to about 30 within a couple of hundred iterations, then hovers above a floor of 29.64 with occasional upward excursions – the hard lower bound with right skew a converged trace should show. Its mean 31.69 is $\bar{D}$ of Equation (13.5) and its floor is $D(\mathbf{y} \mid \widehat{\boldsymbol{\beta}}) = 29.64$, so the gap already gives $p_D \approx 2$, the number of parameters (formalised in Exercise 13.4).

(i) Starting values from `glm`*.*

```
g <- glm(cbind(y, n - y) ~ x, family = binomial(link = 'cloglog'), data = beetle)
coef(g)
fitI <- bugs.mh(centre = FALSE, init = unname(coef(g)))
smry(fitI)
c(corr = cor(fitI$sims[, 1], fitI$sims[, 2]),
  acf1 = acf(fitI$sims[, 2], lag.max = 1, plot = FALSE)$acf[2])
```

```
(Intercept)           x
  -39.57231    22.04117
              mean     sd q2.5.2.5%   median q97.5.97.5%
beta1    -39.3067 1.0640  -41.1120 -39.2347    -37.3687
beta2     21.8923 0.5897   20.8350  21.8556     22.9080
deviance  30.7554 1.3838   29.6638  30.2350     34.6521
      corr       acf1
-0.9972387  0.9977377
```

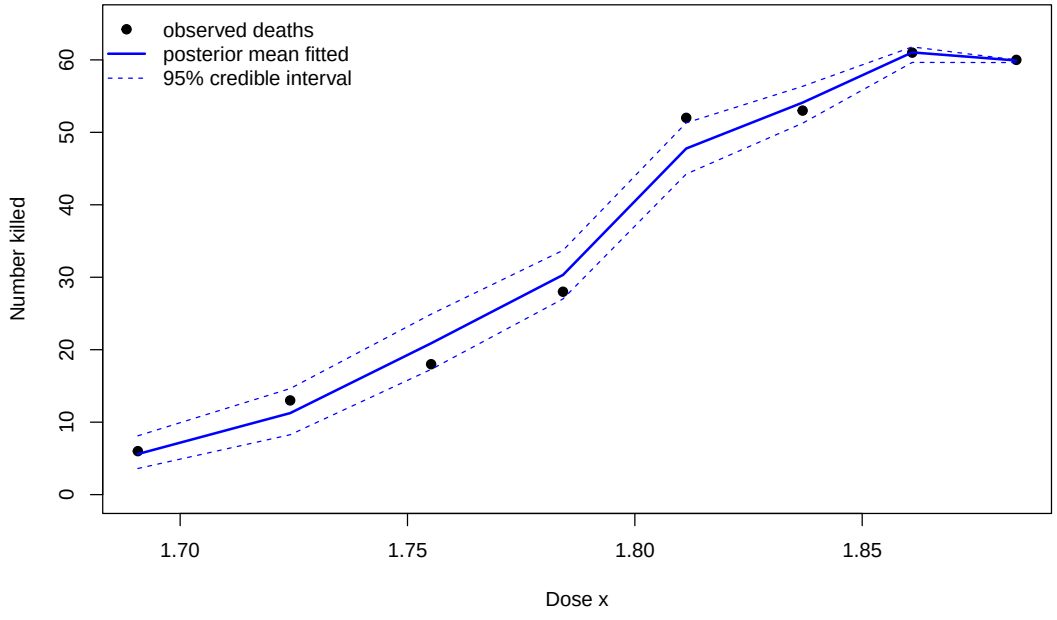
The `glm` fit gives the maximum likelihood solution $\widehat{\beta}_1 = -39.57$, $\widehat{\beta}_2 = 22.04$, and with priors this vague the posterior mode is essentially the MLE, so these are near-perfect starting values. Started there the uncentred chain is immediately in the right region and its deviance summaries ($\bar{D} = 30.8$, floor 29.66) are close to correct, where from $(0, 0)$ it was still 12 units from the mode after 10,000 iterations. What is **not** fixed: posterior correlation -0.997 and lag-1 autocorrelation 0.998 remain, so the chain still crawls along the ridge and its intervals are too narrow (95% for β_2 is $[20.8, 22.9]$ against the correct

centred $[18.7, 25.9]$). Good starting values cure burn-in, not mixing; centring cures both, so do both.
(j) Adding `fitted[i]<-n[i]*pi[i]` to the monitored parameters gives a posterior for each of the eight expected counts, hence mean and 95% credible interval directly – no delta method, only quantiles of the sampled values.

```
fitF <- bugs.mh(centre = TRUE, monitor.fitted = TRUE)
fv <- t(apply(fitF$fitted, 2, function(z) c(mean(z), quantile(z, c(.025, .975)))))
round(cbind(x = beetle$x, observed = beetle$y, fitted = fv[, 1],
            lower = fv[, 2], upper = fv[, 3]), 3)
```

```
      x observed fitted  lower  upper
[1,] 1.691        6  5.601  3.604  8.113
[2,] 1.724       13 11.251  8.264 14.638
[3,] 1.755       18 20.886 17.284 24.906
[4,] 1.784       28 30.320 27.012 33.711
[5,] 1.811       52 47.767 44.245 51.311
[6,] 1.837       53 54.104 51.263 56.353
[7,] 1.861       61 61.034 59.649 61.790
[8,] 1.884       60 59.917 59.631 59.998
```

```
plot(beetle$x, beetle$y, pch = 19, ylim = c(0, 65), xlab = 'Dose x',
     ylab = 'Number killed', main = '')
lines(beetle$x, fv[, 1], col = 'blue', lwd = 2)
lines(beetle$x, fv[, 2], col = 'blue', lty = 2)
lines(beetle$x, fv[, 3], col = 'blue', lty = 2)
legend('topleft', bty = 'n', pch = c(19, NA, NA), lty = c(NA, 1, 2),
       lwd = c(NA, 2, 1), col = c('black', 'blue', 'blue'),
       legend = c('observed deaths', 'posterior mean fitted',
                  '95% credible interval'))
```

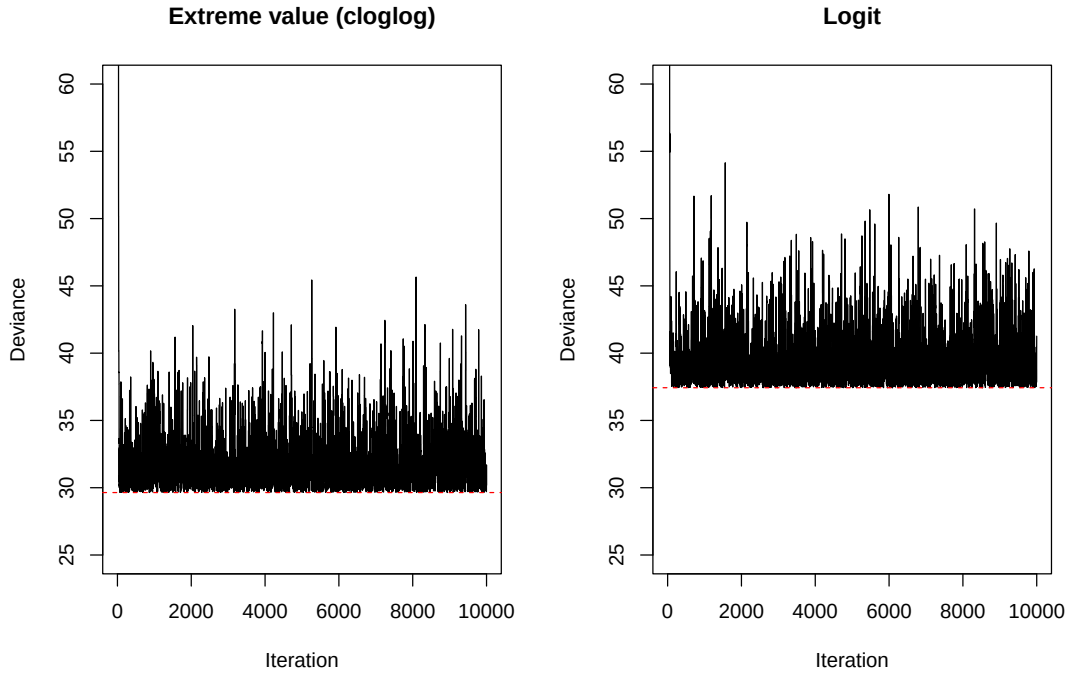


Every observed count lies inside its interval, so the model describes all eight groups adequately. The largest discrepancies are at doses 3 and 5 (over-predicting by 3, under-predicting by 4), the two groups dominating the classical residual deviance 3.45 on 6 d.f. The bands narrow at the top of the dose range because π is pressed against 1: at $x = 1.8839$ the interval is $[59.6, 60.0]$ out of $n = 60$.
(k) The logit link.

```
fitL <- bugs.mh(centre = TRUE, link = 'logit')
smry(fitL)
rbind(cloglog = c(Dbar = mean(fitF$sims[, 3]), Dmin = min(fitF$sims[, 3])),
      logit   = c(Dbar = mean(fitL$sims[, 3]), Dmin = min(fitL$sims[, 3])))
```

```
             mean     sd q2.5.2.5%  median q97.5.97.5%
beta1      0.7464 0.1383    0.4834  0.7419      1.0141
beta2     34.6060 3.0212   28.7253 34.4808     40.8803
deviance 39.4939 2.0472   37.4906 38.8297     45.0683
             Dbar     Dmin
cloglog 31.69374 29.64473
logit   39.49394 37.43073
```

```
par(mfrow = c(1, 2))
plot(fitF$all[, 3], type = 'l', ylim = c(25, 60), xlab = 'Iteration',
     ylab = 'Deviance', main = 'Extreme value (cloglog)')
abline(h = 29.64, col = 'red', lty = 2)
plot(fitL$all[, 3], type = 'l', ylim = c(25, 60), xlab = 'Iteration',
     ylab = 'Deviance', main = 'Logit')
abline(h = 37.43, col = 'red', lty = 2)
```



Both traces converge quickly (centring works for either link) but settle at different levels: the logit floors at 37.43 and averages 39.49, the extreme-value floors at 29.64 and averages 31.69. A gap of 7.8 deviance units at equal parameter count is decisive for the extreme-value link, as classically (residual deviance 3.45 on 6 d.f. against 11.23; AIC 33.64 against 41.43). The logit is symmetric about $\pi = 0.5$, forcing mirror-image approaches to 0 and 1, whereas the observed approach to 1 is far more gradual than the departure from 0; the symmetric curve must compromise, fitting the low doses and the top dose badly. This is the comparison of Section 7.3.1, formalised as DIC in Exercise 13.4(f).

13.4 Problem 13.4 — This exercise is about calculating the deviance information criterion

Problem 13.4. This exercise is about calculating the deviance information criterion (DIC). The two key equations are (13.5) and (13.6) for the number of parameters (p_D) and DIC, respectively.
a. R2WinBUGS calculates the DIC automatically; extract the values by typing `bugs.res$pD` and `bugs.res$DIC`.
b. Use the chains for the deviance and beta parameters to calculate $\overline{D(\mathbf{y} \mid \boldsymbol{\beta})}$ and $D(\mathbf{y} \mid \overline{\boldsymbol{\beta}})$, from which you can estimate p_D and the DIC.
c. Write the results from a. in the first row of the table below and the results from b. in the second row. How well do the calculated results match those calculated by R2WinBUGS? The table has columns $\overline{D(\mathbf{y} \mid \boldsymbol{\beta})}$ (Dbar), $D(\mathbf{y} \mid \widehat{\boldsymbol{\beta}})$ (Dhat), p_D and DIC, and rows labelled "DIC", "Mean of $\boldsymbol{\beta}$",

"Median of $\boldsymbol{\beta}$" and "Half variance of $D(.)$".
d. The mean is just one estimate of the "best possible" deviance; the median could be used instead. Calculate the deviance at the medians of $\boldsymbol{\beta}$, then calculate the alternative values for p_D and DIC. Write these values in the third row of the table.
e. Another alternative calculation for p_D is the variance of $D(\mathbf{y} \mid \widehat{\boldsymbol{\beta}})$ divided by 2. Calculate this alternative p_D and alternative DIC and write the results in the last row of the table. Comment on the differences in the complete table.
f. Re-run exercise 13.4 but this time using a logit link. Which link function gives the best fit? Was the difference consistent regardless of the method used to calculate $D(\mathbf{y} \mid \widehat{\boldsymbol{\beta}})$?
g. Having been through the calculations for the DIC in detail, when might it not work well? (difficulty: ⋆⋆)

Solution. All four ways of estimating $\widehat{D}$ give p_D between 2.04 and 2.17 and a DIC difference between the links of 7.72 to 7.81, so the extreme-value link wins whichever is used. The chains are those of Exercise 13.3 – centred beetle mortality, 10,000 iterations with 5,000 burn-in, run with each link – and the monitored deviance is $D(\mathbf{y} \mid \boldsymbol{\beta}) = -2 \log p(\mathbf{y} \mid \boldsymbol{\beta})$ including the Binomial constant, as WinBUGS reports. Equations (13.5) and (13.6) are

$$p_D = \overline{D(\mathbf{y} \mid \boldsymbol{\beta})} - D(\mathbf{y} \mid \overline{\boldsymbol{\beta}}), \qquad \text{DIC} = \overline{D(\mathbf{y} \mid \boldsymbol{\beta})} + p_D.$$

(a) R2WinBUGS is unavailable here, so its reported `pD` cannot be obtained; but when it computes DIC from the returned simulations it uses not Equation (13.5) but

$$p_D = \tfrac{1}{2}\widehat{\text{var}}\left[D(\mathbf{y} \mid \boldsymbol{\beta})\right], \qquad \text{DIC} = \overline{D} + p_D,$$

the "half variance of $D(.)$" rule of part (e). Rows 1 and 4 of the table are therefore the same calculation and agree exactly, which answers (c): they match row 4 by construction and differ slightly from rows 2 and 3, which use (13.5). (The claim about R2WinBUGS's internals is from documentation, not verified here; the rest of the table is computed from the chains.)
(b)–(e)

```
library(dobson); data(beetle)
xc <- beetle$x - mean(beetle$x)
invlink <- function(eta, link)
  if (link == 'cloglog') 1 - exp(-exp(eta)) else 1 / (1 + exp(-eta))
devf <- function(b, link) {
  pi <- invlink(b[1] + b[2] * xc, link)
  -2 * sum(dbinom(beetle$y, beetle$n, pi, log = TRUE)) }

dic.table <- function(sims, link) {
  D <- sims[, 3]
  Dbar <- mean(D)
  bmean <- colMeans(sims[, 1:2]); bmed <- apply(sims[, 1:2], 2, median)
  Dhat.mean <- devf(bmean, link)
  Dhat.med  <- devf(bmed,  link)
  pD.hv <- var(D) / 2
  rbind(
    'DIC (R2WinBUGS)'      = c(Dbar, Dbar - pD.hv, pD.hv, Dbar + pD.hv),
    'Mean of beta'         = c(Dbar, Dhat.mean, Dbar - Dhat.mean, 2*Dbar - Dhat.mean),
    'Median of beta'       = c(Dbar, Dhat.med,  Dbar - Dhat.med,  2*Dbar - Dhat.med),
    'Half variance of D(.)'= c(Dbar, Dbar - pD.hv, pD.hv, Dbar + pD.hv))
}
colnames.dic <- c('Dbar', 'Dhat', 'pD', 'DIC')
```

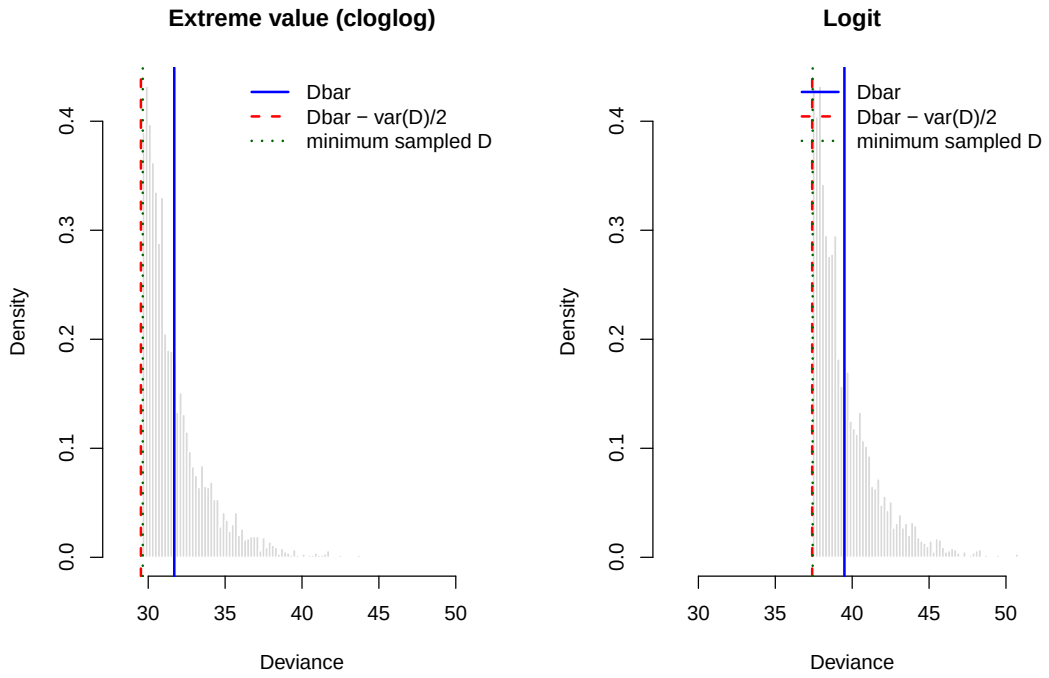
The chains `fitF` (extreme value) and `fitL` (logit) are those built in Exercise 13.3.

```
tabF <- dic.table(fitF$sims, 'cloglog'); colnames(tabF) <- colnames.dic
round(tabF, 3)
round(rbind(mean = colMeans(fitF$sims[, 1:2]),
            median = apply(fitF$sims[, 1:2], 2, median)), 4)
```

```
                        Dbar   Dhat    pD    DIC
DIC (R2WinBUGS)       31.694 29.523 2.170 33.864
Mean of beta          31.694 29.652 2.041 33.735
Median of beta        31.694 29.650 2.044 33.738
Half variance of D(.) 31.694 29.523 2.170 33.864
         beta1   beta2
mean   -0.0449 22.1998
median -0.0461 22.1618
```

- The four versions agree: p_D from 2.04 to 2.17, DIC from 33.74 to 33.86, a spread of 0.13 far below the "less than 5 is small" guideline of Section 13.6.
- $\bar{D} = 31.69$ is identical in every row, depending only on the sampled deviances.
- The mean of $\boldsymbol{\beta}$ gives $p_D = 2.04$, close to the two fitted parameters – the classical justification for (13.5), valid here because the posterior is nearly Normal and the deviance nearly quadratic.
- The median $(-0.0461, 22.16)$ is almost the mean $(-0.0449, 22.20)$, so rows 2 and 3 differ by 0.003: the marginals are near-symmetric. Under skew they separate, and the median is the more robust summary.
- The half-variance rule gives 2.17. The two estimators are only asymptotically equivalent, agreeing exactly when the deviance is quadratic and the posterior Normal, so that $D - D(\widehat{\boldsymbol{\beta}}) \sim \chi^2_p$ with mean p and variance $2p$ and both $\bar{D} - \widehat{D}$ and $\frac{1}{2}\text{var}(D)$ estimate p. The 6% excess reflects mild non-quadratic curvature plus Monte Carlo error, a variance being estimated far less precisely than a mean.
- Equation (13.5) returns a negative p_D whenever $\overline{D} < D(\overline{\boldsymbol{\beta}})$, a symptom of a multimodal or badly skewed posterior; the half-variance rule is a variance and cannot be negative, which is why R2WinBUGS prefers it.

```r
par(mfrow = c(1, 2))
for (nm in list(list(f = fitF, t = 'Extreme value (cloglog)'),
                list(f = fitL, t = 'Logit'))) {
  D <- nm$f$sims[, 3]
  hist(D, breaks = 60, col = 'grey85', border = 'white', xlab = 'Deviance',
       freq = FALSE, main = nm$t, xlim = c(28, 52))
  abline(v = mean(D),               col = 'blue',      lwd = 2)
  abline(v = mean(D) - var(D) / 2,  col = 'red',       lwd = 2, lty = 2)
  abline(v = min(D),                col = 'darkgreen', lwd = 2, lty = 3)
  legend('topright', bty = 'n', lwd = 2, lty = c(1, 2, 3),
         col = c('blue', 'red', 'darkgreen'),
         legend = c('Dbar', 'Dbar - var(D)/2', 'minimum sampled D'))
}
```



The histograms show why the four versions agree: the sampled deviance is approximately $D(\widehat{\boldsymbol{\beta}}) + \chi^2_2$, a hard lower bound with right skew, and $\widehat{D}$ lands at its bottom edge in both cases.

(f) The logit link.

```
tabL <- dic.table(fitL$sims, 'logit'); colnames(tabL) <- colnames.dic
round(tabL, 3)
round(tabL[, 'DIC'] - tabF[, 'DIC'], 3)
```

```
                        Dbar   Dhat    pD    DIC
DIC (R2WinBUGS)       39.494 37.398 2.095 41.589
Mean of beta          39.494 37.444 2.050 41.544
Median of beta        39.494 37.437 2.057 41.551
Half variance of D(.) 39.494 37.398 2.095 41.589
      DIC (R2WinBUGS)          Mean of beta        Median of beta
                7.725                 7.809                 7.813
Half variance of D(.)
                7.725
```

The extreme-value link fits best, DIC about 33.8 against 41.6, and the difference is consistent: all four estimators give between 7.72 and 7.81, a spread of 0.09 against a signal of 7.8, so the choice of estimator affects only the third significant figure. Since $p_D \approx 2$ in both models, DIC here is essentially $D(\widehat{\boldsymbol{\beta}}) + 2 \times 2$, the AIC, and the classical AICs 33.64 and 41.43 are within 0.25 of every DIC in the two tables – with vague priors and a well-behaved two-parameter model DIC reduces to AIC, as Section 13.6 says. A gap of 7.8 sits in that section's intermediate zone, so the extreme-value link is clearly preferred on evidence that is strong rather than overwhelming; the substantive reason is the asymmetry established in Exercise 13.3(c),(k).

(g) The calculations worked because this model is benign – two parameters, unimodal near-Normal posterior, nearly quadratic deviance, vague priors, converged chain – and each condition is a failure point.

1. **Multimodal or badly skewed posteriors** (Section 13.6). With several minima $\overline{\boldsymbol{\beta}}$ can fall between the modes where the deviance is high, so $D(\overline{\boldsymbol{\beta}})$ is not minimal and p_D from (13.5) is too small or negative. Mixture models with label switching are the standard pathology.
2. **Non-invariance to parameterisation.** The mean of $\log\sigma$ is not the log of the mean of σ, so algebraically equivalent parameterisations give different $D(\overline{\boldsymbol{\beta}})$, p_D and DIC; Exercise 13.3(g) shows how routine reparameterisation is. The half-variance p_D avoids this.
3. **Dependence on priors and parameter space** (Section 13.6). Informative or restricting priors change the effective number of parameters, so DIC cannot compare models with different prior

structures.

4. **The focus problem.** In a hierarchical model the deviance may be conditional on the random effects or have them integrated out, giving different p_D and DIC with neither canonically correct; WinBUGS reports the conditional form, which answers about new observations in existing groups.
5. **Unconverged or poorly mixing chains.** All DIC quantities are Monte Carlo averages: Exercise 13.3(f)'s chain gave $\bar{D} = 66.4$ instead of 31.7, with no warning label. The half-variance p_D is the more fragile, a variance needing many more effective samples than a mean.
6. **Missing data and latent variables.** With missing values imputed inside the MCMC, "the data" change between iterations and $\bar{D}$ is not meaningful.
7. **Non-standard likelihoods.** D includes the normalising constant, so comparing likelihood families is safe only if it is retained consistently in both.
8. **Small samples.** The argument tying p_D to the parameter count is asymptotic; at $N = 8$ it worked here partly by luck.

DIC is a guide, not a decision rule: check the deviance trace first, compute p_D both ways and be suspicious if they disagree or if p_D is far from the parameter count, and treat differences below about 5 as inconclusive.

14 Example Bayesian Analyses

Contents

14.1 Problem 14.1 — Confirm that setting $\varphi 1 = 1$ in model (14.1) gives model (8.11).

Problem 14.1. Confirm that setting $\phi_1 = 1$ in model (14.1) gives model (8.11). (difficulty: ⋆)

Solution. The sum $\sum_k \phi_k$ cancels from π_j/π_1, so $\phi_1 = 1$ turns (14.1) into (8.11). Model (14.1), the WinBUGS parameterisation of Section 14.3, introduces non-negative ϕ_1, ϕ_2, ϕ_3 with

$$\log(\phi_j) \;=\; \beta_{0j} + \beta_{1j}x_1 + \beta_{2j}x_2 + \beta_{3j}x_3, \qquad j = 2, 3,$$

$$\pi_j \;=\; \frac{\phi_j}{\sum_{k=1}^{3} \phi_k}, \qquad j = 1, 2, 3.$$

while (8.11) is the nominal logistic regression with "no or little importance" as reference,

$$\log\left(\frac{\pi_j}{\pi_1}\right) \;=\; \beta_{0j} + \beta_{1j}x_1 + \beta_{2j}x_2 + \beta_{3j}x_3, \qquad j = 2, 3.$$

A constraint is needed because $\boldsymbol{\phi} \mapsto \boldsymbol{\pi}$ is invariant to rescaling – $\phi_k \mapsto c\phi_k$ leaves every π_j unchanged – so $\boldsymbol{\phi}$ is identified only up to a positive multiple, and $\phi_1 = 1$ (i.e. $c = 1/\phi_1$) is one free normalisation. Taking the ratio, the common sum cancels:

$$\frac{\pi_j}{\pi_1} \;=\; \frac{\phi_j / \sum_{k=1}^{3} \phi_k}{\phi_1 / \sum_{k=1}^{3} \phi_k} \;=\; \frac{\phi_j}{\phi_1}.$$

and imposing $\phi_1 = 1$ gives $\pi_j/\pi_1 = \phi_j$, so

$$\log\left(\frac{\pi_j}{\pi_1}\right) \;=\; \log(\phi_j) \;=\; \beta_{0j} + \beta_{1j}x_1 + \beta_{2j}x_2 + \beta_{3j}x_3, \qquad j = 2, 3,$$

precisely (8.11) – the line `phi[i,1]<-1; # For identifiability` in the Section 14.3 code. At $j = 1$ both models are degenerate, $\log(\pi_1/\pi_1) = \log 1 = 0$, so $\phi_1 = 1$ says $\beta_{01} = \beta_{11} = \beta_{21} = \beta_{31} = 0$: the corner-point constraint making category 1 the reference. Inverting,

$$\pi_1 = \frac{1}{1 + \phi_2 + \phi_3}, \qquad \pi_j = \frac{\phi_j}{1 + \phi_2 + \phi_3} \quad (j = 2, 3),$$

so $\sum_j \pi_j = 1$ by construction and each $\pi_j > 0$ since $\phi_j = \exp(\cdot) > 0$: the multinomial constraints hold automatically, which is why WinBUGS uses this form – the β's are unconstrained, so vague Normal priors can never propose a $\boldsymbol{\pi}$ outside the simplex. Numerically, for the reference cell (women aged 18–23, $x_1 = x_2 = x_3 = 0$) with the Table 14.5 posterior means:

```r
b02 <- -0.602; b03 <- -1.063
phi <- c(1, exp(b02), exp(b03))
pi.hat <- phi / sum(phi)
round(pi.hat, 4)
round(log(pi.hat[2:3] / pi.hat[1]), 4)   # should return b02, b03
```

```
[1] 0.5282 0.2893 0.1825
[1] -0.602 -1.063
```

The fitted preference probabilities are $(0.53, 0.29, 0.18)$ and the log ratios return β_{02}, β_{03} exactly.

14.2 Problem 14.2 — Prove that the latent variable model (14.2) is equal to the proportional odds

Problem 14.2. Prove that the latent variable model (14.2) is equal to the proportional odds model (8.17). (difficulty: ⋆⋆)

Solution. Negating (14.2) gives (8.14) with $\beta_{0j}^* = C_j - \beta_0$ and $\beta_k^* = -\beta_k$. The latent variable formulation of Section 14.4 has an unobserved continuous z and ordered cutpoints $C_1 < \cdots < C_{J-1}$, the observed category being j when $C_{j-1} < z \le C_j$ ($C_0 = -\infty$, $C_J = +\infty$). With

$$Q_j \;=\; P(z > C_j), \qquad j = 1, \ldots, J-1,$$

model (14.2) is

$$\log\left(\frac{Q_j}{1-Q_j}\right) \;=\; \log\left(\frac{P(z > C_j)}{P(z \le C_j)}\right) \;=\; \mathbf{x}^T\boldsymbol{\beta} - C_j.$$

and $\boldsymbol{\beta}$ carries no j subscript: one slope vector for every cutpoint, only the intercept $-C_j$ varying. Since category j is the event $C_{j-1} < z \le C_j$, telescoping gives

$$P(z \le C_j) \;=\; \sum_{k=1}^{j} \pi_k \;=\; \pi_1 + \cdots + \pi_j, \qquad P(z > C_j) \;=\; \pi_{j+1} + \cdots + \pi_J.$$

(hence also Section 14.4's $\pi_1 = 1 - Q_1$, $\pi_j = Q_{j-1} - Q_j$, $\pi_J = Q_{J-1}$), so

$$\frac{Q_j}{1-Q_j} \;=\; \frac{\pi_{j+1} + \cdots + \pi_J}{\pi_1 + \cdots + \pi_j},$$

the **reciprocal** of the odds in (8.14). Substituting into (14.2) and negating,

$$\log\left(\frac{\pi_{j+1} + \cdots + \pi_J}{\pi_1 + \cdots + \pi_j}\right) \;=\; \mathbf{x}^T\boldsymbol{\beta} - C_j \quad\Longleftrightarrow\quad \log\left(\frac{\pi_1 + \cdots + \pi_j}{\pi_{j+1} + \cdots + \pi_J}\right) \;=\; C_j - \mathbf{x}^T\boldsymbol{\beta}.$$

whose intercept depends on j and whose slopes do not: exactly the proportional odds model (8.14),

$$\log\left(\frac{\pi_1 + \cdots + \pi_j}{\pi_{j+1} + \cdots + \pi_J}\right) \;=\; \beta_{0j}^* + \beta_1^* x_1 + \cdots + \beta_{p-1}^* x_{p-1},$$

under the correspondence

$$\beta_{0j}^* \;=\; C_j - \beta_0, \qquad \beta_k^* \;=\; -\beta_k \quad (k = 1, \ldots, p-1),$$

with β_0 the constant inside $\mathbf{x}^T\boldsymbol{\beta}$. For the car preference data $J = 3$ and x_1, x_2, x_3 are the sex and age dummies of (8.11), so

$$\log\left(\frac{\pi_1}{\pi_2 + \pi_3}\right) = C_1 - \beta_0 - \beta_1 x_1 - \beta_2 x_2 - \beta_3 x_3, \qquad \log\left(\frac{\pi_1 + \pi_2}{\pi_3}\right) = C_2 - \beta_0 - \beta_1 x_1 - \beta_2 x_2 - \beta_3 x_3,$$

model (8.17) with $\beta_{01}^* = C_1 - \beta_0$ and $\beta_{02}^* = C_2 - \beta_0$. Two points.

- β_0 and the cutpoints are confounded – only $C_j - \beta_0$ is estimable – which is why the Section 14.4 code fixes $C_1 \leftarrow 0$ and lets `beta[1]` absorb the location. The ordering $C_1 < \cdots < C_{J-1}$, enforced by the nested Uniform priors $C_j \sim U[C_{j-1}, C_{j+1}]$, gives $Q_1 > Q_2 > \ldots$ and hence non-negative π_j.
- The slopes carry opposite signs in the two orientations: in (14.2) a positive β_k raises $P(z > C_j)$ for every j, so $\exp(\beta_k)$ is the odds ratio for a **higher** category as Table 14.6 says, while the derivation puts $-\beta_k$ on the lower-category side. Table 8.4 nevertheless matches Table 14.6 in sign (-0.576 against -0.580, 1.147 against 1.162, 2.232 against 2.258) because it reports `polr`, which parameterises the cumulative model as logit $P(Y \le j) = \zeta_j - \mathbf{x}^T\boldsymbol{\eta}$ with the minus sign built in. So (8.17) as printed does not match the signs tabulated beneath it; the fitted π_j are identical either way.

Reconstructing the fitted probabilities from $Q_j = \text{expit}(\mathbf{x}^T\boldsymbol{\beta} - C_j)$ with $C_j = \zeta_j$ reproduces `polr`'s own values to machine precision.

```
library(MASS)
sex  <- rep(c("women","men"), each = 3)
age  <- rep(c("18-23","24-40",">40"), 2)
freq <- rbind(c(26,12,7), c(9,21,15), c(5,14,41),
```

```
              c(40,17,8), c(17,15,12), c(8,15,18))
d <- data.frame(sex = factor(sex, levels = c("women","men")),
                age = factor(age, levels = c("18-23","24-40",">40")))
long <- d[rep(1:6, times = rowSums(freq)), ]
long$resp <- factor(unlist(apply(freq, 1, function(r) rep(1:3, r))),
                    levels = 1:3, ordered = TRUE)
fit <- polr(resp ~ sex + age, data = long, Hess = TRUE)
round(c(coef(fit), fit$zeta), 4)
# rebuild pi from the latent-variable model (14.2): Q_j = expit(x'beta - C_j)
X  <- model.matrix(~ sex + age, data = d)[, -1, drop = FALSE]
xb <- as.vector(X %*% coef(fit))
Q  <- sapply(fit$zeta, function(C) plogis(xb - C))
pr <- cbind(1 - Q[, 1], Q[, 1] - Q[, 2], Q[, 2])
round(pr, 4)
max(abs(pr - predict(fit, newdata = d, type = "probs")))
```

```
  sexmen age24-40   age>40      1|2      2|3
 -0.5762   1.1471   2.2325   0.0435   1.6550
       [,1]   [,2]   [,3]
[1,] 0.5109 0.3287 0.1604
[2,] 0.2491 0.3752 0.3757
[3,] 0.1007 0.2588 0.6405
[4,] 0.6502 0.2529 0.0970
[5,] 0.3711 0.3761 0.2527
[6,] 0.1662 0.3335 0.5003
[1] 1.110223e-16
```

The cutpoints $\hat{C}_1 = 0.044$, $\hat{C}_2 = 1.655$ are the intercepts of Table 8.4; the reference-cell probabilities $(0.5109, 0.3287, 0.1604)$ are those quoted in Section 8.4.6; the slopes $(-0.576, 1.147, 2.232)$ match Table 14.6 to within Monte Carlo error. The two are the same model fitted by different algorithms.

14.3 Problem 14.3 — a. Run the Weibull model for the remission times survival data, but this

Problem 14.3. a. Run the Weibull model for the remission times survival data, but this time monitor the DIC.
b. Create an exponential model for the remission times in WinBUGS. Monitor the DIC. Is the exponential model a better model than the Weibull? Compare the results with Section 10.7. (difficulty: ⋆⋆)

Solution. The exponential model is not better, but only just: DIC 221.05 against the Weibull's 219.45. WinBUGS being unavailable, both are fitted with a random walk Metropolis sampler written in R, whose posterior summaries reproduce Table 14.7 to within Monte Carlo error. Following the Section 14.5 code, y_i is Weibull with shape λ and scale ϕ_i, so

$$S(y_i) = \exp\left(-\phi_i y_i^{\lambda}\right), \qquad f(y_i) = \lambda\phi_i y_i^{\lambda-1}\exp\left(-\phi_i y_i^{\lambda}\right), \qquad \log\phi_i = \beta_0 + \beta_1 x_i,$$

with $x_i = 1$ for the 6-mercaptopurine group. The hazard $h(y) = \lambda y^{\lambda-1}\exp(\beta_0 + \beta_1 x)$ is the Weibull proportional hazards model of Section 10.7, so the parameters are comparable with Table 10.3, and $\lambda = 1$ gives the exponential model. With $\delta_i = 1$ for an observed remission and 0 for right censoring,

$$\ell = \sum_{i=1}^{42}\Big[\delta_i\big\{\log\lambda + \log\phi_i + (\lambda-1)\log y_i\big\} - \phi_i y_i^{\lambda}\Big],$$

censored observations contributing only $\log S(y_i) = -\phi_i y_i^{\lambda}$. The priors are the book's, $\beta_0, \beta_1 \sim N(0, 1000)$ and $\lambda \sim \text{Exp}(0.001)$, with sampling on $\log\lambda$ (Jacobian included) so all three parameters live on the line. One difference from WinBUGS: it treats a censored time as missing data from a truncated Weibull and computes the deviance on an augmented likelihood, whereas this sampler integrates the censored times out analytically. The posteriors are identical either way, but the absolute deviance level, hence the numerical DIC, differs; since both models here use the same likelihood, the

DIC **comparison** is unaffected.

(a) Weibull model with DIC.

```
library(dobson)
data(remission)
y <- remission$time
d <- as.numeric(remission$censored == 0)   # 1 = remission observed
x <- as.numeric(remission$group == "T")    # 1 = 6-MP treatment

loglik <- function(p, weib = TRUE) {       # p = c(beta0, beta1, log lambda)
  lam  <- if (weib) exp(p[3]) else 1
  lphi <- p[1] + p[2] * x
  sum(d * (log(lam) + lphi + (lam - 1) * log(y)) - exp(lphi) * y^lam)
}
logpost <- function(p, weib = TRUE) {
  lp <- loglik(p, weib) + sum(dnorm(p[1:2], 0, sqrt(1000), log = TRUE))
  if (weib) lp <- lp + dexp(exp(p[3]), 0.001, log = TRUE) + p[3]
  lp
}
mcmc <- function(weib, init, sd.prop, n.burn = 5000, n.keep = 20000, seed = 1) {
  set.seed(seed)
  k <- if (weib) 3 else 2
  cur <- init; lc <- logpost(cur, weib); out <- matrix(NA, n.keep, k)
  for (it in 1:(n.burn + n.keep)) {
    prop <- cur + rnorm(k, 0, sd.prop)
    lp <- logpost(prop, weib)
    if (log(runif(1)) < lp - lc) { cur <- prop; lc <- lp }
    if (it > n.burn) out[it - n.burn, ] <- cur
  }
  out
}
rhat <- function(ch) sapply(seq_len(ncol(ch[[1]])), function(j) {
  xs <- sapply(ch, function(z) z[, j]); n <- nrow(xs)
  W <- mean(apply(xs, 2, var)); B <- n * var(colMeans(xs))
  sqrt(((n - 1) / n * W + B / n) / W)
})
ch <- lapply(1:2, function(s) mcmc(TRUE, c(-3, -1.7, log(1.4)),
                                   c(0.35, 0.35, 0.11), seed = s))
W <- rbind(ch[[1]], ch[[2]]); W[, 3] <- exp(W[, 3])
colnames(W) <- c("beta0", "beta1", "lambda")
round(t(apply(W, 2, function(z)
      c(mean = mean(z), sd = sd(z), quantile(z, c(.025, .975))))), 3)
round(rhat(ch), 4)
```

```
         mean    sd   2.5%  97.5%
beta0  -3.141 0.587 -4.366 -2.031
beta1  -1.774 0.425 -2.674 -0.990
lambda  1.383 0.210  0.992  1.819
[1] 1.0018 1.0005 1.0014
```

The Gelman-Rubin statistics are all essentially 1, so the chains have converged, and the posterior means reproduce Table 14.7 ($\beta_1 = -1.778$, $\beta_0 = -3.162$, $\lambda = 1.39$). The median survival times follow from $\text{median} = \{\log 2 \cdot \exp(-\log\phi)\}^{1/\lambda}$ applied to every retained draw.

```
med.c <- (log(2) * exp(-W[, 1]))^(1 / W[, 3])
med.t <- (log(2) * exp(-(W[, 1] + W[, 2])))^(1 / W[, 3])
M <- cbind(control = med.c, treatment = med.t, difference = med.t - med.c)
round(t(apply(M, 2, function(z) c(mean = mean(z), quantile(z, c(.025, .975))))), 3)
```

```
             mean   2.5%  97.5%
control     7.463  4.904 10.477
treatment  27.935 17.113 47.693
difference 20.473  9.121 40.772
```

This matches Table 14.7 (7.538, 27.65, difference 20.11, interval 9.367 to 38.12): median remission is about 28 weeks under 6-MP against 7.5 for controls, an extension of some 20 weeks whose interval excludes zero comfortably. The DIC of Section 13.6 is $\bar{D} + p_D$ with $D(\boldsymbol{\theta}) = -2\ell(\boldsymbol{\theta})$ and $p_D = \bar{D} - D(\bar{\boldsymbol{\theta}})$.

```r
dic <- function(S, weib) {
  tr <- function(p) if (weib) c(p[1], p[2], log(p[3])) else p
  D <- -2 * apply(S, 1, function(p) loglik(tr(p), weib))
  Dbar <- mean(D); Dhat <- -2 * loglik(tr(colMeans(S)), weib)
  c(Dbar = Dbar, Dhat = Dhat, pD = Dbar - Dhat, DIC = Dbar + (Dbar - Dhat))
}
round(dic(W, TRUE), 2)
```

```
  Dbar   Dhat     pD    DIC
216.33 213.21   3.12 219.45
```

Here $p_D = 3.12$ is essentially the actual three, as expected with 42 observations, vague priors and a well-identified likelihood.

(b) Setting $\lambda \equiv 1$ removes one parameter; the sampler and DIC function are reused unchanged.

```r
che <- lapply(1:2, function(s) mcmc(FALSE, c(-2.2, -1.5), c(0.22, 0.42), seed = 10 + s))
E <- rbind(che[[1]], che[[2]]); colnames(E) <- c("beta0", "beta1")
round(t(apply(E, 2, function(z)
      c(mean = mean(z), sd = sd(z), quantile(z, c(.025, .975))))), 3)
round(rhat(che), 4)
mec <- log(2) * exp(-E[, 1]); met <- log(2) * exp(-(E[, 1] + E[, 2]))
ME <- cbind(control = mec, treatment = met, difference = met - mec)
round(t(apply(ME, 2, function(z) c(mean = mean(z), quantile(z, c(.025, .975))))), 3)
round(dic(E, FALSE), 2)
```

```
        mean    sd   2.5%  97.5%
beta0 -2.188 0.217 -2.636 -1.787
beta1 -1.556 0.404 -2.380 -0.794
[1] 1.0000 1.0004
             mean   2.5%  97.5%
control     6.332  4.141  9.677
treatment  31.183 15.677 60.791
difference 24.851  8.945 54.360
  Dbar   Dhat     pD    DIC
219.07 217.09   1.98 221.05
```

So the exponential is not better: DIC falls from 221.05 to 219.45, a change of 1.6, conventionally inconsequential. The Weibull buys that with $p_D = 3.12$ against 1.98 effective parameters, so the shape parameter does little work – consistent with the posterior for λ, mean 1.383 but interval $(0.992, 1.819)$, barely excluding $\lambda = 1$. The classical fits:

```r
library(survival)
we <- survreg(Surv(time, censored == 0) ~ group, dist = "weibull", data = remission)
ex <- survreg(Surv(time, censored == 0) ~ group, dist = "exponential", data = remission)
c(lambda = 1 / we$scale, beta0 = -coef(we)[1] / we$scale, beta1 = -coef(we)[2] / we$scale)
c(beta0 = -coef(ex)[1], beta1 = -coef(ex)[2])
c(AIC.weibull = AIC(we), AIC.exponential = AIC(ex))
```

```
          lambda beta0.(Intercept)      beta1.groupT
        1.365758         -3.070704        -1.730872
beta0.(Intercept)      beta1.groupT
        -2.159484         -1.526614
    AIC.weibull AIC.exponential
       219.1590        221.0481
```

The maximum likelihood estimates $\lambda = 1.366$, $\beta_0 = -3.071$, $\beta_1 = -1.731$ are the last row of Table 10.3 and the exponential $\beta_0 = -2.159$, $\beta_1 = -1.527$ the first. The posterior means sit slightly further from zero ($\beta_1 = -1.774$ against -1.731), the usual effect of averaging over a right-skewed likelihood rather than maximising, and λ is centred a little above its MLE for the same reason. The Bayesian standard deviations are honest, where Section 10.7 warns that the Poisson-regression standard errors ignore the uncertainty in $\hat{\lambda}$.

Model choice appears to diverge: Section 10.7 quotes AIC 2.429 (exponential) against 2.782 (Weibull) and prefers the exponential. Those are the AIC of the **Poisson regression surrogate** divided by $n = 42$ – $102.017/42$ for the exponential surrogate and $116.84/42$ for the Weibull one, which uses the offset $\hat{\lambda}\log(y)$. Different offsets put different data-dependent constants into the two Poisson log-likelihoods, so the values are not on a common scale and their ordering is not evidence about the

survival models. On the survival likelihood the AICs are 219.16 (Weibull) and 221.05 (exponential), a difference of 1.9 agreeing with the DIC difference of 1.6 in direction and magnitude.
So the exponential is about as good as the Weibull here, its shape parameter only marginally distinguishable from 1, and it would be chosen for parsimony: its relative hazard $\exp(1.556) = 4.74$ (posterior mean; 4.60 classically) says the control group relapses at about four and a half times the treated rate at every time point.

14.4 Problem 14.4 — a. Fit the random intercepts and slopes model to the stroke recovery data

Problem 14.4. a. Fit the random intercepts and slopes model to the stroke recovery data in WinBUGS. Create a scatter plot of the estimated mean random slopes against the random intercepts. Calculate the Pearson correlation between the intercepts and slopes.
b. Model the random slopes and intercepts so that each subject's intercept is correlated with his or her slope (using a multivariate Normal distribution). Find the mean and 95% posterior interval for the correlation between the intercept and slope. Interpret the correlation and give reasons for the somewhat surprising value.
Hint: To start the MCMC sampling, it may be necessary to use initial values based on the means of the random intercepts and slopes model from part (a). (difficulty: ⋆⋆⋆)

Solution. The fitted correlation is $r = -0.32$ between the posterior mean intercepts and slopes in (a), and $\hat{\rho} = -0.36$ with 95% posterior interval $(-0.68, 0.06)$ in (b); the surprising negative sign is a parameterisation effect (time origin at $t = 0$) reinforced by the ceiling at 100, and it reverses to $+0.27$ once time is centred. The Section 14.6 model for the stroke recovery data (Table 11.1) is

$$Y_{jt} = \alpha_g + a_j + (\beta_g + b_j)t + e_{jt},$$
$$j \le 24,\ t \le 8,\ g = 1, 2, 3,$$

with $e_{jt} \sim N(0, \sigma_e^2)$, taking a_j, b_j independent Normal in (a) and $(a_j, b_j)^T \sim \text{MVN}(\mathbf{0}, \mathbf{G})$ unstructured in (b). In place of WinBUGS a Gibbs sampler is written in R, every full conditional being closed form: the fixed effects given the rest are a Normal linear model on $y - \mathbf{Zu}$; each (a_j, b_j) is bivariate Normal; the book's $U(0, 10^4)$ priors make $\sigma_e^2, \sigma_a^2, \sigma_b^2$ inverse gamma with shape $n/2 - 1$ (the truncation never binds); and the Wishart prior $\mathbf{G}^{-1} \sim W(\mathbf{R}, \nu)$ is conjugate, giving $\mathbf{G}^{-1} \mid \cdot \sim W\big((\mathbf{R} + \sum_j \mathbf{u}_j \mathbf{u}_j^T)^{-1}, \nu + N\big)$ in the scale-matrix convention `rWishart` uses. Part (b) starts from the part (a) values, per the hint; $t = 1, \ldots, 8$ and responses stay on the original scale.
(a) Independent random intercepts and slopes.

```
library(dobson)
data(stroke.wide)
Y <- as.matrix(stroke.wide[, paste0("week", 1:8)])
N <- nrow(Y); T <- ncol(Y); tt <- 1:T
grp <- as.integer(factor(stroke.wide$Group))
y <- as.vector(t(Y)); subj <- rep(1:N, each = T); tidx <- rep(1:T, N)
g <- grp[subj]; time <- tt[tidx]
X <- cbind(outer(g, 1:3, "==") * 1, outer(g, 1:3, "==") * time)  # alphas then betas
Z <- cbind(1, tt); ZtZ <- crossprod(Z)

gibbs <- function(corr, n.burn = 2000, n.keep = 20000, seed = 1,
                  Rprior = diag(2), nu = 2) {
  set.seed(seed); p <- ncol(X); XtX <- crossprod(X)
  th <- as.vector(coef(lm(y ~ X - 1))); U <- matrix(0, N, 2)
  s2 <- 100; G <- diag(c(400, 10))
  keep.th <- matrix(NA, n.keep, p); keep.U <- matrix(0, N, 2)
  keep.G <- matrix(NA, n.keep, 3); keep.s2 <- keep.rho <- numeric(n.keep)
  for (it in 1:(n.burn + n.keep)) {
    ystar <- y - rowSums(Z[tidx, ] * U[subj, ])            # fixed effects
    V <- solve(XtX / s2 + diag(1e-4, p))
    th <- as.vector(V %*% (crossprod(X, ystar) / s2) + t(chol(V)) %*% rnorm(p))
    r <- y - as.vector(X %*% th)                            # random effects
```

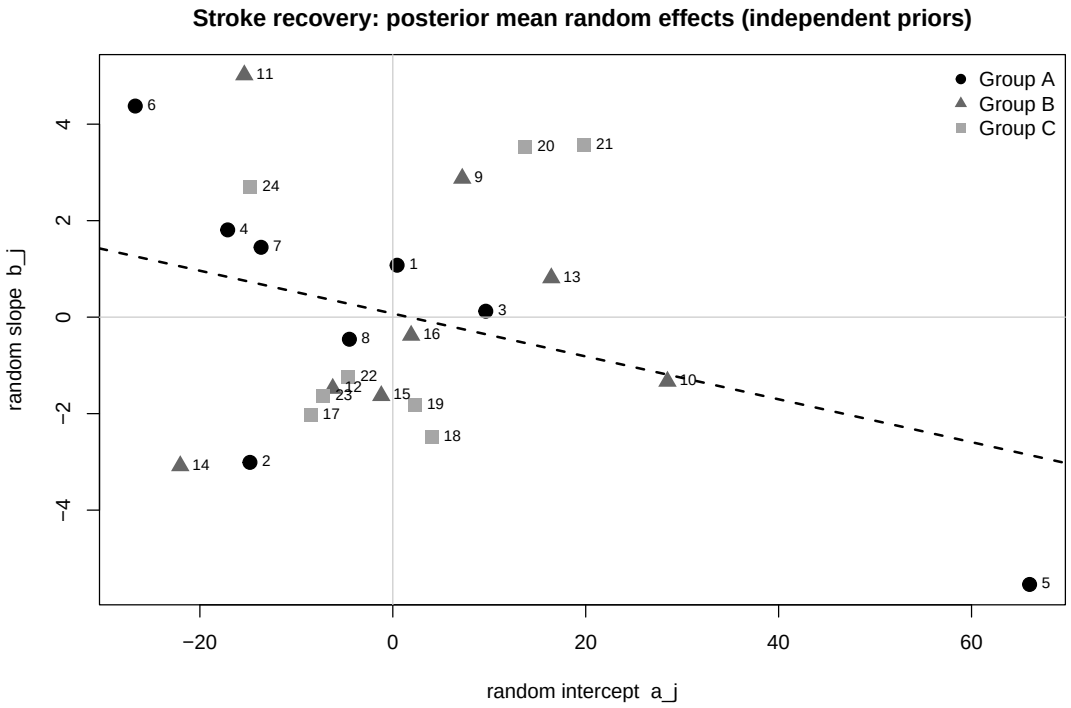
```
    Vu <- solve(ZtZ / s2 + solve(G)); Lu <- t(chol(Vu))
    Mu <- Vu %*% (crossprod(Z, matrix(r, nrow = T)) / s2)
    U <- t(Mu + Lu %*% matrix(rnorm(2 * N), 2, N))
    e <- r - rowSums(Z[tidx, ] * U[subj, ])                # residual variance
    s2 <- 1 / rgamma(1, length(y) / 2 - 1, sum(e^2) / 2)
    if (corr) {
      Wm <- solve(Rprior + crossprod(U))
      G <- solve(rWishart(1, nu + N, (Wm + t(Wm)) / 2)[, , 1])
    } else {
      G <- diag(c(1 / rgamma(1, N / 2 - 1, sum(U[, 1]^2) / 2),
                  1 / rgamma(1, N / 2 - 1, sum(U[, 2]^2) / 2)))
    }
    if (it > n.burn) {
      k <- it - n.burn; keep.th[k, ] <- th; keep.U <- keep.U + U / n.keep
      keep.G[k, ] <- c(G[1, 1], G[2, 2], G[1, 2]); keep.s2[k] <- s2
      keep.rho[k] <- G[1, 2] / sqrt(G[1, 1] * G[2, 2])
    }
  }
  list(th = keep.th, U = keep.U, G = keep.G, s2 = keep.s2, rho = keep.rho)
}
sm <- function(z) c(mean = mean(z), sd = sd(z), quantile(z, c(.025, .975)))
nm <- c("alpha1", "alpha2", "alpha3", "beta1", "beta2", "beta3")
fa <- gibbs(FALSE, seed = 2)
o <- t(apply(fa$th, 2, sm)); rownames(o) <- nm; round(o, 3)
c(sigma.a = mean(sqrt(fa$G[, 1])), sigma.b = mean(sqrt(fa$G[, 2])),
  sigma.e = mean(sqrt(fa$s2)))
```

```
         mean    sd   2.5%  97.5%
alpha1 29.896 8.099 12.854 45.498
alpha2 32.016 8.170 15.050 47.899
alpha3 29.205 8.349 12.509 45.077
beta1   6.349 1.150  4.017  8.548
beta2   4.230 1.130  1.992  6.483
beta3   3.569 1.213  1.022  5.877
  sigma.a   sigma.b   sigma.e
22.716779  3.184529  5.254549
```

These reproduce the "Intercepts + slopes" row of Table 14.8 ($\hat{\alpha}_1 = 30.38$, s.d. 7.988; $\hat{\beta}_1 = 6.378$, s.d. 1.207) and the book's $\hat{\sigma}_a = 22.4$, $\hat{\sigma}_b = 3.3$. Group A (the specialist stroke unit) improves by about 6.3 points per week, B by 4.2, C by 3.6; the differences -2.12 and -2.78 have 95% intervals $(-5.23, 1.05)$ and $(-5.99, 0.52)$, so A's advantage is suggestive but not conclusive once between-subject slope variability is allowed for, while the intercepts are indistinguishable across groups.

The posterior mean random effects, coded by treatment group:

```
par(mar = c(4.5, 4.5, 3, 1))
plot(fa$U[, 1], fa$U[, 2], pch = c(19, 17, 15)[grp],
     col = c("black", "grey40", "grey65")[grp], cex = 1.5,
     xlab = "random intercept  a_j", ylab = "random slope  b_j",
     main = "Stroke recovery: posterior mean random effects (independent priors)")
abline(h = 0, v = 0, col = "grey80")
abline(lm(fa$U[, 2] ~ fa$U[, 1]), lwd = 2, lty = 2)
text(fa$U[, 1], fa$U[, 2], 1:N, pos = 4, cex = 0.75)
legend("topright", pch = c(19, 17, 15), col = c("black", "grey40", "grey65"),
       legend = paste("Group", levels(factor(stroke.wide$Group))), bty = "n")
```




```
ct <- cor.test(fa$U[, 1], fa$U[, 2])
round(c(r = unname(ct$estimate), ct$conf.int, p = ct$p.value), 4)
```

```
     r                       p
-0.3221 -0.6421  0.0935  0.1248
```

So $r = -0.32$ (95% interval -0.64 to 0.09, $p = 0.12$) across the 24 pairs. It is a descriptive summary of shrunken point estimates under a prior that forced $a_j \perp b_j$, not an estimate of a model parameter, and has no honest standard error since the 48 numbers correlated are themselves posterior summaries; hence part (b). The pattern is driven by subject 5, at 100 in all eight weeks, whose largest intercept $\hat{a}_5 = 66.0$ pairs with the most negative slope $\hat{b}_5 = -5.5$ — cancelling almost all the group slope, since there is nowhere to go — while subjects 20 and 21 pair high intercepts with high slopes and subjects 6 and 11 pair low intercepts with the largest slopes.

(b) Correlated random effects. Now $(a_j, b_j)^T \sim \text{MVN}(\mathbf{0}, \mathbf{G})$ with $\mathbf{G}^{-1} \sim W(\mathbf{R}, \nu)$, $\mathbf{R} = \mathbf{I}$, $\nu = 2$ (the smallest degrees of freedom keeping the prior proper in two dimensions), monitoring $\rho = G_{12}/\sqrt{G_{11}G_{22}}$.

```
fb <- gibbs(TRUE, seed = 3)
ob <- t(apply(fb$th, 2, sm)); rownames(ob) <- nm; round(ob, 3)
round(sm(fb$rho), 3)
c(sd.a = mean(sqrt(fb$G[, 1])), sd.b = mean(sqrt(fb$G[, 2])),
  P.rho.neg = mean(fb$rho < 0))
```

```
         mean    sd   2.5%  97.5%
alpha1 29.770 7.304 15.118 44.491
alpha2 32.752 7.809 17.886 47.881
alpha3 29.354 7.606 14.759 44.941
beta1   6.437 1.042  4.423  8.491
beta2   4.322 1.105  2.093  6.538
beta3   3.611 1.075  1.515  5.817
  mean     sd   2.5%  97.5%
-0.355  0.192 -0.682  0.059
     sd.a      sd.b P.rho.neg
21.177021  2.953123  0.954600
```

Thus $\hat{\rho} = -0.36$, 95% interval $(-0.68, 0.06)$, $P(\rho < 0 \mid \mathbf{y}) = 0.96$; the fixed effects barely move. This is not a Wishart artefact: $\nu = 4$, and $\mathbf{R} = \text{diag}(500, 10)$ on the scale of $\mathbf{G}$, give -0.33 to -0.34 with the same interval.

Why the sign is negative. Intuition expects positive — abler patients recovering faster — but two mechanisms push the other way.

(i) **The ceiling.** The ability score is bounded above at 100; ten of the 192 observations are exactly

100 and subject 5 sits there throughout. An intercept near the ceiling cannot carry a large positive slope, so the top right of the plot is structurally empty and the cloud tilts down.
(ii) **Where time zero is**, the larger and purely algebraic effect. The intercept $\alpha_g + a_j$ is the fitted value at $t = 0$, a week before any data; for a line fitted to positive x-values, $\mathrm{Cov}(\hat{a}, \hat{b}) = -\bar{t}\,\mathrm{Var}(\hat{b})$, since a steeper line must come down at $t = 0$ to keep passing through the data. Centring at $t^* = t - 4.5$ reverses the sign.

```
tt <- (1:8) - 4.5; time <- tt[tidx]
X <- cbind(outer(g, 1:3, "==") * 1, outer(g, 1:3, "==") * time)
Z <- cbind(1, tt); ZtZ <- crossprod(Z)
fc <- gibbs(TRUE, n.keep = 10000, seed = 5)
round(sm(fc$rho), 3)
# same thing seen in the raw per-subject least squares lines
raw <- t(apply(Y, 1, function(r) coef(lm(r ~ I(1:8)))))
cen <- t(apply(Y, 1, function(r) coef(lm(r ~ I((1:8) - 4.5)))))
round(c(time.from.zero = cor(raw[, 1], raw[, 2]),
        time.centred   = cor(cen[, 1], cen[, 2])), 3)
```

```
  mean     sd   2.5%  97.5%
 0.269  0.204 -0.162  0.630
time.from.zero   time.centred
        -0.375          0.321
```

With the intercept at week 4.5 the posterior mean correlation is $+0.27$ $(-0.16, 0.63)$, and the flip shows even in per-subject OLS lines: $r = -0.375$ from zero against $r = +0.321$ centred.
Interpretation: patients doing better mid-study did tend to improve somewhat faster, weakly and with an interval covering zero. The negative correlation as specified reports the parameterisation, not stroke recovery — extrapolated week-zero ability and rate of improvement trade off by the algebra of fitting lines, reinforced by the ceiling — so the intercept-slope correlation is interpretable only once the time origin sits somewhere meaningful.

14.5 Problem 14.5 — This exercise illustrates the effect of the choice of the Wishart prior for the

Problem 14.5. This exercise illustrates the effect of the choice of the Wishart prior for the unstructured covariance matrix using the stroke recovery data.
a. Fit a simple linear regression model to the stroke recovery data with terms for treatment and treatment by time. Store the residuals. Use either Bayesian or classical methods to fit the model.
b. Adapt the WinBUGS code for the AR(1) covariance pattern model to an unstructured covariance.
c. Run the model using a vague Wishart prior defined by $\mathbf{R} = \hat{\sigma}^2\mathbf{I}$ and $\nu = 9$. $\mathbf{I}$ is the 8×8 identity matrix and $\hat{\sigma}^2$ is the variance of the residuals from part (a).
d. Run the model using a strong Wishart prior defined by an $\mathbf{R}$ equal to the covariances of the residuals from part (a) and $\nu = 500$. Monitor the intercepts, slopes and covariance and the DIC. Use the same sized burn-in and samples as part (c). What does the prior value of ν of 500 imply?
e. Compare the results from the vague and strong priors. What similarities and differences do you notice for the parameter estimates and covariance matrix? Explain the large difference in the DIC. (difficulty: ⋆⋆⋆)

Solution. The strong prior is worth twenty studies and, because $\mathbf{R}$ is an inverse scale, asserts $\mathbf{V} \approx \mathbf{S}_r/500$: the posterior covariance collapses to $n\mathbf{S}/(n+\nu) = 0.046\,\mathbf{S}$, every posterior standard deviation shrinks by about 4.7, and the DIC explodes from 1358 to 4592.
(a) Ordinary least squares and its residuals. The model is (14.3) with $\mathbf{V} = \sigma^2\mathbf{I}$: a separate intercept and slope per treatment group, independent errors.

```
library(dobson)
data(stroke.wide)
Y <- as.matrix(stroke.wide[, paste0("week", 1:8)])
N <- nrow(Y); T <- ncol(Y); tt <- 1:T
grp <- as.integer(factor(stroke.wide$Group))
long <- data.frame(y = as.vector(t(Y)),
```

```
                  grp = factor(rep(stroke.wide$Group, each = T)),
                  time = rep(tt, N))
m <- lm(y ~ grp + grp:time - 1, data = long)
round(coef(m), 3)
Rmat   <- matrix(residuals(m), nrow = N, byrow = TRUE)   # 24 subjects x 8 weeks
s2.hat <- var(as.vector(Rmat))
Sr     <- cov(Rmat)
s2.hat
round(Sr, 1)
round(mean(cov2cor(Sr)[upper.tri(Sr)]), 3)
```

```
    grpA     grpB     grpC grpA:time grpB:time grpC:time
  29.821   33.170   29.799    6.324    4.330    3.638
[1] 427.7933
      [,1]  [,2]  [,3]  [,4]  [,5]  [,6]  [,7]  [,8]
[1,] 328.4 316.7 315.7 310.5 308.1 269.8 244.1 218.0
[2,] 316.7 362.4 354.7 355.9 358.4 332.5 314.9 289.3
[3,] 315.7 354.7 409.0 411.4 408.2 381.6 362.5 331.1
[4,] 310.5 355.9 411.4 455.7 434.4 411.8 411.9 379.8
[5,] 308.1 358.4 408.2 434.4 486.7 468.8 462.4 439.7
[6,] 269.8 332.5 381.6 411.8 468.8 477.9 479.2 455.3
[7,] 244.1 314.9 362.5 411.9 462.4 479.2 527.4 504.1
[8,] 218.0 289.3 331.1 379.8 439.7 455.3 504.1 502.0
[1] 0.833
```

The estimates are those of Table 11.7 ($\hat{\alpha}_1 = 29.821$, $\hat{\beta}_1 = 6.324$), with $\hat{\sigma}^2 = 427.8$ and a residual covariance $\mathbf{S}_r$ showing the two features of Figure 14.5: variance rising over the eight weeks (328 to 502) and correlations high but decaying with separation (0.89 adjacent, 0.51 between weeks 1 and 8, average 0.83). These are correlations **after** removing treatment and treatment-by-time, so they are the within-subject dependence the covariance pattern model must absorb.

(b) The unstructured model. In the AR(1) code of Section 14.7 the block building `omega.obs` entry by entry from τ, ρ is replaced by a single Wishart draw, as on page 334:

```
omega.obs[1:T,1:T] ~ dwish(R[1:T,1:T], nu)
V[1:T,1:T] <- inverse(omega.obs[1:T,1:T])
```

with `R` and `nu` supplied as data and everything else (likelihood loop, mean structure, Normal priors on `alpha.c` and `beta`) unchanged. In R the same model is a two-block Gibbs sampler, the Wishart being conjugate for the multivariate Normal: given $\mathbf{V}$ the coefficients come from their generalised least squares posterior, and given the coefficients

$$\mathbf{V}^{-1} \mid \cdot \;\sim\; W\left(\left(\mathbf{R} + \sum_{i=1}^{24} \mathbf{e}_i \mathbf{e}_i^T\right)^{-1},\; \nu + 24\right)$$

in the scale-matrix convention of R's `rWishart`, matching WinBUGS's dwish($\mathbf{R}, \nu$) with $\mathbf{R}$ the inverse scale.

```
X8 <- lapply(1:N, function(i) cbind(outer(rep(grp[i], T), 1:3, "==") * 1,
                                    outer(rep(grp[i], T), 1:3, "==") * tt))
Xs <- do.call(rbind, X8); yv <- as.vector(t(Y))
unstr <- function(R, nu, n.burn = 2000, n.keep = 10000, seed = 1) {
  set.seed(seed); p <- 6; V <- Sr; th <- coef(m)
  keep.th <- matrix(NA, n.keep, p); keep.V <- matrix(0, T, T); D <- numeric(n.keep)
  ll <- function(th, V) {
    Vi <- solve(V); ld <- determinant(V, log = TRUE)$modulus
    E <- matrix(yv - Xs %*% th, nrow = T)
    -0.5 * (N * T * log(2 * pi) + N * ld + sum(E * (Vi %*% E)))
  }
  for (it in 1:(n.burn + n.keep)) {
    Vi <- solve(V); A <- matrix(0, p, p); b <- numeric(p)
    for (i in 1:N) {
      Xi <- X8[[i]]; A <- A + t(Xi) %*% Vi %*% Xi; b <- b + t(Xi) %*% Vi %*% Y[i, ]
    }
    Vp <- solve(A + diag(1e-3, p))
    th <- as.vector(Vp %*% b + t(chol(Vp)) %*% rnorm(p))
    E  <- matrix(yv - Xs %*% th, nrow = T)
```

```
    Wm <- solve(R + tcrossprod(E)); Wm <- (Wm + t(Wm)) / 2
    V  <- solve(rWishart(1, nu + N, Wm)[, , 1])
    if (it > n.burn) {
      k <- it - n.burn; keep.th[k, ] <- th; keep.V <- keep.V + V / n.keep
      D[k] <- -2 * ll(th, V)
    }
  }
  Dhat <- -2 * ll(colMeans(keep.th), keep.V)
  list(th = keep.th, V = keep.V,
       dic = c(Dbar = mean(D), Dhat = Dhat, pD = mean(D) - Dhat, DIC = 2 * mean(D) - Dhat))
}
sm <- function(z) c(mean = mean(z), sd = sd(z))
nm <- c("alpha1", "alpha2", "alpha3", "beta1", "beta2", "beta3")
```

(c) Vague prior: $\mathbf{R} = \hat{\sigma}^2\mathbf{I}$, $\nu = 9$. With $p = 8$, $\nu = p + 1$ is the standard vague choice, the smallest degrees of freedom keeping every marginal correlation uniform on $(-1, 1)$.

```
f1 <- unstr(s2.hat * diag(T), 9, seed = 11)
o <- t(apply(f1$th, 2, sm)); rownames(o) <- nm; round(o, 3)
round(rbind("a2-a1" = sm(f1$th[, 2] - f1$th[, 1]), "a3-a1" = sm(f1$th[, 3] - f1$th[, 1]),
            "b2-b1" = sm(f1$th[, 5] - f1$th[, 4]), "b3-b1" = sm(f1$th[, 6] - f1$th[, 4])), 3)
round(diag(f1$V), 1)
round(cov2cor(f1$V), 2)
round(f1$dic, 1)
```

```
         mean    sd
alpha1 33.430 6.660
alpha2 28.512 6.588
alpha3 24.894 6.377
beta1   6.541 1.036
beta2   4.013 1.021
beta3   3.495 0.990
        mean    sd
a2-a1 -4.918 9.588
a3-a1 -8.536 9.737
b2-b1 -2.528 1.491
b3-b1 -3.046 1.521
[1] 370.7 423.8 479.0 532.5 563.7 565.5 610.1 567.1
     [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8]
[1,] 1.00 0.89 0.84 0.78 0.75 0.67 0.58 0.51
[2,] 0.89 1.00 0.89 0.86 0.83 0.78 0.71 0.66
[3,] 0.84 0.89 1.00 0.92 0.89 0.84 0.77 0.72
[4,] 0.78 0.86 0.92 1.00 0.90 0.87 0.83 0.79
[5,] 0.75 0.83 0.89 0.90 1.00 0.94 0.89 0.87
[6,] 0.67 0.78 0.84 0.87 0.94 1.00 0.93 0.91
[7,] 0.58 0.71 0.77 0.83 0.89 0.93 1.00 0.95
[8,] 0.51 0.66 0.72 0.79 0.87 0.91 0.95 1.00
  Dbar   Dhat     pD    DIC
1342.4 1326.8   15.6 1358.0
```

This reproduces the "Unstructured" row of Table 14.8, whose values are $\hat{\alpha}_1 = 34.62$ (6.830), $\hat{\alpha}_2 - \hat{\alpha}_1 = -5.022$ (9.918), $\hat{\alpha}_3 - \hat{\alpha}_1 = -8.946$ (9.966), $\hat{\beta}_1 = 6.436$ (1.042), $\hat{\beta}_2 - \hat{\beta}_1 = -2.533$ (1.507), $\hat{\beta}_3 - \hat{\beta}_1 = -3.023$ (1.526). The covariance rises from 371 at week 1 to 570–610 at weeks 7–8 and the correlations decay away from the diagonal: the surfaces of Figure 14.5. The DIC of 1358.0 with $p_D = 15.6$ sits alongside the book's 1376.9 with $p_D = 34.6$, the discrepancy being the known sensitivity of p_D for a 36-parameter covariance to sampler and prior; no ordering changes.

(d) Strong prior: $\mathbf{R} = \mathbf{S}_r$, $\nu = 500$.

```
f2 <- unstr(Sr, 500, seed = 12)
o2 <- t(apply(f2$th, 2, sm)); rownames(o2) <- nm; round(o2, 3)
round(rbind("a2-a1" = sm(f2$th[, 2] - f2$th[, 1]), "a3-a1" = sm(f2$th[, 3] - f2$th[, 1]),
            "b2-b1" = sm(f2$th[, 5] - f2$th[, 4]), "b3-b1" = sm(f2$th[, 6] - f2$th[, 4])), 3)
round(diag(f2$V), 2)
round(f2$dic, 1)
round(diag(f2$V) / diag(f1$V), 3)
round(N / (N + 500), 4)
```

```
          mean    sd
alpha1 37.163 1.557
alpha2 28.403 1.575
alpha3 21.737 1.506
beta1   6.725 0.225
beta2   3.299 0.231
beta3   2.861 0.223
          mean    sd
a2-a1  -8.760 2.329
a3-a1 -15.426 2.358
b2-b1  -3.426 0.337
b3-b1  -3.864 0.343
[1] 16.25 20.44 23.80 27.11 28.72 29.29 31.52 28.39
  Dbar   Dhat     pD    DIC
4516.9 4441.7   75.1 4592.0
[1] 0.044 0.048 0.050 0.051 0.051 0.052 0.052 0.050
[1] 0.0458
```

What $\nu = 500$ implies. The degrees of freedom are a notional prior sample size, as the posterior mean identity of page 334 makes explicit,

$$\mathbf{V} = \left(n\mathbf{S} + \nu\mathbf{R}^{-1}\right)/(n+\nu),$$

so with $n = 24$ and $\nu = 500$ the data carry weight $24/524 = 0.046$ against the prior's 0.954: the prior is worth twenty studies, and any conflict is settled in its favour. Here the conflict is severe for a second reason, separate from ν: setting **R equal to $\mathbf{S}_r$** is not centring the prior on it. Since $\mathbf{R}$ is the inverse scale, $E(\mathbf{V}^{-1}) = \nu\mathbf{R}^{-1} = 500\,\mathbf{S}_r^{-1}$, asserting $\mathbf{V} \approx \mathbf{S}_r/500$ (centring would need $\mathbf{R} = (\nu - p - 1)\mathbf{S}_r$). Then $\nu\mathbf{R}^{-1}$ is tiny beside $n\mathbf{S}$ and the posterior collapses to $n\mathbf{S}/(n+\nu)$; the last two output lines confirm it, the strong-to-vague variance ratio running 0.044 to 0.052 against the predicted 0.0458.

(e) Comparison.

- **Point estimates shift.** Both priors give group A improving fastest, B and C by 2 to 4 points per week less, but the strong prior pulls estimates apart: $\hat{\alpha}_3 - \hat{\alpha}_1$ from -8.5 to -15.4, $\hat{\beta}_3 - \hat{\beta}_1$ from -3.0 to -3.9. The fixed effects are generalised least squares with weight $\mathbf{V}^{-1}$, so distorting $\mathbf{V}$ reweights the eight repeated measures against one another; the numbers do not merely become more precise.
- **Standard deviations collapse** by $\sqrt{1/0.046} = 4.7$: s.d.$(\hat{\alpha}_1)$ from 6.66 to 1.56, s.d.$(\hat{\beta}_1)$ from 1.04 to 0.23. The precision is spurious — $\hat{\beta}_2 - \hat{\beta}_1$ and $\hat{\beta}_3 - \hat{\beta}_1$, borderline under the vague prior, become overwhelmingly "significant" only because the prior asserted measurements twenty times less noisy than they are.
- **The covariance matrix** keeps its increasing-variance, decaying-correlation structure ($\mathbf{S}$ enters both posteriors) but its scale is wrong by a factor of about 22: diagonal entries 16 to 32 in place of 371 to 610.
- **The DIC** rises from 1358 to 4592. Since $-2\ell = n\log|\mathbf{V}| + \sum_i \mathbf{e}_i^T\mathbf{V}^{-1}\mathbf{e}_i + \text{const}$, shrinking $\mathbf{V}$ by $c = 0.046$ reduces the log-determinant term by $nT\log c$ but multiplies the quadratic form by $1/c \approx 22$, and at the observed residual sizes the quadratic form dominates: the strong-prior model predicts week-1 scores to within $\sqrt{16} = 4$ points when residuals run $\sqrt{330} = 18$, making every observation a five-sigma outlier. Correspondingly p_D rises to 75.1 rather than falling, the usual symptom of gross misspecification, since p_D measures deviance variation over the posterior and stops counting parameters once the model is this far from the data.

14.6 Problem 14.6 — a. Find the inverse of the variance–covariance matrix

Problem 14.6. a. Find the inverse of the variance–covariance matrix

$$\mathbf{V} = \begin{bmatrix} \sigma^2 & \rho\sigma^2 & 0 & 0 & 0 & 0 & 0 \\ \rho\sigma^2 & \sigma^2 & \rho\sigma^2 & 0 & 0 & 0 & 0 \\ 0 & \rho\sigma^2 & \sigma^2 & \rho\sigma^2 & 0 & 0 & 0 \\ 0 & 0 & \rho\sigma^2 & \sigma^2 & \rho\sigma^2 & 0 & 0 \\ 0 & 0 & 0 & \rho\sigma^2 & \sigma^2 & \rho\sigma^2 & 0 \\ 0 & 0 & 0 & 0 & \rho\sigma^2 & \sigma^2 & \rho\sigma^2 \\ 0 & 0 & 0 & 0 & 0 & \rho\sigma^2 & \sigma^2 \end{bmatrix}$$

(that is, a symmetric tridiagonal matrix with σ^2 on the diagonal, $\rho\sigma^2$ on the two adjacent diagonals and zeros elsewhere).
b. Fit the model to the stroke recovery data as a covariance pattern model. Compare the parameter estimates and overall fit (using the DIC) to the results in Tables 14.8 and 14.9.
c. What does the matrix assume about the correlation between responses from the same subject? (difficulty: ⋆⋆⋆)

Solution. (a) The inverse. Writing $\mathbf{V} = \sigma^2\mathbf{T}_m(\rho)$ with $\mathbf{T}_m(\rho)$ the symmetric tridiagonal Toeplitz matrix carrying 1 on the diagonal and ρ beside it ($m = 7$ as printed, $m = 8$ for the stroke data), $\mathbf{V}^{-1}$ is dense: here the **covariance** is tridiagonal, the reverse of the AR(1) case of Section 14.7. Put

$$\theta_0 = 1, \qquad \theta_1 = 1, \qquad \theta_i = \theta_{i-1} - \rho^2\theta_{i-2} \quad (i \geq 2),$$

so $\theta_i = \det \mathbf{T}_i(\rho)$, the trailing minors coinciding with the leading ones by Toeplitz symmetry. The standard tridiagonal inversion formula gives, for $j \leq k$,

$$\left(\mathbf{V}^{-1}\right)_{jk} = \frac{(-1)^{j+k}\,\rho^{k-j}\,\theta_{j-1}\,\theta_{m-k}}{\sigma^2\,\theta_m},$$

with $(\mathbf{V}^{-1})_{kj} = (\mathbf{V}^{-1})_{jk}$. The recursion's characteristic equation $x^2 - x + \rho^2 = 0$ has roots $x_\pm = (1 \pm \delta)/2$, $\delta = \sqrt{1-4\rho^2}$, whence

$$\theta_i = \frac{x_+^{i+1} - x_-^{i+1}}{\delta} = \frac{1}{\sqrt{1-4\rho^2}}\left[\left(\frac{1+\sqrt{1-4\rho^2}}{2}\right)^{i+1} - \left(\frac{1-\sqrt{1-4\rho^2}}{2}\right)^{i+1}\right].$$

real for $|\rho| < 1/2$, and for $|\rho| > 1/2$ the same expression with imaginary roots, better written $\theta_i = \rho^i \sin\{(i+1)\psi\}/\sin\psi$ with $\cos\psi = 1/(2\rho)$. Two consequences carry into (b).

- **Dense with alternating signs.** The factor $(-1)^{j+k}\rho^{k-j}$ alternates along each row and decays like $\rho^{|j-k|}$ without vanishing, so one codes this model in WinBUGS by building $\mathbf{V}$ and calling `inverse()`, not by writing $\mathbf{V}^{-1}$ out as the AR(1) code does.
- **Positive definiteness is restricted.** The eigenvalues of $\mathbf{T}_m$ are $1+2\rho\cos\{k\pi/(m+1)\}$, so $\mathbf{V} \succ 0$ only for $|\rho| < 1/\{2\cos(\pi/(m+1))\}$, namely 0.5321 at $m = 8$ and 0.5412 at $m = 7$; adjacent correlation 0.6 is unattainable. Since $\theta_m \to 0$ at the bound, the inverse blows up exactly where the data push.

Checking the formula against a numerical inverse:

```
Tmat <- function(rho, n = 8) {
  M <- diag(n); for (j in 1:(n - 1)) { M[j, j + 1] <- rho; M[j + 1, j] <- rho }; M
}
theta <- function(i, rho) {
  th <- c(1, 1)                          # th[k+1] = theta_k
  if (i >= 2) for (k in 2:i) th <- c(th, th[k] - rho^2 * th[k - 1])
  th[i + 1]
}
inv.formula <- function(rho, s2, n = 8) {
  M <- matrix(0, n, n); tn <- theta(n, rho)
  for (j in 1:n) for (k in 1:n) {
    a <- min(j, k); b <- max(j, k)
    M[j, k] <- (-1)^(j + k) * rho^(b - a) * theta(a - 1, rho) * theta(n - b, rho) / (s2 * tn)
  }
```

```
  M
}
for (r in c(0.2, 0.35, -0.4, 0.5))
  cat("rho =", r, " max abs difference from solve():",
      format(max(abs(inv.formula(r, 3.7) - solve(3.7 * Tmat(r)))), digits = 3), "\n")
# closed form for theta_i against the recursion, rho = 0.35
d <- sqrt(1 - 4 * 0.35^2); xp <- (1 + d) / 2; xm <- (1 - d) / 2
round(rbind(recursion = sapply(0:8, theta, rho = 0.35),
            closed    = sapply(0:8, function(i) (xp^(i + 1) - xm^(i + 1)) / d)), 5)
c(pd.bound = 1 / (2 * cos(pi / 9)),
  min.eigen.at.0.53 = min(eigen(Tmat(0.53))$values),
  min.eigen.at.0.54 = min(eigen(Tmat(0.54))$values))
```

```
rho = 0.2  max abs difference from solve(): 5.55e-17
rho = 0.35  max abs difference from solve(): 1.67e-16
rho = -0.4  max abs difference from solve(): 1.67e-16
rho = 0.5  max abs difference from solve(): 7.77e-16
          [,1] [,2]   [,3]  [,4]    [,5]    [,6]   [,7]    [,8]    [,9]
recursion    1    1 0.8775 0.755 0.64751 0.55502 0.4757 0.40771 0.34944
closed       1    1 0.8775 0.755 0.64751 0.55502 0.4757 0.40771 0.34944
        pd.bound min.eigen.at.0.53 min.eigen.at.0.54
      0.532088886       0.003925822      -0.014868030
```

(b) Fitting it to the stroke recovery data. The model is (14.3), $\mathbf{Y}_i = \alpha_g + \beta_g t_i + \mathbf{e}_i$, $\mathbf{e}_i \sim \mathrm{MVN}(\mathbf{0}, \mathbf{V})$, $\mathbf{V} = \sigma^2 \mathbf{T}_8(\rho)$, fitted alongside the book's four patterns so that all DICs come from one sampler. Coefficients are drawn from their generalised least squares posterior given (σ^2, ρ), which are themselves updated by random walk Metropolis on $(\log \sigma^2, \rho)$ under $\sigma^2 \sim U(0, 10^4)$ and ρ Uniform on the positive definite region.

```
Vbuild <- list(
  independent  = function(s2, rho) s2 * diag(T),
  exchangeable = function(s2, rho) s2 * ((1 - rho) * diag(T) + rho),
  ar1          = function(s2, rho) s2 * rho^abs(outer(1:T, 1:T, "-")),
  banded       = function(s2, rho) s2 * Tmat(rho, T))
rng <- list(independent = c(0, 0), exchangeable = c(-1 / (T - 1) + 1e-6, 0.999),
            ar1 = c(-0.99, 0.99), banded = c(-0.5321, 0.5321))
fit <- function(str, n.burn = 2000, n.keep = 20000, seed = 1, sdp = c(0.12, 0.05)) {
  set.seed(seed); Vf <- Vbuild[[str]]; lo <- rng[[str]][1]; hi <- rng[[str]][2]
  p <- 6; s2 <- 400; rho <- if (hi > 0) 0.5 else 0; th <- coef(lm(yv ~ Xs - 1))
  ll <- function(th, V) {
    Vi <- solve(V); ld <- determinant(V, log = TRUE)$modulus
    E <- matrix(yv - Xs %*% th, nrow = T)
    -0.5 * (N * T * log(2 * pi) + N * ld + sum(E * (Vi %*% E)))
  }
  ok <- function(s2, rho) {
    if (rho < lo || rho > hi || s2 <= 0 || s2 > 1e4) return(FALSE)
    min(eigen(Vf(s2, rho), only.values = TRUE)$values) > 1e-8
  }
  keep.th <- matrix(NA, n.keep, p); keep <- matrix(NA, n.keep, 2); D <- numeric(n.keep)
  for (it in 1:(n.burn + n.keep)) {
    V <- Vf(s2, rho); Vi <- solve(V); A <- matrix(0, p, p); b <- numeric(p)
    for (i in 1:N) {
      Xi <- X8[[i]]; A <- A + t(Xi) %*% Vi %*% Xi; b <- b + t(Xi) %*% Vi %*% Y[i, ]
    }
    Vp <- solve(A + diag(1e-3, p)); th <- as.vector(Vp %*% b + t(chol(Vp)) %*% rnorm(p))
    s2p <- s2 * exp(rnorm(1, 0, sdp[1])); rhop <- if (hi > 0) rho + rnorm(1, 0, sdp[2]) else
    ↪  0
    if (ok(s2p, rhop)) {
      la <- ll(th, Vf(s2p, rhop)) - ll(th, V) + log(s2p) - log(s2)   # flat prior + Jacobian
      if (log(runif(1)) < la) { s2 <- s2p; rho <- rhop }
    }
    if (it > n.burn) {
      k <- it - n.burn; keep.th[k, ] <- th; keep[k, ] <- c(s2, rho)
      D[k] <- -2 * ll(th, Vf(s2, rho))
    }
  }
  Dhat <- -2 * ll(colMeans(keep.th), Vf(mean(keep[, 1]), mean(keep[, 2])))
```

```
  list(th = keep.th, par = keep,
       dic = c(Dbar = mean(D), Dhat = Dhat, pD = mean(D) - Dhat, DIC = 2 * mean(D) - Dhat))
}
for (s in names(Vbuild)) {
  f <- fit(s, seed = which(names(Vbuild) == s)); cat("###", s, "\n")
  o <- t(apply(f$th, 2, sm)); rownames(o) <- nm; print(round(o, 3))
  print(round(rbind("a2-a1" = sm(f$th[, 2] - f$th[, 1]), "a3-a1" = sm(f$th[, 3] - f$th[, 1]),
                    "b2-b1" = sm(f$th[, 5] - f$th[, 4]), "b3-b1" = sm(f$th[, 6] - f$th[,
                    ↪  4])), 3))
  cat("sigma2:", round(sm(f$par[, 1]), 2), " rho:",
      round(c(sm(f$par[, 2]), quantile(f$par[, 2], c(.025, .975))), 3), "\n")
  print(round(f$dic, 1))
}
```

```
### independent
         mean    sd
alpha1 28.826 5.741
alpha2 32.127 5.768
alpha3 28.896 5.736
beta1   6.498 1.143
beta2   4.511 1.144
beta3   3.796 1.148
         mean    sd
a2-a1  3.301 8.132
a3-a1  0.070 8.109
b2-b1 -1.987 1.615
b3-b1 -2.703 1.621
sigma2: 449.07 47.34  rho: 0 0 0 0
  Dbar   Dhat     pD    DIC
1714.3 1707.5    6.8 1721.2
### exchangeable
         mean    sd
alpha1 28.111 7.565
alpha2 31.331 7.520
alpha3 28.160 7.589
beta1   6.352 0.470
beta2   4.362 0.471
beta3   3.668 0.469
         mean     sd
a2-a1  3.220 10.595
a3-a1  0.049 10.693
b2-b1 -1.990  0.668
b3-b1 -2.684  0.659
sigma2: 511.11 150.22  rho: 0.842 0.044 0.751 0.919
  Dbar   Dhat     pD    DIC
1463.1 1456.4    6.7 1469.8
### ar1
         mean    sd
alpha1 31.295 7.921
alpha2 31.236 7.980
alpha3 25.425 7.902
beta1   6.178 0.846
beta2   4.030 0.853
beta3   3.918 0.835
         mean     sd
a2-a1 -0.059 11.270
a3-a1 -5.870 11.212
b2-b1 -2.147  1.197
b3-b1 -2.260  1.186
sigma2: 488.96 122.18  rho: 0.949 0.013 0.922 0.971
  Dbar   Dhat     pD    DIC
1333.9 1327.1    6.8 1340.7
### banded
         mean    sd
alpha1 31.366 5.645
alpha2 33.530 5.664
alpha3 27.259 5.668
```

```
beta1   6.019 1.087
beta2   4.147 1.082
beta3   4.033 1.083
        mean    sd
a2-a1  2.164 7.934
a3-a1 -4.106 8.034
b2-b1 -1.872 1.527
b3-b1 -1.986 1.545
sigma2: 302.32 33.6  rho: 0.512 0.006 0.498 0.521
  Dbar   Dhat     pD    DIC
1543.2 1535.5    7.7 1550.8
```

Validation. The three replicated structures track the book: DICs 1721.2, 1469.8, 1340.7 against Table 14.9's 1721.3, 1471.1, 1342.0, with p_D of 6.7–6.8 against 7.0–8.1; exchangeable $\hat{\rho} = 0.842$ $(0.751, 0.919)$ against 0.856 $(0.764, 0.923)$, AR(1) 0.949 $(0.922, 0.971)$ against 0.946 $(0.915, 0.971)$; intercepts and slopes reproduce Table 14.8 throughout, e.g. exchangeable $\hat{\beta}_1 = 6.352$ (0.470) against 6.320 (0.472). The banded numbers therefore read on the same scale.

Comparison. Ranking the six models, the unstructured value taken from Exercise 14.5:

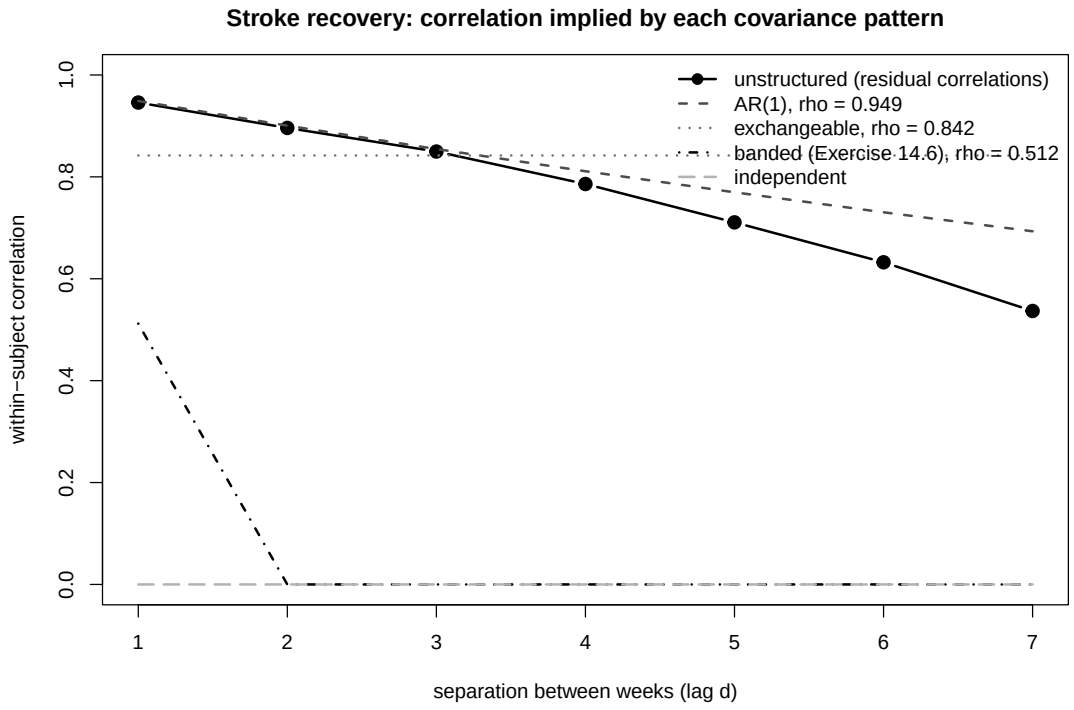
Covariance pattern	p_D	DIC (mine)	DIC (Table 14.9)
Independent	6.8	1721.2	1721.3
Banded (this exercise)	7.7	1550.8	–
Exchangeable	6.7	1469.8	1471.1
Unstructured	15.6	1358.0	1376.9
AR(1)	6.8	1340.7	1342.0

The banded model improves on independence by 170 in DIC for one extra parameter, but is worse than every other correlated structure — 81 worse than exchangeable, 210 worse than AR(1) — so it is second-worst of the six, and model averaging (Section 14.8) would still put essentially all posterior probability on AR(1).

The estimates $\hat{\beta}_1 = 6.02$, $\hat{\beta}_2 - \hat{\beta}_1 = -1.87$, $\hat{\beta}_3 - \hat{\beta}_1 = -1.99$ sit in line with the other rows of Table 14.8, so group A improving fastest by roughly 2 points per week is robust to the covariance choice; the precision is not. The banded model gives s.d.$(\hat{\beta}_2 - \hat{\beta}_1) = 1.53$, twice the exchangeable 0.67, because a structure denying correlation beyond one week cannot exploit within-subject replication when comparing slopes.

Most informative is $\hat{\rho} = 0.512$ with interval $(0.498, 0.521)$ against the positive definiteness limit 0.5321: the posterior is jammed against the boundary, since the lag-1 residual correlation is 0.95 and the structure cannot deliver it. Hence $\hat{\sigma}^2 = 302$ is deflated against the other models' 450–510, the sampler trading variance for a correlation it cannot raise.

```r
C <- cov2cor(cov(Rmat)); lag <- abs(outer(1:T, 1:T, "-"))
emp <- sapply(1:7, function(d) mean(C[lag == d]))
par(mar = c(4.5, 4.5, 3, 1))
plot(1:7, emp, type = "b", pch = 19, ylim = c(0, 1), lwd = 2, cex = 1.3,
     xlab = "separation between weeks (lag d)", ylab = "within-subject correlation",
     main = "Stroke recovery: correlation implied by each covariance pattern")
lines(1:7, 0.949^(1:7), col = "grey30", lwd = 2, lty = 2)
lines(1:7, rep(0.842, 7), col = "grey45", lwd = 2, lty = 3)
lines(1:7, c(0.512, rep(0, 6)), col = "black", lwd = 2, lty = 4)
lines(1:7, rep(0, 7), col = "grey70", lwd = 2, lty = 5)
legend("topright", bty = "n", lwd = 2, lty = c(1, 2, 3, 4, 5), pch = c(19, NA, NA, NA, NA),
       col = c("black", "grey30", "grey45", "black", "grey70"),
       legend = c("unstructured (residual correlations)", "AR(1), rho = 0.949",
                  "exchangeable, rho = 0.842", "banded (Exercise 14.6), rho = 0.512",
                  "independent"))
```




```
round(emp, 3)
```

```
[1] 0.946 0.896 0.850 0.786 0.711 0.632 0.537
```

(c) What the matrix assumes. Two responses from the same subject are correlated, with correlation ρ, exactly when they fall in adjacent weeks; anything two or more weeks apart is uncorrelated. This is a one-dependent or MA(1) structure, the opposite of the AR(1) model of Section 14.7 whose ρ^d decays but never vanishes, and for these data it is implausible: it says week 1 carries no information whatever about week 3, or week 8, once the fitted line accounts for week 2.

The figure shows the failure. Residual correlations decay smoothly from 0.95 at lag 1 to 0.54 at lag 7, tracking 0.949^d, whereas the banded model can only fit a spike at lag 1 and flat zero after, missing six of the seven lags, and the positive definiteness constraint caps even lag 1 at 0.53 against the observed 0.95. That is the whole explanation of its DIC: a short-memory structure applied to data whose defining feature is a persistent subject-level effect, which a random intercept (exchangeable, constant across lags) or AR(1) captures far better.