THE SINGULAR VALUE DECOMPOSITION

This week we will learn about:

- The singular value decomposition (SVD),
- Orthogonality of the fundamental matrix subspaces, and
- How the SVD relates to other matrix decompositions,

Extra reading and watching:

- Section 2.3.1 and 2.3.2 in the textbook
- Lecture videos 34, 35, 36, and 37 on YouTube
- Singular value decomposition at Wikipedia
- Fundamental Theorem of Linear Algebra at Wikipedia

Extra textbook problems:

- \star 2.3.1, 2.3.4(a,b,c,f,g,i)
- $\star \star 2.3.3, 2.3.5, 2.3.7$
- $\star \star \star 2.3.14, 2.3.20$
 - **2** 2.3.26

If the Schur decomposition theorem from last week was "big", then the upcoming theorem is "super-mega-gigantic". The singular value decomposition is possibly the biggest and most widely-used theorem in all of linear algebra (and is my personal favourite), so we're going to spend some time focusing on it.

Theorem 9.1 — Singular Value Decomposition (SVD)

Suppose $\mathbb{F} = \mathbb{R}$ or $\mathbb{F} = \mathbb{C}$, and $A \in \mathcal{M}_{m,n}(\mathbb{F})$. Then there exist unitary matrices $U \in \mathcal{M}_m(\mathbb{F})$ and $V \in \mathcal{M}_n(\mathbb{F})$ and a diagonal matrix $\Sigma \in \mathcal{M}_{m,n}(\mathbb{R})$ with non-negative entries such that

Furthermore, the diagonal entries of Σ (called the **singular values** of A) are the non-negative square roots of the eigenvalues of A^*A .

Let's compare how this decomposition theorem is good and bad compared to our previous decomposition theorems:

- · Good: applies to every matrix (even rectangular)
- · Good: matrix Z in the middle is diagonal (not just triangular), real, non-negative
- Kinda good, kinda bad: need two unitaries V and V. Better than invertible?

Proof. Consider the matrix A^*A and assume that $m \ge n$... (if m < n, use AA^*)

since A*A is PSD, we can find a spectral decomposition of it: A*A=VDV*

Let Z=JD, but of size mxn (pad with zero rows).

Then
$$(ZV^*)^*(ZV^*) = VZ^*ZV^* = VDV^* = A^*A$$
.

Yay!

Some notes about the SVD are in order:

• The singular values of A are exactly the square roots of the eigenvalues of A^*A . Alternatively...

square roots of eigenvalues of

• Even though the singular values are uniquely determined by A, the diagonal matrix Σ isn't.

Can permute the diagonal entries (usually: 0,2022...)

• The unitary matrices U and V are often not uniquely determined by A. Example:

For any unitary U, I=UV* is an SVD of I.

Example. Let's find the singular values of a matrix. $A = \begin{bmatrix} 2 & 3 & i \\ -1 & 2 & -i \end{bmatrix}$

eigenstuff to $AA^* = \begin{bmatrix} 2 & 3 & i \\ -1 & 2 & -i \end{bmatrix} \begin{bmatrix} 2 & -1 \\ 3 & 2 \\ -i & i \end{bmatrix} = \begin{bmatrix} 14 & 3 \\ 3 & 6 \end{bmatrix}$.

Eigenvalues: $O = det(AA^* - \lambda I) = det(\begin{bmatrix} 14 - \lambda & 3 \\ 3 & 6 - \lambda \end{bmatrix})$ $=(14-\lambda)(6-\lambda)-9=\lambda^2-20\lambda+75$ That quadratic has roots 15 and 5, so those are the eigenvalues of AA^* .

A has singular values $\sigma_1 = \sqrt{15}$ and $\sigma_2 = \sqrt{5}$.

To compute a full singular value decomposition (not just the singular values), we again leech off of diagonalization. Notice that

if
$$A = U E V^*$$
 is an SVD then $A^*A = V E^*E V^*$ is a spectral decomposition.
... Columns of V are eigenvectors of A^*A .

Similarly, the columns of U are eigenvectors of AA^* , but a slightly quicker (and slightly more correct) way to compute the columns of U is to notice that

$$A = U \Sigma V^*$$
, so $AV = U \Sigma$ which means $[AV_1 | AV_2 | \cdots | AV_n] = [\sigma_1 \vec{u}_1 | \sigma_2 \vec{u}_2 | \cdots | \sigma_n \vec{u}_n]$. If $\sigma_1 \neq 0$ then $\sigma_2 = \sigma_1 + \sigma_2 = \sigma_2 + \sigma_3 = \sigma_3 + \sigma_4 = \sigma_3 = \sigma_3$

Example. Compute a singular value decomposition of the matrix

$$A = \begin{bmatrix} 1 & 2 & 3 \\ -1 & 0 & 1 \\ 3 & 2 & 1 \end{bmatrix}.$$

$$D \text{ Eigenstuff for } A^*A = \begin{bmatrix} 1 & 8 & 5 \\ 8 & 8 & 8 \\ 5 & 8 & 1 \end{bmatrix};$$

$$\lambda_1 = 24, \quad \lambda_2 = b, \quad \lambda_3 = 0 \quad \text{and}$$

$$\vec{V}_1 = (1,1,1), \quad \vec{V}_2 = (1,0,-1), \quad \vec{V}_3 = (1,-2,1).$$

② Construct
$$\Sigma$$
 and V :
$$\Sigma = \begin{bmatrix} 255 & 0 & 0 \\ 0 & 55 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \text{and} \quad V = \begin{bmatrix} 55 & 55 & 55 \\ 55 & 55 & 55 \\ 55 & 55 & 55 \end{bmatrix}.$$

3) Construct
$$U:$$

$$\vec{U}_{1} = \frac{1}{5} \cdot A\vec{V}_{1} = \frac{1}{216} \begin{bmatrix} 1 & 2 & 3 \\ -1 & 0 & 1 \\ 3 & 2 & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{12} \\ \frac{1}{13} \end{bmatrix} = \frac{1}{52} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} \times Better have$$

$$\vec{U}_{2} = \frac{1}{52} \cdot A\vec{V}_{2} = \frac{1}{16} \begin{bmatrix} 1 & 2 & 3 \\ -1 & 0 & 1 \\ 3 & 2 & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{12} \\ 0 \\ \frac{1}{12} \end{bmatrix} = \frac{1}{13} \begin{bmatrix} -1 \\ -1 \\ 1 \end{bmatrix} \times norm 1!$$

Since
$$\sigma_3 = 0$$
, \vec{U}_3 can be ANY unit vector that is orthogonal to \vec{U}_1 and \vec{U}_2 . E.g., use Gram-Schmidt or cross product: $\vec{U}_1 \times \vec{U}_2 = \frac{1}{12}(1,0,1) \times \frac{1}{12}(-1,-1,1) = \frac{1}{12}(1,-2,-1)$.

$$... U = \begin{bmatrix} \frac{1}{12} & \frac{1}{12} & \frac{1}{12} \\ 0 & \frac{1}{12} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{12} & \frac{1}{12} \end{bmatrix}$$

Before delving into what makes the singular value decomposition so useful, it is worth noting that if $A \in \mathcal{M}_{m,n}(\mathbb{F})$ has singular value decomposition $A = U\Sigma V^*$ then A^T and A^* have singular value decompositions

$$A^{T} = \overline{V} Z^{T} U^{T}$$
 and $A^{*} = V Z^{*} U^{*}$

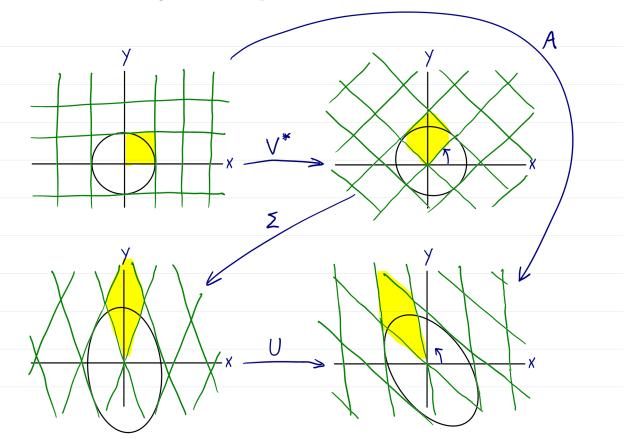
In particular,

Geometric Interpretation

Recall that we think of unitary matrices as arbitrary-dimensional rotations and/or reflections. Using this intuition gives the singular value decomposition a simple geometric interpretation. Specifically, it says that every matrix $A = U\Sigma V^* \in \mathcal{M}_{m,n}(\mathbb{F})$ acts as a linear transformation from \mathbb{F}^n to \mathbb{F}^m in the following way:

- · First, capply V*: rotate and/or reflect F.
- Then, apply Σ : stretch F^n along its coordinate axes and embed in F^m .
- · Finally, apply U: rotate and/or reflect Fm

Let's illustrate this geometric interpretation in the m=n=2 case:



In particular, it is worth keeping track not only of how the linear transformation changes a unit square grid on \mathbb{R}^2 into a parallelogram grid, but also how it transforms...

the unit circle into an ellipse

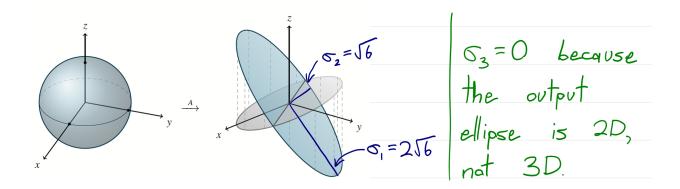
Furthermore, the two radii of the ellipse are exactly

the singular values of A (5, long radius, 5, short)

In higher dimensions, linear transformations send (hyper-)ellipsoids to (hyper-)ellipsoids. For example, the matrix

$$A = \begin{bmatrix} 1 & 2 & 3 \\ -1 & 0 & 1 \\ 3 & 2 & 1 \end{bmatrix}$$

from earlier deforms the unit sphere as follows:



The fact that the unit sphere is turned into a 2D ellipse by this matrix corresponds to the fact that...

In fact, the first two left singular vectors \mathbf{u}_1 and \mathbf{u}_2 (which point in the directions of the major and minor axes of the ellipse) form an orthonormal basis of the range.

Similarly, the 3rd right sing. Vector
$$\vec{V}_3$$
 has $A\vec{V}_3 = U\Sigma V^*\vec{V}_3 = U\Sigma \vec{e}_3 = U(\sigma_3 \vec{e}_3) = \vec{O}$ (i.e., $\vec{V}_3 \in \text{null}(A)$).

This same type of argument works in general and leads to the following theorem:

Theorem 9.2 — Bases of the Fundamental Subspaces

Let $A \in \mathcal{M}_{m,n}$ be a matrix with rank r and singular value decomposition $A = U\Sigma V^*$, where

$$U = [\mathbf{u}_1 \mid \mathbf{u}_2 \mid \cdots \mid \mathbf{u}_m]$$
 and $V = [\mathbf{v}_1 \mid \mathbf{v}_2 \mid \cdots \mid \mathbf{v}_n]$.

Then

- a) $\{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_r\}$ is an orthonormal basis of range(A),
- **b)** $\{\mathbf{u}_{r+1}, \mathbf{u}_{r+2}, \dots, \mathbf{u}_m\}$ is an orthonormal basis of $\text{null}(A^*)$,
- c) $\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_r\}$ is an orthonormal basis of range (A^*) , and
- d) $\{\mathbf{v}_{r+1}, \mathbf{v}_{r+2}, \dots, \mathbf{v}_n\}$ is an orthonormal basis of null(A).

Proof. Let's compute $A\mathbf{v}_i$:

Corollary 9.3 — Orthogonality of the Fundamental Subspaces

Suppose $\mathbb{F} = \mathbb{R}$ or $\mathbb{F} = \mathbb{C}$, and $A \in \mathcal{M}_{m,n}(\mathbb{F})$. Then

- a) range(A) is orthogonal to $null(A^*)$, and
- **b)** null(A) is orthogonal to $\text{range}(A^*)$.

In this corollary, when we say that one subspace is orthogonal to another, we mean that

Example. Compute a singular value decomposition of the matrix

$$A = \begin{bmatrix} 1 & 1 & 1 & -1 \\ 0 & 1 & 1 & 0 \\ -1 & 1 & 1 & 1 \end{bmatrix},$$

and use it to construct bases of the four fundamental subspaces of A.

① Eigenstuff for
$$AA^* = \begin{bmatrix} \frac{1}{2} & \frac{2}{2} & \frac{2}{2} \\ 0 & \frac{2}{2} & \frac{4}{2} \end{bmatrix}$$
: $(AA^* \text{ is } 3 \times 3)$, $A^*A \text{ is } 4 \times 4$)

eigenvalues are $6, 4, 0$, with corresponding eigenvectors $(1,1,1), (1,0,-1), (1,-2,1), \text{ respectively.}$

② $Z = \begin{bmatrix} \frac{1}{6} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$ and $U = \begin{bmatrix} \frac{1}{6} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{bmatrix}$

We used AA^* (not A^*A), so we get U (not V).

③ $V_1 = \frac{1}{6} A^* \overrightarrow{U}_1 = \frac{1}{6} \begin{bmatrix} 1 & 0 & 1 \\ 1 & 1 & 1 \\ -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{6} & 1 \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ 0 & \frac{1}{4} & \frac{1}{4} \end{bmatrix} \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ 0 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ 0 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{bmatrix} \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ 0 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{bmatrix} \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ 0 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{bmatrix} \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ 0 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{bmatrix} \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ 0 & \frac{1}{4} & \frac{1$

By inspection:
$$\vec{V}_3 = \vec{J}_2 \begin{bmatrix} 0 \\ -1 \\ 0 \end{bmatrix}$$
 and $\vec{V}_4 = \vec{J}_2 \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ work. (Can also find via Gram-Schmidt, for example)

Relationship With Other Matrix Decompositions

We now make sure that we really understand where the SVD fits into our world of matrix decompositions. For example, one way of rephrasing the singular value decomposition is as saying that we can always write a rank-r matrix as a sum of r rank-1 matrices in a very special way:

Theorem 9.4 — Orthogonal Rank-One Sum Decomposition

Suppose $\mathbb{F} = \mathbb{R}$ or $\mathbb{F} = \mathbb{C}$, and $A \in \mathcal{M}_{m,n}(\mathbb{F})$ is a matrix with rank(A) = r. Then there exist orthonormal sets of vectors $\{\mathbf{u}_i\}_{i=1}^r \subset \mathbb{F}^m$ and $\{\mathbf{v}_i\}_{i=1}^r \subset \mathbb{F}^n$ such that

$$A = \sum_{j=1}^{r} \sigma_j \vec{u_j} \vec{v_j}^* \qquad (= U \Sigma V^*)$$

where $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$ are the non-zero singular values of A.

- This formulation is sometimes useful because... it lets us break

 A into r "pieces": one for each of
- In fields other than $\mathbb R$ and $\mathbb C$, ... the same theorem holds, but with "lin. indep." instead of "orthonormal".

Proof. For simplicity, we again assume that $m \leq n$ throughout this proof, and then we just do block matrix multiplication in the singular value decompositon:

$$A = U \geq V^* = \begin{bmatrix} \vec{u}_1 & \vec{u}_2 & \cdots & \vec{u}_m \end{bmatrix} \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix} \underbrace{\begin{bmatrix} \vec{\nabla}_1^* \\ \vec{\nabla}_2^* \\ \vdots \\ \vec{\nabla}_n^* \end{bmatrix}}_{= \vec{v}_1^* = \vec{v}_1^* \vec{v}_1^* \vec{v}_2^* = \vec{v}_2^* \vec{v}_1^* \vec{v}_2^* \vec{v}_2$$

In fact the singular value decomposition and the orthogonal rank-one sum decomposition are "equivalent" in the sense that you can prove one to quickly prove the other, and viceversa. Sometimes they are both just called the singular value decomposition.

Example. Compute an orthogonal rank-one sum decomposition of the matrix

$$A = \begin{bmatrix} 1 & 1 & 1 & -1 \\ 0 & 1 & 1 & 0 \\ -1 & 1 & 1 & 1 \end{bmatrix}.$$

We computed the following SVD
$$A = U \Sigma V^*$$
 earlier this week:

$$U = \begin{bmatrix} \frac{1}{15} & \frac{1}{15} & \frac{1}{15} \\ \frac{1}{15} & 0 & \frac{1}{2} & \frac{1}{15} \end{bmatrix}, \quad \Sigma = \begin{bmatrix} \frac{1}{15} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad V = \frac{1}{15} \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}.$$
Then $A = \sigma_1 \vec{u}_1 \vec{v}_1^* + \sigma_2 \vec{u}_2 \vec{v}_2^* = \sqrt{5} \left(\frac{1}{15} \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix} \right) + 2 \left(\frac{1}{2} \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 \end{bmatrix} \right).$

Similarly, the singular value decomposition is also "essentially equivalent" to the polar decomposition:

If
$$A \in M_n$$
 has SVD $A = U \le V^*$ then
$$A = (UV^*)(V \le V^*)$$
 is a polar decomposition of A .

In the opposite direction,

If
$$A \in M_n$$
 has polar decomposition $A = UP$
and P has spectral decomposition $P = VDV^*$
then $A = (UV)DV^*$ is an SVD of A .

If $A \in \mathcal{M}_n$ is positive semidefinite, then the singular value decomposition coincides exactly with the spectral decomposition:

Spectral decomp.:
$$A = UDU^*$$
, with diagonal entries of D real and non-negative. This is an $SVD!$.: Sing. values are eigenvalues.

A slight generalization of this type of argument leads to the following theorem:

Theorem 9.5 — Singular Values of Normal Matrices

Suppose $A \in \mathcal{M}_n$ is a normal matrix. Then the singular values of A are the absolute values of its eigenvalues.

Proof. Since A is normal, we can use the spectral decomposition to write $A = UDU^*$, where U is unitary and D is diagonal...

(but the diagonal entries of D can be negative/complex). Each diagonal entry
$$d_j$$
 of D can be written in polar form: $d_j = r_j e^{i\theta_j}$. Then

$$A = UDU^* = U\begin{bmatrix} e^{i\theta_1} & 0 & 0 \\ 0 & e^{i\theta_2} & 0 \\ 0 & 0 & e^{i\theta_n} \end{bmatrix} \begin{bmatrix} r_1 & 0 & 0 & 0 \\ 0 & r_2 & 0 & 0 \\ 0 & 0 & r_n \end{bmatrix}$$

$$V^* = Z$$

$$SVD \quad \text{of} \quad A.$$

The singular values of A are
$$r_1 = |d_1|$$
, $r_2 = |d_2|$, $r_n = |d_n|$.

To see that the above theorem does not hold for non-normal matrices, consider the following example:

Example. Compute the eigenvalues and singular values of the matrix

$$A = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}.$$

Eigenvalues: 1 and 1 (diagonal entries)

Singular values: $A^*A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 2 \\ 1 & 2 \end{bmatrix}$, which has eigenvalues $\frac{1}{2}(3\pm\sqrt{5})$.

The singular values of A are thus $\sigma_1 = \sqrt{\frac{1}{2}(3+\sqrt{5})}$ and $\sigma_2 = \sqrt{\frac{1}{2}(3-\sqrt{5})}$, which do not equal 1.