

Math 221: LINEAR ALGEBRA

Chapter 8. Orthogonality

§8-6. Singular Value Decomposition

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Emory University, 2020 Fall

(last updated on 11/16/2020)



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¹Slides are adapted from those by Karen Seyffarth from University of Calgary.

Singular Value Decomposition

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Singular Value Decomposition

$$\mathbf{M}_{m \times n} = \mathbf{U}_{m \times m} \mathbf{\Sigma}_{m \times n} \mathbf{V}^*_{n \times n}$$

$$\mathbf{U}_{m \times m} \mathbf{U}^*_{m \times m} = \mathbf{I}_m$$

$$\mathbf{V}_{n \times n} \mathbf{V}^*_{n \times n} = \mathbf{I}_n$$

Definition

Let A be an $m \times n$ matrix. The **singular values** of A are the square roots of the nonzero eigenvalues of $A^T A$. **Singular Value Decomposition (SVD)** can be thought of as a generalization of orthogonal diagonalization of a symmetric matrix to an arbitrary $m \times n$ matrix.

Given an $m \times n$ matrix A , we will see how to express A as a product

$$A = U\Sigma V^T$$

where

- ▶ U is an $m \times m$ orthogonal matrix whose columns are eigenvectors of AA^T .
- ▶ V is an $n \times n$ orthogonal matrix whose columns are eigenvectors of $A^T A$.
- ▶ Σ is an $m \times n$ matrix whose only nonzero values lie on its main diagonal, and are the square roots of the eigenvalues of both AA^T and $A^T A$.

Theorem

If A is an $m \times n$ matrix, then $A^T A$ and AA^T have the same nonzero eigenvalues.

Proof.


Suppose A is an $m \times n$ matrix, and suppose that λ is a nonzero eigenvalue of $A^T A$. Then there exists a nonzero vector $\vec{x} \in \mathbb{R}^n$ such that

$$(A^T A)\vec{x} = \lambda\vec{x}. \quad (1)$$

Multiplying both sides of this equation by A :

$$\begin{aligned} A(A^T A)\vec{x} &= A\lambda\vec{x} \\ (AA^T)(A\vec{x}) &= \lambda(A\vec{x}). \end{aligned}$$

Since $\lambda \neq 0$ and $\vec{x} \neq \vec{0}_n$, $\lambda\vec{x} \neq \vec{0}_n$, and thus by equation (1), $(A^T A)\vec{x} \neq \vec{0}_n$; thus $A^T(A\vec{x}) \neq \vec{0}_n$, implying that $A\vec{x} \neq \vec{0}_m$.

Therefore $A\vec{x}$ is an eigenvector of AA^T corresponding to eigenvalue λ . An analogous argument can be used to show that every nonzero eigenvalue of AA^T is an eigenvalue of $A^T A$, thus completing the proof. 

Examples

Example

Let $A = \begin{bmatrix} 1 & -1 & 3 \\ 3 & 1 & 1 \end{bmatrix}$. Then

$$AA^T = \begin{bmatrix} 1 & -1 & 3 \\ 3 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 3 \\ -1 & 1 \\ 3 & 1 \end{bmatrix} = \begin{bmatrix} 11 & 5 \\ 5 & 11 \end{bmatrix}.$$

$$A^TA = \begin{bmatrix} 1 & 3 \\ -1 & 1 \\ 3 & 1 \end{bmatrix} \begin{bmatrix} 1 & -1 & 3 \\ 3 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 10 & 2 & 6 \\ 2 & 2 & -2 \\ 6 & -2 & 10 \end{bmatrix}.$$

Example (continued)

Since AA^T is 2×2 while A^TA is 3×3 , and AA^T and A^TA have the same nonzero eigenvalues, compute $c_{AA^T}(x)$ (because it's easier to compute than $c_{A^TA}(x)$).

$$\begin{aligned}c_{AA^T}(x) &= \det(xI - AA^T) = \begin{vmatrix} x - 11 & -5 \\ -5 & x - 11 \end{vmatrix} \\&= (x - 11)^2 - 25 \\&= x^2 - 22x + 121 - 25 \\&= x^2 - 22x + 96 \\&= (x - 16)(x - 6).\end{aligned}$$

Therefore, the eigenvalues of AA^T are $\lambda_1 = 16$ and $\lambda_2 = 6$.

Example (continued)

The eigenvalues of $A^T A$ are $\lambda_1 = 16$, $\lambda_2 = 6$, and $\lambda_3 = 0$, and the singular values of A are $\sigma_1 = \sqrt{16} = 4$ and $\sigma_2 = \sqrt{6}$. By convention, we list the eigenvalues (and corresponding singular values) in nonincreasing order (i.e., from largest to smallest).

To find the matrix V , find eigenvectors for $A^T A$. Since the eigenvalues of AA^T are distinct, the corresponding eigenvectors are orthogonal, and we need only normalize them.

$\lambda_1 = 16$: solve $(16I - A^T A)\vec{y}_1 = \vec{0}$.

$$\left[\begin{array}{ccc|c} 6 & -2 & -6 & 0 \\ -2 & 14 & 2 & 0 \\ -6 & 2 & 6 & 0 \end{array} \right] \rightarrow \left[\begin{array}{ccc|c} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right], \text{ so } \vec{y}_1 = \begin{bmatrix} t \\ 0 \\ t \end{bmatrix} = t \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, t \in \mathbb{R}.$$

$\lambda_2 = 6$: solve $(6I - A^T A)\vec{y}_2 = \vec{0}$.

$$\left[\begin{array}{ccc|c} -4 & -2 & -6 & 0 \\ -2 & 4 & 2 & 0 \\ -6 & 2 & -4 & 0 \end{array} \right] \rightarrow \left[\begin{array}{ccc|c} 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right], \text{ so } \vec{y}_2 = \begin{bmatrix} -s \\ -s \\ s \end{bmatrix} = s \begin{bmatrix} -1 \\ -1 \\ 1 \end{bmatrix}, s \in \mathbb{R}.$$

Example (continued)

$\lambda_3 = 0$: solve $(-A^T A)\vec{y}_3 = \vec{0}$.

$$\left[\begin{array}{ccc|c} -10 & -2 & -6 & 0 \\ -2 & -2 & 2 & 0 \\ -6 & 2 & -10 & 0 \end{array} \right] \rightarrow \left[\begin{array}{ccc|c} 1 & 0 & 1 & 0 \\ 0 & 1 & -2 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right], \text{ so } \vec{y}_3 = \begin{bmatrix} -r \\ 2r \\ r \end{bmatrix} = r \begin{bmatrix} -1 \\ 2 \\ 1 \end{bmatrix}, r \in \mathbb{R}.$$

Let

$$\vec{v}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \vec{v}_2 = \frac{1}{\sqrt{3}} \begin{bmatrix} -1 \\ -1 \\ 1 \end{bmatrix}, \vec{v}_3 = \frac{1}{\sqrt{6}} \begin{bmatrix} -1 \\ 2 \\ 1 \end{bmatrix}.$$

Then

$$V = \frac{1}{\sqrt{6}} \begin{bmatrix} \sqrt{3} & -\sqrt{2} & -1 \\ 0 & -\sqrt{2} & 2 \\ \sqrt{3} & \sqrt{2} & 1 \end{bmatrix}.$$

Also,

$$\Sigma = \begin{bmatrix} 4 & 0 & 0 \\ 0 & \sqrt{6} & 0 \end{bmatrix},$$

and we use A , V^T , and Σ to find U .

Example (continued)

Since V is orthogonal and $A = U\Sigma V^T$, it follows that $AV = U\Sigma$. Let $V = \begin{bmatrix} \vec{v}_1 & \vec{v}_2 & \vec{v}_3 \end{bmatrix}$, and let $U = \begin{bmatrix} \vec{u}_1 & \vec{u}_2 \end{bmatrix}$, where \vec{u}_1 and \vec{u}_2 are the two columns of U . Then we have

$$\begin{aligned} A \begin{bmatrix} \vec{v}_1 & \vec{v}_2 & \vec{v}_3 \end{bmatrix} &= \begin{bmatrix} \vec{u}_1 & \vec{u}_2 \end{bmatrix} \Sigma \\ \begin{bmatrix} A\vec{v}_1 & A\vec{v}_2 & A\vec{v}_3 \end{bmatrix} &= \begin{bmatrix} \sigma_1\vec{u}_1 + 0\vec{u}_2 & 0\vec{u}_1 + \sigma_2\vec{u}_2 & 0\vec{u}_1 + 0\vec{u}_2 \end{bmatrix} \\ &= \begin{bmatrix} \sigma_1\vec{u}_1 & \sigma_2\vec{u}_2 & \vec{0} \end{bmatrix} \end{aligned}$$

which implies that $A\vec{v}_1 = \sigma_1\vec{u}_1 = 4\vec{u}_1$ and $A\vec{v}_2 = \sigma_2\vec{u}_2 = \sqrt{6}\vec{u}_2$. Thus,

$$\vec{u}_1 = \frac{1}{4}A\vec{v}_1 = \frac{1}{4} \begin{bmatrix} 1 & -1 & 3 \\ 3 & 1 & 1 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} = \frac{1}{4\sqrt{2}} \begin{bmatrix} 4 \\ 4 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix},$$

and

$$\vec{u}_2 = \frac{1}{\sqrt{6}}A\vec{v}_2 = \frac{1}{\sqrt{6}} \begin{bmatrix} 1 & -1 & 3 \\ 3 & 1 & 1 \end{bmatrix} \frac{1}{\sqrt{3}} \begin{bmatrix} -1 \\ -1 \\ 1 \end{bmatrix} = \frac{1}{3\sqrt{2}} \begin{bmatrix} 3 \\ -3 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$

Example (continued)

Therefore,

$$\mathbf{U} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix},$$

and

$$\begin{aligned} \mathbf{A} &= \begin{bmatrix} 1 & -1 & 3 \\ 3 & 1 & 1 \end{bmatrix} \\ &= \left(\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \right) \begin{bmatrix} 4 & 0 & 0 \\ 0 & \sqrt{6} & 0 \end{bmatrix} \left(\frac{1}{\sqrt{6}} \begin{bmatrix} \sqrt{3} & 0 & \sqrt{3} \\ -\sqrt{2} & -\sqrt{2} & \sqrt{2} \\ -1 & 2 & 1 \end{bmatrix} \right). \end{aligned}$$

Problem

Find an SVD for $A = \begin{bmatrix} -1 \\ 2 \\ 2 \end{bmatrix}$.

Solution

Since A is 3×1 , $A^T A$ is a 1×1 matrix whose eigenvalues are easier to find than the eigenvalues of the 3×3 matrix AA^T .

$$A^T A = \begin{bmatrix} -1 & 2 & 2 \end{bmatrix} \begin{bmatrix} -1 \\ 2 \\ 2 \end{bmatrix} = \begin{bmatrix} 9 \end{bmatrix}.$$

Thus $A^T A$ has eigenvalue $\lambda_1 = 9$, and the eigenvalues of AA^T are $\lambda_1 = 9$, $\lambda_2 = 0$, and $\lambda_3 = 0$. Furthermore, A has only one singular value, $\sigma_1 = 3$.

To find the matrix V , find an eigenvector for $A^T A$ and normalize it. In this case, finding a unit eigenvector is trivial: $\vec{v}_1 = \begin{bmatrix} 1 \end{bmatrix}$, and

$$V = \begin{bmatrix} 1 \end{bmatrix}.$$

Solution (continued)

Also, $\Sigma = \begin{bmatrix} 3 \\ 0 \\ 0 \end{bmatrix}$, and we use A , V^T , and Σ to find U .

Now $AV = U\Sigma$, with $V = \begin{bmatrix} \vec{v}_1 \end{bmatrix}$, and $U = \begin{bmatrix} \vec{u}_1 & \vec{u}_2 & \vec{u}_3 \end{bmatrix}$, where \vec{u}_1 , \vec{u}_2 , and \vec{u}_3 are the columns of U . Thus

$$\begin{aligned} A \begin{bmatrix} \vec{v}_1 \end{bmatrix} &= \begin{bmatrix} \vec{u}_1 & \vec{u}_2 & \vec{u}_3 \end{bmatrix} \Sigma \\ \begin{bmatrix} A\vec{v}_1 \end{bmatrix} &= \begin{bmatrix} \sigma_1 \vec{u}_1 + 0\vec{u}_2 + 0\vec{u}_3 \end{bmatrix} \\ &= \begin{bmatrix} \sigma_1 \vec{u}_1 \end{bmatrix} \end{aligned}$$

This gives us $A\vec{v}_1 = \sigma_1 \vec{u}_1 = 3\vec{u}_1$, so

$$\vec{u}_1 = \frac{1}{3}A\vec{v}_1 = \frac{1}{3} \begin{bmatrix} -1 \\ 2 \\ 2 \end{bmatrix} \begin{bmatrix} 1 \end{bmatrix} = \frac{1}{3} \begin{bmatrix} -1 \\ 2 \\ 2 \end{bmatrix}.$$

Solution (continued)

The vectors \vec{u}_2 and \vec{u}_3 are eigenvectors of AA^T corresponding to the eigenvalue $\lambda_2 = \lambda_3 = 0$. Instead of solving the system $(0I - AA^T)\vec{x} = \vec{0}$ and then using the Gram-Schmidt orthogonalization algorithm on the resulting set of two basic eigenvectors, the following approach may be used.

Find vectors \vec{u}_2 and \vec{u}_3 by first extending $\{\vec{u}_1\}$ to a basis of \mathbb{R}^3 , then using the Gram-Schmidt algorithm to orthogonalize the basis, and finally normalizing the vectors.

Starting with $\{3\vec{u}_1\}$ instead of $\{\vec{u}_1\}$ makes the arithmetic a bit easier. It is easy to verify that

$$\left\{ \begin{bmatrix} -1 \\ 2 \\ 2 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \right\}$$

is a basis of \mathbb{R}^3 . Set

$$\vec{f}_1 = \begin{bmatrix} -1 \\ 2 \\ 2 \end{bmatrix}, \vec{x}_2 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \vec{x}_3 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix},$$

and apply the Gram-Schmidt orthogonalization algorithm to $\{\vec{f}_1, \vec{x}_2, \vec{x}_3\}$.

Solution (continued)

This gives us

$$\vec{f}_2 = \begin{bmatrix} 4 \\ 1 \\ 1 \end{bmatrix} \quad \text{and} \quad \vec{f}_3 = \begin{bmatrix} 0 \\ 1 \\ -1 \end{bmatrix}.$$

Therefore,

$$\vec{u}_2 = \frac{1}{\sqrt{18}} \begin{bmatrix} 4 \\ 1 \\ 1 \end{bmatrix}, \quad \vec{u}_3 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ -1 \end{bmatrix},$$

and

$$U = \begin{bmatrix} -\frac{1}{3} & \frac{4}{\sqrt{18}} & 0 \\ \frac{2}{3} & \frac{1}{\sqrt{18}} & \frac{1}{\sqrt{2}} \\ \frac{2}{3} & \frac{1}{\sqrt{18}} & -\frac{1}{\sqrt{2}} \end{bmatrix}.$$

Finally,

$$A = \begin{bmatrix} -1 \\ 2 \\ 2 \end{bmatrix} = \begin{bmatrix} -\frac{1}{3} & \frac{4}{\sqrt{18}} & 0 \\ \frac{2}{3} & \frac{1}{\sqrt{18}} & \frac{1}{\sqrt{2}} \\ \frac{2}{3} & \frac{1}{\sqrt{18}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 3 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 1 \end{bmatrix}.$$



Problem

Find a singular value decomposition of $A = \begin{bmatrix} 1 & 4 \\ 2 & 8 \end{bmatrix}$.

Solution

$$\begin{bmatrix} 1 & 4 \\ 2 & 8 \end{bmatrix} = \left(\frac{1}{\sqrt{5}} \begin{bmatrix} 1 & -2 \\ 2 & 1 \end{bmatrix} \right) \begin{bmatrix} \sqrt{85} & 0 \\ 0 & 0 \end{bmatrix} \left(\frac{1}{\sqrt{17}} \begin{bmatrix} 1 & -4 \\ 4 & 1 \end{bmatrix} \right).$$



Remark

Since there is only one non-zero eigenvalue, \vec{u}_2 (the second column of U) can not be found using the formula $\vec{u}_2 = \frac{1}{\sigma_2} A \vec{v}_2$. However, \vec{u}_2 can be chosen to be any unit vector orthogonal to \vec{u}_1 ; in this case, $\vec{u}_2 = \frac{1}{\sqrt{5}} \begin{bmatrix} -2 \\ 1 \end{bmatrix}$.

Problem

Find a singular value decomposition of $A = \begin{bmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix}$.

Solution

$$\begin{bmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \\ \parallel \\ \left(\frac{1}{\sqrt{2}} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} \right) \begin{bmatrix} \sqrt{3} & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \left(\frac{1}{\sqrt{6}} \begin{bmatrix} 1 & -2 & 1 \\ -\sqrt{3} & 0 & \sqrt{3} \\ \sqrt{2} & \sqrt{2} & \sqrt{2} \end{bmatrix} \right)$$



Fundamental Subspaces

Full Singular Value Decomposition

$$\begin{array}{c}
 \begin{array}{c} n \\ m \end{array} \begin{array}{|c|} \hline A \\ \hline \end{array} = \begin{array}{c} k \\ \begin{array}{|c|} \hline U \\ \hline \end{array} \end{array} \begin{array}{c} \Sigma \\ \begin{array}{|c|} \hline \diagdown \\ \hline \end{array} \end{array} \begin{array}{c} V^T \\ \begin{array}{|c|} \hline \equiv \\ \hline \end{array} \end{array} \\
 \\
 = \begin{array}{c} k \\ \begin{array}{|c|c|} \hline U \\ \hline \end{array} \end{array} \begin{array}{c} \Sigma \\ \begin{array}{|c|} \hline \diagdown \\ \hline 0 \\ \hline \end{array} \end{array} \begin{array}{c} V^T \\ \begin{array}{|c|} \hline \\ \hline \end{array} \end{array}
 \end{array}$$

Full

Singular Value Decomposition

$$\begin{array}{c} n \\ m \end{array} \begin{array}{|c|} \hline A \\ \hline \end{array} = \begin{array}{c} u \\ \begin{array}{|c|} \hline U \\ \hline \end{array} \end{array} \begin{array}{c} \Sigma \\ \begin{array}{|c|} \hline \diagdown \\ \hline \end{array} \end{array} \begin{array}{c} V^T \\ \begin{array}{|c|} \hline \equiv \\ \hline \end{array} \end{array}$$

Applications

Example (Polar Decomposition)

$$a + bi = \underbrace{\sqrt{a^2 + b^2}}_{\text{radius}} \underbrace{e^{i\theta}}_{\text{rotation}}.$$

Similarly, any square matrix

$$A = U\Sigma V^T = \underbrace{U\Sigma U^T}_{\text{nonneg. def.}} \underbrace{UV^T}_{\text{rotation}}$$

Definition

A real $n \times n$ matrix G is **nonnegative definite** (or **positive** in the book) if it is symmetric and for all $\vec{x} \in \mathbb{R}^n$

$$\vec{x}^T G \vec{x} \geq 0.$$

Example (Generalized inverse)

$$\boxed{A} \mid = \mid$$



$$\mid = \boxed{A^{-1}} \mid$$

$$\boxed{A} \mid = \mid$$



Example (Image of unit ball under linear transform A)

Let $A = U\Sigma V^T$ be the full SVD for an $m \times n$ matrix A. We will see how the unit ball will be mapped:

$$\{A\vec{x} \mid \|\vec{x}\| \leq 1\}$$

The linear map $\vec{y} = A\vec{x}$ is trying to do the following things:

1. Rotate the n-vector \vec{x} by V^T
2. Stretch along axes by σ_i with $\sigma_i = 0$ for $i > \text{rank}(A)$
3. Zero-pad for tall matrix (i.e., $m > n$) or truncate for fat matrix (i.e., $m < n$) to get m-vector
4. Rotate the m-vector by U^T

Example (Image of unit ball under linear transform A – continued)

