MA60053 - Computational Linear Algebra Singular Value Decomposition(SVD) (To be updated)

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March 5, 2020

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and $U \in \mathbb{R}^{n \times n}$ and $V \in \mathbb{R}^{m \times m}$ are orthogonal.

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and $U \in \mathbb{R}^{n \times n}$ and $V \in \mathbb{R}^{m \times m}$ are orthogonal.

The matrix U is called a left singular vector matrix, V is called a right singular vector matrix, and the scalars σ_j are called singular values.

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and $U \in \mathbb{R}^{n \times n}$ and $V \in \mathbb{R}^{m \times m}$ are orthogonal.

Condensed SVD

Let $A \in \mathbb{R}^{n \times m}$ be a nonzero matrix of rank r. Then, there exist $\widehat{U} \in \mathbb{R}^{n \times r}$, $\widehat{\Sigma} \in \mathbb{R}^{r \times r}$ and $\widehat{V} \in \mathbb{R}^{m \times r}$ such that $\widehat{U}^T \widehat{U} = \widehat{V}^T \widehat{V} = I_r$, $\widehat{\Sigma}$ is a diagonal matrix with main diagonal entries $\sigma_1 \geq \cdots \geq \sigma_r > 0$, and $A = \widehat{U} \widehat{\Sigma} \widehat{V}^T$.

Existence of SVD

Theorem

Every matrix has an singular value decomposition.

Proof.

- Let A be an $n \times m$ matrix with rank r and $n \leq m$.

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- Let A be an $n \times m$ matrix with rank r and $n \leq m$.
- Then the matrix AA^T is a symmetric matrix with rank r.
- By Spectral theorem, we have $AA^T = U \Lambda U^T$, where $\Lambda = \mathrm{diag}(d_1, \ldots, d_r, 0, \ldots, 0)$ and $U^T U = I$.

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- Take $B = A^T U$, then $B^T B = \Lambda$.

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- Take $B = A^T U$, then $B^T B = \Lambda$.
- Define $V = BG$ where $G = \text{diag}(\frac{1}{\sqrt{d_1}}, \ldots, \frac{1}{\sqrt{d_r}}, 0, \ldots, 0(m\text{-times}))$.

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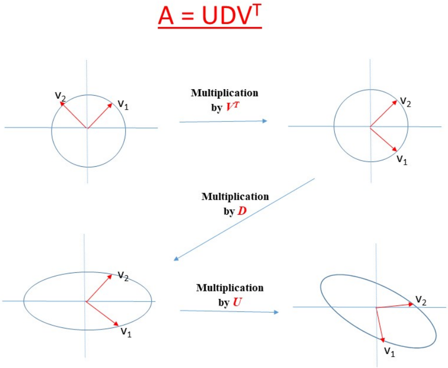
- Define $V = BG$ where $G = \mathrm{diag}(\frac{1}{\sqrt{d_1}}, \ldots, \frac{1}{\sqrt{d_r}}, 0, \ldots, 0(m\text{-times}))$.
- Let $\Sigma = (\sqrt{\Lambda}\ 0)$ Verify $U\Sigma V^T$ is a singular value decomposition for A.

$\square$

SVD geometry



Computing SVD

Example

Let us compute SVD for the following 2×3 matrix,

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

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Next, we have to find the eigenvalues and corresponding eigenvectors of AA^T. After calculating, we get the following eigenvalues and their corresponding eigenvectors.

$$\lambda = 10; \quad u_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\lambda = 12; \quad u_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

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Thus the matrix A has singular values $\sigma_1 = \sqrt{12}$ and $\sigma_2 = \sqrt{10}$. Now after normalizing u_1 and u_2, we put $U = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix}$.

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The calculation of V is similar. V is based on $A^T A$, so we have

$$A^T A = \begin{pmatrix} 3 & -1 \\ 1 & 3 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 3 & 1 & 1 \\ -1 & 3 & 1 \end{pmatrix} = \begin{pmatrix} 10 & 0 & 2 \\ 0 & 10 & 4 \\ 2 & 4 & 2 \end{pmatrix}.$$

Eigenvalues and their corresponding eigenvectors are as follows

$$\textit{for } \lambda = 12; \quad v_1 = \begin{pmatrix} 1 \\ 2 \\ 1 \end{pmatrix}$$

$$\textit{for } \lambda = 10; \quad v_2 = \begin{pmatrix} 2 \\ -1 \\ 0 \end{pmatrix}$$

$$\textit{for } \lambda = 0; \quad v_3 = \begin{pmatrix} 1 \\ 2 \\ -5 \end{pmatrix}.$$

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After normalization, we get $V = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{5}} & \frac{1}{\sqrt{30}} \\ \frac{2}{\sqrt{6}} & \frac{-1}{\sqrt{5}} & \frac{2}{\sqrt{30}} \\ \frac{1}{\sqrt{6}} & 0 & \frac{-5}{\sqrt{30}} \end{pmatrix}$ i.e.,

$$V^T = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{5}} & \frac{-1}{\sqrt{5}} & 0 \\ \frac{1}{\sqrt{30}} & \frac{2}{\sqrt{30}} & \frac{-5}{\sqrt{30}} \end{pmatrix}$$

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Geometric form of SVD

Let $A \in \mathbb{R}^{n \times m}$ with $n \leq m$. Then, $\mathbb{R}^n$ has an orthonormal basis $\{u_1, \dots, u_n\}$, $\mathbb{R}^m$ has an orthonormal basis $\{v_1, \dots, v_m\}$ and there exists $\sigma_1 \geq \sigma_2 \geq \dots, \geq \sigma_r > 0$ such that

$$Av_i = \begin{cases} \sigma_i u_i, & \text{if } i = 1, \dots, r, \\ 0 & \text{if } i \geq r+1, \end{cases}$$

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and

$$A^T u_i = \begin{cases} \sigma_i v_i, & \text{if } i = 1, \ldots, r, \\ 0 & \text{if } i \geq r+1. \end{cases}$$

Proof.

$A = U\Sigma V^T$ implies $AV = U\Sigma$, and $A^T U = V\Sigma$. □

Four fundamental subspaces

For an $n \times m$ matrix A, the following subspaces are called fundamental subspaces.

- ***Range space of** A**:*** $R(A) = \{x \in \mathbb{R}^n : x = Ay \text{ for some } y \in \mathbb{R}^m\}$. (span of columns of A)

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Basis for fundamental subspaces

If $A \in \mathbb{R}^{n \times m}$ is a matrix of rank r, and $A = U\Sigma V^T$ is the SVD of A, then

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By products

- $R(A)^\perp = N(A^T)$ and $N(A)^\perp = R(A^T)$,
- If $A \in \mathbb{R}^{n \times m}$, then $\dim(R(A)) + \dim(N(A)) = m$.

Illustration

$$A = \begin{pmatrix} 3 & 1 & 1 \\ -1 & 3 & 1 \end{pmatrix} =$$

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \sqrt{12} & 0 & 0 \\ 0 & \sqrt{10} & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{5}} & \frac{-1}{\sqrt{5}} & 0 \\ \frac{1}{\sqrt{30}} & \frac{2}{\sqrt{30}} & \frac{-5}{\sqrt{30}} \end{pmatrix}.$$

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- $R(A) = span \left\{ \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix}, \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \right\},$

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- $R(A^T) = span \left\{ \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} \\ \frac{2}{\sqrt{5}} & \frac{-1}{\sqrt{5}} \\ \frac{1}{\sqrt{30}} & \frac{2}{\sqrt{30}} \end{pmatrix} \right\},$

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SVD - equivalent (and useful) form

Theorem

Let $A \in \mathbb{R}^{m \times n}$, and let $\sigma_1, \ldots, \sigma_r$ be the nonzero singular values of A, with associated right and left singular vectors $v_1, \ldots, v_r$ and $u_1, \ldots, u_r$, respectively. Then

$$A = \sum_{j=1}^{r} \sigma_j u_j v_j^T.$$

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If $A = \begin{pmatrix} 3 & 1 & 1 \\ -1 & 3 & 1 \end{pmatrix}$, then

$$A = (\sqrt{12}) \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \left(\frac{1}{\sqrt{6}}, \frac{2}{\sqrt{5}}, \frac{1}{\sqrt{30}} \right) + (\sqrt{10}) \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix} \left(\frac{2}{\sqrt{6}}, \frac{-1}{\sqrt{5}}, \frac{2}{\sqrt{30}} \right).$$

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3. Let $A \in \mathbb{R}^{n \times m}$ with $n \geq m$. If $A = U \begin{pmatrix} \Sigma \\ 0 \end{pmatrix} V^T$ is an SVD of A, then $A^T = V(\Sigma\ 0)U^T$ is an SVD of A^T. Therefore, A and A^T have the same singular values.

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5. If $A = U \Sigma V^T$ is an SVD of A, then $A^{-1} = V \Sigma^{-1} U^T$ is an SVD of A^{-1}.

Theorem

If $A \in \mathbb{R}^{n \times m}$ *has singular values* $\sigma_1 \geq \ldots \geq \sigma_p$, *where* $p = min\{m, n\}$, *then* $\|A\|_2 = \max_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2} = \sigma_1$, *and* $\|A\|_2 = \|A^T\|_2$.

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Theorem

$\|A\|_F = (\sigma_1^2 + \cdots + \sigma_r^2)^{\frac{1}{2}}$.

Properties

Theorem (Condition number)

If $A \in \mathbb{R}^{n\times n}$ *is nonsingular, then* $\kappa_2(A) = \frac{\sigma_1}{\sigma_n} = \frac{\text{maxmag}(A)}{\text{minmag}(A)}$.

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Let $A \in \mathbb{R}^{n\times m}$. *Then* $\|A^T A\|_2 = \|A\|_2^2$, *and* $\kappa_2(A^T A) = \kappa(A)^2$.

Theorem

Let $A \in \mathbb{R}^{n \times m}$, $n \geq m$, $\mathrm{rank}(A) = m$, *with singular values* $\sigma_1 \geq \ldots \sigma_m > 0$. *Then,*

1. $\|(A^T A)^{-1}\|_2 = \frac{1}{\sigma_m^2}$,
2. $\|(A^T A)^{-1} A^T\|_2 = \frac{1}{\sigma_m}$,
3. $\|A^T (A^T A)^{-1}\|_2 = \frac{1}{\sigma_m}$, *and*
4. $\|A^T (A^T A)^{-1} A^T\|_2 = 1$.

Full rank matrices are dense

Theorem

Let $A \in \mathbb{R}^{n \times m}$ with rank r such that $r < \min\{n, m\}$. Then for every $\epsilon > 0$, there exists a full rank matrix $A_\epsilon \in \mathbb{R}^{n \times m}$ such that $\|A - A_\epsilon\|_2 = \epsilon$.

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Corollary

Full column rank matrices are dense on $\mathbb{R}^{n \times m}$*, for* $n \leq m$*.*

Low rank approximation using SVD

Theorem (Eckart and Young (1936))

Let $A \in \mathbb{R}^{n\times m}$ have a SVD as in previous definition. If $k < \mathrm{rank}(A)$, then the absolute distance of A to the set of rank k matrices is

$$\sigma_{k+1} = \min_{B\in\mathbb{R}^{n\times m}, \mathrm{rank}(B)=k} \|A - B\|_2 = \|A - A_k\|_2,$$

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Let $A \in \mathbb{R}^{n\times m}$ has full rank. Let $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$, where $r = \min\{n, m\}$. If $B \in \mathbb{R}^{n\times m}$ and $\|A - B\|_2 < \sigma_r$. Then B has full rank.

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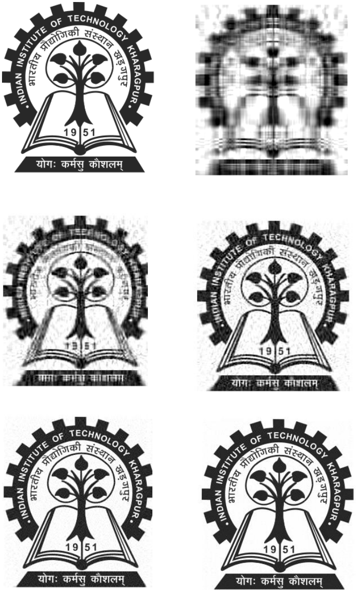
Relative distance to singular matrices

Theorem

Let $A \in \mathbb{R}^{n \times n}$ be a nonsingular matrix. Let A_s be the singular matrix closest to A in the sense that $\|A - A_s\|_2$ is as small as possible. Then, $\|A - A_s\|_2 = \sigma_n$ and

$$\frac{\|A - A_s\|_2}{\|A\|_2} = \frac{\sigma_n}{\|A\|_2} = \frac{1}{\|A\|_2 \|A^{-1}\|_2} = \frac{1}{\kappa_2(A)}.$$

Applications of SVD - I - Image compression



Applications of SVD - II - Least squares problems

Applications of SVD - III - Handwritten digit classification

Problem: How to classify unknown digit?

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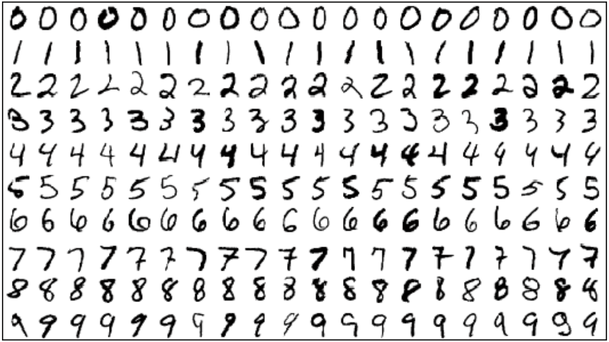

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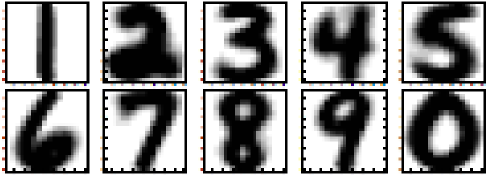
- Ideally the clusters are well separated, and the separation between the clusters depends on how well written the training digits are.

The means (“averages“) of all digits in the training set.



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Using singular value decomposition(SVD), we will see a classification algorithm, for which the success rate is around 93%.

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Algorithm

Training: For the training set of known digits, compute the SVD of each set of digits of one kind.
Classification: For a given test digit, compute its relative residual in all 10 bases. If one residual is significantly smaller than all the others, classify as that. Otherwise give up.