The Matrix Singular Value Decomposition

Singular Value Decomposition(SVD)

The Singular Value Decomposition (SVD) of a matrix $A \in \mathbb{R}^{n \times m}$ is a decomposition of the form

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

where $U \in \mathbb{R}^{n \times n}$ and $V \in \mathbb{R}^{m \times m}$ are orthogonal matrices and $\Sigma := \mathrm{diag}(\sigma_1, \sigma_2, \ldots \sigma_p) \in \mathbb{R}^{n \times m}$ is a diagonal matrix with

$$\sigma_1 \geq \sigma_2 \geq \cdots \sigma_p \geq 0$$

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The numbers $\sigma_1, \sigma_2, \dots, \sigma_p$ are called the singular values of A.

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Every matrix has an SVD. For example, the SVD of

$$A := \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}^T,$$

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Clearly if $A = U\mathrm{diag}(\sigma_1, \sigma_2, \ldots \sigma_p)V^T$ is the SVD of A and $\mathrm{rank}\, A = r$, then the first r singular values $\sigma_1 \geq \cdots \geq \sigma_r > 0$ with $\sigma_k = 0$ for $k = r+1, \ldots, p$ if $r < p$.

Singular Value Decomposition(SVD)

If $U = [u_1 \cdots u_n]$ and $V = [v_1 \cdots v_m]$, then for $i = 1, \ldots, p$,

$$Av_i = \sigma_i u_i \text{ and } u_i^* A = \sigma_i v_i^*$$

Hence u_i and v_i are respectively left and right singular vectors of A corresponding to σ_i.

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Theorem Let $A = U\Sigma V^*$ be an SVD of $A \in \mathbb{F}^{n\times m}$ with $\operatorname{rank} A = r$.

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(c)

$$R(A) = \operatorname{span}\{u_1, \ldots, u_r\}, \qquad N(A) = \operatorname{span}\{v_{r+1}, \ldots, v_m\}$$
$$R(A^*) = \operatorname{span}\{v_1, \ldots, v_r\} \qquad N(A^*) = \operatorname{span}\{u_{r+1}, \ldots, u_n\}.$$

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(d) $\|A\|_2 = \sigma_1$.

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$$\begin{aligned} R(A) &= \mathrm{span}\{u_1, \ldots, u_r\}, \qquad & N(A) &= \mathrm{span}\{v_{r+1}, \ldots, v_m\} \\ R(A^*) &= \mathrm{span}\{v_1, \ldots, v_r\} \qquad & N(A^*) &= \mathrm{span}\{u_{r+1}, \ldots, u_n\}. \end{aligned}$$

(d) $\|A\|_2 = \sigma_1$.

(e) $\|A\|_F = \sqrt{\Sigma_{k=1}^r \sigma_k^2}$.

(Here $\mathbb{F} = \mathbb{R}$ or $\mathbb{F} = \mathbb{C}$.)

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Corollary Let $A = U\Sigma V^*$ be an SVD of $A \in \mathbb{F}^{n\times m}$.

(a) If A is square and nonsingular, then $A^{-1} = (VF)(F\Sigma^{-1}F)(UF)^*$ is an SVD of A^{-1} and where F is the $n \times n$ 'flip' matrix and $\|A^{-1}\|_2 = \frac{1}{\sigma_n}$.

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(b) If $p = \min\{m, n\}$, then assuming $\kappa_2(A) = \frac{\operatorname{maxmag} A^T}{\operatorname{minmag} A^T}$ if $n < m$,

$$\kappa_2(A) = \begin{cases} \frac{\sigma_1}{\sigma_p} & \text{if } \operatorname{rank} A = p, \\ \infty & \text{otherwise} \end{cases}$$

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(d) If $n = m$ and A is a singular matrix, then for any $\epsilon > 0$, there exists a nonsingular matrix $B \in \mathbb{F}^{n\times n}$ such that $\|A - B\|_2 < \epsilon$.

Condensed Singular Value Decomposition

Let $A = U\Sigma V^*$ be an SVD of $A \in \mathbb{F}^{n\times m}$ with $\mathrm{rank}\, A = r$. Let $U = [u_1\, u_2 \cdots u_r] \in \mathbb{F}^{n\times r}$, $V_r = [v_1\, v_2 \cdots v_r] \in \mathbb{F}^{m\times r}$ and $\Sigma_r = \mathrm{diag}(\sigma_1, \ldots \sigma_r) \in \mathbb{F}^{r\times r}$. Then

$$A = U_r \Sigma_r V_r^*$$

is called the Condensed Singular Value Decomposition of A.

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Computing the Condensed SVD for small matrices:

1. Find the nonzero eigenvalues, say λ_i, $i = 1, \ldots, r$, of A^*A or AA^*, whichever is smaller in size and corresponding eigenvectors. Here $\operatorname{rank} A = r$.
2. Set $\Sigma_r = \operatorname{diag}(\sigma_1 \ \cdots \ \sigma_r)$ where $\sigma_i = \sqrt{\lambda_i}$, $i = 1, \ldots, r$.
3. If the eigenvectors of A^*A were found, call them $v_i, i = 1, \ldots, r$. Compute $u_i = \frac{v_i}{\sigma_i}$, $i = 1, \ldots, r$ and set $U_r = \begin{bmatrix} u_1 & \cdots & u_r \end{bmatrix}$. Otherwise if the eigenvectors of AA^* were found, call them u_i, $i = 1, \ldots, r$. Compute $v_i = \frac{u_i}{\sigma_i}$, $i = 1, \ldots, r$, and set $V_r = \begin{bmatrix} v_1 & \cdots & v_r \end{bmatrix}$.
4. Then $A = U_r \Sigma_r V_r^*$ is a Condensed SVD of A.

Moore-Penrose Pseudoinverse

Let $A = U\Sigma V^*$ be an SVD of $A \in \mathbb{F}^{n\times m}$ with $\operatorname{rank} A = r$. The Moore-Penrose pseudoinverse $A^\dagger$ of A is defined as

$$A^\dagger := V\Sigma^\dagger U^*$$

where $\Sigma^\dagger = \operatorname{diag}(\sigma_1^{-1}, \ldots, \sigma_r^{-1}, 0, \ldots 0) \in \mathbb{R}^{m\times n}$.

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Examples: The SVD of

$$A := \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}^T.$$

Therefore,

$$A^\dagger = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{3} & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}^T = \begin{bmatrix} -1/3 & 2/3 \\ -2/3 & -1/3 \end{bmatrix} = A^{-1}.$$

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The SVD of

$$B := \begin{bmatrix} 1 & 2 \end{bmatrix} = [1] \begin{bmatrix} \sqrt{5} & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{5}} & -\frac{2}{\sqrt{5}} \\ \frac{2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{bmatrix}^T .$$

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Finally the SVD of

$$D := \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \sqrt{2} \\ 0 \end{bmatrix} [1]^T .$$

Therefore,

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Properties of the Moore-Penrose Pseudoinverse

Theorem Let $A \in \mathbb{F}^{n\times m}$. Then,

(a) $A^{-1} = A^\dagger$ if $n = m$ and A is nonsingular. (Exercise!)

(b) $A^\dagger = (A^*A)^{-1}A^*$ if $\operatorname{rank} A = m$ (Exercise!)

(c) $A^\dagger = A^*(AA^*)^{-1}$ if $\operatorname{rank} A = n$. (Exercise!)

(d) $(AA^\dagger)^* = AA^\dagger, \quad (A^\dagger A)^* = A^\dagger A, \quad AA^\dagger A = A, \quad A^\dagger AA^\dagger = A^\dagger$.
Also, if $B \in \mathbb{F}^{m\times n}$, such that
$(AB)^* = AB, \quad (BA)^* = BA, \quad ABA = A, \quad BAB = B$, then
$B = A^\dagger$. (Exercise!)

(f) $(A^\dagger)^* = (A^*)^\dagger$. (Exercise!)

(g) $A^\dagger = V_r\Sigma_r^{-1}U_r^*$. (Exercise!)

Moore-Penrose Pseudoinverse and the LSP

Theorem Let $Ax = b$ where $A \in \mathbb{R}^{n \times m}$ and $b \in \mathbb{R}^n$ with $n \geq m$. Then $x_0 = A^\dagger b$ is the unique least squares solution of the system $Ax = b$ if $\operatorname{rank} A = m$.

If $\operatorname{rank} A < m$, then x_0 is the least squares solution of the system with the smallest 2-norm.

Moore-Penrose Pseudoinverse and the LSP

Theorem Let $Ax = b$ where $A \in \mathbb{R}^{n\times m}$ and $b \in \mathbb{R}^n$ with $n \geq m$. Then $x_0 = A^\dagger b$ is the unique least squares solution of the system $Ax = b$ if $\operatorname{rank} A = m$.

If $\operatorname{rank} A < m$, then x_0 is the least squares solution of the system with the smallest 2-norm.

The main flop count of solving the LSP problem associated with an overdetermined system $Ax = b$ is that of computing the Condensed SVD of A.

Eckart-Young Theorem

Theorem[Schmidt, 1907], [Eckart & Young, 1936]
Let $A \in \mathbb{F}^{n\times m}$ with $\operatorname{rank} A = r$. Let $A = U\Sigma V^*$ be an SVD of A. For $k = 1, \ldots r-1$, define

$$A_k = U\Sigma_k V^*$$

where $\Sigma_k = \operatorname{diag}(\sigma_1, \ldots, \sigma_k, 0, \ldots, 0) \in \mathbb{R}^{n\times m}$ is a diagonal matrix.
Then $\operatorname{rank} A_k = k$ and

$$\|A - A_k\|_2 = \min\{\|A - B\|_2 : B \in \mathbb{F}^{n\times m} \text{ with } \operatorname{rank} B \leq k\} = \sigma_{k+1}.$$

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Corollary Let $A \in \mathbb{F}^{n\times n}$ be nonsingular. Let $A = U\Sigma V^*$ be an SVD of A. Then,

$$\sigma_n = \min\{\|A - B\|_2 : B \in \mathbb{F}^{n\times n} \text{ is singular}\}.$$

(Exercise!)

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Corollary Let $A \in \mathbb{F}^{n\times n}$ be nonsingular. Let $A = U\Sigma V^*$ be an SVD of A. Then,

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Corollary Let $A \in \mathbb{F}^{n\times n}$ be nonsingular. Then,

$$\frac{1}{\kappa_2(A)} = \min\left\{\frac{\|\Delta A\|_2}{\|A\|_2} : A + \Delta A \text{ is singular}\right\}$$

(Exercise!)

Numerical rank determination via SVD

Let $A = U\Sigma V^*$ be an SVD of an $n \times m$ real or complex matrix A with

$$\Sigma := \mathrm{diag}(\sigma_1, \sigma_2, \dots \sigma_p) \in \mathbb{R}^{n \times m}$$

where $\sigma_1 \geq \sigma_2 \geq \cdots \sigma_p \geq 0$ for $p = \min\{n, m\}$. If $\mathrm{rank}\, A = r$, then $r \leq p$. In particular if $r < p$, then

$$\sigma_1 \geq \sigma_2 \geq \cdots \sigma_r > 0 = \sigma_{r+1} = \cdots = \sigma_p.$$

However, due to rounding error, the computed singular values of A are likely to satisfy

$$\sigma_1 \geq \sigma_2 \geq \cdots \sigma_k > \epsilon >> \sigma_{k+1} \geq \cdots \geq \sigma_p \geq 0$$

for some $1 \leq k \leq p$, where $0 < \epsilon << 1$.

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In such cases, we may set $\sigma_j = 0$, for $j = k+1, \ldots, p$, and state that the *numerical rank* of A is k.

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If the entries of A are affected only by rounding error, then we may set $\epsilon = 2\max\{n, m\}u\|A\|_2$. This is the default threshold for Matlab's `rank` command which can be modified by the user.