

CS 357 - 18 Singular Value Decompositions

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Overview of SVD: A more general factorization for any $m \times n$ matrix, there exists a Singular Value Decomposition $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$.

- \mathbf{U} is composed of the eigenvectors of $\mathbf{A}\mathbf{A}^T$ as its columns, the vectors are called left singular vectors of \mathbf{A} . \mathbf{U} is an orthogonal basis of \mathbb{R}^m . \mathbf{U} is an $m \times m$ orthogonal matrix.

$$\begin{aligned}\mathbf{A}\mathbf{A}^T &= (\mathbf{U}\mathbf{\Sigma}\mathbf{V}^T)(\mathbf{U}\mathbf{\Sigma}\mathbf{V}^T)^T \\ (\mathbf{U}\mathbf{\Sigma}\mathbf{V}^T)(\mathbf{V}^T)^T\mathbf{\Sigma}^T\mathbf{U}^T &= \mathbf{U}\mathbf{\Sigma}(\mathbf{V}^T\mathbf{V})\mathbf{\Sigma}^T\mathbf{U}^T = \mathbf{U}(\mathbf{\Sigma}\mathbf{\Sigma}^T)\mathbf{U}^T\end{aligned}$$

- \mathbf{V} is composed of the eigenvectors of $\mathbf{A}^T\mathbf{A}$ as its columns, the vectors are called right singular vectors of \mathbf{A} . \mathbf{V} is an orthogonal basis of \mathbb{R}^n . \mathbf{V} is an $n \times n$ orthogonal matrix.

$$\begin{aligned}\mathbf{A}^T\mathbf{A} &= (\mathbf{U}\mathbf{\Sigma}\mathbf{V}^T)^T(\mathbf{U}\mathbf{\Sigma}\mathbf{V}^T) \\ &= \mathbf{V}(\mathbf{\Sigma}^T\mathbf{\Sigma})\mathbf{V}^T \\ &= \mathbf{V}\mathbf{\Sigma}^2\mathbf{V}^T\end{aligned}$$

- $\mathbf{\Sigma}$ is a $m \times n$ diagonal matrix composed of square roots of the eigenvalues of $\mathbf{A}^T\mathbf{A}$, called singular values. The diagonal of $\mathbf{\Sigma}$ is ordered by non-increasing singular values and the columns of \mathbf{U} and \mathbf{V} are ordered respectively.

$$\mathbf{\Sigma} = \begin{bmatrix} \sigma_1 & & & \\ & \ddots & & \\ & & \sigma_s & \\ 0 & & 0 & \\ \vdots & \ddots & \vdots & \\ 0 & & 0 & \end{bmatrix} \text{ when } m > n, \text{ and } \mathbf{\Sigma} = \begin{bmatrix} \sigma_1 & & 0 & \dots & 0 \\ & \ddots & & \ddots & \\ & & \sigma_s & 0 & \dots & 0 \end{bmatrix} \text{ when } m < n.$$

Note: $\sigma_1 \geq \sigma_2 \dots \geq \sigma_s \geq 0$.

Time complexity: All of the computation cost of SVD, matrix-matrix production and LU decomposition is $\mathcal{O}(n^3)$. But the cost ranking is SVD > Matrix-Matrix Production > LU.

Reduced SVD: SVD of a non-square matrix \mathbf{A} of size $m \times n$ can be represented in a reduced format:

- For $m \geq n$: \mathbf{U} is $m \times n$, $\mathbf{\Sigma}$ is $n \times n$, and \mathbf{V} is $n \times n$.
- For $m \leq n$: \mathbf{U} is $m \times m$, $\mathbf{\Sigma}$ is $m \times m$, and \mathbf{V} is $n \times m$. (\mathbf{V}^T is $m \times n$)

In general we will represent the reduced SVD as: $\mathbf{A} = \mathbf{U}_R\mathbf{\Sigma}_R\mathbf{V}_R^T$, where \mathbf{U}_R is a $m \times k$ matrix, \mathbf{V}_R is a $n \times k$ matrix, $\mathbf{\Sigma}_R$ is a $k \times k$ matrix, $k = \min(m, n)$.

Important concepts about SVD: For a $m \times n$ matrix $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$:

- **Rank of a matrix:** Let $s = \min(m, n)$, if there are r non-zero singular values, $\text{rank}(\mathbf{A}) = r$, if $r = s$, the matrix is full rank, if $r < s$, the matrix is rank deficient.
- **Nullspace:** $\text{null}(\mathbf{A}) = \text{span}(\mathbf{v}_{r+1}, \mathbf{v}_{r+2}, \dots, \mathbf{v}_n)$; solve space for \mathbf{A} when $\mathbf{A}\mathbf{x} = \vec{0}$.
- **Range:** $\text{range}(\mathbf{A}) = \text{span}(\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_r)$
- **Rank-nullity theorem:** $\text{rank}(\mathbf{A}) + \text{null}(\mathbf{A}) = n$.
- **Pseudoinverse:** If the matrix $\mathbf{\Sigma}$ is rank deficient, we cannot get its inverse. We define instead the pseudoinverse: $(\mathbf{\Sigma}^+)_{ii} = \begin{cases} 1/\sigma_i & \sigma_i \neq 0 \\ 0 & \sigma_i = 0 \end{cases}$. So the pseudoinverse of \mathbf{A} is defined as $\mathbf{A}^+ = \mathbf{V}\mathbf{\Sigma}^+\mathbf{U}^T$. Here are some true concepts that might be useful for the quiz:

- ✓ If \mathbf{A} is orthogonal, then \mathbf{A}^{-1} and \mathbf{A}^+ exist and are equal.
- ✓ If \mathbf{A}^{-1} exists, then \mathbf{A}^+ also exists and they are equal.
- ✓ It is possible for \mathbf{A}^+ to exist when \mathbf{A}^{-1} does not exist.
- ✓ For any matrix, the pseudoinverse always exists.

- **Euclidean Norm of a matrix / inverse:**

- $\|\mathbf{A}\|_2 = \sigma_1$ - The largest singular value.
- If the matrix is full-rank, $\|\mathbf{A}^{-1}\|_2 = 1/\sigma_n$ - Inverse of the smallest singular value.
- If the rank is rank-deficient, $\|\mathbf{A}^+\|_2 = 1/\sigma_r$ - Inverse of the smallest non-zero singular value.
- For a zero matrix, $\|\mathbf{A}^+\|_2 = 0$
- For a full-rank matrix, the 2-norm condition number is $\sigma_{\max}/\sigma_{\min}$. If the matrix is rank-deficient, the 2-norm condition number is ∞ .

- **Low-rank approximation:** $\|\mathbf{A} - \mathbf{A}_k\|_2 = \left\| \sum_{i=k+1}^n \sigma_i \mathbf{u}_i \mathbf{v}_i^T \right\|_2 = \sigma_{k+1}$

- **Using SVD to solve system of equation:** Cost to solve $\mathcal{O}(n^2)$

1. $\mathbf{\Sigma y} = \mathbf{U}^T \mathbf{b}$
2. $\mathbf{x} = \mathbf{V y}$

```
import numpy as np
import numpy.linalg as la
U1, S1, VT1 = np.linalg.svd(A, full_matrices=True)    # Full SVD
U2, S2, VT2 = np.linalg.svd(B, full_matrices=False)  # Reduced SVD
```

Link to course textbook for more detailed information.