Mathematical Foundations for Machine Learning and Data Science

Singular Value Decomposition, Column Space and Null Space

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Outline

- Positive/negative definite and semi-definite matrices
- Singular Value Decomposition (SVD)
  - Formulation
  - Interpretation
  - Application examples
- Column space and Null Space
Positive/Negative Definite/Semi-Definite Matrices

Definition:

For a matrix $A \in \mathbb{R}^{n \times n}$, if

- $x^T Ax \geq 0 \quad \forall \ x \in \mathbb{R}^n$ \quad $A$ is positive semi-definite (PSD)
- $x^T Ax > 0 \quad \forall \ x \in \mathbb{R}^n$ \quad $A$ is positive definite (PD)
- $x^T Ax \leq 0 \quad \forall \ x \in \mathbb{R}^n$ \quad $A$ is negative semi-definite (NSD)
- $x^T Ax < 0 \quad \forall \ x \in \mathbb{R}^n$ \quad $A$ is negative definite (ND)
**Interpretation:**

A is positive semi-definite (PSD)

\[ x^T Ax \geq 0 \]

- Let \( y = Ax \)
  - \( y \) is a linear transformation defined by the matrix \( A \).
- \( x^T y \geq 0 \) implies angle between \( x \) and \( y \) is less than or equal to \( \frac{\pi}{2} \).
- \( x^T y \geq 0 \) implies angle between \( x \) and linearly transformed \( x \), that is, \( Ax \) is less than or equal to \( \frac{\pi}{2} \).

Graphically, a vector \( x \) when transformed by a matrix \( A \), that is, \( Ax \) can be anywhere in the green region including the dashed boundary where \( x^T Ax = 0 \)
Interpretation:

A is positive definite (PD)

\[ x^T A x > 0 \]

- Let \( y = Ax \)
  - \( y \) is a linear transformation defined by the matrix \( A \).
- \( x^T y > 0 \) implies angle between \( x \) and \( y \) is less than \( \frac{\pi}{2} \).
- \( x^T y \geq 0 \) implies angle between \( x \) and linearly transformed \( x \), that is, \( Ax \) is less than \( \frac{\pi}{2} \).

Graphically, a vector \( x \) when transformed by a matrix \( A \), that is, \( Ax \) can be anywhere in the green region excluding the dashed boundary where \( x^T A x = 0 \).
Positive Definite and Semi-Definite Matrices

**Eigenvalues of symmetric PSD/PD matrix:**
For a symmetric and PD matrix $A$, eigenvalues are positive.

**How?**
- We already know that the eigenvalues of a symmetric matrix are real.
- For a PD symmetric, we require $x^T A x > 0$
- If we take $x = q$, where $q$ is an eigenvector with an associated eigenvalue $\lambda$
  $$q^T A q > 0 \Rightarrow \lambda q^T q > 0 \Rightarrow \lambda \|q\|^2 > 0 \Rightarrow \lambda > 0$$

**Similarly, we can show the following:**
For a symmetric and PSD matrix $A$, eigenvalues are non-negative.
For a symmetric and NSD matrix $A$, eigenvalues are non-positive.
For a symmetric and ND matrix $A$, eigenvalues are negative.
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Singular Value Decomposition

Overview:

- The singular value decomposition (SVD) of a matrix is a central matrix decomposition method in linear algebra.

- It has been referred to as the “fundamental theorem of linear algebra” (Strang, 1993) because it can be applied to all matrices, not only to square matrices, and it always exists.

- For $A \in \mathbb{R}^{m \times n}$, we have

$$x \in \mathbb{R}^n \quad \xrightarrow{A} \quad A \, x \in \mathbb{R}^m$$

- SVD explains the underlying geometry of this linear transformation.
Singular Value Decomposition

**Formulation:**

- For any matrix $A \in \mathbb{R}^{m \times n}$, we have a singular value decomposition (SVD) given by

\[
A = U \Sigma V^T
\]

- Matrix $U \in \mathbb{R}^{m \times m}$ is an orthonormal matrix.
- Matrix $V \in \mathbb{R}^{n \times n}$ is an orthonormal matrix.
- Matrix $\Sigma \in \mathbb{R}^{m \times n}$ is a (special) diagonal matrix.

\[
\begin{align*}
\Sigma &= \begin{bmatrix}
\sigma_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\
0 & \sigma_2 & \cdots & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \sigma_m & 0 & \cdots & 0
\end{bmatrix} & m < n \\
\Sigma &= \begin{bmatrix}
\sigma_1 & 0 & \cdots & 0 \\
0 & \sigma_2 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \sigma_n
\end{bmatrix} & m = n \\
\Sigma &= \begin{bmatrix}
\sigma_1 & 0 & \cdots & 0 \\
0 & \sigma_2 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \sigma_n \\
0 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 0
\end{bmatrix} & m > n
\end{align*}
\]
Singular Value Decomposition

Formulation:

\[ A = U \Sigma V^T \]

- Columns of \( U \) are referred to as left singular vectors of matrix \( A \).
- Columns of \( V \) are referred to as right singular vectors of matrix \( A \).
- \( \sigma_1, \sigma_2, \ldots, \sigma_{\min(m,n)} \) are singular values of matrix \( A \), which are (usually) indexed such that

\[ \sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_{\min(m,n)} \geq 0 \]
Singular Value Decomposition

How to Compute SVD?

- For a matrix $A \in \mathbb{R}^{m \times n}$, we define a matrix $G = AA^T$.
- Using $A = U \Sigma V^T$, we can write $G$ as

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

- What is special about matrix $G$?
  - $G$ is symmetric by definition.
  - $G$ is positive semi-definite. \textbf{How? You are fully equipped to show this.}

- We note that $\Sigma \Sigma^T$ is a diagonal matrix of size $m \times m$.
- Eigenvalue decomposition of $G$ gives columns of $U$ as eigenvectors and diagonal entries of $\Sigma \Sigma^T$ as eigenvalues.
- In other words, left singular vectors of $A$ are eigenvectors of $AA^T$ and $\sigma^2 = \lambda$ (eigenvalue of $AA^T$). Furthermore, $\lambda \geq 0$ since $G = AA^T$ is PSD.

Eigenvalue decomposition of $AA^T$ gives $m$ left singular vectors of $A$ and first $m$ singular values.
Singular Value Decomposition

**How to Compute SVD?**

- Now we define a matrix $G = A^T A$.
- Using $A = U \Sigma V^T$, we can write $G$ as

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

- What is special about matrix $G$?
  - $G$ is symmetric by definition.
  - $G$ is positive semi-definite. **How? You are fully equipped to show this.**
- We note that $\Sigma^T \Sigma$ is a diagonal matrix of size $n \times n$.
- Eigenvalue decomposition of $G$ gives columns of $V$ as eigenvectors and diagonal entries of $\Sigma^T \Sigma$ as eigenvalues.
- In other words, right singular vectors of $A$ are eigenvectors of $A^T A$ and

  $$\sigma^2 = \lambda \text{ (eigenvalue of } A^T A).$$

  Furthermore, $\lambda \geq 0$ since $G$ is PSD.

  **Eigenvalue decomposition of $A^T A$ gives $n$ right singular vectors of $A$ and first $n$ singular values.**

Now you can explain the non-negativity of the singular values.
**Singular Value Decomposition**

**SVD Summary**

- Singular value decomposition (SVD) of a matrix $A \in \mathbb{R}^{m\times n}$ is given by

\[
A = U \Sigma V^T
\]

- EVD of $AA^T$ gives $U$ and first $m$ singular values.

- EVD of $A^TA$ gives $V$ and first $n$ singular values.

- $U$ and $V$ are always orthogonal.

- SVD always exists.

- Singular values are non-negative, that is,

\[
\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_{\min(m,n)} \geq 0
\]
Singular Value Decomposition

Geometric Interpretation

\[ x \in \mathbb{R}^n \rightarrow A \rightarrow A x \in \mathbb{R}^m \]

Transformation (Change of Basis)

\[ x \in \mathbb{R}^n \rightarrow V^T \rightarrow \Sigma \rightarrow U \rightarrow A x \in \mathbb{R}^m \]

Scaling (In new Basis)

Transformation (Change of Basis)

Change of basis in \( \mathbb{R}^n \)

Change of basis in \( \mathbb{R}^m \)

Scaling along the new basis by singular values.

- \( m < n \) - Drop the last \( n - m \) basis (impact of columns of zeros in \( \Sigma \))
- \( m > n \) - Append \( m - n \) basis (impact of rows of zeros in \( \Sigma \))
Singular Value Decomposition

Geometric Interpretation

\[ V_2 \]

\[ V_1 \]

\[ A \]

\[ U \]

\[ V^\top \]

\[ e_2 \]

\[ e_1 \]

\[ \sigma_2 u_2 \]

\[ \sigma_1 u_1 \]

\[ \sum \]

\[ \sigma_2 e_2 \]

\[ \sigma_1 e_1 \]
Singular Value Decomposition

Geometric Interpretation - Example

\[
A = \begin{bmatrix}
1 & -0.8 \\
0 & 1 \\
1 & 0
\end{bmatrix} = U \Sigma V^T
\]

\[
= \begin{bmatrix}
-0.79 & 0 & -0.62 \\
0.38 & -0.78 & -0.49 \\
-0.48 & -0.62 & 0.62
\end{bmatrix}
\begin{bmatrix}
1.62 & 0 \\
0 & 1.0 \\
0 & 0
\end{bmatrix}
\begin{bmatrix}
-0.78 & 0.62 \\
-0.62 & -0.78
\end{bmatrix}
\]

Change of basis in \( \mathbb{R}^2 \)

Change of basis in \( \mathbb{R}^3 \)

- Append 1 more basis (impact of a row of zeros in \( \Sigma \))
Singular Value Decomposition

**Rank of a Matrix:**
- The rank of a matrix is equal to the number of non-zero singular values.

**How?**
- Since $A^T A$ and $A$ have the same rank and we know that the rank of any square matrix equals the number of nonzero eigenvalues.

**Application Example – Rank Estimation:**

*We use SVD for the estimation of rank while analyzing data.* **How?**
- Suppose that we have $n$ data points $a_1, a_2, \ldots, a_n$, all of which live in $\mathbb{R}^m$, where $n$ is much larger than $m$. Let $A$ be the $m \times n$ matrix with columns $a_1, a_2, \ldots, a_n$.

- Assume that the the data points satisfy some linear relations, such that $a_1, a_2, \ldots, a_n$ all lie in an $r$ dimensional subspace of $\mathbb{R}^m$. Then we would expect the matrix $A$ to have rank $r$.

- If the data points are obtained from measurements with errors, then the matrix $A$ will probably have full rank $m$. But only $r$ of the singular values of $A$ will be large, and the other singular values will be close to zero.

- Using SVD, we can can estimate an “approximate rank” of $A$ by counting the number of singular values which are much larger than the others.
Singular Value Decomposition

**Application: Matrix Approximation**

- A matrix $A \in \mathbb{R}^{m \times n}$ can be decomposed using SVD as

  $$A = U \Sigma V^T = \sum_{i=1}^{\min(m,n)} u_i \sigma_i v_i^T$$

- If rank of a matrix is $r \leq \min(m,n)$, we can truncate the summation at $r$

  $$A = \sum_{i=1}^{r} u_i \sigma_i v_i^T$$

- Using SVD formulation, we can define $k$ rank approximation of the matrix $A$ by including first $k$ singular vectors and associated singular values in the representation, that is,

  $$A \approx \sum_{i=1}^{k} u_i \sigma_i v_i^T \quad \text{(k-rank approximation)}$$
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**Column Space:**

- For a matrix $A \in \mathbb{R}^{m \times n}$, the column space, denoted by $\mathcal{C}(A)$, is the span of the columns of $A$.

- If $a_1, a_2, \ldots, a_n \in \mathbb{R}^m$ are the columns of $A$, column space is given by
  $$\mathcal{C}(A) = \text{span}(a_1, a_2, \ldots, a_n)$$
  $$\mathcal{C}(A) = \{Ax | x \in \mathbb{R}^n\} \quad (\text{all possible linear combinations of columns of } A)$$

- In other words, column space is a linear transformation of every point in $\mathbb{R}^n$, that is,
  $$x \in \mathbb{R}^n \quad \xrightarrow{A} \quad A x \in \mathbb{R}^m$$

- Consequently, $\mathcal{C}(A)$ is the subspace of $\mathbb{R}^m$.

- What is the dimension of column space $\mathcal{C}(A)$? Number of linearly independent columns of $A=\text{rank}(A)$. 
Column Space and Null Space

**Null Space:**
- For a matrix $A \in \mathbb{R}^{m \times n}$, the null space, denoted by $\mathcal{N}(A)$, is the subspace of $\mathbb{R}^n$ such that
  \[ \mathcal{N}(A) = \{ x \in \mathbb{R}^n \mid Ax = 0 \} \] (all points that are mapped to zero by matrix $A$)
- In other words, null space is an inverse linear transformation of $0 \in \mathbb{R}^m$.

- Nullity of the matrix, that is, the dimension of the null-space $\mathcal{N}(A)$ is given by the following rank-nullity theorem (also known as rank-nullity theorem).
  \[ \text{rank}(A) + \text{nullity}(A) = \text{number of columns of } A \]
Column Space and Null Space

Example:

\[ A = \begin{bmatrix} 1 & 1 & 2 \\ 2 & 1 & 3 \\ 3 & 1 & 4 \\ 4 & 1 & 5 \end{bmatrix} \]

- \( m = 4, \ n = 3 \)
- \( \mathcal{C}(A) \) is a subspace of \( \mathbb{R}^4 \).
- \( \mathcal{N}(A) \) is a subspace of \( \mathbb{R}^3 \).

- Note that a third column is a sum of first two columns and therefore number of linearly independent columns is equal to 2.

- Consequently, \( \mathcal{C}(A) \) is a 2-dimensional subspace of \( \mathbb{R}^4 \).