Singular Value Decomposition (matrix factorization)

Singular Value Decomposition

The SVD is a factorization of a $m \times n$ matrix into

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

where \boldsymbol{U} is a $m \times m$ orthogonal matrix, $\boldsymbol{V}^{\boldsymbol{T}}$ is a $n \times n$ orthogonal matrix and $\boldsymbol{\Sigma}$ is a $m \times n$ diagonal matrix.

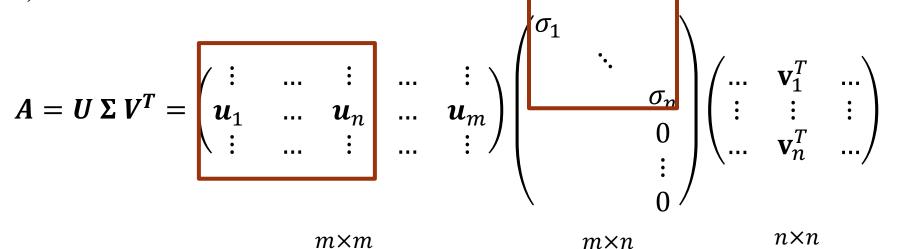
For a square matrix
$$(m = n)$$
:

$$\begin{aligned}
\sigma_1 &\geq \sigma_2 \geq \sigma_3 \dots \\
& \sigma_1 &= \begin{pmatrix} \vdots & \dots & \vdots \\ u_1 & \dots & u_n \\ \vdots & \dots & \vdots \end{pmatrix} \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix} \begin{pmatrix} \dots & \mathbf{v}_1^T & \dots \\ \vdots & \vdots & \vdots \\ \dots & \mathbf{v}_n^T & \dots \end{pmatrix} \\
& A &= \begin{pmatrix} \vdots & \dots & \vdots \\ u_1 & \dots & u_n \\ \vdots & \dots & \vdots \end{pmatrix} \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix} \begin{pmatrix} \vdots & \dots & \vdots \\ v_1 & \dots & v_n \\ \vdots & \dots & \vdots \end{pmatrix}^T
\end{aligned}$$

Reduced SVD

What happens when \boldsymbol{A} is not a square matrix?

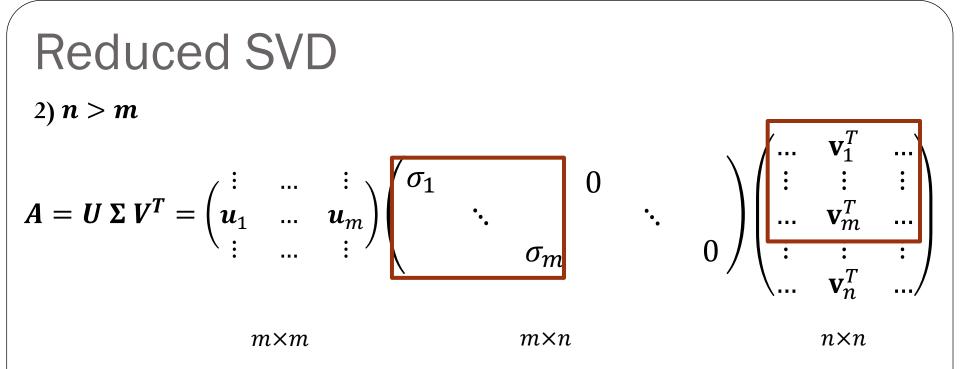
1) m > n



We can instead re-write the above as:

 $A = U_R \Sigma_R V^T$

Where $\boldsymbol{U}_{\boldsymbol{R}}$ is a $m \times n$ matrix and $\boldsymbol{\Sigma}_{\boldsymbol{R}}$ is a $n \times n$ matrix



We can instead re-write the above as:

 $A = U \Sigma_R V_R^T$

where $\boldsymbol{V_R}$ is a $n \times m$ matrix and $\boldsymbol{\Sigma_R}$ is a $m \times m$ matrix

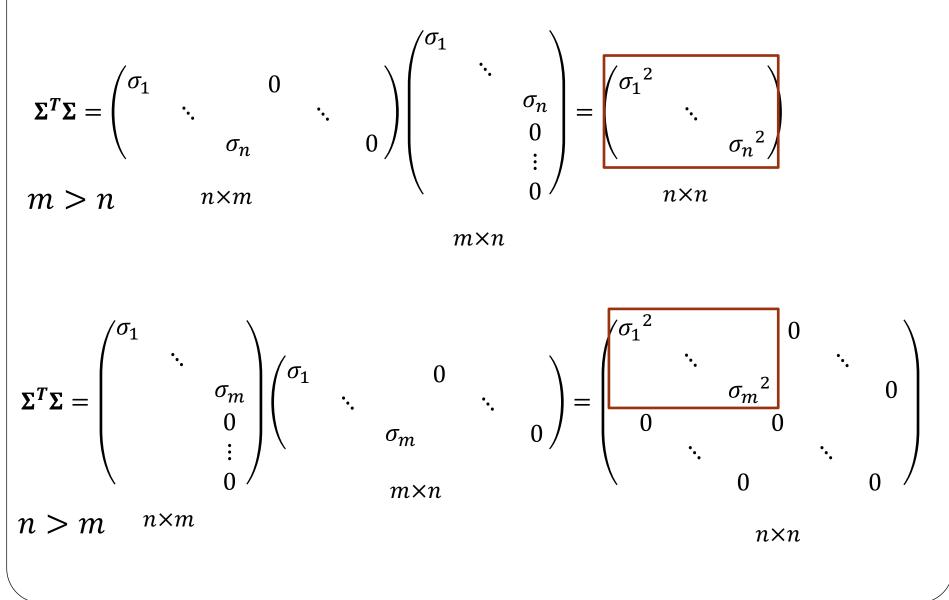
In general:

$$A = U_R \Sigma_R V_R^T$$

 U_R is a $m \times k$ matrix Σ_R is a $k \times k$ matrix V_R is a $n \times k$ matrix

$$k = \min(m, n)$$

Let's take a look at the product $\Sigma^T \Sigma$, where Σ has the singular values of a A, a $m \times n$ matrix.



Assume **A** with the singular value decomposition $A = U \Sigma V^T$. Let's take a look at the eigenpairs corresponding to $A^T A$:

$$A^{T}A = (U \Sigma V^{T})^{T} (U \Sigma V^{T})$$
$$(V^{T})^{T} (\Sigma)^{T} U^{T} (U \Sigma V^{T}) = V\Sigma^{T} U^{T} U \Sigma V^{T} = V \Sigma^{T} \Sigma V^{T}$$

Hence $A^T A = V \Sigma^2 V^T$

Recall that columns of **V** are all linear independent (orthogonal matrix), then from diagonalization ($B = XDX^{-1}$), we get:

- the columns of V are the eigenvectors of the matrix $A^T A$
- The diagonal entries of Σ^2 are the eigenvalues of $A^T A$

Let's call λ the eigenvalues of $A^T A$, then $\sigma_i^2 = \lambda_i$

In a similar way,

$$AA^{T} = (U \Sigma V^{T}) (U \Sigma V^{T})^{T}$$
$$(U \Sigma V^{T}) (V^{T})^{T} (\Sigma)^{T} U^{T} = U \Sigma V^{T} V \Sigma^{T} U^{T} = U \Sigma \Sigma^{T} U^{T}$$

Hence $AA^T = U \Sigma^2 U^T$

Recall that columns of U are all linear independent (orthogonal matrices), then from diagonalization ($B = XDX^{-1}$), we get:

• The columns of \boldsymbol{U} are the eigenvectors of the matrix $\boldsymbol{A}\boldsymbol{A}^T$

How can we compute an SVD of a matrix A?

- 1. Evaluate the *n* eigenvectors \mathbf{v}_i and eigenvalues λ_i of $\mathbf{A}^T \mathbf{A}$
- 2. Make a matrix V from the normalized vectors v_i . The columns are called "right singular vectors".

$$V = \begin{pmatrix} \vdots & \dots & \vdots \\ \mathbf{v}_1 & \dots & \mathbf{v}_n \\ \vdots & \dots & \vdots \end{pmatrix}$$

3. Make a diagonal matrix from the square roots of the eigenvalues.

$$\boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix} \quad \sigma_i = \sqrt{\lambda_i} \quad \text{and} \quad \sigma_1 \ge \sigma_2 \ge \sigma_3 \dots$$

4. Find $U: A = U \Sigma V^T \Longrightarrow U \Sigma = A V \Longrightarrow U = A V \Sigma^{-1}$. The columns are called the "left singular vectors".

True or False?

A has the singular value decomposition $A = U \Sigma V^T$.

- The matrices \boldsymbol{U} and \boldsymbol{V} are not singular
- The matrix Σ can have zero diagonal entries
- $\|\boldsymbol{U}\|_2 = 1$
- The SVD exists when the matrix **A** is singular
- The algorithm to evaluate SVD will fail when taking the square root of a negative eigenvalue

Singular values are always non-negative

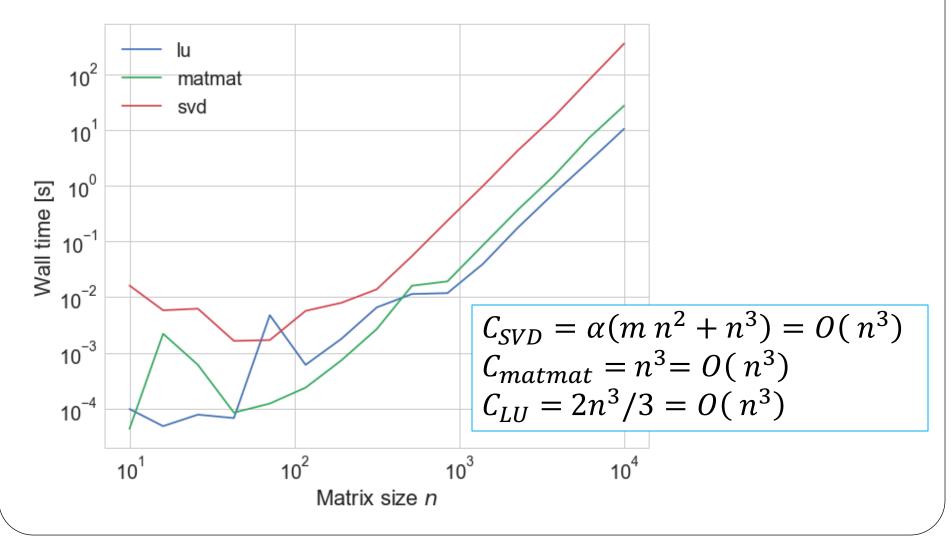
Singular values cannot be negative since $A^T A$ is a positive semidefinite matrix (for real matrices A)

- A matrix is positive definite if $x^T B x > 0$ for $\forall x \neq 0$
- A matrix is positive semi-definite if $x^T B x \ge 0$ for $\forall x \neq 0$
- What do we know about the matrix $A^T A$? $x^T A^T A x = (Ax)^T A x = ||Ax||_2^2 \ge 0$
- Hence we know that $A^T A$ is a positive semi-definite matrix
- A positive semi-definite matrix has non-negative eigenvalues

$$Bx = \lambda x \Longrightarrow x^T B x = x^T \lambda x = \lambda ||x||_2^2 \ge 0 \Longrightarrow \lambda \ge 0$$

Cost of SVD

The cost of an SVD is proportional to $m n^2 + n^3$ where the constant of proportionality constant ranging from 4 to 10 (or more) depending on the algorithm.



SVD summary:

- The SVD is a factorization of a $m \times n$ matrix into $A = U \Sigma V^T$ where U is a $m \times m$ orthogonal matrix, V^T is a $n \times n$ orthogonal matrix and Σ is a $m \times n$ diagonal matrix.
- In reduced form: $A = U_R \Sigma_R V_R^T$, where U_R is a $m \times k$ matrix, Σ_R is a $k \times k$ matrix, and V_R is a $n \times k$ matrix, and $k = \min(m, n)$.
- The columns of V are the eigenvectors of the matrix $A^T A$, denoted the right singular vectors.
- The columns of U are the eigenvectors of the matrix AA^T , denoted the left singular vectors.
- The diagonal entries of Σ^2 are the eigenvalues of $A^T A$. $\sigma_i = \sqrt{\lambda_i}$ are called the singular values.
- The singular values are always non-negative (since $A^T A$ is a positive semi-definite matrix, the eigenvalues are always $\lambda \ge 0$)

Singular Value Decomposition (applications)

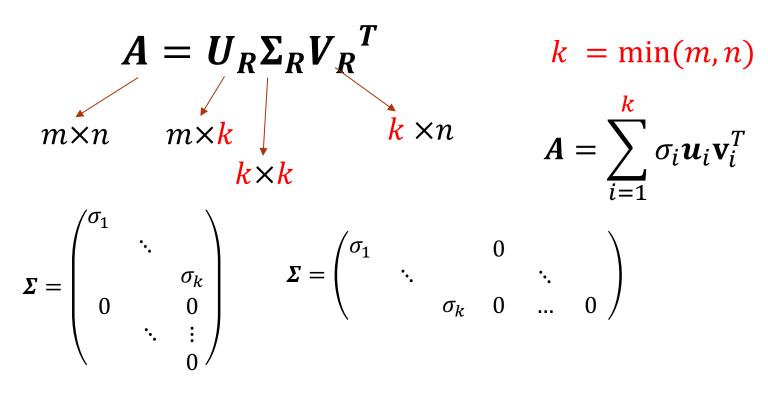
1) Determining the rank of a matrix

Suppose **A** is a $m \times n$ rectangular matrix where m > n:

$$A = \begin{pmatrix} \vdots & \dots & \vdots & \dots & \vdots \\ u_1 & \dots & u_n & \dots & u_m \\ \vdots & \dots & \vdots & \dots & \vdots \end{pmatrix} \begin{pmatrix} \sigma_1 & & & \\ & \ddots & & \\ & & \sigma_n \\ & & 0 \end{pmatrix} \begin{pmatrix} \dots & v_1^T & \dots \\ & \vdots & \vdots \\ & \dots & v_n^T & \dots \end{pmatrix}$$
$$A = \begin{pmatrix} \vdots & \dots & \vdots \\ u_1 & \dots & u_n \\ \vdots & \vdots & \vdots \\ \vdots & \dots & \vdots \end{pmatrix} \begin{pmatrix} \dots & \sigma_1 \mathbf{v}_1^T & \dots \\ \vdots & \vdots & \vdots \\ \dots & \sigma_n \mathbf{v}_n^T & \dots \end{pmatrix} = \sigma_1 u_1 \mathbf{v}_1^T + \sigma_2 u_2 \mathbf{v}_2^T + \dots + \sigma_n u_n \mathbf{v}_n^T$$
$$A = \sum_{i=1}^n \sigma_i u_i \mathbf{v}_i^T$$
$$A_1 = \sigma_1 u_1 \mathbf{v}_1^T \text{ what is rank} (A_1) = ?$$
$$A) 1$$
$$B) n$$
$$C) \text{ depends on the matrix}$$
$$D) \text{ NOTA}$$

Rank of a matrix

For general rectangular matrix A with dimensions $m \times n$, the reduced SVD is:



If $\sigma_i \neq 0 \forall i$, then rank(A) = k (Full rank matrix)

In general, rank(A) = r, where r is the number of non-zero singular values σ_i

r < k (Rank deficient)

Rank of a matrix

- The rank of **A** equals the number of non-zero singular values which is the same as the number of non-zero diagonal elements in Σ .
- Rounding errors may lead to small but non-zero singular values in a rank deficient matrix, hence the rank of a matrix determined by the number of non-zero singular values is sometimes called "effective rank".
- The right-singular vectors (columns of V) corresponding to vanishing singular values span the null space of A.
- The left-singular vectors (columns of **U**) corresponding to the non-zero singular values of **A** span the range of **A**.

2) Pseudo-inverse

- **Problem:** if **A** is rank-deficient, Σ is not be invertible
- How to fix it: Define the Pseudo Inverse
- Pseudo-Inverse of a diagonal matrix:

$$(\mathbf{\Sigma}^{+})_{i} = \begin{cases} \frac{1}{\sigma_{i}}, & \text{if } \sigma_{i} \neq 0\\ 0, & \text{if } \sigma_{i} = 0 \end{cases}$$

• Pseudo-Inverse of a matrix *A*:

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

3) Matrix norms

The Euclidean norm of an orthogonal matrix is equal to 1

$$\|\boldsymbol{U}\|_{2} = \max_{\|\boldsymbol{x}\|_{2}=1} \|\boldsymbol{U}\boldsymbol{x}\|_{2} = \max_{\|\boldsymbol{x}\|_{2}=1} \sqrt{(\boldsymbol{U}\boldsymbol{x})^{T}(\boldsymbol{U}\boldsymbol{x})} = \max_{\|\boldsymbol{x}\|_{2}=1} \sqrt{\boldsymbol{x}^{T}\boldsymbol{x}} = \max_{\|\boldsymbol{x}\|_{2}=1} \|\boldsymbol{x}\|_{2} = 1$$

The Euclidean norm of a matrix is given by the largest singular value

$$\|A\|_{2} = \max_{\|x\|_{2}=1} \|Ax\|_{2} = \max_{\|x\|_{2}=1} \|U\Sigma V^{T}x\|_{2} = \max_{\|x\|_{2}=1} \|\Sigma V^{T}x\|_{2} =$$
$$= \max_{\|V^{T}x\|_{2}=1} \|\Sigma V^{T}x\|_{2} = \max_{\|y\|_{2}=1} \|\Sigma y\|_{2} = \max(\sigma_{i})$$

Where we used the fact that $\|\boldsymbol{U}\|_2 = 1$, $\|\boldsymbol{V}\|_2 = 1$ and $\boldsymbol{\Sigma}$ is diagonal

$$\|A\|_2 = \max(\sigma_i) = \sigma_{max} \qquad \qquad \sigma_{max} \text{ is the largest singular value}$$

4) Norm for the inverse of a matrix

The Euclidean norm of the inverse of a square-matrix is given by:

Assume here A is full rank, so that A^{-1} exists

$$\|A^{-1}\|_{2} = \max_{\|x\|_{2}=1} \|(U \Sigma V^{T})^{-1} x\|_{2} = \max_{\|x\|_{2}=1} \|V \Sigma^{-1} U^{T} x\|_{2}$$

Since $\|\boldsymbol{U}\|_2 = 1$, $\|\boldsymbol{V}\|_2 = 1$ and $\boldsymbol{\Sigma}$ is diagonal then

 $\|A^{-1}\|_2 = \frac{1}{\sigma_{min}}$

 σ_{min} is the smallest singular value

5) Norm of the pseudo-inverse matrix

The norm of the pseudo-inverse of a $m \times n$ matrix is:

$$\|\boldsymbol{A}^+\|_2 = \frac{1}{\sigma_r}$$

where σ_r is the smallest **non-zero** singular value. This is valid for any matrix, regardless of the shape or rank.

Note that for a full rank square matrix, $\|A^+\|_2$ is the same as $\|A^{-1}\|_2$.

Zero matrix: If A is a zero matrix, then A^+ is also the zero matrix, and $||A^+||_2 = 0$

6) Condition number of a matrix

The condition number of a matrix is given by

 $cond_2(A) = \|A\|_2 \|A^+\|_2$

If the matrix is full rank: rank(A) = min(m, n)

$$cond_2(\mathbf{A}) = \frac{\sigma_{max}}{\sigma_{min}}$$

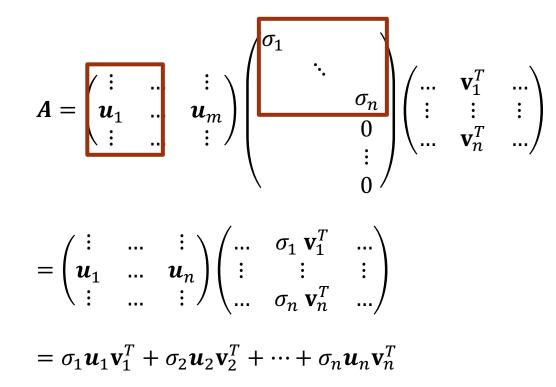
where σ_{max} is the largest singular value and σ_{min} is the smallest singular value

If the matrix is rank deficient: rank(A) < min(m, n)

 $cond_2(\mathbf{A}) = \infty$

7) Low-Rank Approximation

Another way to write the SVD (assuming for now m > n for simplicity)



The SVD writes the matrix A as a sum of outer products (of left and right singular vectors).

7) Low-Rank Approximation (cont.)

The best **rank-**k approximation for a $m \times n$ matrix A, (where $k \leq min(m, n)$) is the one that minimizes the following problem:

$$\min_{A_k} \|A - A_k\|$$

such that $\operatorname{rank}(A_k) \le k$.

When using the induced 2-norm, the best **rank-***k* approximation is given by:

$$A_k = \sigma_1 \boldsymbol{u}_1 \mathbf{v}_1^T + \sigma_2 \boldsymbol{u}_2 \mathbf{v}_2^T + \dots + \sigma_k \boldsymbol{u}_k \mathbf{v}_k^T$$
$$\sigma_1 \ge \sigma_2 \ge \sigma_3 \dots \ge 0$$

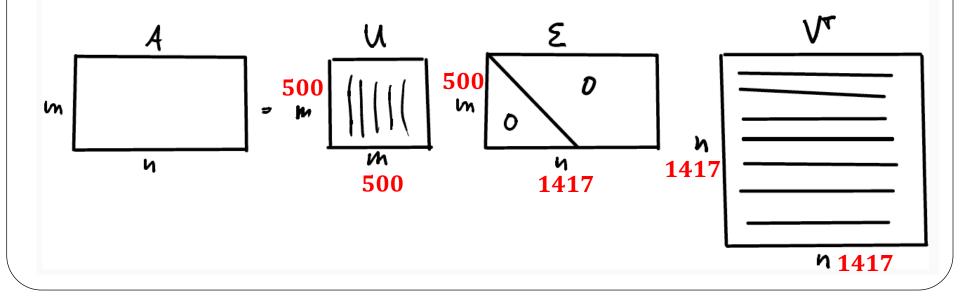
Note that rank(A) = n and $rank(A_k) = k$ and the norm of the difference between the matrix and its approximation is

$$\|\boldsymbol{A} - \boldsymbol{A}_{k}\|_{2} = \|\sigma_{k+1}\boldsymbol{u}_{k+1}\boldsymbol{v}_{k+1}^{T} + \sigma_{k+2}\boldsymbol{u}_{k+2}\boldsymbol{v}_{k+2}^{T} + \dots + \sigma_{n}\boldsymbol{u}_{n}\boldsymbol{v}_{n}^{T}\|_{2} = \sigma_{k+1}\boldsymbol{u}_{k+1}\boldsymbol{v}_{k+1}^{T} + \sigma_{k+2}\boldsymbol{u}_{k+2}\boldsymbol{v}_{k+2}^{T} + \dots + \sigma_{n}\boldsymbol{u}_{n}\boldsymbol{v}_{n}^{T}\|_{2}$$

Example: Image compression



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Example: Image compression





Image using rank-50 approximation



8) Using SVD to solve square system of linear equations

If **A** is a $n \times n$ square matrix and we want to solve A = b, we can use the SVD for **A** such that

 $U \Sigma V^T x = b$ $\Sigma V^T x = U^T b$

Solve: $\Sigma y = U^T b$ (diagonal matrix, easy to solve!) Evaluate: x = V y

Cost of solve: $O(n^2)$ Cost of decomposition $O(n^3)$ (recall that SVD and LU have the same cost asymptotic behavior, however the number of operations - constant factor before n^3 - for the SVD is larger than LU)