

Linear Algebra for Computer Science

Lecture 28

SVD (cont.)

Remember: SVD



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

A is $m \times n$, U is orthogonal $m \times m$, Σ is diagonal $m \times n$, and V is orthogonal $n \times n$.

$U^T U = U^T U = I_m$
 $V V^T = V^T V = I_n$

$$\Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_{\min(m,n)} \end{bmatrix}$$
$$\sigma_1 \geq \sigma_2 \geq \sigma_3 \geq \dots \geq \sigma_{\min(m,n)} \geq 0$$

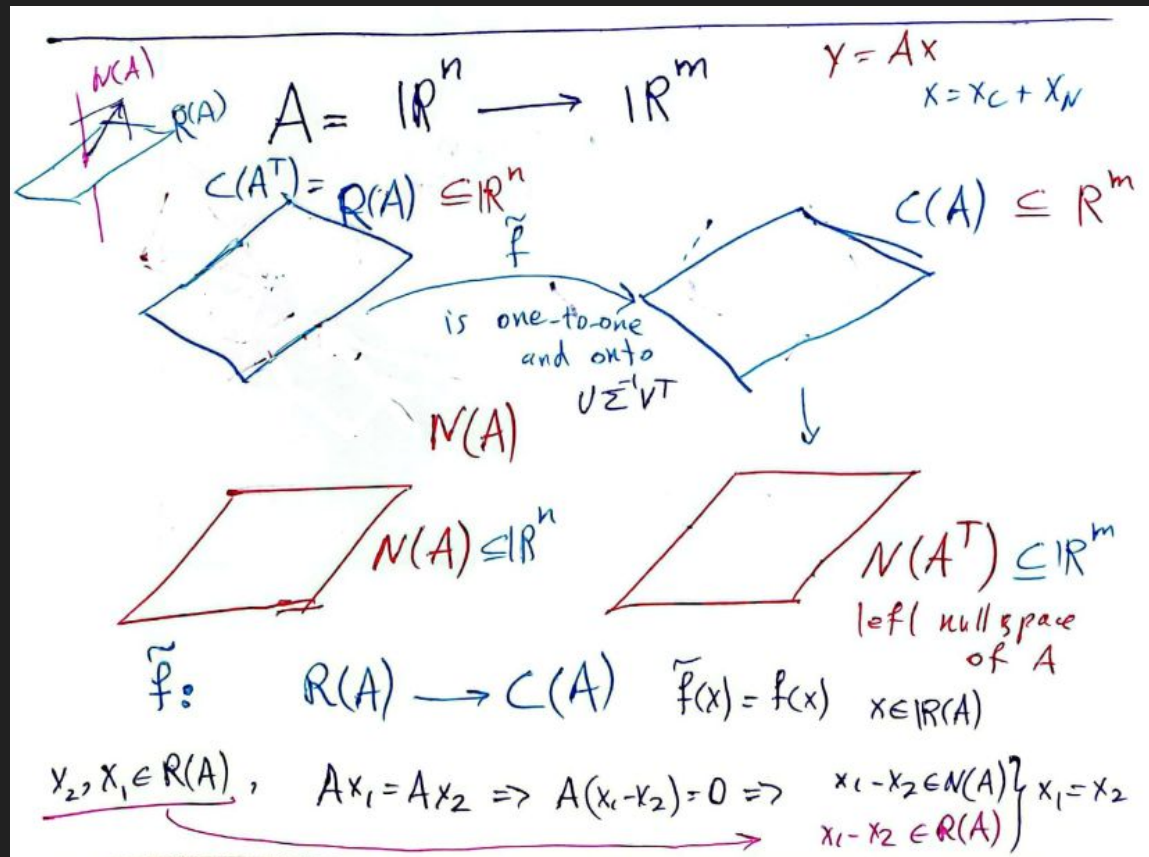
$U = [u_1 \ u_2 \ \dots \ u_m]$ left singular vectors

$V = [v_1 \ v_2 \ \dots \ v_n]$ right singular vectors

$\sigma_1 \ \sigma_2 \ \dots \ \sigma_{\min(m,n)}$ singular values

$$A u_i = \sigma_i v_i$$
$$A = \begin{bmatrix} u_1 & u_2 & \dots & u_m \\ \min(m,n) \end{bmatrix} \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_{\min(m,n)} \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \\ \vdots \\ v_n^T \end{bmatrix}$$
$$= \sum_{i=1}^{\min(m,n)} \sigma_i u_i v_i^T = U \Sigma V^T$$

Bijjective Map between Row space and Column Space



Choose a basis



m $\begin{bmatrix} n \\ A \end{bmatrix}$ $A \in \mathbb{R}^{m \times n}$ $f(x) = Ax$ (II) 30

orthonormal basis

$R(A)$

$N(A) \perp R(A)$

$C(A)$

$N(A^T) \perp C(A)$

$N(A)$

$N(A^T)$

Choose a basis



$R(A) \subseteq \mathbb{R}^n$

$C(A) \subseteq \mathbb{R}^m$

$r = \dim(R(A)) = \text{rank}(A) = \dim(C(A))$

$N(A) \subseteq \mathbb{R}^n$

$N(A^T) \subseteq \mathbb{R}^m$

v_1, v_2, \dots, v_r	is	an	orthonormal	basis	for	$R(A)$
u_1, u_2, \dots, u_r	form	an	orthonormal	basis	for	$C(A)$
v_{r+1}, \dots, v_n	form	an	orthonormal	basis	for	$N(A)$
u_{r+1}, \dots, u_m	form	an	"	"	"	$N(A^T)$
v_1, v_2, \dots, v_n	"	"	"	"	"	\mathbb{R}^n
u_1, u_2, \dots, u_m	"	"	"	"	"	\mathbb{R}^m

Singular Values and Singular Vectors

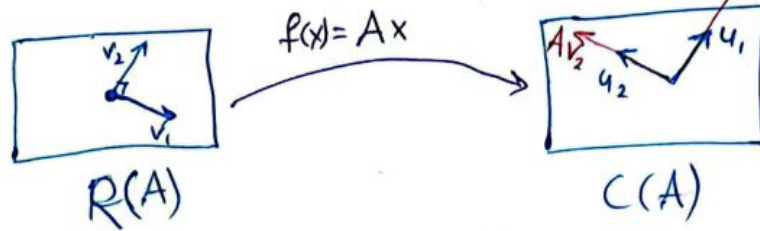


for a matrix $A \in \mathbb{R}^{m \times n}$ choose v_1, v_2, \dots, v_r and u_1, u_2, \dots, u_r such that

$$A v_i = \sigma_i u_i \quad i=1, 2, \dots, r$$

$$\sigma_1 \geq \sigma_2 \geq \sigma_3 \geq \dots \geq \sigma_r > 0$$

$$\sigma_i \geq 0$$



$\sigma_1, \sigma_2, \dots, \sigma_r$ are called singular values
تعداد منفرد

v_1, v_2, \dots, v_r : right singular vectors

u_1, u_2, \dots, u_r : left singular vectors

Singular Values and Singular Vectors



How to compute $v_1, v_2, \dots, v_r, u_1, \dots, u_r, \sigma_1, \dots, \sigma_r$?

$$A v_i = \sigma_i u_i \quad i=1 \dots r$$

$$A \underbrace{\begin{bmatrix} v_1 & v_2 & \dots & v_r \end{bmatrix}}_V = \underbrace{\begin{bmatrix} u_1 & u_2 & \dots & u_r \end{bmatrix}}_U \underbrace{\begin{bmatrix} \sigma_1 & \emptyset & \emptyset & \emptyset \\ \emptyset & \sigma_2 & \emptyset & \emptyset \\ \emptyset & \emptyset & \dots & \emptyset \\ \emptyset & \emptyset & \emptyset & \sigma_r \end{bmatrix}}_{\Sigma}$$

diag($\sigma_1, \sigma_2, \dots, \sigma_r$)

$$AV = U\Sigma$$

$m \times n \quad n \times r \quad m \times r \quad r \times r$

$$V^T V = I$$

$$U^T U = I$$

$$\begin{bmatrix} u_1^T \\ u_2^T \\ \vdots \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Singular Values and Singular Vectors



$$A \begin{bmatrix} v_1 & v_2 & \dots & v_r \end{bmatrix} = \begin{bmatrix} u_1 & u_2 & \dots & u_r \end{bmatrix} \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_r \end{bmatrix}$$

(JV)
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$$\begin{matrix} m \times n \\ A \end{matrix} \underbrace{\begin{bmatrix} v_1 & v_2 & \dots & v_r & v_{r+1} & v_{r+2} & \dots & v_n \end{bmatrix}}_{V \in \mathbb{R}^{n \times n}} = \begin{bmatrix} u_1 & u_2 & \dots & u_r \end{bmatrix} \begin{bmatrix} \sigma_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sigma_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \ddots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sigma_r & 0 & 0 & 0 \end{bmatrix}$$

$V \in \mathbb{R}^{n \times n}$
 $m \times r$
 r
 $n-r$

$v_{r+1}, \dots, v_n \in N(A)$

$V^T V = V V^T = I$
 V : orthogonal

Singular Values and Singular Vectors



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

$m \times n$ $m \times m$ $m \times n$ $n \times n$

Singular Value decomposition
(SVD)

U, V orthogonal

$$U^T U = V V^T = I$$

$$V^T V = V V^T = I$$

Σ diagonal

Singular Values and Singular Vectors



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$$\begin{matrix} m \\ \left[\begin{array}{c} A \\ \cdot \\ \cdot \\ \cdot \end{array} \right] \\ n \\ m \leq n \\ \text{rank}(A) = r \end{matrix} = \begin{matrix} \left[U \right] \\ m \times m \\ \sigma_1 \geq \sigma_2 \geq \sigma_3 \geq \dots \geq \sigma_r > 0 \\ \sigma_{r+1} = \sigma_{r+2} = \dots = \sigma_m = 0 \end{matrix} \begin{matrix} \left[\begin{array}{c} \sigma_1 \\ \sigma_2 \\ \vdots \\ \sigma_m \end{array} \right] \\ m \times n \end{matrix} \begin{matrix} \left[V^T \right] \\ n \times n \end{matrix}$$

Singular Values and Singular Vectors



$$\begin{matrix}
 m & & n \\
 \left[\begin{matrix} A \\ \vdots \\ \vdots \end{matrix} \right] & = & \left[\begin{matrix} \text{wavy lines} \\ U \end{matrix} \right] & \left[\begin{matrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_r \end{matrix} \right] & \left[\begin{matrix} \text{wavy lines} \\ V^T \end{matrix} \right] \\
 m \geq n & & m \times m & m \times n & n \times n
 \end{matrix}$$

$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$$

$$\sigma_{r+1} = \sigma_{r+2} = \dots = \sigma_n = 0$$

$$\begin{aligned}
 A &= \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \dots + \sigma_k u_k v_k^T \\
 &= \sum_{i=1}^{\min(m,n)} \sigma_i u_i v_i^T = \sum_{i=1}^r \sigma_i u_i v_i^T \quad k = \min(m,n)
 \end{aligned}$$

check: $A v_j = \sigma_j u_j \quad u_j^T A = \sigma_j v_j^T$

Pseudo-inverse



LA28

$$f(x) = Ax$$
$$A = U \Sigma V^T = U \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_l & & \\ & & & & & 0 & \dots & 0 \end{bmatrix} V^T$$

$m \times n$

$$\Sigma^+ = \begin{bmatrix} 1/\sigma_1 & & & \\ & 1/\sigma_2 & & \\ & & \ddots & \\ & & & 1/\sigma_l & & \\ & & & & & 0 & \dots & 0 \end{bmatrix} \rightarrow \text{if not zero}$$

$n \times m$

$$A^+ = V \Sigma^+ U^T$$
$$A^+ A = V \Sigma^+ \underbrace{U^T U}_{I} \Sigma V^T = V \Sigma^+ \Sigma V^T$$
$$= V \begin{bmatrix} \sigma_1^{-1} & & & \\ & \sigma_2^{-1} & & \\ & & \ddots & \\ & & & 0 & \dots & 0 \end{bmatrix} \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & 0 & \dots & 0 \end{bmatrix} V^T$$

Pseudo-inverse



$$\begin{aligned} \uparrow \\ A^{\dagger} &= V \Sigma^{\dagger} U^T \quad n \times m \\ A^{\dagger} A &= V \Sigma^{\dagger} U^T U \Sigma V^T = V \Sigma^{\dagger} \Sigma V^T \\ &= V \begin{bmatrix} \sigma_1^{-1} & & & \\ & \sigma_2^{-1} & & \\ & & 0 & \\ & & & 0 \end{bmatrix} \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & 0 & \\ & & & 0 \end{bmatrix} V^T \\ &= V \begin{bmatrix} 1 & & \\ & 1 & \\ & & 0 \end{bmatrix} V^T = [v_1 \ v_2 \ v_3] \begin{bmatrix} 1 & \\ & 1 & \\ & & 0 \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \\ v_3^T \end{bmatrix} \\ &= [v_1 \ v_2] \begin{bmatrix} 1 & \\ & 1 \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \end{bmatrix} = [v_1 \ v_2] \begin{bmatrix} v_1^T \\ v_2^T \end{bmatrix} \end{aligned}$$

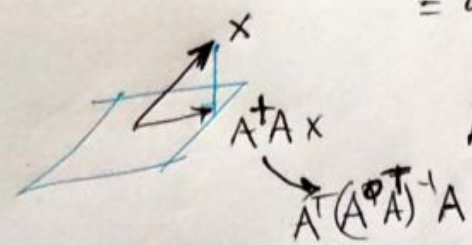
Pseudo-inverse



$$\begin{aligned}
 &= V \begin{bmatrix} 1 & 1 & 0 \end{bmatrix} V^T = [v_1 \ v_2 \ v_3] \begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \\ v_3^T \end{bmatrix} \\
 &= [v_1 \ v_2] \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \end{bmatrix} = [v_1 \ v_2] \begin{bmatrix} v_1^T \\ v_2^T \end{bmatrix}
 \end{aligned}$$

$x \in R(A) \Rightarrow \alpha v_1 + \beta v_2$

$$x \in R(A) \Rightarrow A^+ A x = [v_1 \ v_2] \begin{bmatrix} v_1^T \\ v_2^T \end{bmatrix} (\alpha v_1 + \beta v_2) = [v_1 \ v_2] \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \alpha v_1 + \beta v_2 = x$$



A full ~~column~~ rank $\Rightarrow A^+ = A^T (A A^T)^{-1}$

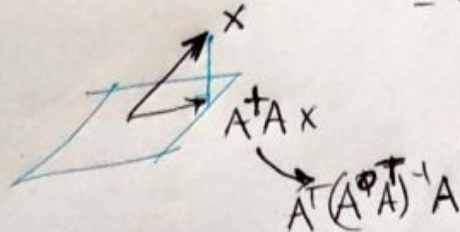
Pseudo-inverse



$$\begin{aligned}
 &= V \begin{bmatrix} 1 & 1 & 0 \end{bmatrix} V^T = [v_1 \ v_2 \ v_3] \begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \\ v_3^T \end{bmatrix} \\
 &= [v_1 \ v_2] \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \end{bmatrix} = [v_1 \ v_2] \begin{bmatrix} v_1^T \\ v_2^T \end{bmatrix}
 \end{aligned}$$

$x \in R(A) \Rightarrow \alpha v_1 + \beta v_2$

$$\begin{aligned}
 x \in R(A) \Rightarrow A^+ A x &= [v_1 \ v_2] \begin{bmatrix} v_1^T \\ v_2^T \end{bmatrix} (\alpha v_1 + \beta v_2) = [v_1 \ v_2] \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \\
 &= \alpha v_1 + \beta v_2 = x
 \end{aligned}$$



A full ~~column~~ rank $\Rightarrow A^+ = A^T (A A^T)^{-1}$

SVD for tall and fat matrices



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$$m > n \quad [A] = \begin{bmatrix} U \\ 0 \end{bmatrix} \begin{bmatrix} \sigma_1 & & \\ & \sigma_2 & \\ & & \ddots \\ & & & \sigma_n \\ & & & & \emptyset \end{bmatrix} [V^T]$$

$m \times m$ $m \times n$ $n \times n$

$$\begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_m \end{bmatrix} = \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_m \end{bmatrix}$$

$m \times n$ $m \times n$

$\sigma_1 \dots \sigma_{\min(m, n)}$

How to find singular values and singular vectors



The bad way!

$$\begin{bmatrix} \sigma_1 & \sigma_2 \\ & \sigma_3 \end{bmatrix} = \begin{bmatrix} \sigma_1 & & \\ & \sigma_1 & \\ & & \emptyset \end{bmatrix} \begin{bmatrix} \sigma_1 & & \\ & \sigma_2 & \\ & & \emptyset \end{bmatrix}$$

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

$$A^T A = V \Sigma^T \underbrace{U^T U}_I \Sigma V^T = V \Sigma^T \Sigma V^T = V \Lambda V^T$$

symmetric

$$= V \Lambda V^{-1}$$

$n \times n$ $m \times n$ $n \times n$

$$\lambda_i = \sigma_i^2$$

$v_1, v_2, \dots, v_n, \sigma_1^2, \sigma_2^2, \dots, \sigma_n^2 = \text{eigenvector \& eigenvalue}$

$u_1, \dots, u_m \leftarrow \text{erg}(AA^T)$ of $A^T A$

Obtain SVD from Eigendecomposition



$$A = \underset{m \times m}{U} \underset{m \times n}{\Sigma} \underset{n \times n}{V^T}$$
$$AA^T = U \Sigma \underbrace{V^T V}_{I} \Sigma^T U^T$$
$$= U \Sigma \Sigma^T U^T$$

$m=3$

$$= [u_1 \ u_2 \ u_3] \begin{bmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_3 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_3 \end{bmatrix} \begin{bmatrix} u_1^T \\ u_2^T \\ u_3^T \end{bmatrix}$$
$$AA^T = [u_1 \ u_2 \ u_3] \begin{bmatrix} \sigma_1^2 & & \\ & \sigma_2^2 & \\ & & \sigma_3^2 \end{bmatrix} \begin{bmatrix} u_1^T \\ u_2^T \\ u_3^T \end{bmatrix}$$
$$AA^T = U \begin{bmatrix} \sigma_1^2 & & \\ & \sigma_2^2 & \\ & & \sigma_3^2 \end{bmatrix} U^T$$

symmetric & positive semi def

eigen decomposition

$\rightarrow U^{-1}$

Obtain SVD from Eigendecomposition



$AA^T = U \begin{bmatrix} \sigma_1^2 & & \\ & \sigma_2^2 & \\ & & \sigma_3^2 \end{bmatrix} U^T$

symmetric & positive semi def

eigen decomposition

$\Rightarrow (AA^T)u_i = \sigma_i^2 u_i$ For symmetric matrices

u_1, \dots, u_m eigenvectors of AA^T

$\sigma_1^2, \sigma_2^2, \dots, \sigma_m^2$ eigenvalues of AA^T

$AA^T =$

v_1, v_2, \dots, v_n eigenvectors of $A^T A$

SVD, Rank, Column Space, Row Space, Null Space



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$$A = [u_1 \ u_2 \ \dots \ u_m] \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_r & & \\ & & & & & 0 \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \\ \vdots \\ v_n^T \end{bmatrix} \quad (VI)$$

Compute svd (e.g. using `np.linalg.svd`)

$r = \text{rank}(A)$: no. of non-zero $\sigma_i = \max_i \text{st } \sigma_i > 0$

column space: $\text{span}(u_1, u_2, \dots, u_r)$

orthonormal basis for $C(A)$

row space: $\text{span}(v_1, v_2, \dots, v_r)$

orthonormal basis for $R(A)$

null space: $\text{span}(v_{r+1}, \dots, v_n)$

orthonormal basis for $N(A)$

left null space: $\text{span}(u_{r+1}, \dots, u_m)$

orthonormal basis for $N(A^T)$

Problems with full SVD



Assume that we have a lot of data $x_1, x_2, \dots, x_n \in \mathbb{R}^d$ LA28
 $d=100$ $n=10000000$ (VI)

arrange them in a matrix

$$X = \begin{bmatrix} x_1^T \\ x_2^T \\ \vdots \\ x_n^T \end{bmatrix} \in \mathbb{R}^{n \times d}$$

np.linalg.svd(A)

$$X = U \Sigma V^T \rightarrow \text{Full SVD}$$

$n \times n$ $n \times d$ $d \times d$
 10000000×10000000 100×100

float32 $\Rightarrow 4 \times 10^{12}$ bytes

4000 GB

represented as

$$\vec{\sigma} = \begin{bmatrix} \sigma_1 \\ \vdots \\ \sigma_d \end{bmatrix} \rightarrow 100$$

$\min(\text{rows}, \text{cols}) \Rightarrow d$

Skinny (thin) SVD



4000 GB

$$X = U \Sigma V^T = \begin{bmatrix} u_1 & u_2 & \dots & u_d & \dots & u_n \\ \vdots & \vdots & & \vdots & & \vdots \\ \vdots & \vdots & & \vdots & & \vdots \\ \vdots & \vdots & & \vdots & & \vdots \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \vdots \\ \sigma_d \\ \vdots \\ \sigma_n \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \\ \vdots \\ v_n^T \end{bmatrix}$$

$m \times n$
 $m \gg n$

$$= \begin{bmatrix} u_1 & u_2 & \dots & u_d \\ \vdots & \vdots & & \vdots \\ \vdots & \vdots & & \vdots \end{bmatrix} \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_d \end{bmatrix} V^T$$

\downarrow
 $4 \times 1000000 \times 100 = 400 \text{ MB}$

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

$$A = U \Sigma V^T = U_{1:l} \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_l \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \\ \vdots \\ v_l^T \end{bmatrix}$$

skinny SVD, thin SVD

Thin (Skinny) SVD



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$$\begin{aligned} \begin{matrix} m \\ \left[\begin{array}{c} n \\ A \end{array} \right] \end{matrix} &= \begin{matrix} \left[\begin{array}{c} u_1 \ u_2 \ \dots \ u_n \end{array} \right] \\ m \times n \end{matrix} \begin{matrix} \left[\begin{array}{c} \sigma_1 \ \dots \ \sigma_n \end{array} \right] \\ n \times n \end{matrix} \begin{matrix} \left[\begin{array}{c} v_1^T \\ v_2^T \\ \vdots \\ v_n^T \end{array} \right] \\ n \times n \end{matrix} \end{aligned} \quad \left. \begin{array}{l} \text{thin} \\ \text{svd} \end{array} \right\} \\ \begin{matrix} m \\ \left[\begin{array}{c} n \\ A \end{array} \right] \end{matrix} &= \begin{matrix} \left[\begin{array}{c} u_1 \ \dots \ u_m \end{array} \right] \\ m \times m \end{matrix} \begin{matrix} \left[\begin{array}{c} \sigma_1 \ \dots \ \sigma_m \end{array} \right] \\ m \times m \end{matrix} \begin{matrix} \left[\begin{array}{c} v_1^T \\ \vdots \\ v_m^T \end{array} \right] \\ m \times n \end{matrix} \end{aligned} \quad \left. \begin{array}{l} \text{skinny} \\ \text{svd} \end{array} \right\}$$

Compact SVD



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$$\begin{bmatrix} A \end{bmatrix} = \begin{bmatrix} u_1 & u_2 & \dots & u_r \end{bmatrix} \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_r \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \\ \vdots \\ v_r^T \end{bmatrix}$$

$\text{rank}(A) = r$
 $A: m \times n$

$m \times r$

$r \times r$
invertible

$r \times n$

compact
svd

$$\Sigma^{-1} = \begin{bmatrix} 1/\sigma_1 & & & \\ & 1/\sigma_2 & & \\ & & \ddots & \\ & & & 1/\sigma_r \\ & & & & \phi \end{bmatrix}$$