Math Refresher for DS

Lecture 5

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Last Time

- Eigenvalues & eigenvectors
- Eigendecomposition
  - Matrix diagonalization;
  - PCA.

Today

- Singular Value Decomposition

Reminder: Eigenvalues & Eigenvectors

- Let A be an $n \times n$ matrix.
- $v \in \mathbb{R}^n$ – eigenvector with eigenvalue λ if

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  There are n roots in total (incl. repetitions).

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n_i – algebraic multiplicity of λ_i.

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- $E_{\lambda_i} = span\,\{v : Av = \lambda_i v\}, \;\; dimE_{\lambda_i} \leq n_i$ – geometric multiplicity.

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

where $V = [v_1 \mid v_2 \mid \dots \mid v_n]$, $\quad \Lambda = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix}$

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- If A is symmetric, then V is orthogonal and $A = V\Lambda V^T$.

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Reminder: PCA

$X - m \times n$ data matrix (m features, n examples)

$S = \frac{1}{n-1} X X^T$ – data covariance matrix ($m \times m$)

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

$$\begin{bmatrix} \mathbf{s_{11}} & s_{12} & \cdots & s_{1m} \\ s_{21} & \mathbf{s_{22}} & \cdots & s_{2m} \\ \vdots & \vdots & \cdots & \vdots \\ s_{n1} & s_{n2} & \cdots & \mathbf{s_{mm}} \end{bmatrix} = \begin{bmatrix} v_{11} & v_{12} & \cdots & v_{1m} \\ v_{21} & v_{22} & \cdots & v_{2m} \\ \vdots & \vdots & \cdots & \vdots \\ v_{n1} & v_{n2} & \cdots & v_{mm} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda_1} & 0 & \cdots & 0 \\ 0 & \boldsymbol{\lambda_2} & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & \boldsymbol{\lambda_m} \end{bmatrix} \begin{bmatrix} v_{11} & v_{12} & \cdots & v_{1m} \\ v_{21} & v_{22} & \cdots & v_{2m} \\ \vdots & \vdots & \cdots & \vdots \\ v_{n1} & v_{n2} & \cdots & v_{mm} \end{bmatrix}^T$$

Total variance of the data $\mathrm{T} = tr(S) = s_{11} + \cdots + s_{nn} = \lambda_1 + \cdots \lambda_m$

Orthogonal eigenvectors $v_1, \dots, v_n$ – principal components of the data

Direction of v_i describes λ_i out of the total variance T.

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- We can show that $\boldsymbol{\lambda_i \geq 0}$:

$$0 \leq \|Av_i\|^2 = (Av_i, Av_i) = (Av_i)^T Av_i = v_i^T A^T A v_i = v_i^T \lambda_i v_i = \lambda_i \|v_i\|^2$$

$$\Leftrightarrow$$

$$\lambda_i \geq 0.$$

Eigenvalues of AA^T

- Let A be an $m \times n$ matrix.

- AA^T is an $m \times m$ symmetric matrix. Therefore, AA^T has m linearly independent eigenvectors $u_1, \dots, u_m$ with eigenvalues $\lambda_1, \dots, \lambda_n$.

- We can show that $\lambda_i \geq 0$:

$$0 \leq \|A^T u_i\|^2 = (A^T u_i, A^T u_i) = (A^T u_i)^T A^T u_i = u_i^T A A^T u_i = v_i^T \lambda_i u_i = \lambda_i \|u_i\|^2$$

$$\Leftrightarrow$$

$$\lambda_i \geq 0.$$

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Positive Definite Matrices

- Square matrices with non-negative eigenvalues $\lambda_i \geq 0$ are called positive semi-definite.

$$A \text{ is positive definite} \Leftrightarrow x^T A x \geq 0 \ \forall x \in \mathbb{R}^n$$

- Square matrices with positive eigenvalues $\lambda_i > 0$ are called positive definite.

$$A \text{ is positive definite} \Leftrightarrow x^T A x > 0 \ \forall x \neq 0 \in \mathbb{R}^n$$

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Eigenvalues of $A^T A$ and AA^T

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- What is the relationship between eigenvalues of $A^T A$ and AA^T?

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$$\color{green}{A}A^T Av = \lambda \color{green}{A}v$$

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$$AA^T Av = \lambda Av$$

$v \neq 0$ is an eigenvector of $A^T A$ with $\lambda \neq 0 \iff$
$Av \neq 0$ is an eigenvalue of AA^T with the same eigenvalue $\lambda \neq 0$.

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Matrices $\boldsymbol{A^T A}$ and $\boldsymbol{AA^T}$ share the same set of non-zero eigenvalues!

$$(AA^T)u = \lambda u, \qquad \lambda \neq 0$$

$$A^T AA^T u = \lambda A^T u$$

$u \neq 0$ is an eigenvector of AA^T with $\lambda \neq 0 \iff$
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$$v \neq 0 \text{ is an eigenvector of } A^T A \text{ with } \lambda \neq 0 \iff$$
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$$u \neq 0 \text{ is an eigenvector of } AA^T \text{ with } \lambda \neq 0 \iff$$
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- Why this is useful? Imagine that A is a 1000×2 matrix.

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- You need to find eigenvalues of AA^T which is a 1000×1000 matrix.

Trick: compute eigenvalues of $A^T A$ instead!

SVD: Motivation

Eigendecomposition: Problems

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$$A = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{pmatrix} = ?$$

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Singular Value Decomposition : generalization of eigendecomposition for all matrices.

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SVD:
Main Idea

SVD: Main Idea

- Let A be an $m \times n$ matrix.
- *(SVD)*: A can be decomposed as

$$A_{m\times n} = U_{m\times m}\Sigma_{m\times n}(V_{n\times n})^T, \text{ where}$$

$$U = [u_1 \,|\ldots|\, u_m], \;\; V = [v_1 \,|\ldots|\, v_n] - \text{orthogonal matrices},$$

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$$m \geq n: \quad \Sigma = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \sigma_n \\ & & 0 & \end{bmatrix}$$

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$\boldsymbol{n-m}$ zero columns

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- Unlike in eigendecomposition, U and V are (generally) not the same.

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$$m \geq n: \quad \Sigma = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \sigma_n \\ & & 0 & \end{bmatrix}, \qquad m < n: \quad \Sigma = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 & \\ 0 & \sigma_2 & \cdots & 0 & \\ \vdots & \vdots & \vdots & \vdots & 0 \\ 0 & 0 & \cdots & \sigma_m & \end{bmatrix}$$

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$$A =$$

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$$A = u_1\sigma_1 v_1^T + u_2\sigma_2 v_2^T + \cdots + u_r\sigma_r v_r^T.$$

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- *(Reduced SVD)*:

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- *(Reduced SVD)*: A can be decomposed as

$$A_{m\times n} = U^r_{m\times r}\Sigma^r_{r\times r}(V^r_{n\times r})^T, \text{ where}$$

$$U^r = [u_1 | \ldots | u_r],\ \ V^r = [v_1 | \ldots | v_r] - \text{orthogonal matrices,}$$

$$\Sigma^r - \text{diagonal matrix with } \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$$

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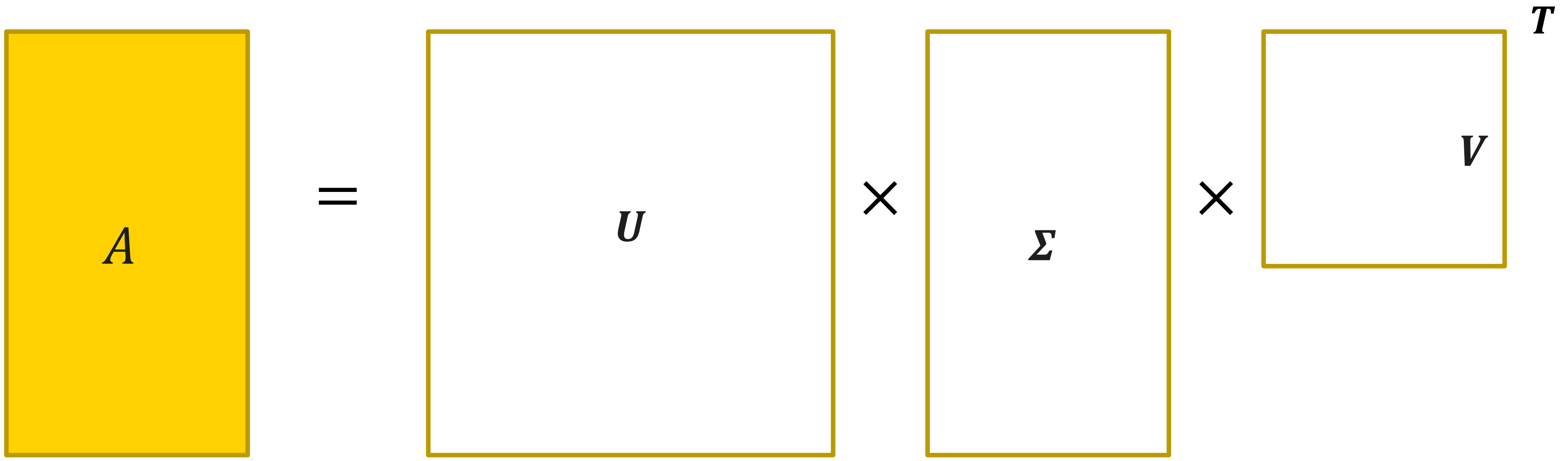

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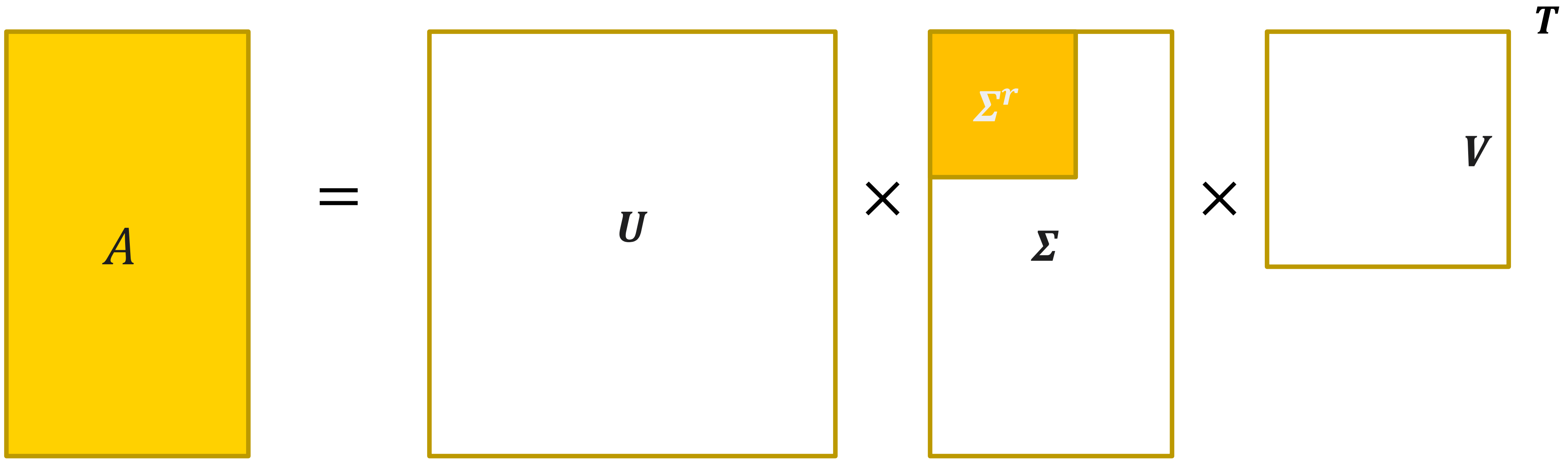
Σ – "diagonal matrix" with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$,
$\sigma_{r+1} = \cdots = \sigma_{\max(m,n)} = 0$



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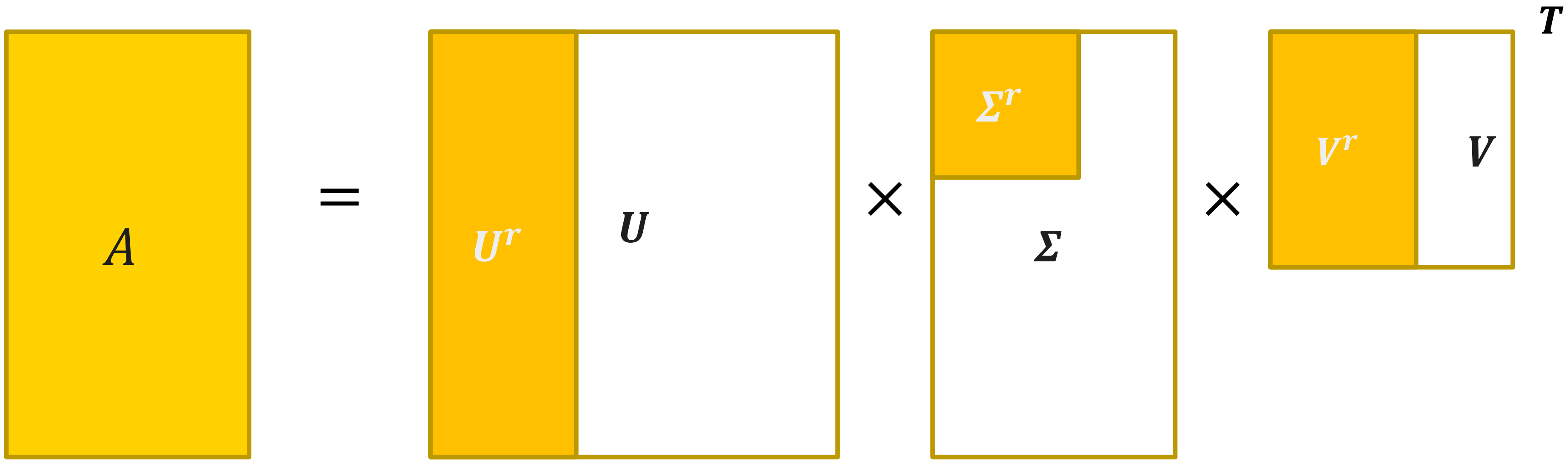
Reduced SVD: Main Idea

$$A_{m\times n} = U^r_{m\times r}\Sigma^r_{r\times r}(V^r_{n\times r})^T,$$ where

$U^r = [u_1 | \ldots | u_r]$, $V^r = [v_1 | \ldots | v_r]$ – orthogonal matrices,

Σ^r – diagonal matrix with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$.



SVD: Derivation

SVD: Main Idea

- Let A be an $m \times n$ matrix.
- *(SVD)*: A can be decomposed as

$$A_{m\times n} = U_{m\times m}\Sigma_{m\times n}(V_{n\times n})^T, \text{ where}$$

$$U = [u_1 \,|\ldots|\, u_m],\ \ V = [v_1 \,|\ldots|\, v_n] - \text{orthogonal matrices,}$$

Σ – "diagonal matrix" with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0,\ \sigma_{r+1} = \cdots = \sigma_{\max(m,n)} = 0$

SVD: Main Idea

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$$\Sigma \text{ – "diagonal matrix" with } \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0, \;\; \sigma_{r+1} = \cdots = \sigma_{\max(m,n)} = 0$$

How do we arrive to this?

SVD

- Let A be an $m \times n$ matrix:

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$$

SVD

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$row(A) = span\{A_1, \dots, A_m\} \subseteq \mathbb{R}^n$, $\{v_1, \dots, v_r\}$ – orthonormal basis

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Key idea: let's find $\boldsymbol{v_i}, \boldsymbol{u_i}$ such that $\boldsymbol{Av_i} = \boldsymbol{\sigma_i u_i}$.

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SVD

- Let A be an $m \times n$ matrix.

- $\{v_1, \dots, v_r\}$ – orthonormal basis of $row(A)$,
  $\{u_1, \dots, u_r\}$ – orthonormal basis of $col(A)$

SVD

- Let A be an $m \times n$ matrix.

- $\{v_1, \dots, v_r\}$ – orthonormal basis of $row(A)$, $v_{r+1}, \dots, v_n \in null(A)$,
$\{u_1, \dots, u_r\}$ – orthonormal basis of $col(A)$

- $\{v_1, \dots, v_r, v_{r+1}, \dots, v_n\}$ – orthonormal basis of $\mathbb{R}^n$,

SVD

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Let's find v_i, u_i such that $Av_i = \sigma_i u_i$

$$\Leftrightarrow$$

$A_{m\times n} V_{n\times n} = U_{m\times m} \Sigma_{m\times n}$, where

$U = [u_1 | \dots | u_m]$, $V = [v_1 | \dots | v_n]$ – orthogonal matrices,

Σ – "diagonal matrix" with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$, $\sigma_{r+1} = \cdots = 0$

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SVD

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$$A = U\Sigma\mathrm{V}^{-1} = U\Sigma\mathrm{V}^{\mathrm{T}}$$ (V is orthogonal)

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$$V = [v_1\,|\ldots|v_n] - \text{eigenvectors of } A^T A$$

SVD

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$$V = [v_1\,|\ldots|v_n] - \text{eigenvectors of } A^T A$$

$$m \geq n:\quad \Sigma = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \sigma_n \\ & & 0 & \end{bmatrix},\; m < n:\quad \Sigma = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 & \\ 0 & \sigma_2 & \cdots & 0 & \\ \vdots & \vdots & \vdots & \vdots & 0 \\ 0 & 0 & \cdots & \sigma_m & \end{bmatrix}$$

$$\Sigma^T\Sigma = \begin{bmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \sigma_n^2 \end{bmatrix},\quad \sigma_i^2 = \lambda_i - \text{eigenvalues of } A^T A.$$

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SVD

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

By multiplying by A^T on the left we got that
$V = [v_1 | \dots | v_n]$ – eigenvectors of $A^T A$,
$\sigma_1^2, \dots, \sigma_n^2$ – corresponding eigenvalues *(some of them possibly 0s).*

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$$AA^T = U\Sigma \mathrm{V}^{\mathrm{T}} \cdot \left(U\Sigma \mathrm{V}^{\mathrm{T}}\right)^T = U\Sigma V^T V \Sigma^T U^T = U_{m\times m}(\Sigma\Sigma^T)_{m\times m}(U_{m\times m})^T$$

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SVD

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SVD: Example

Example

- Let's find SVD and reduced SVD of

$$A = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{pmatrix}$$

$$A_{2\times3} = U_{2\times2}\,\Sigma_{2\times3}(V_{3\times3})^T$$

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Singular values = (non-zero) eigenvalues of AA^T:

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Singular values = (non-zero) eigenvalues of AA^T:

$$AA^T = \begin{pmatrix} 17 & 8 \\ 8 & 17 \end{pmatrix}, \qquad \det(AA^T - \lambda E) = (\lambda - 25)(\lambda - 9) = 0 \Leftrightarrow$$

$$\sigma_1 = \sqrt{25} = 5, \qquad \sigma_2 = \sqrt{9} = 3$$

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$$\boldsymbol{\Sigma} = \begin{pmatrix} \mathbf{5} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{3} & \mathbf{0} \end{pmatrix}, \qquad V = ?, \qquad U = ?$$

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$$A_{2\times 3} = U_{2\times 2}\Sigma_{2\times 3}(V_{3\times 3})^T, \qquad \Sigma = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 3 & 0 \end{pmatrix}$$

Columns of V are eigenvectors of $A^T A$.
Eigenvalues of $A^T A$ are 25, 9 and 0.

$$A^T A - 25E = \begin{pmatrix} -12 & 12 & 2 \\ 12 & -12 & -2 \\ 2 & -2 & -17 \end{pmatrix} \sim \ldots \to v_1 = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}^T$$

Example

- Let's find SVD and reduced SVD of

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Columns of V are eigenvectors of $A^T A$.
Eigenvalues of $A^T A$ are 25, 9 and 0.

$$A^T A - 9E = \begin{pmatrix} 4 & 12 & 2 \\ 12 & 4 & -2 \\ 2 & -2 & -1 \end{pmatrix} \sim \ldots \to v_2 = \left(\frac{1}{3\sqrt{2}} \quad \frac{-1}{3\sqrt{2}} \quad \frac{4}{3\sqrt{2}}\right)^T$$

Example

- Let's find SVD and reduced SVD of

$$A = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{pmatrix}$$

$$A_{2\times3} = U_{2\times2}\Sigma_{2\times3}(V_{3\times3})^T, \qquad \Sigma = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 3 & 0 \end{pmatrix}$$

Columns of V are eigenvectors of A^TA.
Eigenvalues of A^TA are 25, 9 and 0.

$$A^TA - 0E = \begin{pmatrix} 13 & 12 & 2 \\ 12 & 13 & -2 \\ 2 & -2 & 10 \end{pmatrix} \sim \dots \to v_3 = \begin{pmatrix} \frac{2}{3} & \frac{-2}{3} & \frac{-1}{3} \end{pmatrix}^T$$

Example

- Let's find SVD and reduced SVD of

$$A = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{pmatrix}$$

$$A_{2\times 3} = U_{2\times 2}\Sigma_{2\times 3}(V_{3\times 3})^T,$$

$$\Sigma = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 3 & 0 \end{pmatrix}, \qquad \boldsymbol{V} = \begin{pmatrix} \mathbf{1/\sqrt{2}} & \mathbf{1/3\sqrt{2}} & \mathbf{2/3} \\ \mathbf{-1/\sqrt{2}} & \mathbf{-1/3\sqrt{2}} & \mathbf{-2/3} \\ \mathbf{0} & \mathbf{4/3\sqrt{2}} & \mathbf{-1/3} \end{pmatrix}, \qquad U = ?$$

Example

- Let's find SVD and reduced SVD of

$$A = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{pmatrix}$$

$$A_{2\times 3} = U_{2\times 2}\Sigma_{2\times 3}(V_{3\times 3})^T,$$

$$\Sigma = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 3 & 0 \end{pmatrix}, \qquad V = \begin{pmatrix} 1/\sqrt{2} & 1/3\sqrt{2} & 2/3 \\ -1/\sqrt{2} & -1/3\sqrt{2} & -2/3 \\ 0 & 4/3\sqrt{2} & -1/3 \end{pmatrix}, \qquad U =?$$

Remember: $\boldsymbol{Av_i = \sigma_i u_i}$

Example

- Let's find SVD and reduced SVD of

$$A = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{pmatrix}$$

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$$\begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{pmatrix}\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{pmatrix} = 5u_1 \Rightarrow u_1 = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$

Example

- Let's find SVD and reduced SVD of

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$$u_1 = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}, \qquad \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{pmatrix}\begin{pmatrix} 1/3\sqrt{2} \\ -1/3\sqrt{2} \\ 4/3\sqrt{2} \end{pmatrix} = 3u_1 \Rightarrow u_2 = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}$$

Example

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$$\Sigma = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 3 & 0 \end{pmatrix}, \qquad V = \begin{pmatrix} 1/\sqrt{2} & 1/3\sqrt{2} & 2/3 \\ -1/\sqrt{2} & -1/3\sqrt{2} & -2/3 \\ 0 & 4/3\sqrt{2} & -1/3 \end{pmatrix}, \qquad \boldsymbol{U} = \begin{pmatrix} \mathbf{1/\sqrt{2}} & \mathbf{1/\sqrt{2}} \\ \mathbf{1/\sqrt{2}} & \mathbf{-1/\sqrt{2}} \end{pmatrix}$$

Example

- SVD of

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From SVD to Reduced SVD

$$A = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{pmatrix}$$

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From SVD to Reduced SVD

$$A = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{pmatrix}$$

$$A_{2\times3} = U_{2\times2}\Sigma_{2\times3}(V_{3\times3})^T,$$

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Reduced SVD:

$$A_{2\times 3} = U_{2\times 2}\Sigma_{2\times \mathbf{2}}(V_{3\times \mathbf{2}})^T,$$

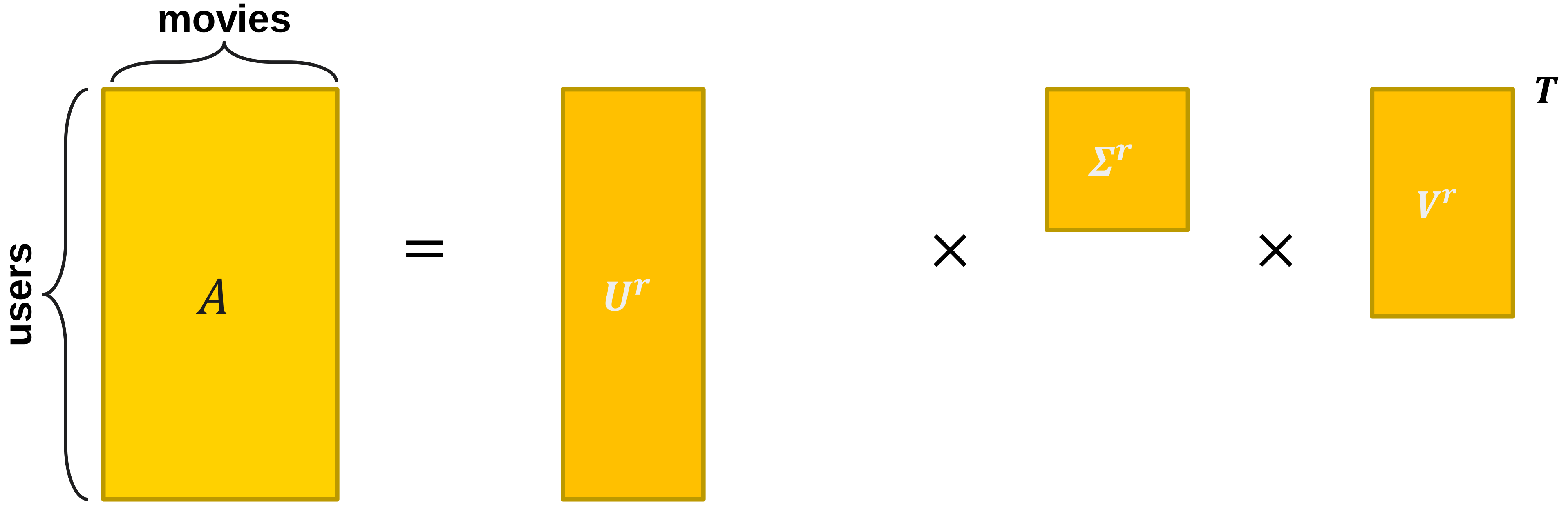
$$A = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \cdot \begin{pmatrix} 5 & 0 \\ 0 & 3 \end{pmatrix} \cdot \begin{pmatrix} 1/\sqrt{2} & 1/3\sqrt{2} \\ -1/\sqrt{2} & -1/3\sqrt{2} \\ 0 & 4/3\sqrt{2} \end{pmatrix}^T$$

Reduced SVD: Main Idea

$$A_{m\times n} = U^r_{m\times \mathbf{r}}\Sigma^r_{\mathbf{r}\times \mathbf{r}}(V^r_{n\times \mathbf{r}})^T,$$ where

$U^r = [u_1 \,|\ldots|\, u_r],\ \ V^r = [v_1 \,|\ldots|\, v_r]$ – orthogonal matrices,

Σ^r – diagonal matrix with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$.



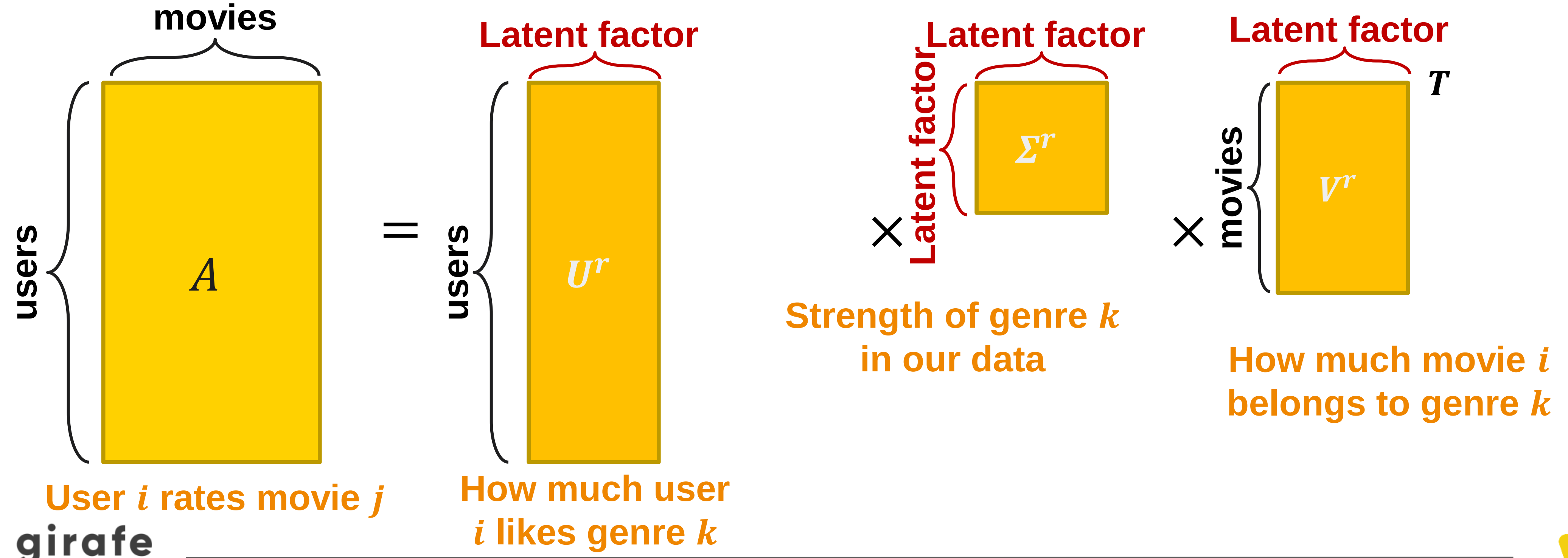
User i rates movie j

Reduced SVD: Main Idea

$$A_{m\times n} = U^r_{m\times r}\Sigma^r_{r\times r}(V^r_{n\times r})^T, \text{ where}$$

$$U^r = [u_1\,|\ldots|u_r],\ \ V^r = [v_1\,|\ldots|v_r] - \text{orthogonal matrices},$$

$$\Sigma^r - \text{diagonal matrix with } \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0.$$



To sum up

- SVD: a generalization of eigendecomposition.
- Computing SVD: an example.
- Application: recommender systems.