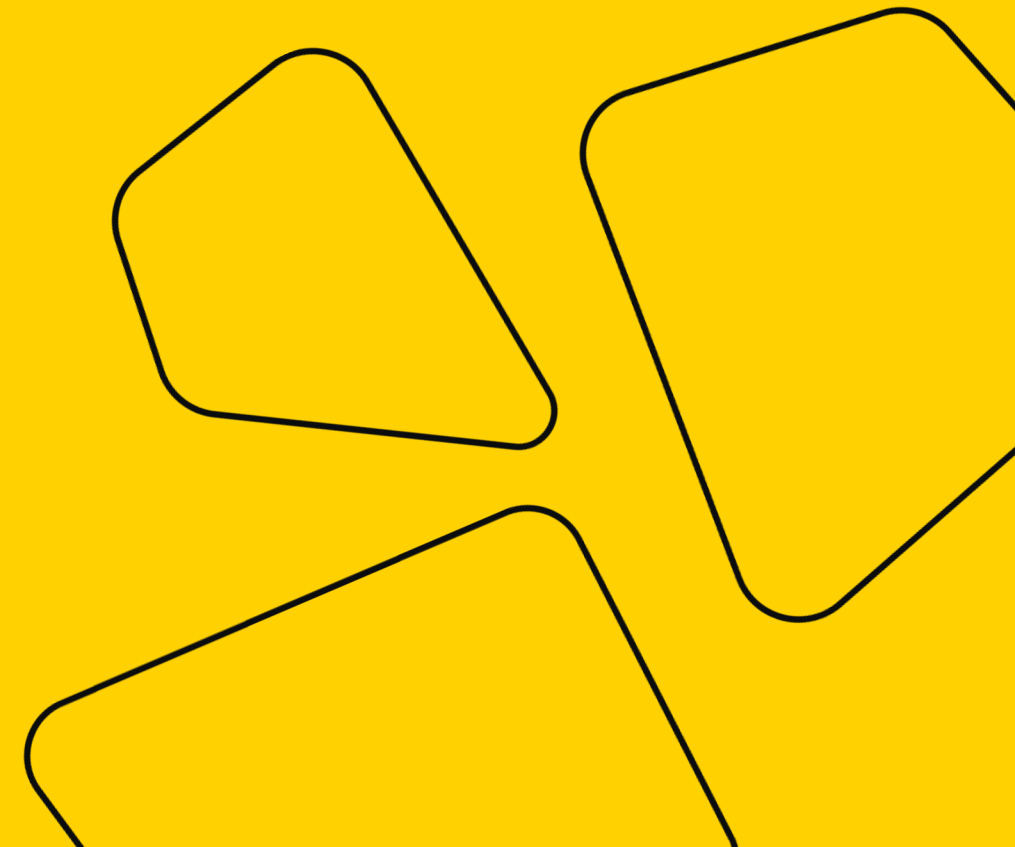


Math Refresher for DS

Lecture 5



girafe
ai



Last Time

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

Today

- Singular Value Decomposition

Reminder: Eigenvalues & Eigenvectors

- Let A be an $n \times n$ matrix.
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- $E_{\lambda_i} = \text{span} \{v : Av = \lambda_i v\}$, $\dim E_{\lambda_i} \leq n_i$ – geometric multiplicity.

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

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

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

Reminder: PCA

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

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

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

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

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

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 $\lambda_i \geq 0$:

$$\begin{aligned} 0 \leq \|Av_i\|^2 &= (Av_i, Av_i) = (Av_i)^T Av_i = v_i^T A^T Av_i = v_i^T \lambda_i v_i = \lambda_i \|v_i\|^2 \\ &\Leftrightarrow \\ &\lambda_i \geq 0. \end{aligned}$$

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 $\lambda_i \geq 0$:

$$\begin{aligned} 0 \leq \|A^T u_i\|^2 &= (A^T u_i, A^T u_i) = (A^T u_i)^T A^T u_i = u_i^T A A^T u_i = \lambda_i \|u_i\|^2 \\ &\Leftrightarrow \\ &\lambda_i \geq 0. \end{aligned}$$

Positive Definite Matrices

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

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

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

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

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

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$v \neq 0$ is an eigenvector of $A^T A$ with $\lambda \neq 0 \iff$

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

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- Why this is useful? Imagine that A is a 1000×2 matrix.

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

SVD: Motivation



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Singular Value Decomposition : generalization of eigendecomposition for all matrices.

SVD:

Main Idea



SVD: Main Idea

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

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- u_1, \dots, u_m – left singular vectors of A .
 v_1, \dots, v_n – right singular vectors of A .
- $\sigma_1, \dots, \sigma_r$ – singular values of A .
- Unlike in eigendecomposition, U and V are (generally) not the same.

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$$A =$$

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

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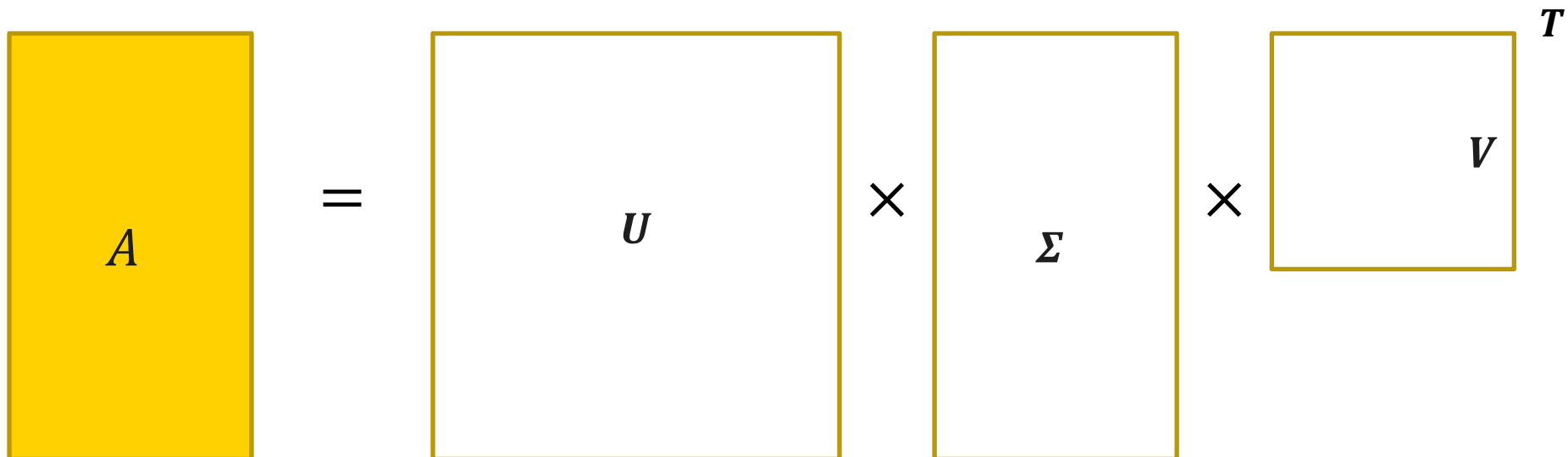
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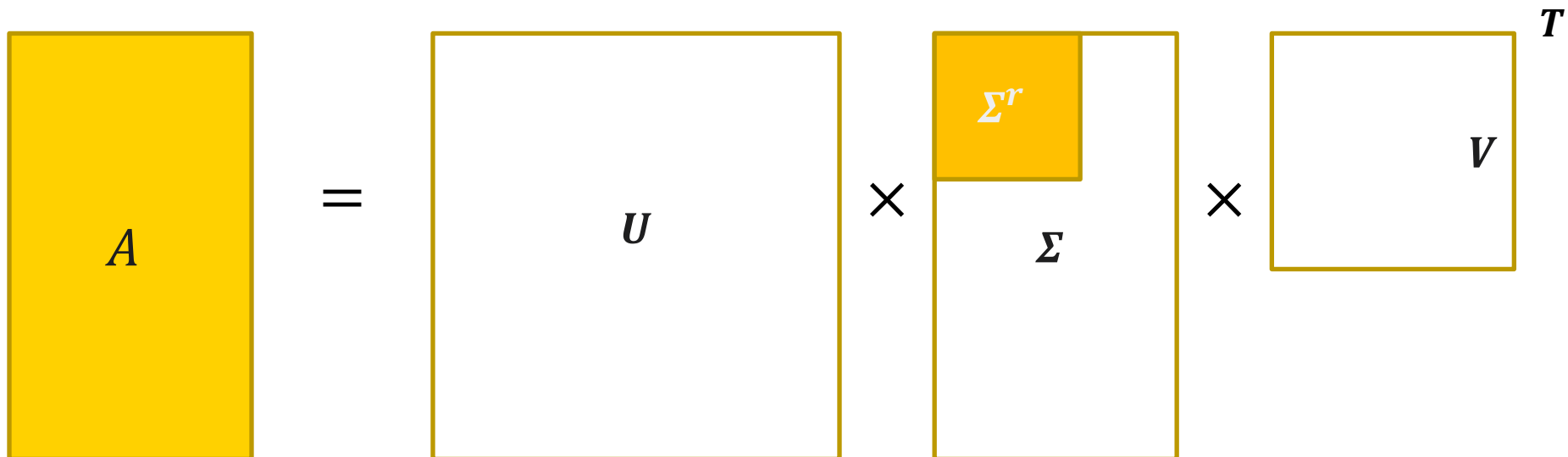
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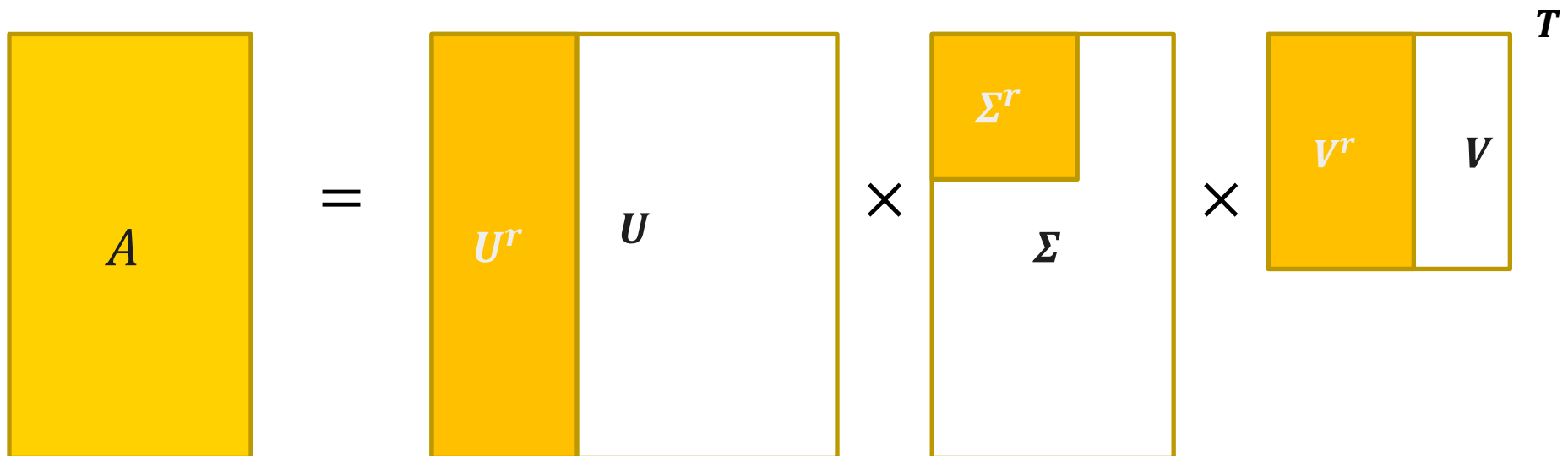


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SVD: Derivation



SVD: Main Idea

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

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

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

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

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How do we arrive to this?

SVD

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

SVD

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 $v_{r+1}, \dots, v_n \in \text{null}(A)$,
- $\{v_1, \dots, v_r, v_{r+1}, \dots, v_n\}$ – orthonormal basis of \mathbb{R}^n ,

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

\Leftrightarrow

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

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

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

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

By multiplying by A^T on the left we got that

$V = [v_1 \mid \dots \mid v_n]$ – eigenvectors of $A^T A$,
 $\sigma_1^2, \dots, \sigma_n^2$ – corresponding eigenvalues (*some of them possibly 0s*).

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SVD: Example



Example

- Let's find SVD and reduced SVD of

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

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

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

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

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

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

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Columns of V are eigenvectors of $A^T A$.

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

$$A^T A - 25E = \begin{pmatrix} -12 & 12 & 2 \\ 12 & -12 & -2 \\ 2 & -2 & -17 \end{pmatrix} \sim \dots \rightarrow v_1 = \left(\frac{1}{\sqrt{2}} \quad \frac{1}{\sqrt{2}} \quad 0 \right)^T$$

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

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

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

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Remember: $Av_i = \sigma_i u_i$

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

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

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

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Reduced SVD:

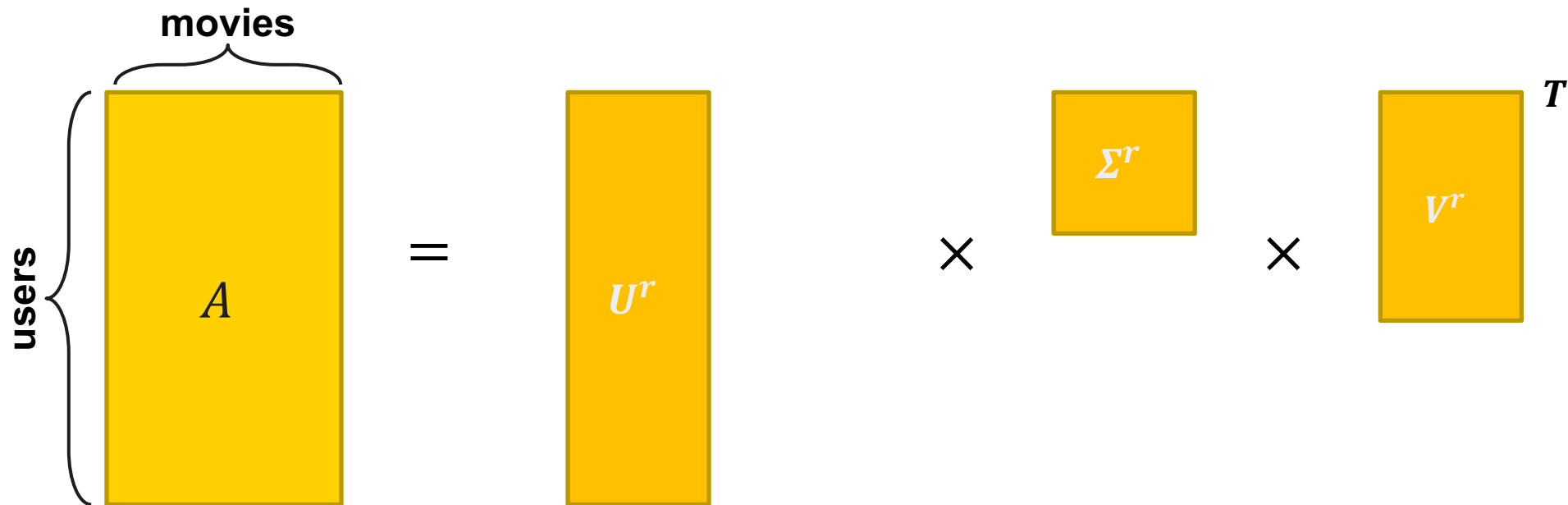
$$A = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \cdot \begin{pmatrix} 5 & 0 \\ 0 & 3 \end{pmatrix} \cdot \begin{pmatrix} 1/\sqrt{2} & 1/3\sqrt{2} \\ -1/\sqrt{2} & -1/3\sqrt{2} \\ 0 & 4/3\sqrt{2} \end{pmatrix}^T$$

Reduced SVD: Main Idea

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

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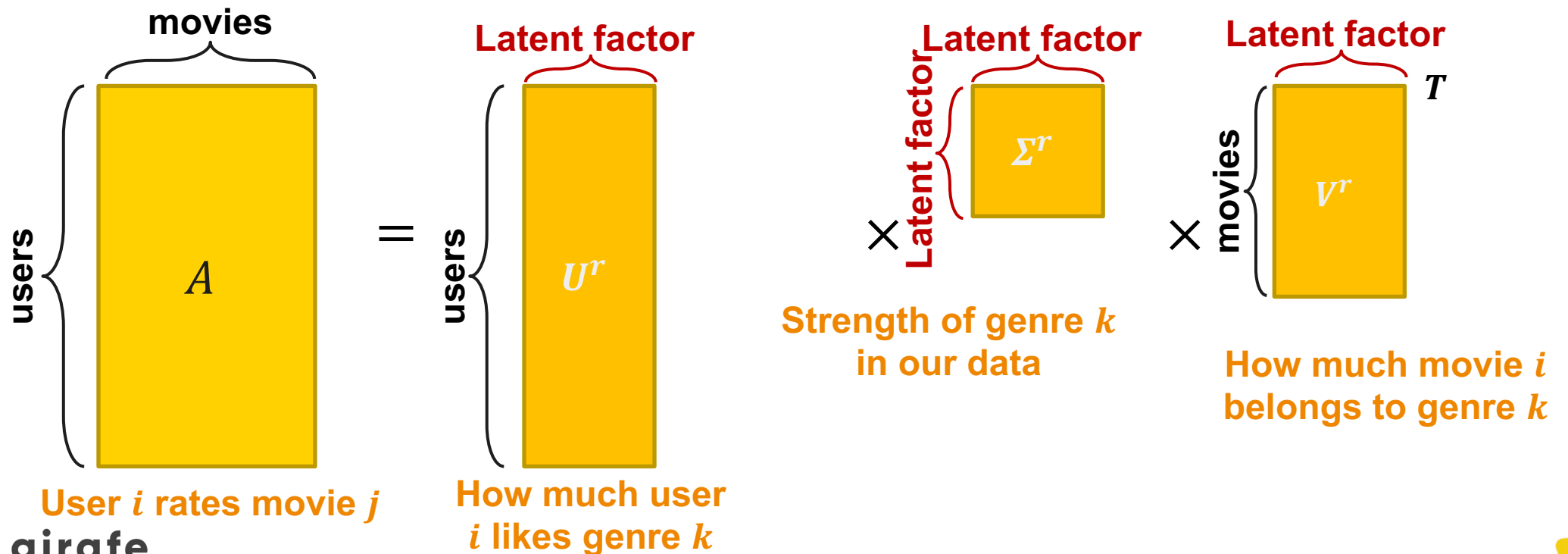
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To sum up



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