Singular Values and Singular Vectors

Reminder: Eigendecomposition

- Consider an $n \times n$ symmetric matrix A.

- Eigendecomposition of A:

$$A_{n \times n} = V_{n \times n} \Lambda_{n \times n} V^T_{n \times n}$$

Columns of V – eigenvectors of A,
V – orthogonal matrix: $V^T = V^{-1}$.

Λ – diagonal matrix,
diagonal elements $\lambda_1, \dots, \lambda_n$ – eigenvalues of A.

SVD: Motivation

- Eigendecomposition is great ☺
- But it only works for square and symmetric matrices ☹

Singular Value Decomposition:
generalization of eigendecomposition
for *any* rectangular matrix.

Singular Values and Singular Vectors

- For square matrices: eigenvalue + eigenvector:

$$Av = \lambda v$$

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- For non-square matrices:

$$u, v \ -\text{ unit vectors, } \ \sigma > 0 - \text{ some number such that}$$
$$Av = \sigma u, \qquad A^T u = \sigma v$$

u – left singular vector, v – right singular vector, σ – singular number

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What are those vectors and numbers?

SVD

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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$\boldsymbol{m} - \boldsymbol{n}$ zero rows

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$\boldsymbol{m-n}$ zero rows

$\boldsymbol{n-m}$ zero columns

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

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

$\boldsymbol{m-n}$ zero rows

$\boldsymbol{n-m}$ zero columns

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SVD: Main Ingredients

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

$U = [u_1 \,|\ldots|\, u_m]$ – eigenvectors of AA^T,

$V = [v_1 \,|\ldots|\, v_n]$ – eigenvectors of A^TA,

$\sigma_1^2, \ldots, \sigma_r^2$ – corresponding non-zero eigenvalues of of A^TA / AA^T.

Full SVD

$$A_{m\times n} = U_{m\times m}\Sigma_{m\times n}V_{n\times n}^T$$

U, V – orthogonal matrices

Σ – "diagonal" matrix

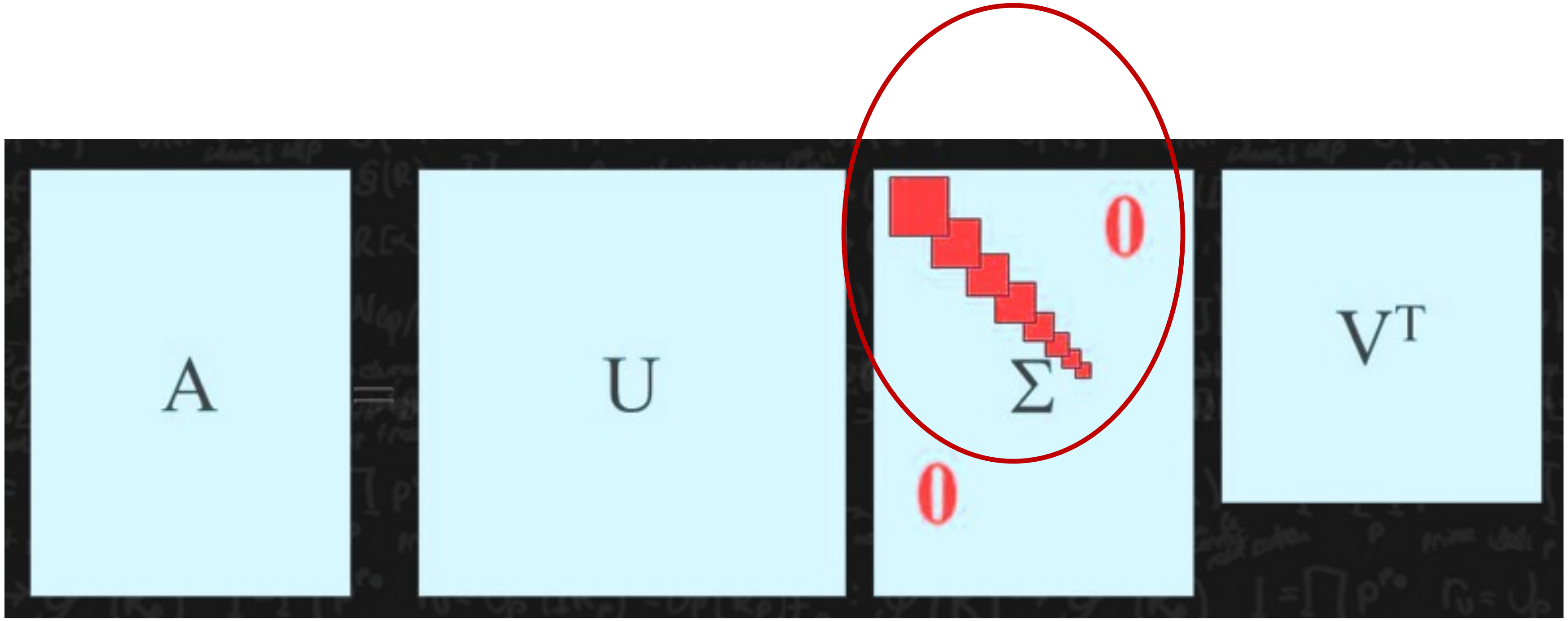
$$m \geq n: \quad \Sigma = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \sigma_n \\ & \boxed{0} & & \end{bmatrix} \qquad m < n: \quad \Sigma = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 & \\ 0 & \sigma_2 & \cdots & 0 &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

$\boldsymbol{m-n}$ zero rows

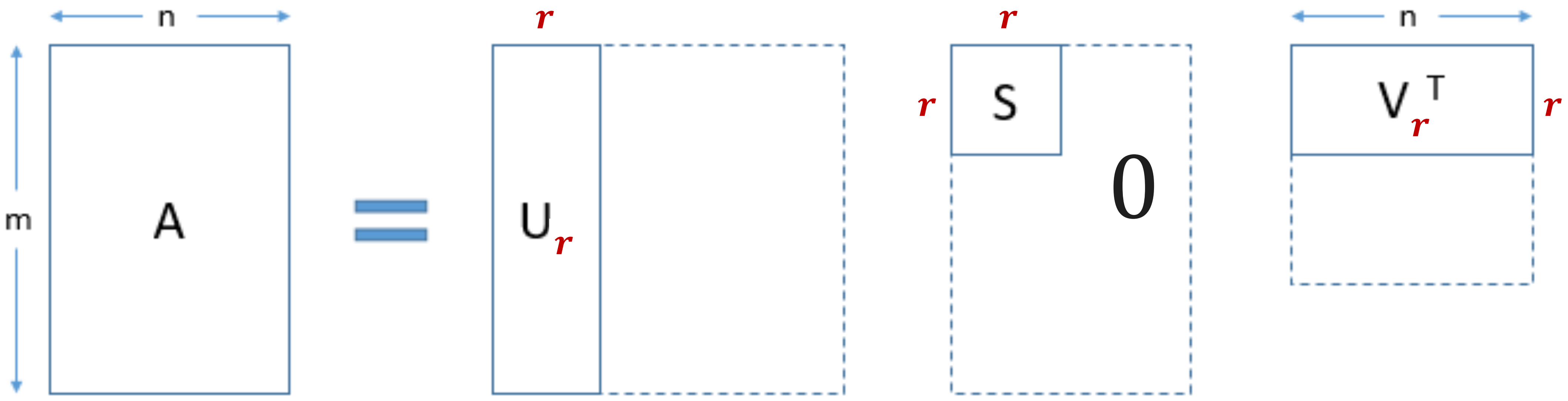
$\boldsymbol{n-m}$ zero columns

Full SVD

Only r non-zero diagonal elements!



Reduced SVD



Reduced SVD

$$A_{m\times n} = U_{m\times \mathbf{r}}\Sigma_{\mathbf{r}\times \mathbf{r}}V^T_{n\times \mathbf{r}}$$

$U_{m\times k}, V_{n\times k}$ – orthogonal matrices

$u_1, \dots u_r$ – left singular vectors *= eigenvectors of* AA^T

$v_1, \dots v_r$ – right singular vectors *= eigenvectors of* A^TA

$\Sigma_{r\times r}$ – diagonal matrix

$\sigma_1, \dots \sigma_r > 0$ – singular values of A

$\sigma_1^2, \dots \sigma_r^2$ *- non-zero eigenvalues of* AA^T *and* A^TA

$$Av_i = \sigma_i u_i$$

Singular Values: Example

- Find singular values of $A = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{pmatrix}$.

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

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$A^T A$ is a 3×3 matrix while AA^T is only 2×2 but has the same non-zero eigenvalues.

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$$AA^T = \begin{pmatrix} 17 & 8 \\ 8 & 17 \end{pmatrix},$$

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A^TA is a 3×3 matrix while AA^T is only 2×2 but has the same non-zero eigenvalues.

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

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

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

$$\Sigma = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 3 & 0 \end{pmatrix}$$

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.

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

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

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

$$A^T A - 9E = \begin{pmatrix} 4 & 12 & 2 \\ 12 & 4 & -2 \\ 2 & -2 & -1 \end{pmatrix} \sim \dots \to v_2 = \begin{pmatrix} \frac{1}{3\sqrt{2}} & \frac{-1}{3\sqrt{2}} & \frac{4}{3\sqrt{2}} \end{pmatrix}^T$$

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

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

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

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Remember: $\boldsymbol{A v_i} = \boldsymbol{\sigma_i u_i}$

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

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Example

- SVD of

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

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

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

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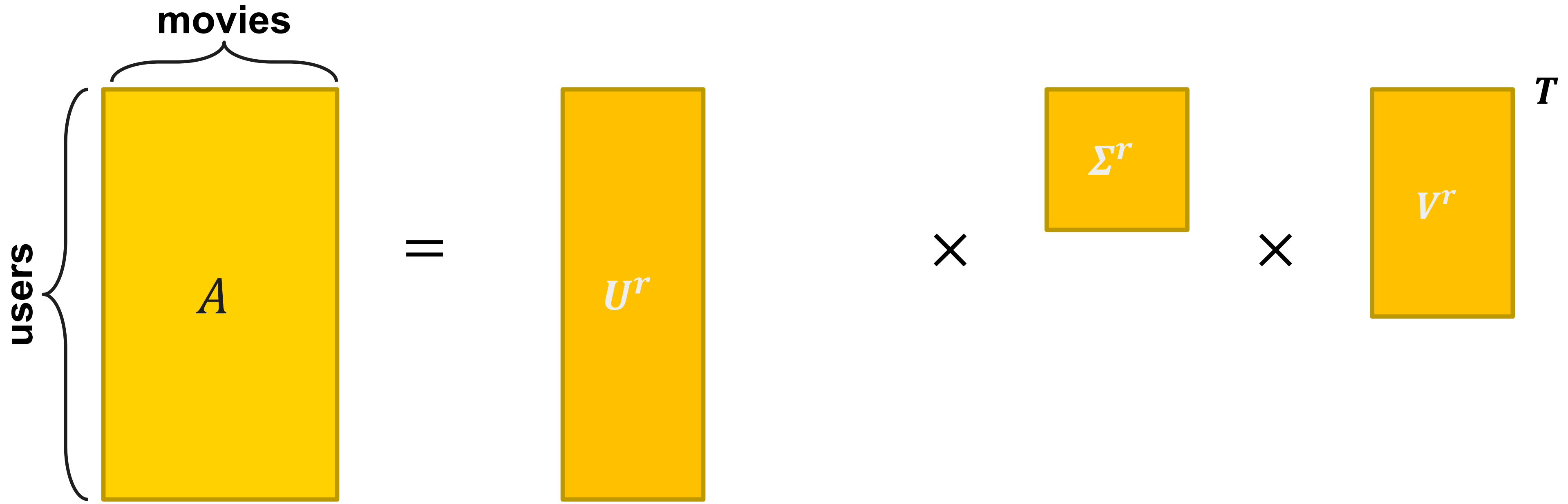

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Reduced SVD: Main Idea

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

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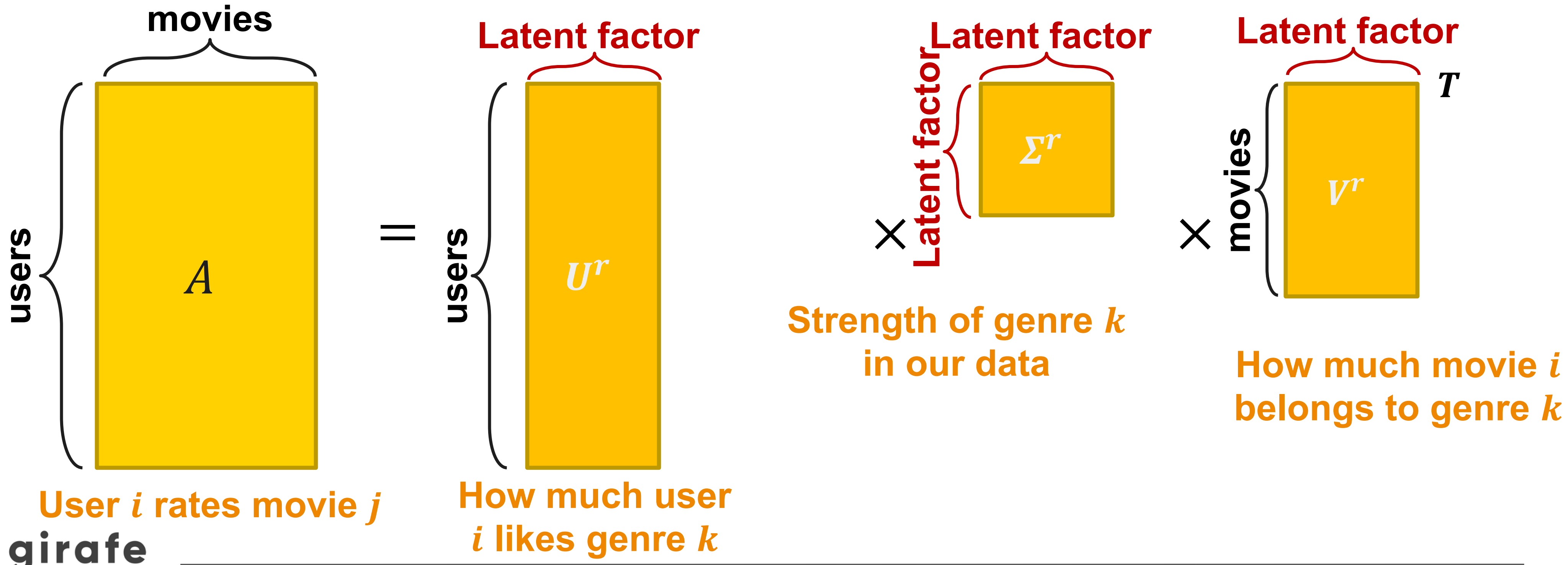

SVD: Dimensionality Reduction

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

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