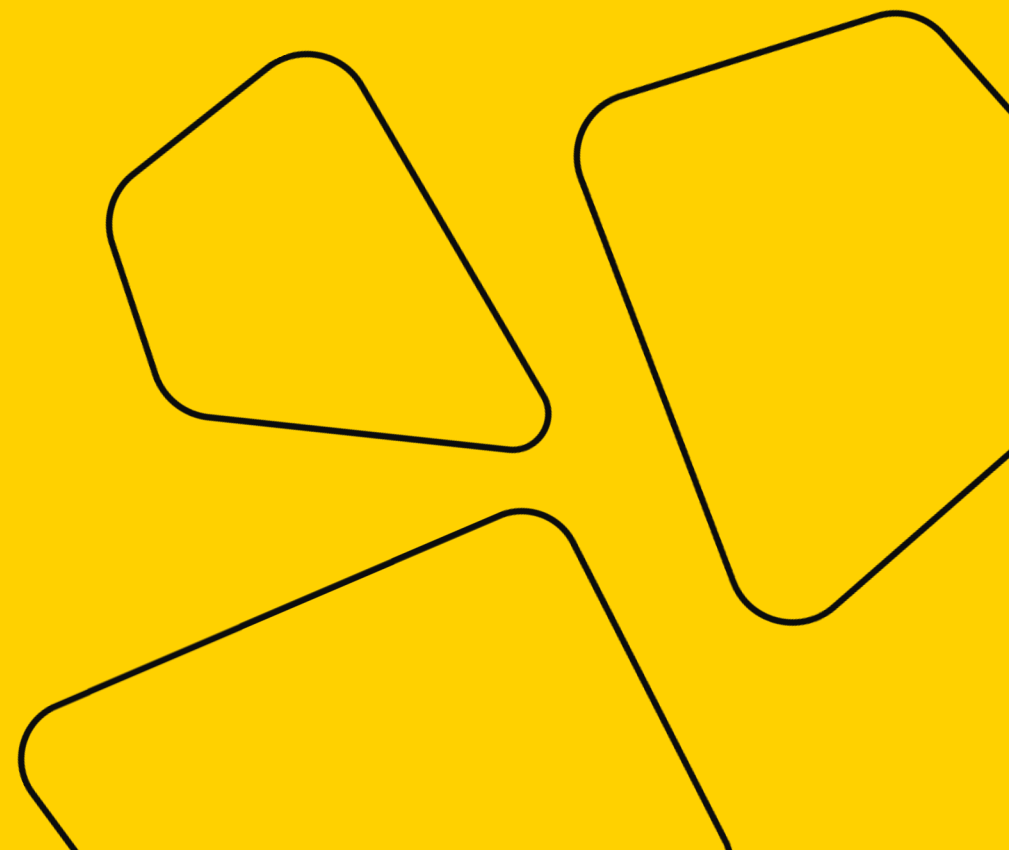




Math Refresher for DS

Practical Session 6



Plan for Today

- Logistics
- Short Quiz
- PCA: final overview
- Intro to SVD



Logistics for Next Weeks

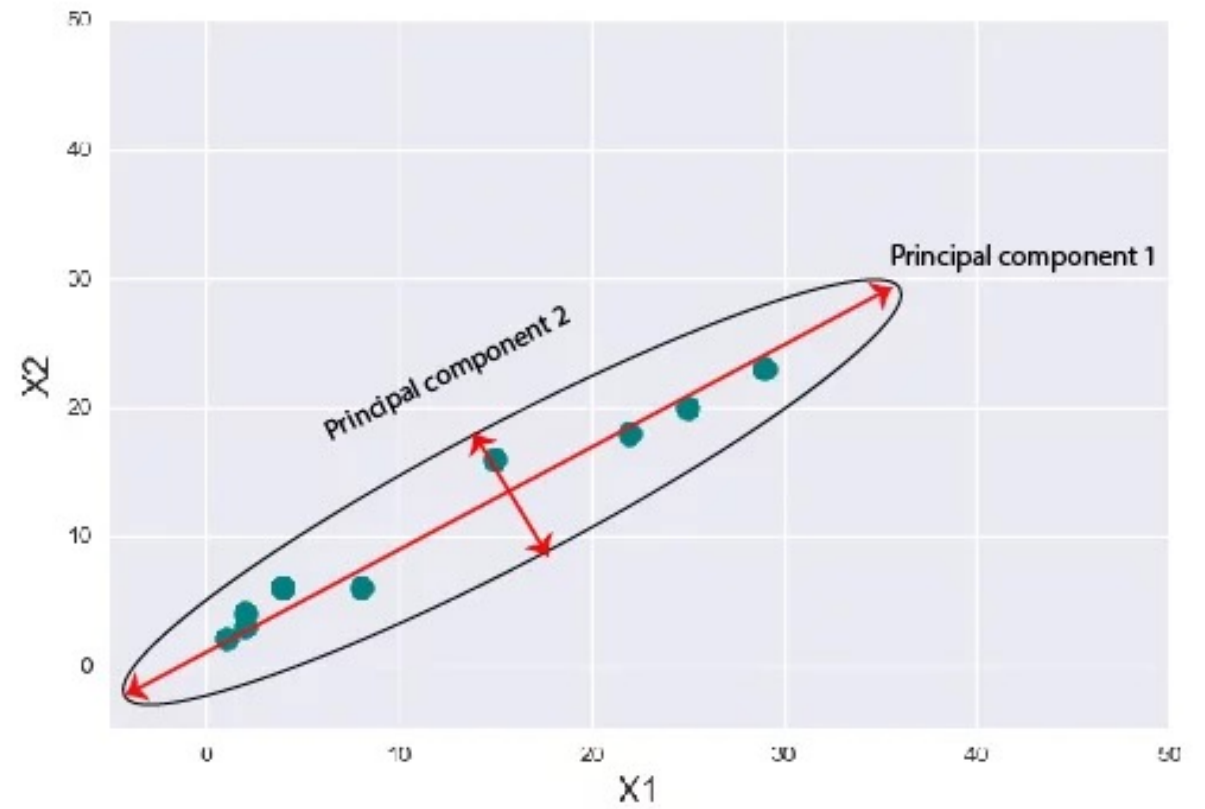
- No class on Wednesday
- Tomorrow:
 - Submission deadline Graded Assignment 2
 - Graded Assignment 3 will be out
- Next Monday: starting Calculus
- Single final exam (still 2 parts)



Short Quiz

<https://forms.gle/ohsrDkAJPCwDTZGaA>

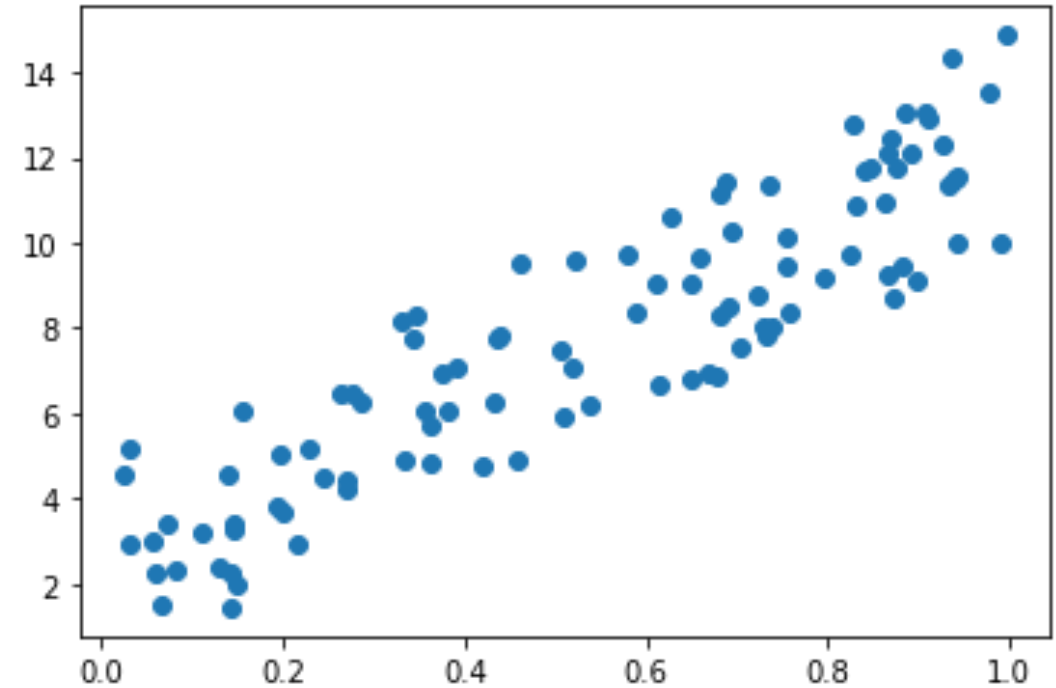
PCA STEP-BY- STEP



PCA STEP 1: COLLECT THE DATA

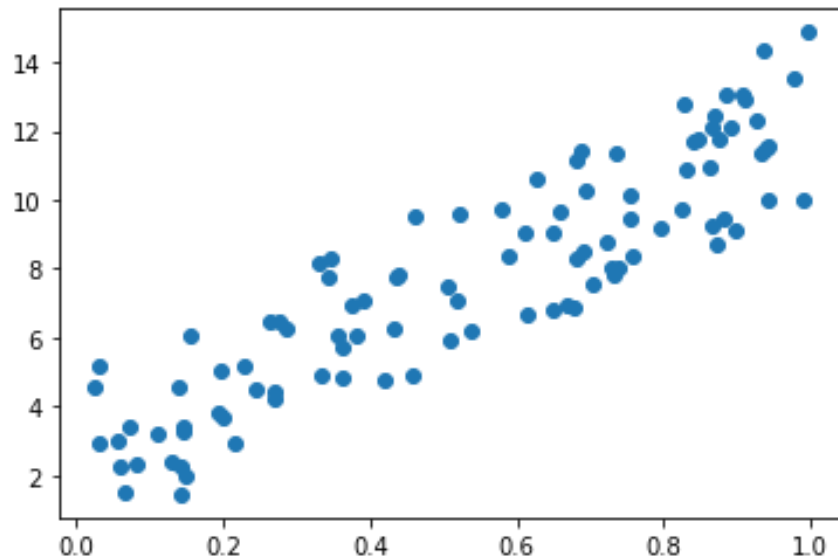


- X – $m \times n$ matrix.
 m features, n examples.
- Columns = examples,
rows = features.
- Each example = a point
in an m –dimensional space.



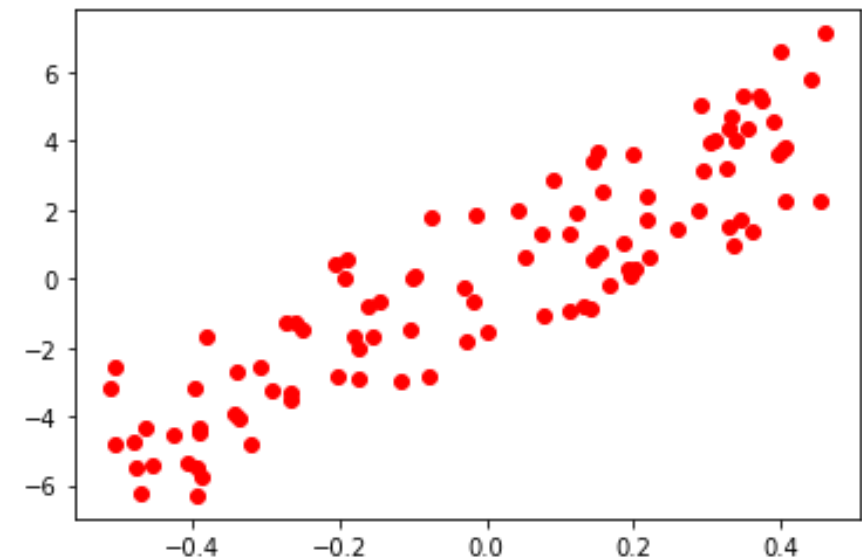
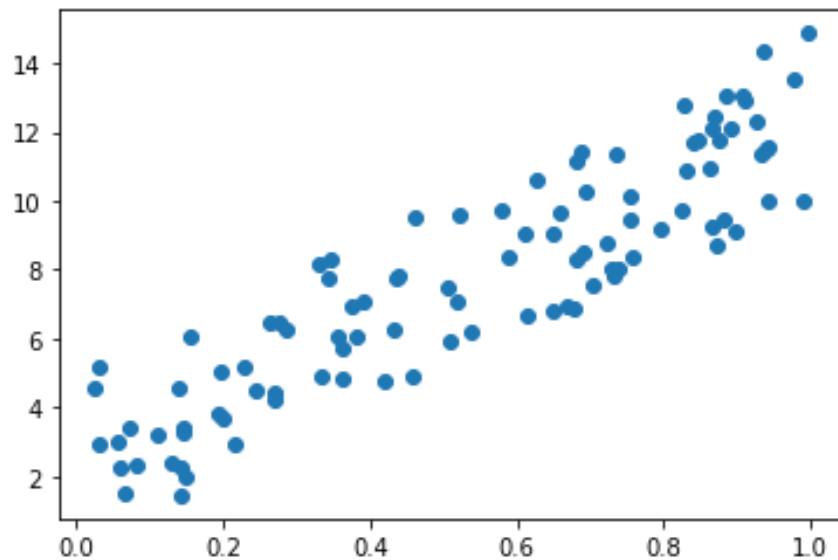
PCA STEP 2: CENTER THE DATA

- (This is needed to construct the covariance matrix)
- From each feature (*row*), subtract its mean.



PCA STEP 2: CENTER THE DATA

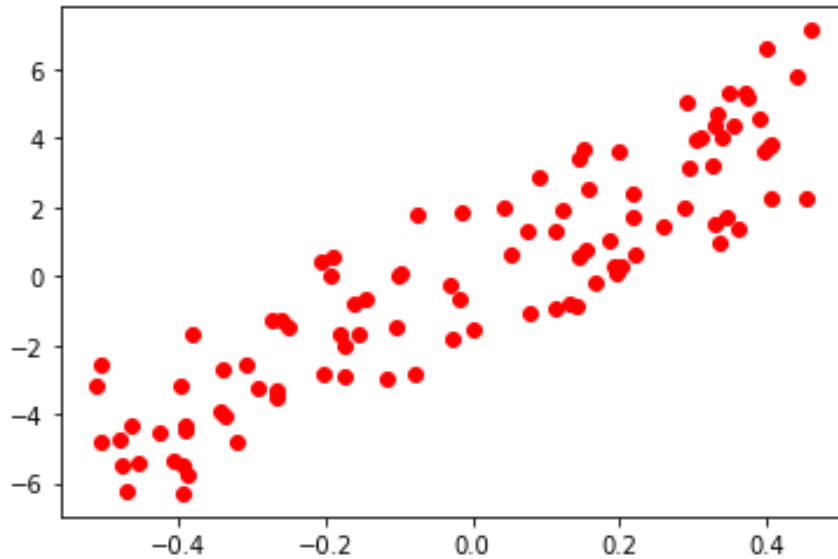
- (This is needed to construct the covariance matrix)
- From each feature (*row*), subtract its mean.



PCA STEP 3: BUILD COVARIANCE MATRIX S

- Sample covariance matrix with centered X :

$$S = \frac{1}{n-1}XX^t - n \times n \text{ matrix.}$$

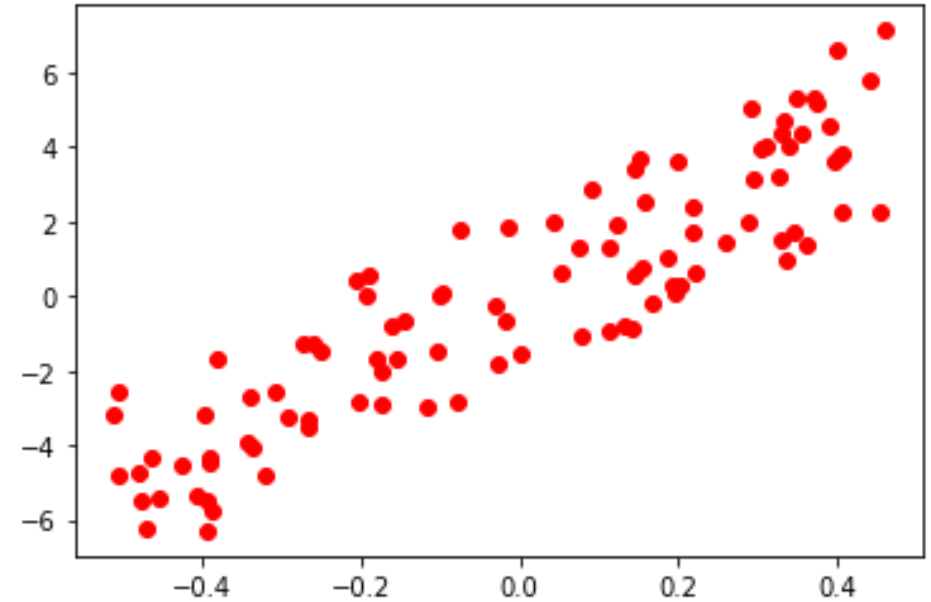


```
(1./(n-1))*np.matmul(X_centered, X_centered.transpose())  
  
array([[ 0.08830318,  0.88570231],  
       [ 0.88570231, 10.93980675]])
```

PCA STEP 4: DECOMPOSE S

- S is a symmetric matrix, so it has an eigendecomposition:

$$S = V\Lambda V^T$$



PCA STEP 4: DECOMPOSE S

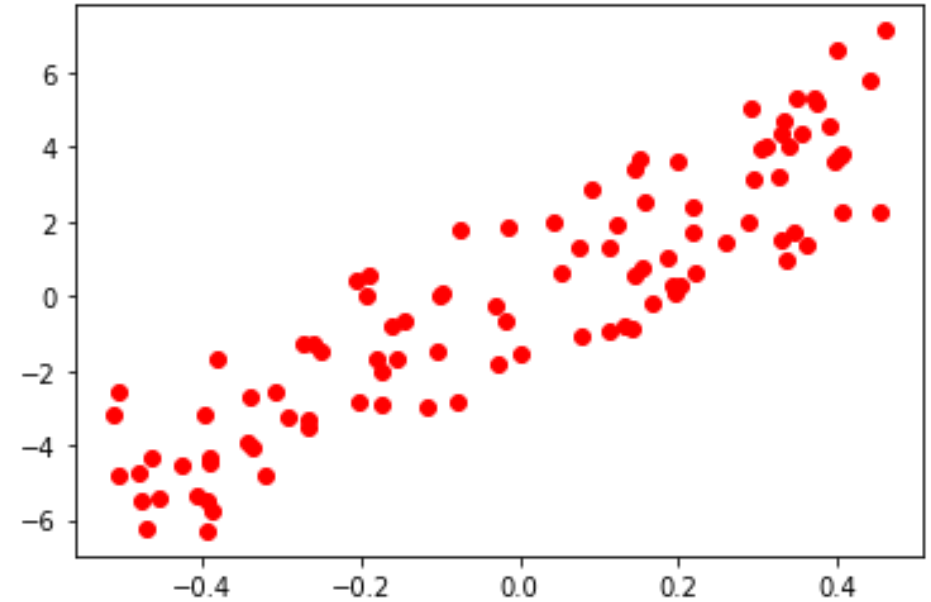
- S is a symmetric matrix, so it has an eigendecomposition:

$$S = V\Lambda V^T$$

- Eigenvalues of S (ordered from large to small):

```
l, V = np.linalg.eig(S)
ind = np.argsort(l)[::-1]
l[ind]

array([11.0116227 ,  0.01648723])
```



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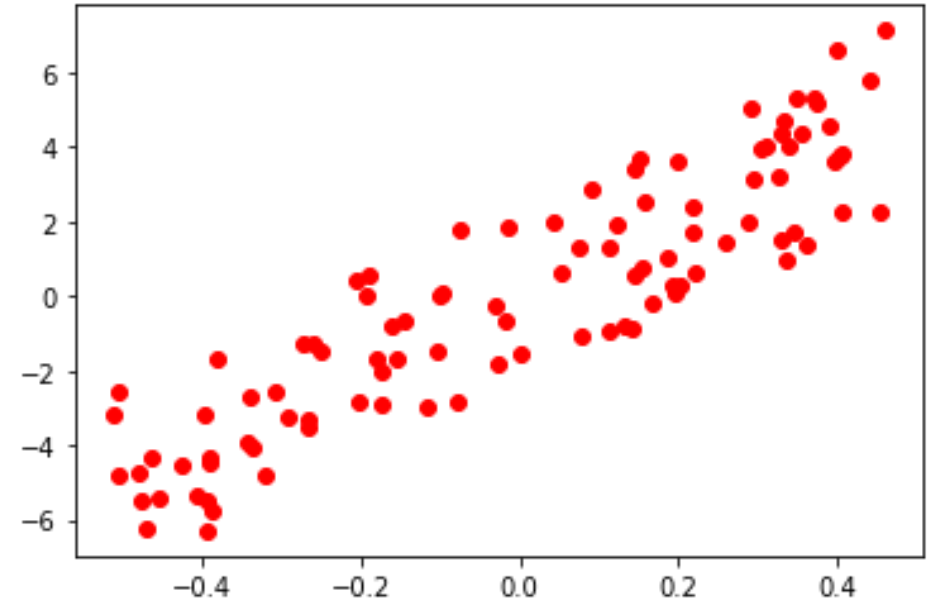
```
l, V = np.linalg.eig(S)
ind = np.argsort(l)[::-1]
l[ind]

array([11.0116227 ,  0.01648723])
```

- Corresponding eigenvectors of S
(= principal components of the data):

```
V[:,ind]

array([[ -0.08081839, -0.99672884],
       [-0.99672884,  0.08081839]])
```



PCA STEP 5: PROJECT THE DATA

- Let's project the data onto the first principal component.
- We know orthogonal projections from the first lecture!

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Projecting a single example (= one column):

$$x_{v_1} =$$

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Projecting a single example (= one column):

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Projecting the whole data matrix (= all columns):

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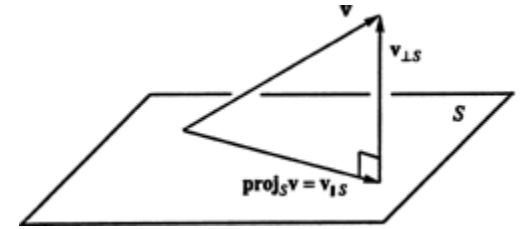
$$x_{v_1} = \frac{(x, v_1)}{(v_1, v_1)} v_1 = (x, v_1) \cdot v_1$$

Projecting the whole data matrix (= all columns):

$$X_{v_1} = v_1^T X$$

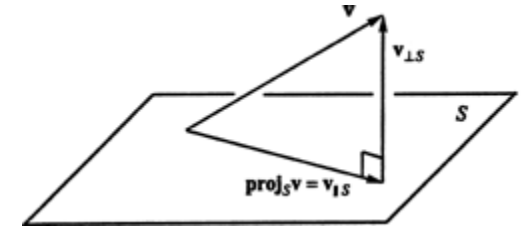
PCA STEP 5: PROJECT THE DATA

- Let's project the data onto p principal components.
- How to project onto a subspace spanned by these p principal components (= its orthonormal basis)?



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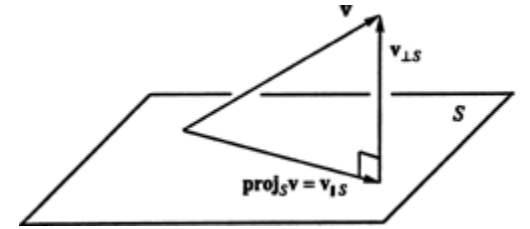
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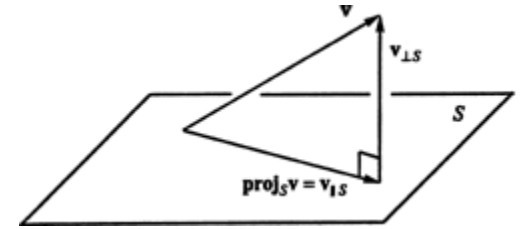
Projecting one example (= a single column):

$$x_{proj} = [(x, v_1), (x, v_2), \dots, (x, v_p)]^T = V_p^T x$$

Projecting the whole data (= every column):

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Projecting one example (= a single column):

$$x_{proj} = [(x, v_1), (x, v_2), \dots, (x, v_p)]^T = V_p^T x$$

Projecting the whole data (= every column):

$$X_{proj} = V_p^T X, \quad X_{proj} - p \times n \text{ matrix.}$$

Singular Values and Singular Vectors



Reminder: Eigendecomposition

- Consider an $n \times n$ symmetric matrix A .
- Eigendecomposition of A :

$$A_{n \times n} = V_{n \times n} \Lambda_{n \times n} V_{n \times n}^T$$

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:

$$Av = \lambda v$$



Singular Values and Singular Vectors

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$$Av = \lambda v$$

- For non-square matrices:

u, v – unit vectors, $\sigma > 0$ – some number such that

$$Av = \sigma u, \quad A^T u = \sigma v$$

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

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

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

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

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$m - n$ zero rows

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$n - m$ zero columns

$m - n$ zero rows

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

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

$m - n$ zero rows $n - m$ zero columns

SVD: Main Ingredients

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

$$U = [u_1 \mid \dots \mid u_m] - \text{eigenvectors of } AA^T,$$

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

$\sigma_1^2, \dots, \sigma_r^2$ – corresponding non-zero eigenvalues of $A^T A$ / 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

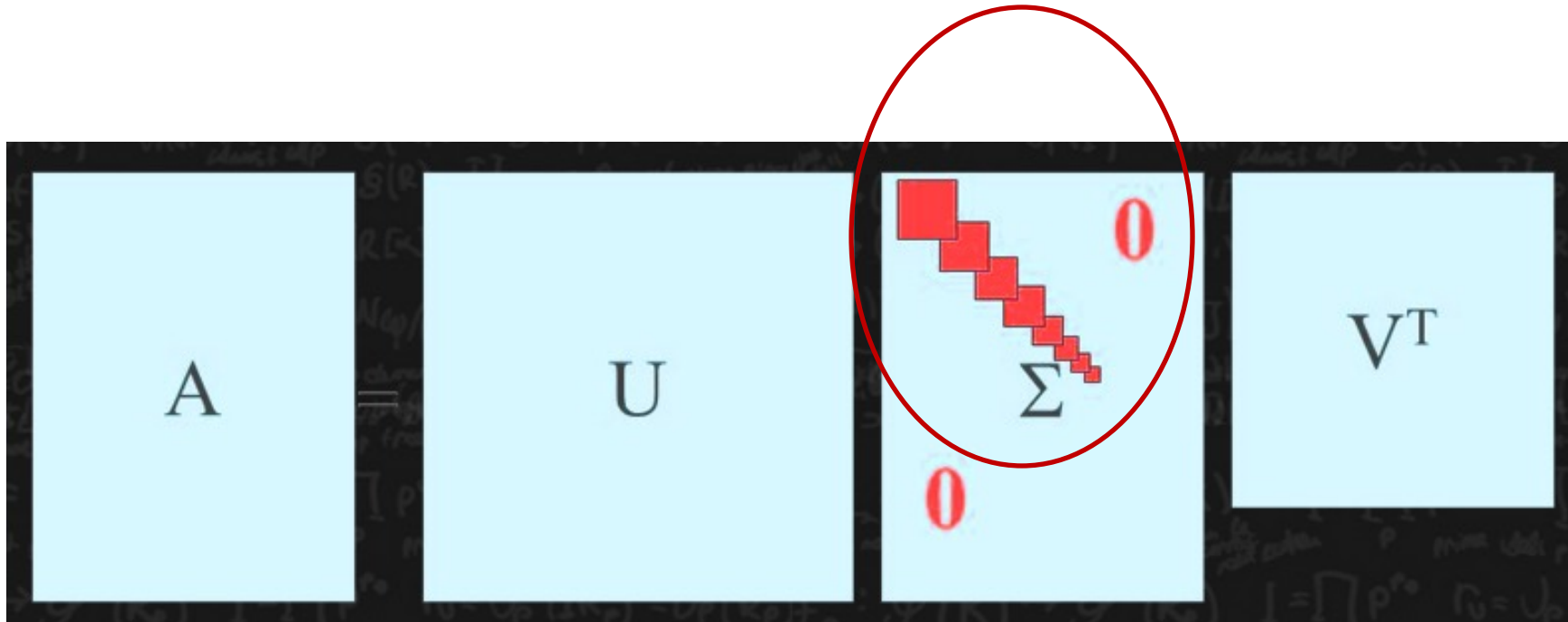
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$m - n$ zero rows

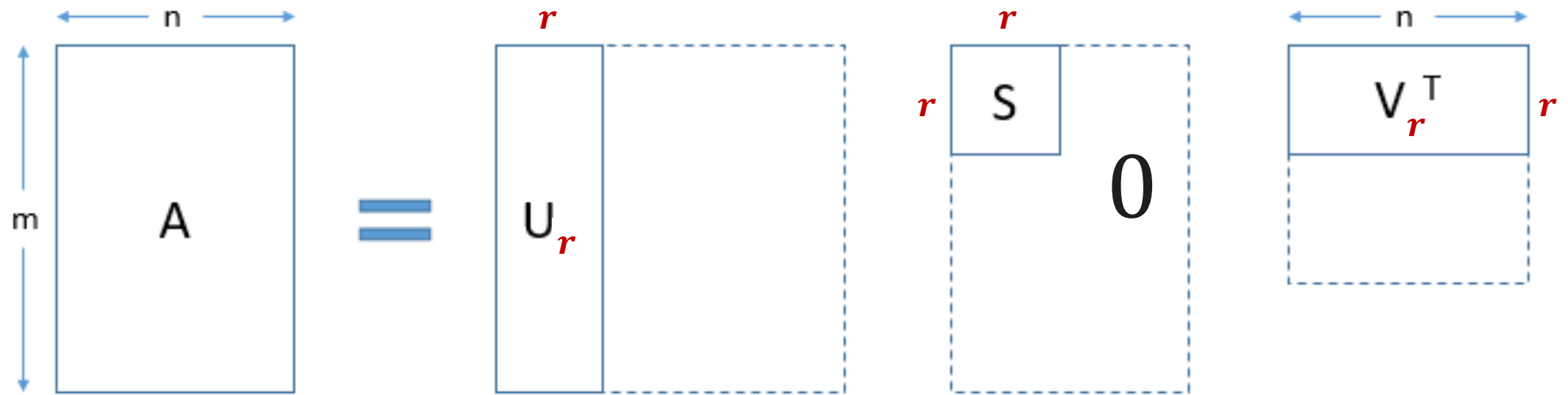
$n - m$ zero columns

Full SVD

Only r non-zero diagonal elements!



Reduced SVD



Reduced SVD

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

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

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

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

$\Sigma_{r \times r}$ – 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 $A^T A$*

$$Av_i = \sigma_i u_i$$

Singular Values: Example

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

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



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

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



Example

- Let's find SVD and reduced SVD of

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

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

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

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

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

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

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.

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

Example

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

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Example

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Remember: $Av_i = \sigma_i u_i$

Example

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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

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

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

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

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

Example

- Let's find SVD and reduced SVD of

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

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

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

Example

- SVD of

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

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

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

From SVD to Reduced SVD

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

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

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

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

Reduced SVD:

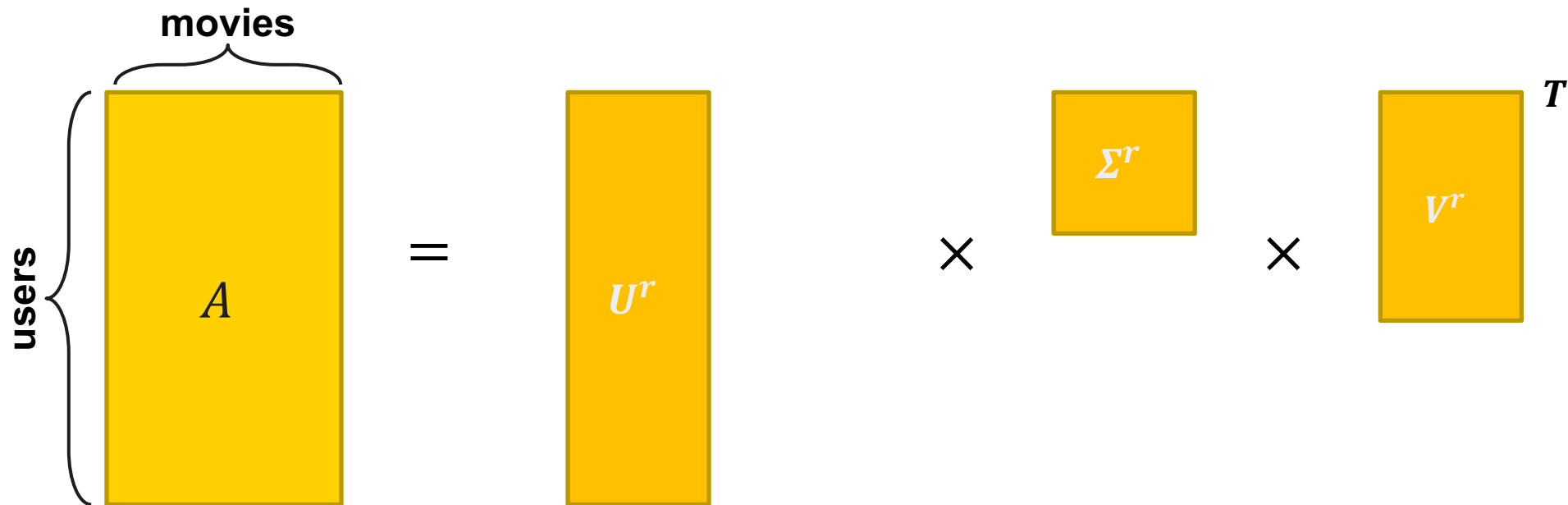
$$A = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \cdot \begin{pmatrix} 5 & 0 \\ 0 & 3 \end{pmatrix} \cdot \begin{pmatrix} 1/\sqrt{2} & 1/3\sqrt{2} \\ -1/\sqrt{2} & -1/3\sqrt{2} \\ 0 & 4/3\sqrt{2} \end{pmatrix}^T$$

Reduced SVD: Main Idea

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

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

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



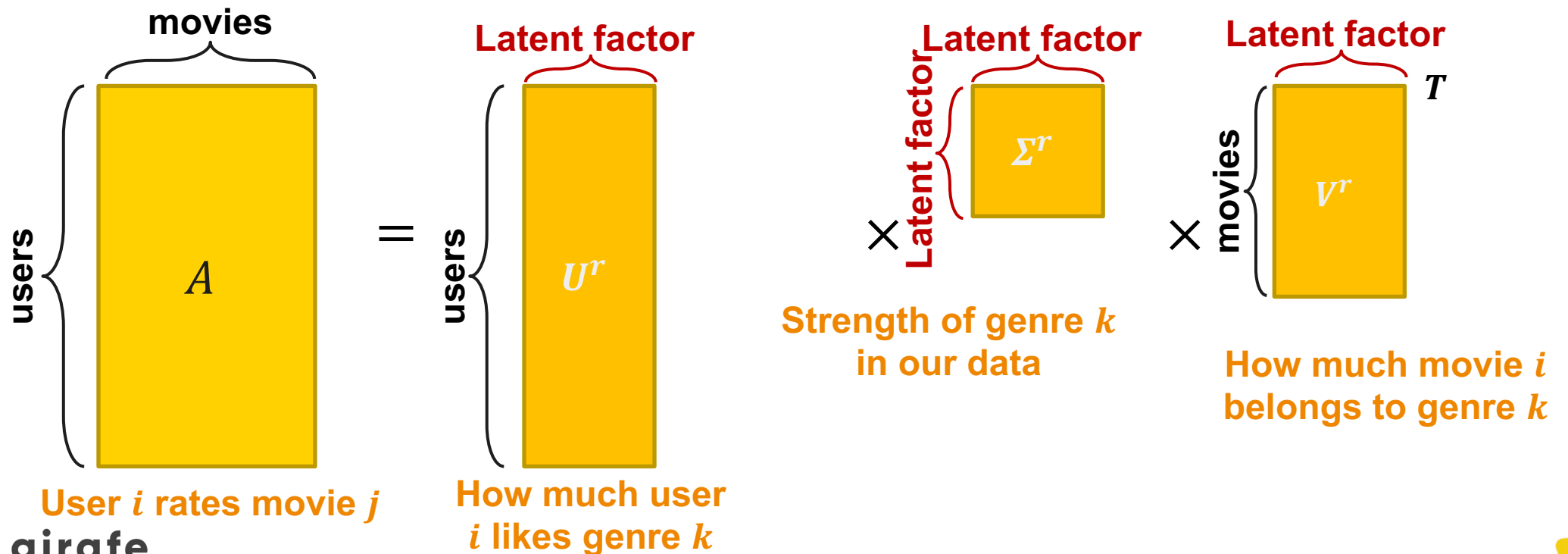
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Reduced SVD: Main Idea

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

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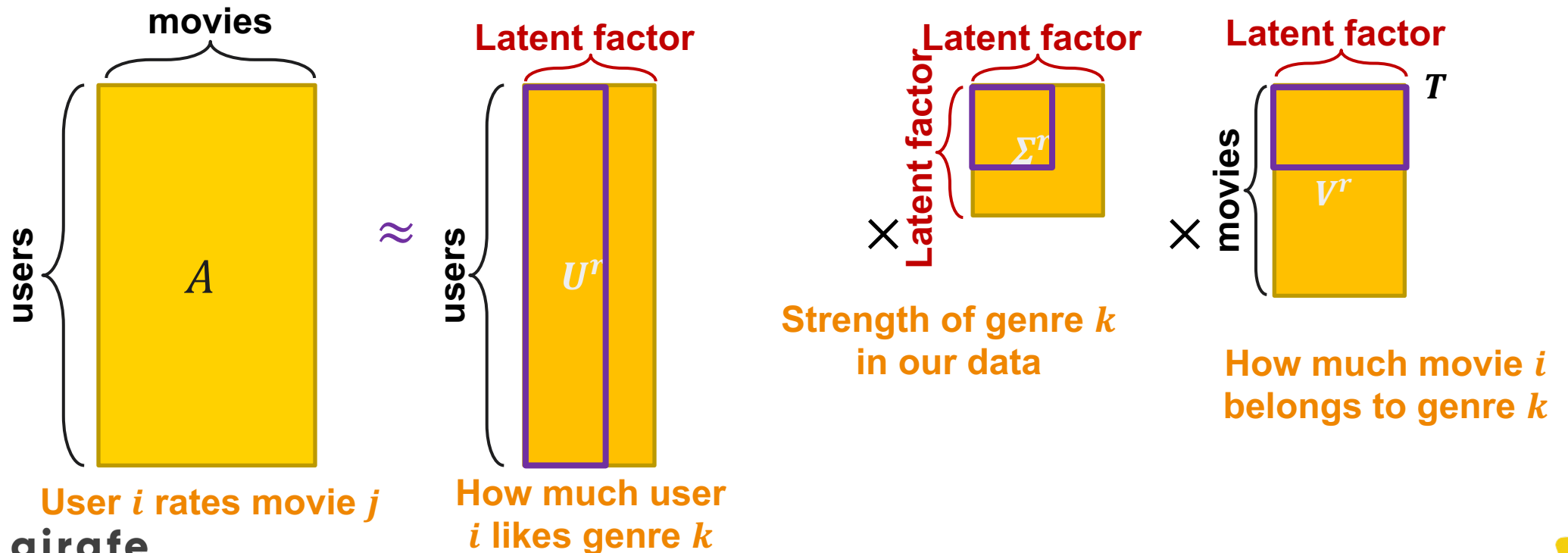


SVD: Dimensionality Reduction

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

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

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



Practice!

<https://colab.research.google.com/drive/1faLfFmMHZbxtpzgZxxT6MCBuy57CE7Po?usp=sharing>