EE16B, Spring 2018
UC Berkeley EECS

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Lectures 8A, 8B & 9A: Overview Slides

Data Analysis

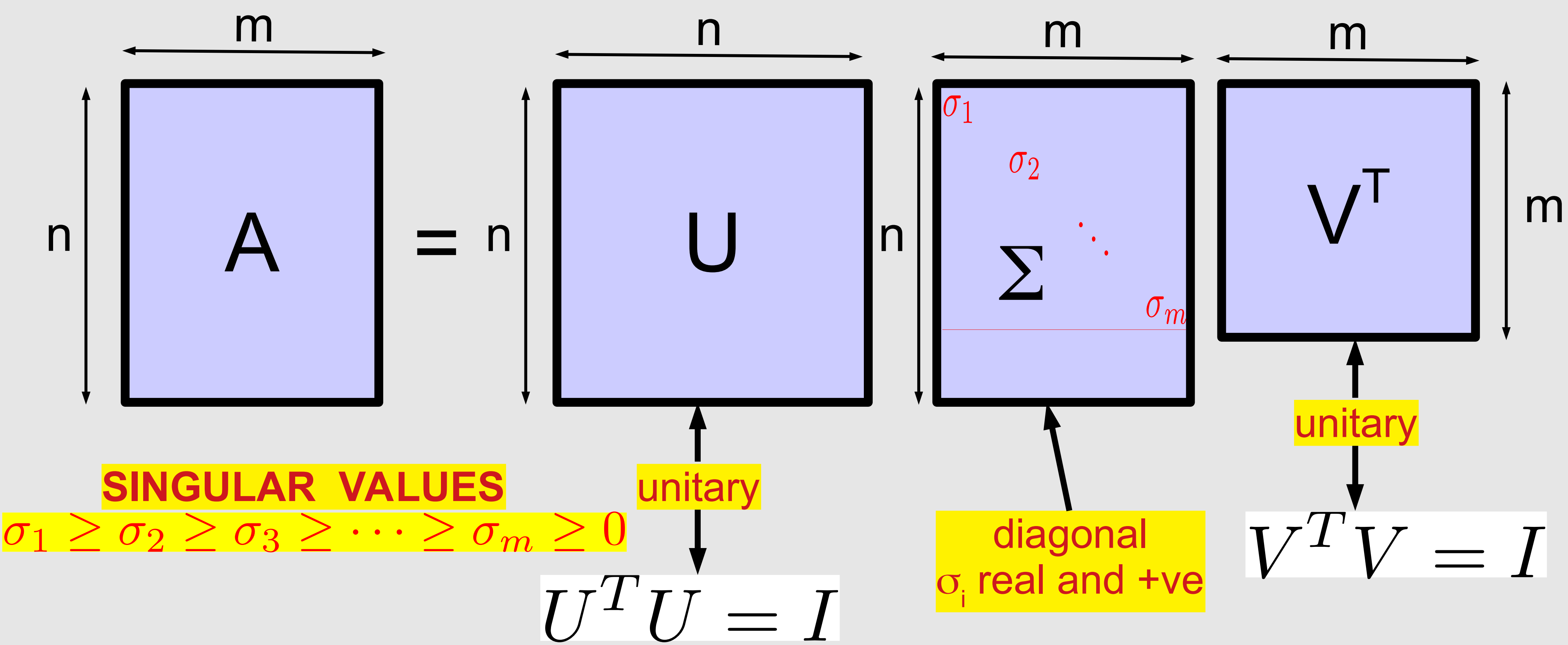
Singular Value Decomposition
and
Principal Component Analysis

The SVD
(Singular Value Decomposition)

Singular Value Decomposition

- Looks like eigendecomposition, **but is different**
  - **Any matrix A** (no exceptions) can be decomposed as

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



Unitary Matrices: Orthonormality

$$\underbrace{\begin{bmatrix} \longleftarrow & \vec{u}_1^T & \longrightarrow \\ \longleftarrow & \vec{u}_2^T & \longrightarrow \\ \longleftarrow & \vec{u}_3^T & \longrightarrow \\ & \vdots & \\ \longleftarrow & \vec{u}_n^T & \longrightarrow \end{bmatrix}}_{\mathrm{U^T}} \underbrace{\begin{bmatrix} \uparrow & \uparrow & \uparrow & & \uparrow \\ \vec{u}_1 & \vec{u}_2 & \vec{u}_3 & \cdots & \vec{u}_n \\ \downarrow & \downarrow & \downarrow & & \downarrow \end{bmatrix}}_{\mathrm{U}} = \underbrace{\begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix}}_{\mathrm{I}}$$

$$\begin{matrix} \vec{u}_1^T\vec{u}_1 = 1 & \vec{u}_1^T\vec{u}_2 = 0 & \vec{u}_1^T\vec{u}_3 = 0 & \cdots & \vec{u}_1^T\vec{u}_n = 0 \\ \vec{u}_2^T\vec{u}_1 = 0 & \vec{u}_2^T\vec{u}_2 = 1 & \vec{u}_3^T\vec{u}_3 = 0 & \cdots & \vec{u}_2^T\vec{u}_n = 0 \\ & \vdots & & \vdots & \\ \vec{u}_n^T\vec{u}_1 = 0 & \vec{u}_n^T\vec{u}_2 = 0 & \vec{u}_n^T\vec{u}_3 = 0 & \cdots & \vec{u}_n^T\vec{u}_n = 1 \end{matrix}$$

$\vec{u}_1, \vec{u}_2, \cdots, \vec{u}_n$
called **ORTHONORMAL**

$$\vec{u}_i^T\vec{u}_j = \begin{cases} 1, & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

$\|\vec{u}_i\| = 1$

Similarly,
$\vec{v}_1, \vec{v}_2, \cdots, \vec{v}_m$
are **ORTHONORMAL**

$\|\vec{v}_j\| = 1$

Rank 1 Matrices and Outer Products

- Consider $\underbrace{A = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 3 & 3 & 3 & 3 & 3 \\ 2 & 2 & 2 & 2 & 2 \end{bmatrix}}_{\text{rank=1}} = \underbrace{\begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix}}_{\text{col}} \underbrace{\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \end{bmatrix}}_{\text{row}}$
  - rank-1 matrix can be written as $\vec{x}\vec{y}^T$: an **outer product**
- outer product: product of col and row vectors
  - $\begin{bmatrix} x \\ y \\ z \end{bmatrix} \begin{bmatrix} a & b & c & d & e \end{bmatrix} = \underbrace{\begin{bmatrix} xa & xb & xc & xd & xe \\ ya & yb & yc & yd & ye \\ za & zb & zc & zd & ze \end{bmatrix}}_{\text{rank=1}}$
- rank-1: a very "simple" type of matrix
  - its "data" can be "compressed" very easily
    - can be written as outer product: $\underbrace{A}_{\substack{n\times m \\ \text{nm numbers}}} = \underbrace{\underbrace{\vec{x}}_{n\times 1} \underbrace{\vec{y}^T}_{1\times m}}_{\text{n+m numbers}}$

n+m << nm: **data compression**

Where We Were Before

SVDs

the decomposition
unitary matrices and orthonormal sets of vectors
rank-1 matrices as outer products

TODAY

SVDs for identifying features of images
SVDs for identifying features of general data
start Principal Component analysis

Matrix Multiplication using Outer Products

$$X = \begin{bmatrix} \uparrow & \uparrow & \uparrow & & \uparrow \\ \vec{x}_1 & \vec{x}_2 & \vec{x}_3 & \cdots & \vec{x}_n \\ \downarrow & \downarrow & \downarrow & & \downarrow \end{bmatrix} \quad Y^T = \begin{bmatrix} \longleftarrow & \vec{y}_1^T & \longrightarrow \\ \longleftarrow & \vec{y}_2^T & \longrightarrow \\ \longleftarrow & \vec{y}_3^T & \longrightarrow \\ & \vdots & \\ \longleftarrow & \vec{y}_n^T & \longrightarrow \end{bmatrix}$$

each of these is a rank-1 OUTER PRODUCT

$$= \vec{x}_1\vec{y}_1^T + \vec{x}_2\vec{y}_2^T + \vec{x}_3\vec{y}_3^T + \cdots + \vec{x}_n\vec{y}_n^T$$

- Example:

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} x & y & z \\ p & q & r \end{bmatrix} = \begin{bmatrix} ax+bp & ay+bq & az+br \\ cx+dp & cy+dq & cz+dr \end{bmatrix}$$

$$\begin{bmatrix} a \\ c \end{bmatrix} \begin{bmatrix} x & y & z \end{bmatrix} = \begin{bmatrix} ax & ay & az \\ cx & cy & cz \end{bmatrix}$$

$$\begin{bmatrix} b \\ d \end{bmatrix} \begin{bmatrix} p & q & r \end{bmatrix} = \begin{bmatrix} bp & bq & br \\ dp & dq & dr \end{bmatrix}$$

$$\boxed{\begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} x & y & z \\ p & q & r \end{bmatrix} = \begin{bmatrix} a \\ c \end{bmatrix} \begin{bmatrix} x & y & z \end{bmatrix} + \begin{bmatrix} b \\ d \end{bmatrix} \begin{bmatrix} p & q & r \end{bmatrix}}$$

SVD: Sum of Outer Products Form

$$A = \underbrace{\begin{bmatrix} \uparrow & \uparrow & \uparrow & & \uparrow \\ \vec{u}_1 & \vec{u}_2 & \vec{u}_3 & \cdots & \vec{u}_n \\ \downarrow & \downarrow & \downarrow & & \downarrow \end{bmatrix}}_{U} \underbrace{\begin{bmatrix} \sigma_1 & & & & \\ & \sigma_2 & & & \\ & & \sigma_3 & & \\ & & & \ddots & \\ & & & & \sigma_m \end{bmatrix}}_{\Sigma} \underbrace{\begin{bmatrix} \longleftarrow & \vec{v}_1^T & \longrightarrow \\ \longleftarrow & \vec{v}_2^T & \longrightarrow \\ & \vdots & \\ \longleftarrow & \vec{v}_m^T & \longrightarrow \end{bmatrix}}_{V^T}$$

biggest weight

next biggest weight

smallest weight

$$= \sigma_1 \begin{bmatrix} \uparrow \\ \vec{u}_1 \\ \downarrow \end{bmatrix} \begin{bmatrix} \longleftarrow & \vec{v}_1^T & \longrightarrow \end{bmatrix} + \sigma_2 \begin{bmatrix} \uparrow \\ \vec{u}_2 \\ \downarrow \end{bmatrix} \begin{bmatrix} \longleftarrow & \vec{v}_2^T & \longrightarrow \end{bmatrix} + \ldots + \sigma_m \begin{bmatrix} \uparrow \\ \vec{u}_m \\ \downarrow \end{bmatrix} \begin{bmatrix} \longleftarrow & \vec{v}_m^T & \longrightarrow \end{bmatrix}$$

outer product nxm rank-1 matrix $\vec{u}_1\vec{v}_1^T$

outer product nxm rank-1 matrix $\vec{u}_2\vec{v}_2^T$

outer product nxm rank-1 matrix $\vec{u}_m\vec{v}_m^T$

Frobenius norm (sqrt(sum of squares) = 1)

SVD splits a matrix into a **weighted sum of rank-1 matrices of norm 1**

Using the SVD for Image Analysis and Compression

Example: B&W Polish Flag as a Matrix

- size: 281x450

A =

original: 3.2MB

rank=1: 58kB

$$\sigma_1 \begin{bmatrix} \uparrow \\ \vec{u}_1 \\ \downarrow \end{bmatrix} \begin{bmatrix} \longleftarrow & \vec{v}_1^T & \longrightarrow \end{bmatrix}$$

6.75x10^4

$$\sigma_2 \simeq 10^{-10}$$

$$\begin{bmatrix} 1 \\ \vdots \\ 1 \\ 0.2 \\ \vdots \\ 0.2 \end{bmatrix}$$

$$\begin{bmatrix} 1 & \cdots & 1 \end{bmatrix}$$

(actual values are normalized)

(actual values are normalized)

This is a RANK-1 FLAG

Example: Polish Flag as a Matrix

- size: 281x450 (x 3 colours: R, G, B)

A = 

original: 10MB

rank 1: 17.5kB

$$\sigma_1 \begin{bmatrix}\uparrow\\ \vec{u}_1\\ \downarrow\end{bmatrix}\begin{bmatrix}\longleftarrow & \vec{v}_1^T & \longrightarrow\end{bmatrix}$$

(8.5,6.4,6.6)x10^4

$$\begin{bmatrix}1,1,1\\ \vdots\\ 1,1,1\\ 1,0,0\\ \vdots\\ 1,0,0\end{bmatrix} \qquad \begin{bmatrix}1,1,1 & \cdots & 1,1,1\end{bmatrix}$$

RGB components
(actual ones are normalized)

RGB components
(actual ones are normalized)

$\sigma_2 \simeq 10^{-10}$ for R, G, B

This is a RANK-1 FLAG

Example: SVD of the Austrian Flag

- size: 281x450 (x 3 colours: R, G, B)

A =

original: 73MB

rank 1: 48.5kB

$$\sigma_1 \begin{bmatrix} \uparrow \\ \vec{u}_1 \\ \downarrow \end{bmatrix} \begin{bmatrix} \longleftarrow & \vec{v}_1^T & \longrightarrow \end{bmatrix}$$

2.3x10^5

$$\vec{u}_1 = \begin{bmatrix} 1,0,0 \\ \vdots \\ 1,0,0 \\ 1,1,1 \\ \vdots \\ 1,1,1 \\ 1,0,0 \\ \vdots \\ 1,0,0 \end{bmatrix} \qquad \vec{v}_1^T = \begin{bmatrix} 1,1,1 & \cdots & 1,1,1 \end{bmatrix}$$

RGB components
(actual ones are normalized)

RGB components
(actual ones are normalized)

This is ALSO a RANK-1 FLAG

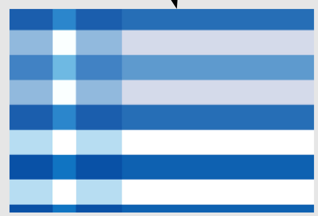
$\sum_{i=1}^{3} \sigma_i \vec{u}_i \vec{v}_i^T$

Example: SVD of the Greek Flag

- size: 295x450 (x 3 colours: R, G, B)

original: 10.1MB

strongest "feature"



rank 1: 18kb

$\sigma_1 \vec{u}_1 \vec{v}_1^T$

2nd strongest "feature"

$\sigma_2 \vec{u}_2 \vec{v}_2^T$

3rd strongest "feature"

$\sigma_3 \vec{u}_3 \vec{v}_3^T$

rank 3: 54kb

$\sum_{i=1}^{3} \sigma_i \vec{u}_i \vec{v}_i^T$

rank 2: 36kB

$\sigma_1 \vec{u}_1 \vec{v}_1^T +$
$\sigma_2 \vec{u}_2 \vec{v}_2^T$

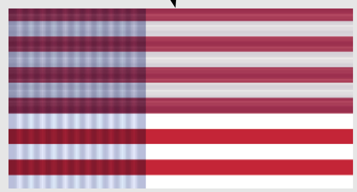
This is a RANK-3 FLAG

Example: SVD of the US Flag

- size: 450x237 (x 3 colours: R, G, B)

original: 8.8MB

strongest **"feature"**



$\sigma_1 \vec{u}_1 \vec{v}_1^T$

$\sum_{i=1}^{5} \sigma_i \vec{u}_i \vec{v}_i^T$

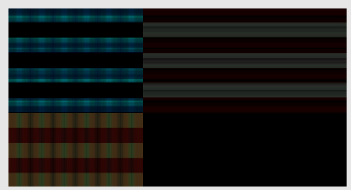
rank 5: 83kB

$\sum_{i=1}^{10} \sigma_i \vec{u}_i \vec{v}_i^T$

rank 10: 167kB

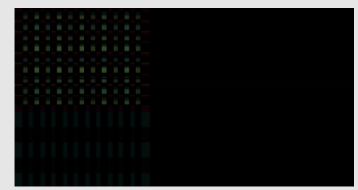
$\sum_{i=1}^{15} \sigma_i \vec{u}_i \vec{v}_i^T$

rank 15: 253kB

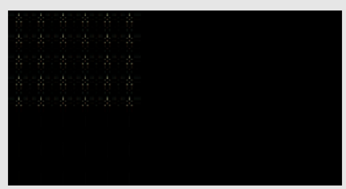


$\sigma_2 \vec{u}_2 \vec{v}_2^T$ 16.5kb

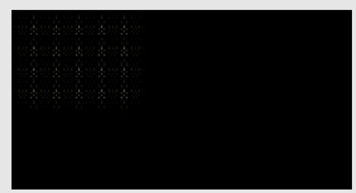
$\sigma_3 \vec{u}_3 \vec{v}_3^T$ 16.5kB



$\sigma_4 \vec{u}_4 \vec{v}_4^T$ 16.5kB



$\sigma_5 \vec{u}_5 \vec{v}_5^T$ 16.5kb



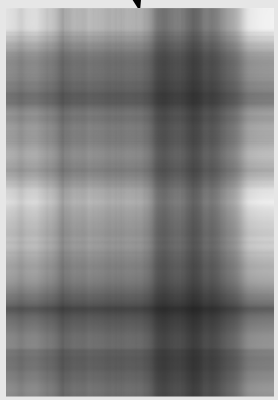
$\sigma_6 \vec{u}_6 \vec{v}_6^T$ 16.5kb

Example: SVD of Michel Maharbiz

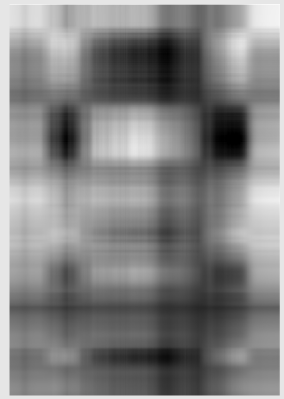
- size: 1100x757 (grayscale)

original

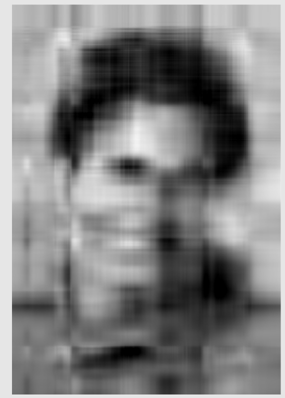
strongest **“feature” ?!**



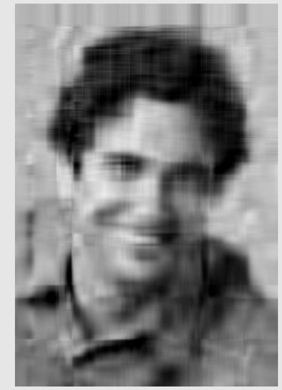
$\sigma_1\vec{u}_1\vec{v}_1^T$ 15kB



$\sum_{i=1}^{2}\sigma_i\vec{u}_i\vec{v}_i^T$



$\sum_{i=1}^{5}\sigma_i\vec{u}_i\vec{v}_i^T$



$\sum_{i=1}^{10}\sigma_i\vec{u}_i\vec{v}_i^T$

$\sum_{i=1}^{300}\sigma_i\vec{u}_i\vec{v}_i^T$

$\sum_{i=1}^{20}\sigma_i\vec{u}_i\vec{v}_i^T$

$\sum_{i=1}^{50}\sigma_i\vec{u}_i\vec{v}_i^T$

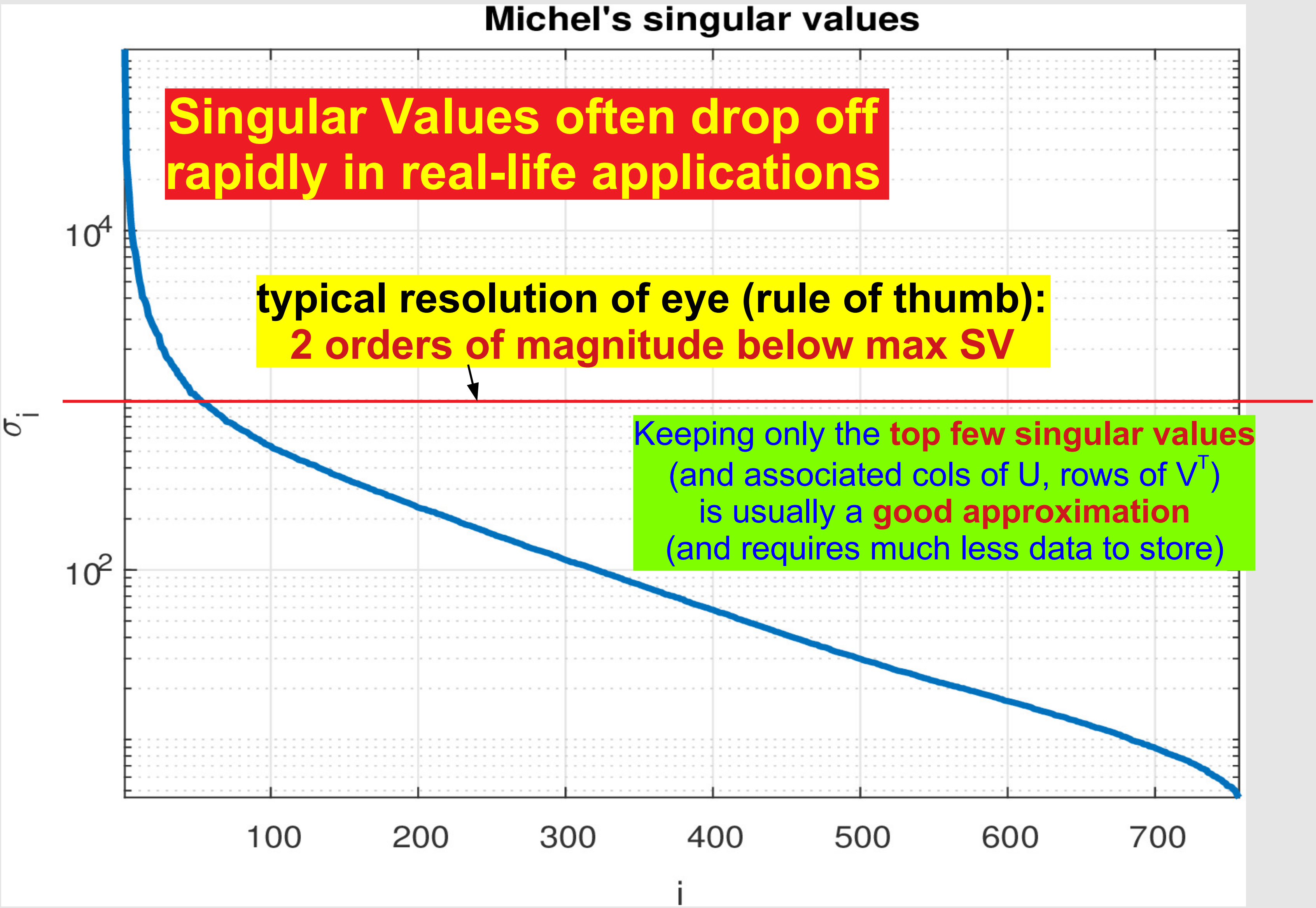
$\sum_{i=1}^{100}\sigma_i\vec{u}_i\vec{v}_i^T$

$\sum_{i=1}^{200}\sigma_i\vec{u}_i\vec{v}_i^T$

Features not always intuitive

Michel's Singular Values

- How Michel's singular values drop off



Geometric View of Orthogonality

Projection onto Orthonormal Bases

Geometric View of Unitary Operations

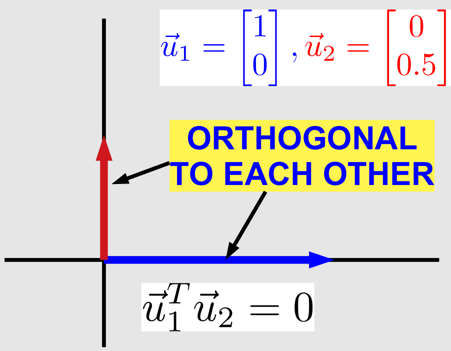
Geometric View of Orthogonality

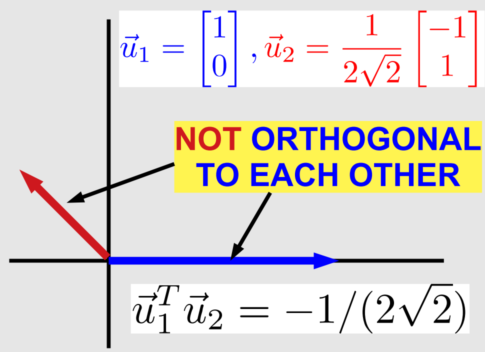
- recall: $$\vec{u}_i^T \vec{u}_j = \begin{cases} 1, & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

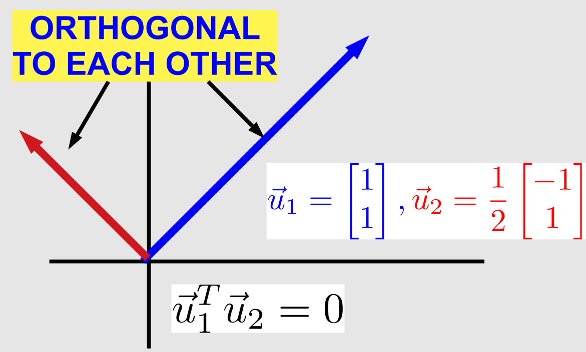
if not necessarily = 1 (but ≠ 0): then called **ORTHOGONAL**

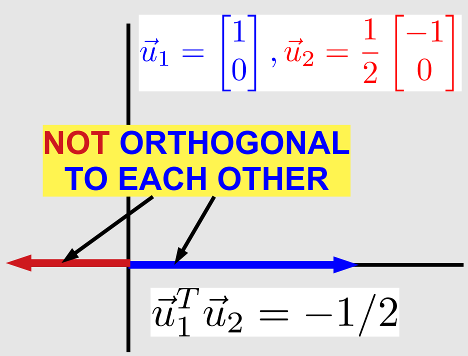
$\vec{u}_1, \vec{u}_2, \cdots, \vec{u}_n$ called **ORTHONORMAL**

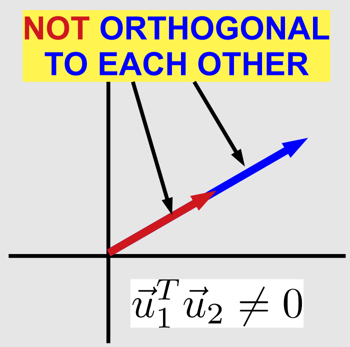
- In 2D:

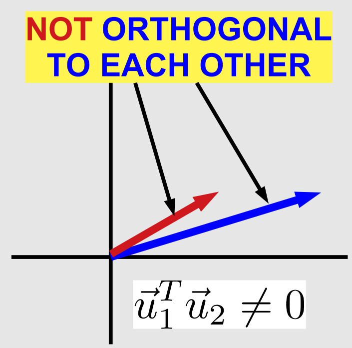








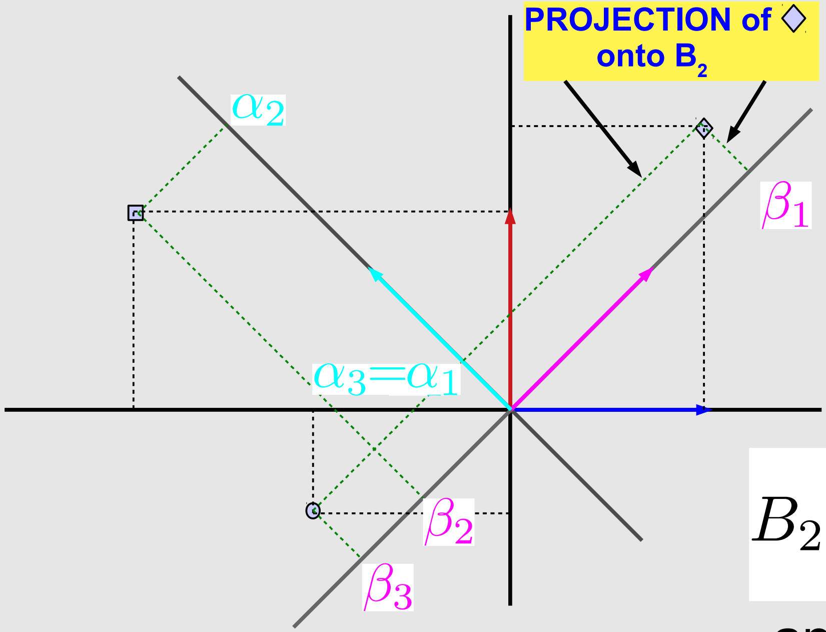




3D: orthogonality also means **at right angles**

4D and higher: "**right angles**" **means orthogonality!**

Projection onto Orthonormal Bases



orthonormal basis

$$B_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

SAMPLES

$$\begin{array}{ccc} & \mathbf{x} & \mathbf{y} \\ D = & \begin{bmatrix} 1 & \diamond & 1.5 \\ -2 & \square & 1 \\ -1 & \circ & -0.5 \end{bmatrix} \end{array}$$

$$B_2 = \frac{1}{\sqrt{2}} \begin{array}{c} \vec{p}_1 \quad \vec{p}_2 \\ \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \end{array} \qquad \|\vec{p}_i\| = 1 \qquad \vec{p}_1^T \vec{p}_2 = 0$$

another orthonormal basis

- How can we calculate the projections?
  - data point: $\begin{bmatrix} x \\ y \end{bmatrix} = \alpha \vec{p}_1 + \beta \vec{p}_2$, or $\begin{bmatrix} x & y \end{bmatrix} = \alpha \vec{p}_1^T + \beta \vec{p}_2^T$
  - post-multiply by basis vectors: $\begin{bmatrix} x & y \end{bmatrix} \vec{p}_1 = \alpha$, $\begin{bmatrix} x & y \end{bmatrix} \vec{p}_2 = \beta$
    - ➔ or: $\begin{bmatrix} \alpha & \beta \end{bmatrix} = \begin{bmatrix} x & y \end{bmatrix} B_2$; or, for all the data $D_2 = \begin{bmatrix} \alpha_1 & \beta_1 \\ \alpha_2 & \beta_2 \\ \alpha_3 & \beta_3 \end{bmatrix} = \boxed{DB_2}$

projecting the data D onto the basis B_2

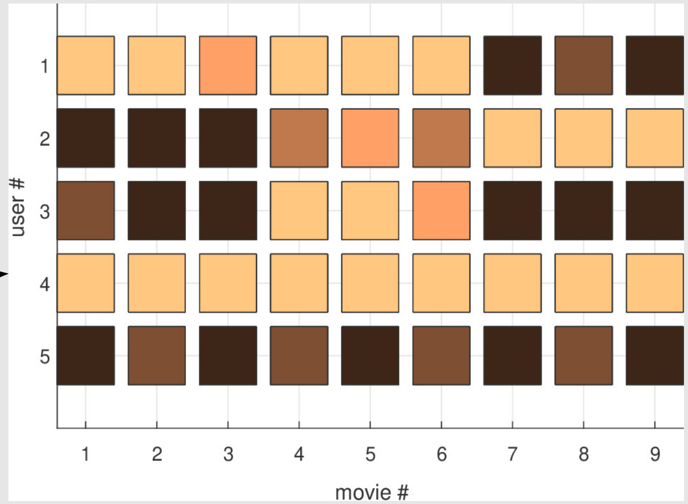
Using the SVD for Data Analysis, Feature Extraction and Clustering

Matrices Representing Ratings

- Movies rated by Users (eg, Netflix, Amazon Video)

Movie → User Name ↓	Full Metal Jacket	Die Hard	Yojimbo	2001: A Space Odyssey	The Quiet Earth	On The Beach	Would I Lie to You	Dr. Strangelove	Hokkabaz
A	5	5	4	5	5	5	1	2	1
B	1	1	1	3	4	3	5	5	5
C	2	1	1	5	5	4	2	1	1
D	5	5	5	5	5	5	5	5	5
E	1	2	1	2	1	2	2	2	1

lighter colours = stronger ratings



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

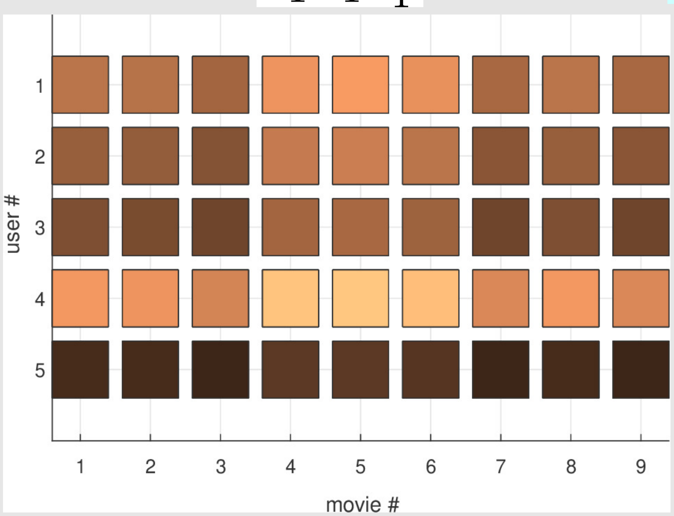
Features of Rating Matrices

Movie → User Name ↓	Full Metal Jacket	Die Hard	Yojimbo	2001: A Space Odyssey	The Quiet Earth	On The Beach	Would I Lie to You	Dr. Strangelove	Hokkabaz
A	5	5	4	5	5	5	1	2	1
B	1	1	1	3	4	3	5	5	5
C	2	1	1	5	5	4	2	1	1
D	5	5	5	5	5	5	5	5	5
E	1	2	1	2	1	2	2	2	1

"most typical" col (movie) feature:
65% like D's choices, 50% like A's,
40% like B's, 35% like C's
20% E's

"most typical" row (user) feature:
likes SF more;
action somewhat less;
and comedy even less

$\sigma_1 \vec{u}_1 \vec{v}_1^T$



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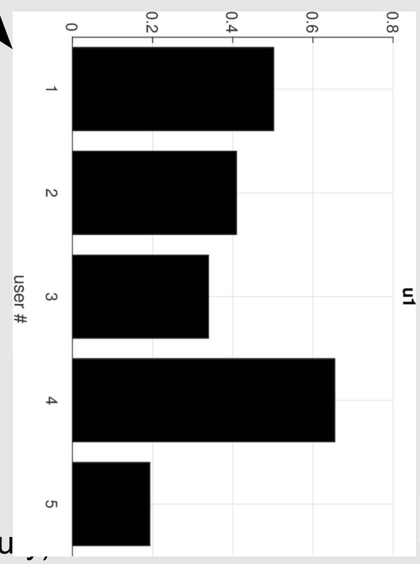
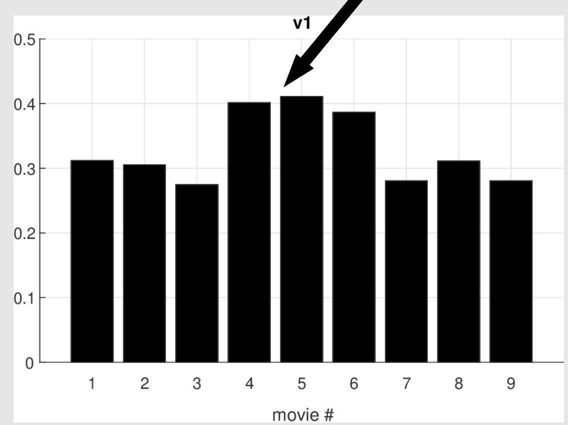


$\vec{u}_1$



$\vec{v}_1^T$

$\sigma_1 = 22.6$

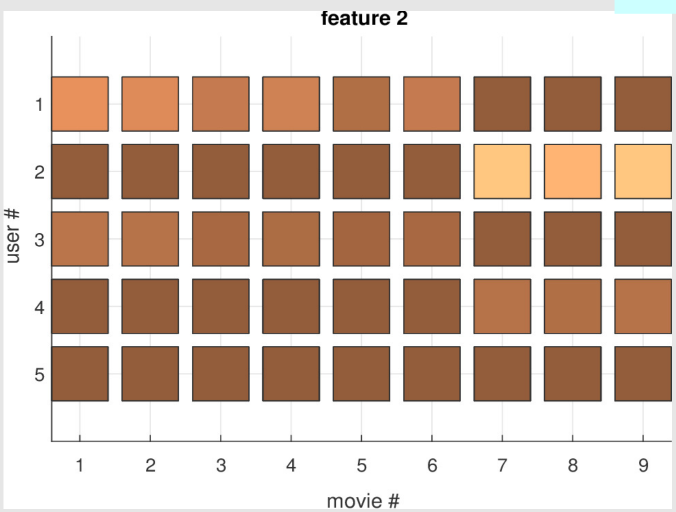
Features of Rating Matrices (contd.)

Movie → User Name ↓	Full Metal Jacket	Die Hard	Yojimbo	2001: A Space Odyssey	The Quiet Earth	On The Beach	Would I Lie to You	Dr. Strangelove	Hokkabaz
A	5	5	4	5	5	5	1	2	1
B	1	1	1	3	4	3	5	5	5
C	2	1	1	5	5	4	2	1	1
D	5	5	5	5	5	5	5	5	5
E	1	2	1	2	1	2	2	2	1

2nd most typical col (movie) feature:
55% like A's choices, 70% unlike B's, 35% like C's, 15% unlike D's, negligibly like E's

2nd most typical row (user) feature:
likes mostly action;
a bit less SF;
strongly anti-comedy

$\sigma_2 \vec{u}_2 \vec{v}_2^T$



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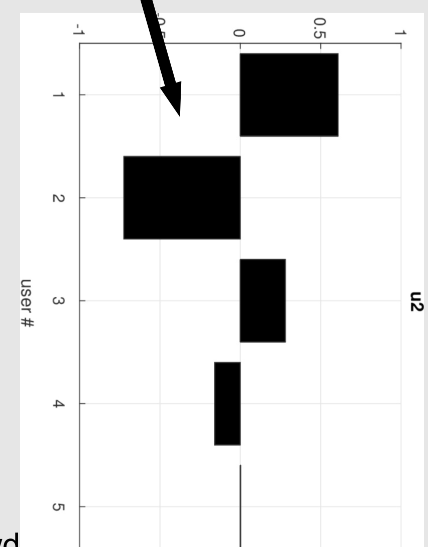
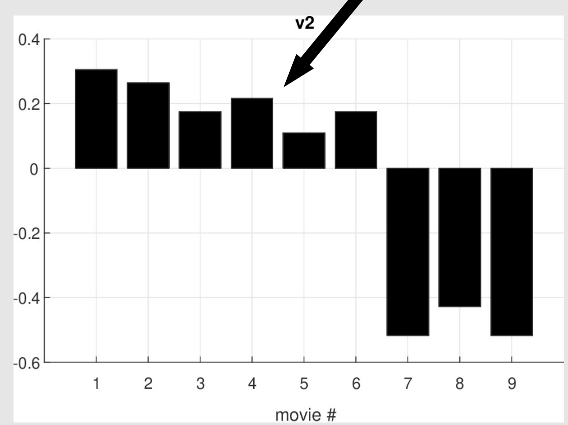


$\vec{u}_2$



$\vec{v}_2^T$

$\sigma_2 = 6.8$

Projection in the Feature Basis

Movie → User Name ↓	Full Metal Jacket	Die Hard	Yojimbo	2001: A Space Odyssey	The Quiet Earth	On The Beach	Would I Lie to You	Dr. Strangelove	Hokkabaz
A	5	5	4	5	5	5	1	2	1
B	1	1	1	3	4	3	5	5	5
C	2	1	1	5	5	4	2	1	1
D	5	5	5	5	5	5	5	5	5
E	1	2	1	2	1	2	2	2	1

- Express each col of A (movie column) as a linear combination of col. features
  - e.g., **Full Metal Jacket** column:

col.(movie) features

$$\begin{bmatrix}5\\1\\2\\5\\1\end{bmatrix} = \alpha_{11}\vec{u}_1 + \alpha_{21}\vec{u}_2 + \alpha_{31}\vec{u}_3 + \cdots + \alpha_{51}\vec{u}_5$$

"how much FMJ is like the most typical movie"

"how much FMJ is like the 3rd most typical movie"

➔ $$\alpha_{i1} = \vec{u}_i^T \begin{bmatrix}5\\1\\2\\5\\1\end{bmatrix}, \quad i = 1, \cdots, 5$$

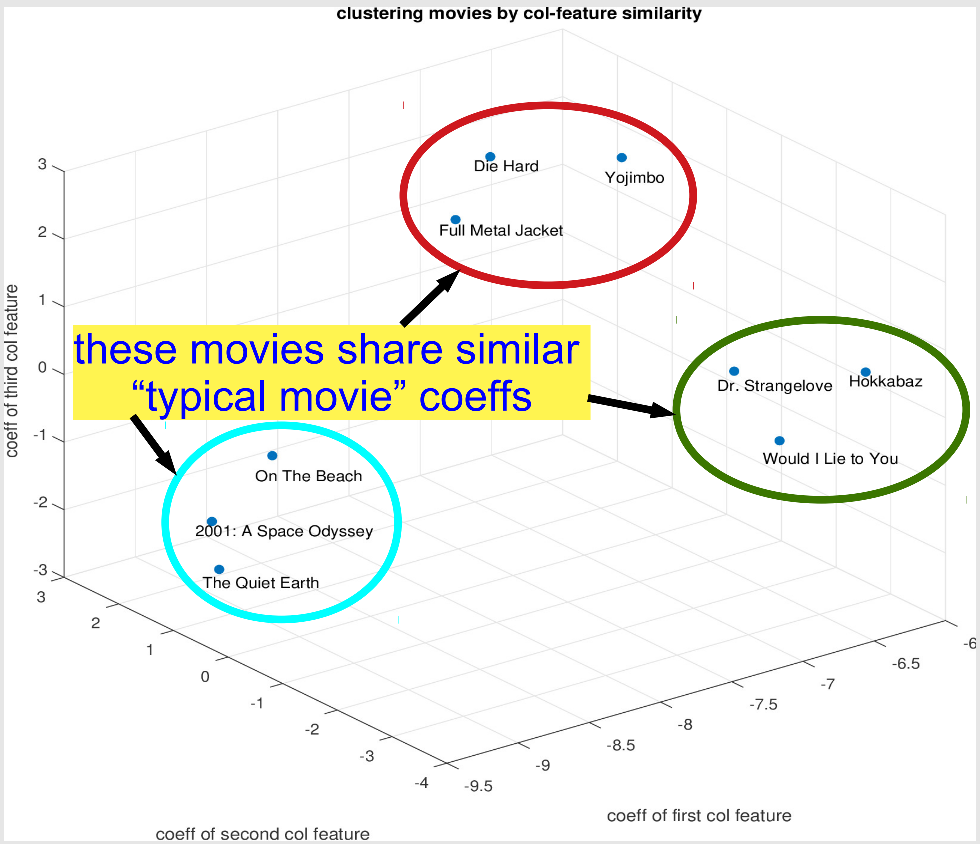
Projections of 1st col (FMJ) onto column feature basis

Clustering in Feature Bases

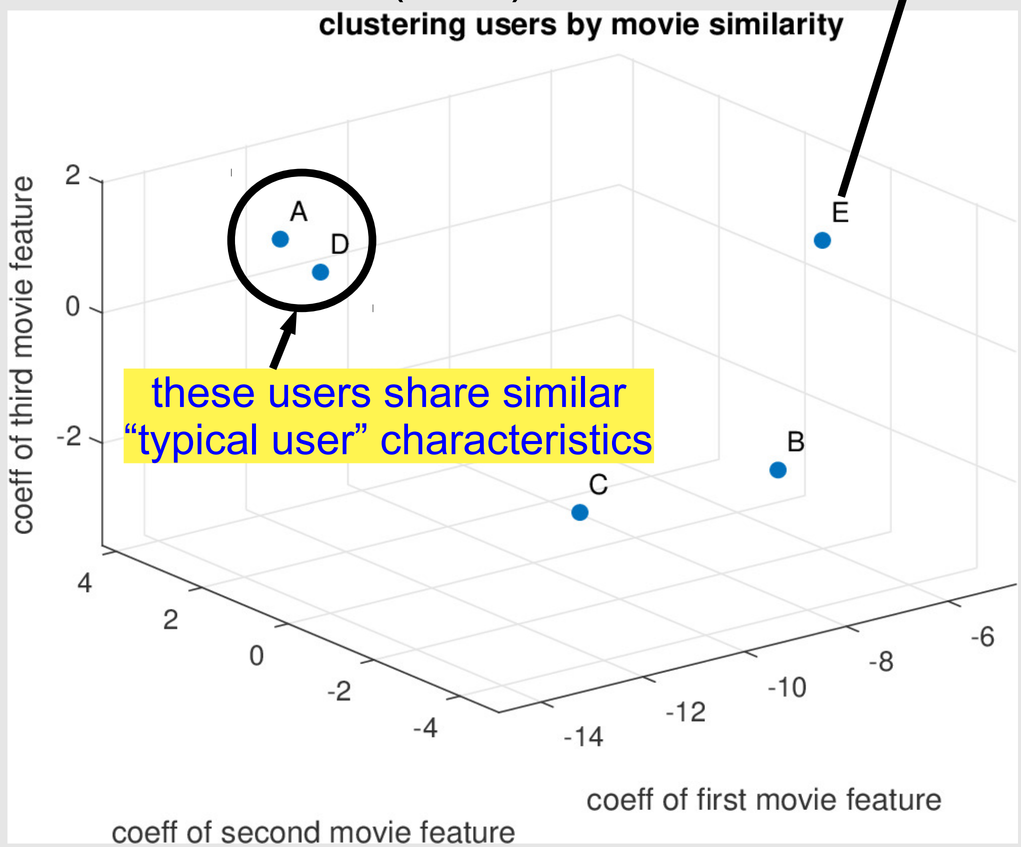
- Scatter plot of α_{11}, α_{21}, and α_{31} for all movies

$$\text{user E row} = \begin{bmatrix} 1 & 2 & 1 & 2 & 1 & 2 & 2 & 2 & 1 \end{bmatrix}$$
$$= \beta_{51}\vec{v}_1^T + \beta_{52}\vec{v}_2^T + \beta_{53}\vec{v}_3^T + \cdots + \beta_{55}\vec{v}_5^T$$

Movies classified by projections on column (movie) features

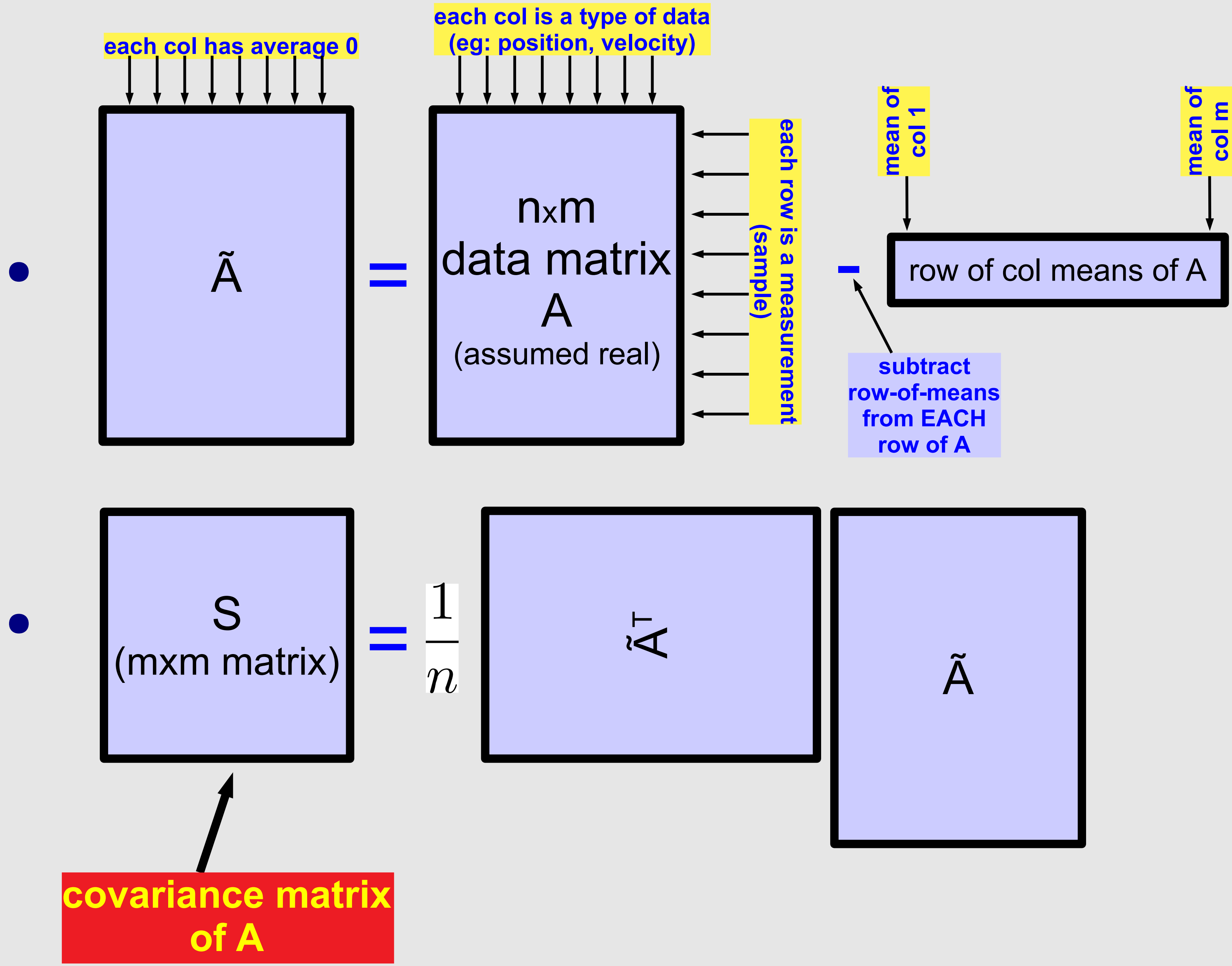


Users classified by projection on row (user) features



Principal Component Analysis (PCA)

Covariance Matrices



Covariance Matrix – example

- 3 x 2 example

Covariance Matrices: Properties

- $S \triangleq \dfrac{1}{n} \tilde{A}^T \tilde{A}$
- S is square and **symmetric**: $S = S^T$ or $s_{ij} = s_{ji}$
- The **diagonal entries of S** are **real and ≥ 0**
  - $s_i^2 \triangleq s_{ii} = \dfrac{1}{n} \sum_{j=1}^{n} \tilde{a}_{ji}^2 \geq 0$: **variance of i^th col of A**
  - $S = \begin{bmatrix} s_1^2 & s_{12} & s_{13} & \cdots & s_{1m} \\ s_{21} & s_2^2 & s_{23} & \cdots & s_{2m} \\ s_{31} & s_{32} & s_3^2 & \cdots & s_{3m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ s_{m1} & s_{m2} & s_{m3} & \cdots & s_m^2 \end{bmatrix}$ **covariance matrix**
  - **can also show:** $|s_{ij}| \leq s_i s_j$
    - using the **Cauchy-Schwartz inequality**

The Correlation Matrix

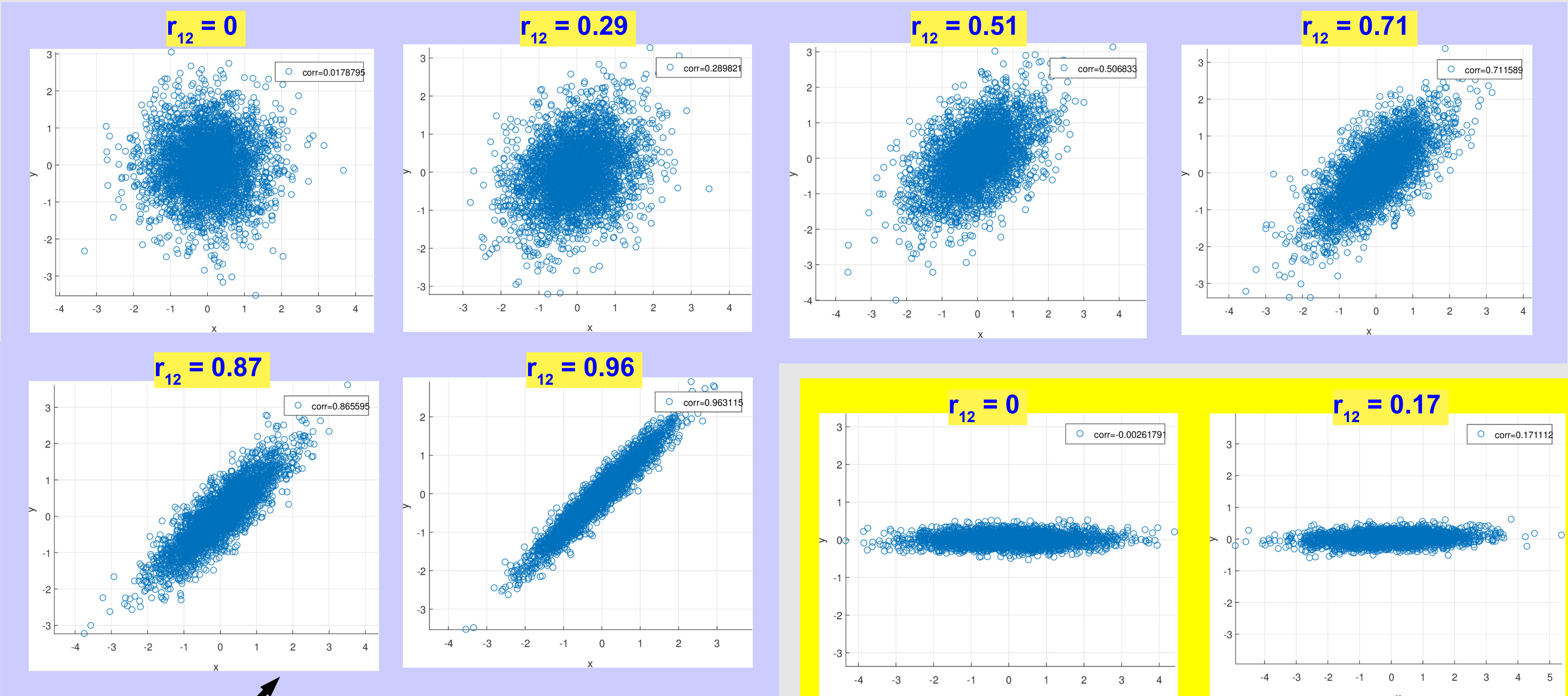
- $r_{ij} \triangleq \dfrac{s_{ij}}{s_i s_j}$; $r_{ij} = r_{ji}$ (symmetry); $\Rightarrow r_{ii} = 1$ why? $\Rightarrow |r_{ij}| <= 1$

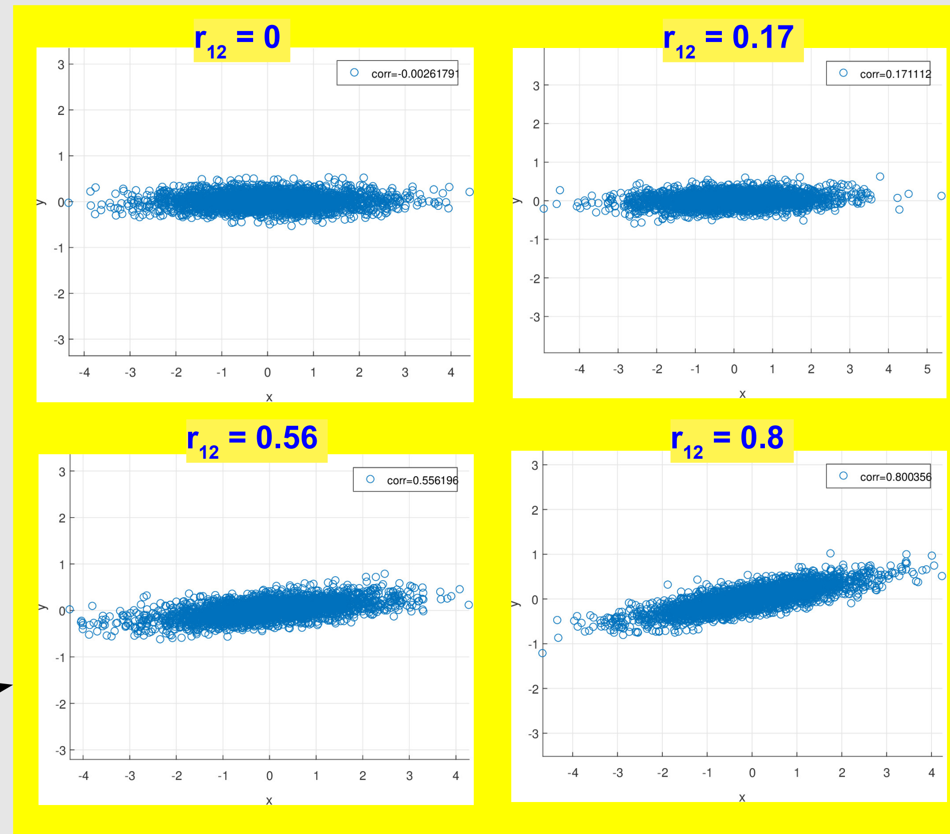
correlation

- $$R = \begin{bmatrix} 1 & r_{12} & r_{13} & \cdots & r_{1m} \\ r_{21} & 1 & r_{23} & \cdots & r_{2m} \\ r_{31} & r_{32} & 1 & \cdots & r_{3m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ r_{m1} & r_{m2} & r_{m3} & \cdots & 1 \end{bmatrix}$$

correlation matrix

Correlation: Geometric Intuition





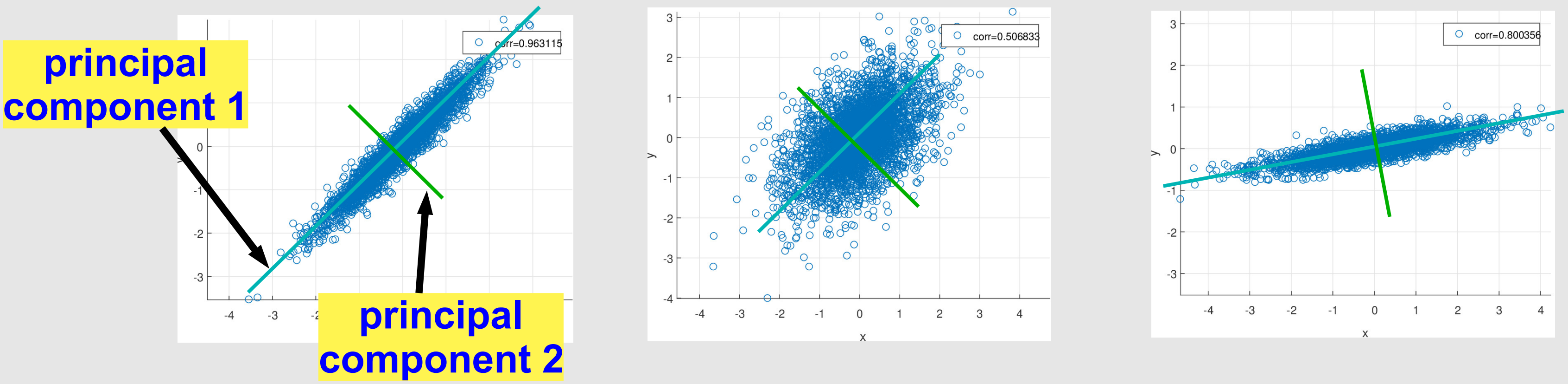
5000 x 2 matrices
(each point is a row)

correlation provides some insight ...

... but it leaves a lot out

The Intuition behind PCA

- PCA: finds (orthogonal) "**main axes** along which the data lie": the **principal components**
  - provides weights indicating "strength" of each axis



- starting point for PCA: the covariance matrix S

PCA: The Procedure

- **Eigendecompose** the covariance matrix
  - $$S = \begin{bmatrix} s_1^2 & s_{12} & s_{13} & \cdots & s_{1m} \\ s_{21} & s_2^2 & s_{23} & \cdots & s_{2m} \\ s_{31} & s_{32} & s_3^2 & \cdots & s_{3m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ s_{m1} & s_{m2} & s_{m3} & \cdots & s_m^2 \end{bmatrix} = P \Lambda P^{-1}$$

$$P = \begin{bmatrix} \uparrow & \uparrow & \uparrow & & \uparrow \\ \vec{p}_1 & \vec{p}_2 & \vec{p}_3 & \cdots & \vec{p}_n \\ \downarrow & \downarrow & \downarrow & & \downarrow \end{bmatrix}$$

cols will be orthonormal

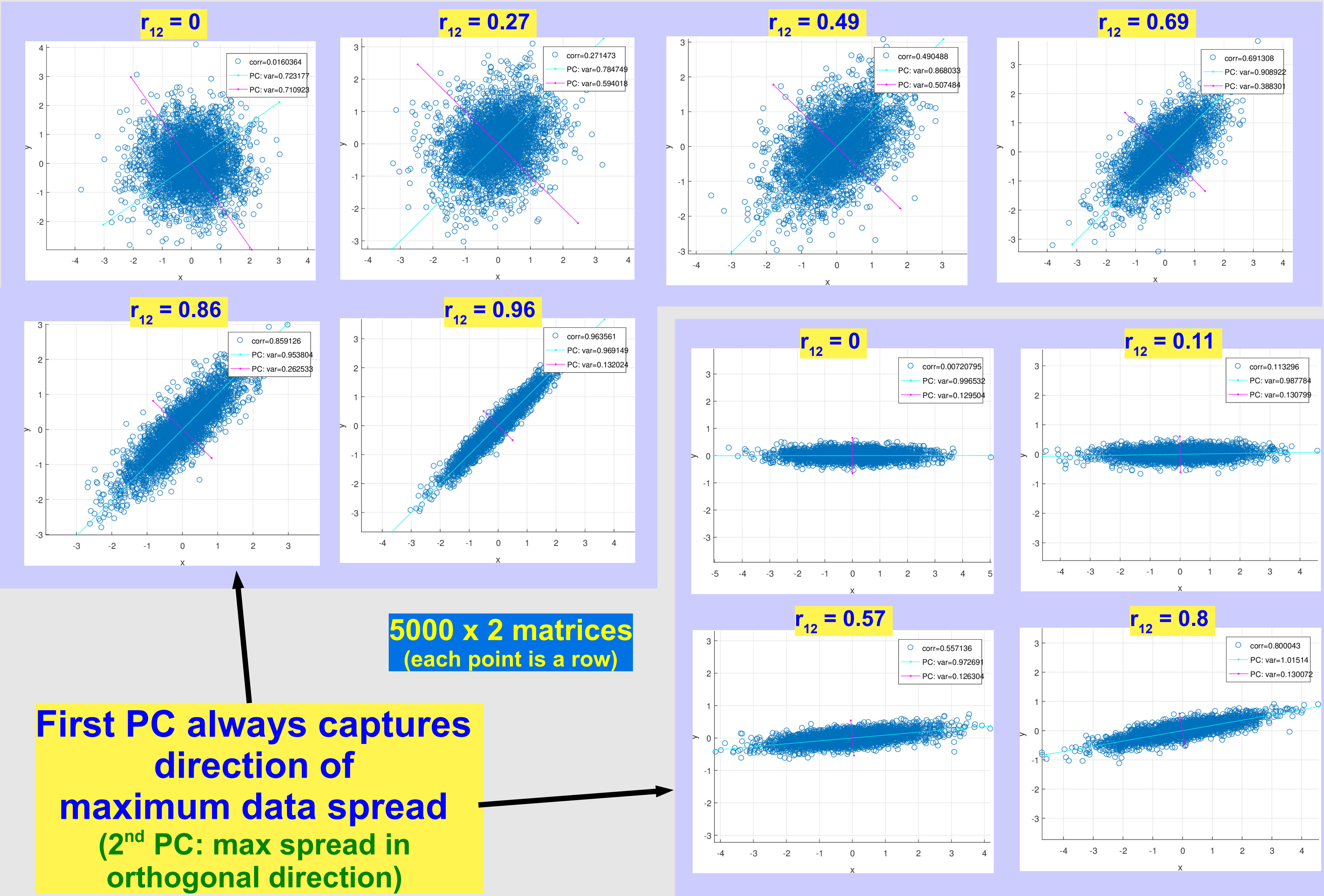
these are the PCs

$$\Lambda = \begin{bmatrix} \lambda_1 & & & & \\ & \lambda_2 & & & \\ & & \lambda_3 & & \\ & & & \ddots & \\ & & & & \lambda_m \end{bmatrix}$$

will be real and ≥0

- $\sqrt{\lambda_i}$ = the **weights**
  - (i.e., the variances)
  - with $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \cdots \geq \lambda_m \geq 0$
- eigenvectors $\vec{p}_i$ = the **principal components**

Principal Components of the Data

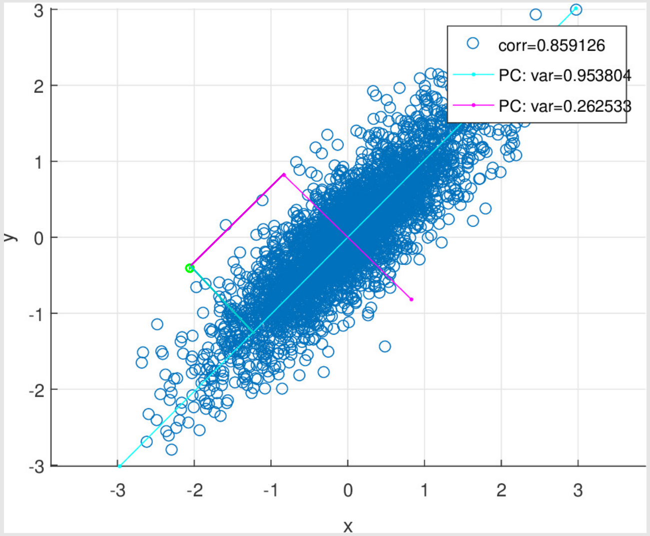


5000 x 2 matrices
(each point is a row)

First PC always captures direction of maximum data spread
(2^{nd} PC: max spread in orthogonal direction)

PCA: Why it Works: The Flow

- First: establish some properties of P and Λ
  - properties of real symmetric matrices
    - ➔ real eigenvalues
    - ➔ real set of orthonormal eigenvectors
  - properties of real $A^T A$
    - ➔ eigenvalues ≥ 0



- Express data in eigenvector basis
  - project each data point onto eigenvectors
- Show that the covariance matrix of the projected data is diagonal
  - the variances of the projections along each axis/PC
- First PC maximizes variance along any 1D projection
  - 2^{nd} PC maximizes remaining variance; and so on

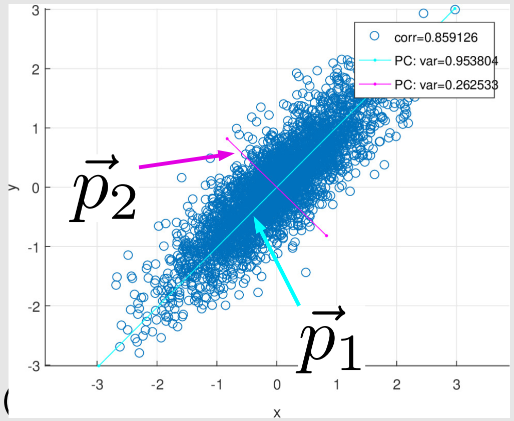
Properties of Covariance Matrices

- If S is a real mxm symmetric matrix ($s_{ij} = s_{ji}$)
  - 1. its eigenvalues are all real
    - $S\vec{p} = \lambda\vec{p}$. S symmetric $\rightarrow$ $\vec{p}^T S = \lambda\vec{p}^T$. $\rightarrow$ $\vec{p}^T S\overline{\vec{p}} = \lambda\vec{p}^T\overline{\vec{p}} = \lambda\|\vec{p}\|^2$
    - S real $\rightarrow$ $S\overline{\vec{p}} = \overline{\lambda}\,\overline{\vec{p}}$. $\rightarrow$ $\vec{p}^T S\overline{\vec{p}} = \overline{\lambda}\vec{p}^T\overline{\vec{p}} = \overline{\lambda}\|\vec{p}\|^2$.
    - hence $\lambda\|\vec{p}\|^2 = \overline{\lambda}\|\vec{p}\|^2$ $\rightarrow$ $\lambda = \overline{\lambda}$ $\rightarrow$ λ is real.
  - 2. A set of real eigenvectors can be found (see the notes)
  - 3. The eigenvectors form an orthonormal set (basis).
    - (see the notes)
- If S is in the form A^TA (A real)
  - 4. its eigenvalues are all ≥ 0.
    - $A^T A\vec{p} = \lambda\vec{p}$ $\rightarrow$ $\vec{p}^T A^T A\vec{p} = \lambda\vec{p}^T\vec{p}$ $\rightarrow$ $(A\vec{p})^T A\vec{p} = \lambda\vec{p}^T\vec{p}$
    - $\rightarrow$ $\|A\vec{p}\|^2 = \lambda\|\vec{p}\|^2$ $\rightarrow$ $\lambda = \dfrac{\|A\vec{p}\|^2}{\|\vec{p}\|^2} \geq 0$.

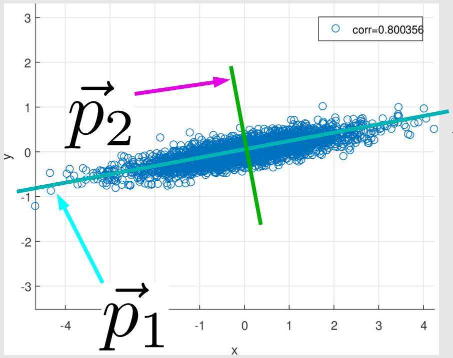
PCA Basis Diagonalises the Data

- eigenvectors orthonormal $\longrightarrow$ $PP^T = I \longrightarrow P^T = P^{-1}$
- eigendecomposition of S: $S = P\Lambda P^T$
- project rows of (zero-mean) A in basis P: $F = \tilde{A}P$
  - columns of F are the projections along $\vec{p}_i$
- Let G be the co-variance matrix of F: $G \triangleq (F^T F)/n$
  - $nG = F^T F = P^T \tilde{A}^T \tilde{A} P = nP^T S P = nP^T P\Lambda P^T P = n\Lambda$

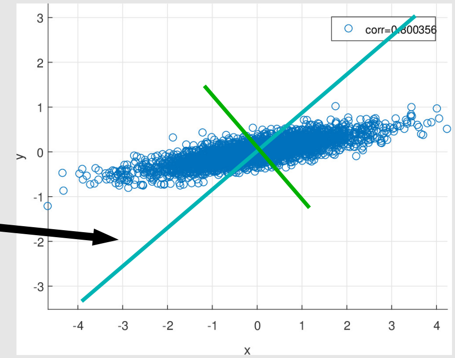
    = Λ (diagonal) ← **Data projected on PC basis becomes UNCORRELATED**
  - the diagonal entries are the variances of the data projected along $\vec{p}_i$ (recall: from defn. of covariance matrix)



Why do PCs Align with Visual Axes?



Why this? and not this?



- So far: have shown that PCs are orthonormal
  - data projected onto them becomes uncorrelated
- but why is the first **PC aligned with the direction of maximum spread**?
- Key property of PCA ⟵ **proof → notes**
  - consider **any** norm-1 vector ("direction") $\vec{p}$
  - project the data along it: $\tilde{A}\vec{p}$
  - find the variance of the projected data: $\frac{1}{n}(\tilde{A}\vec{p})^T(\tilde{A}\vec{p})$
  - **the first PC $\vec{p}_1$ maximizes this variance** (the max is $\vec{\lambda}_1$)
    - ➔ 2nd PC: maximizes variance along directions orthogonal to $\vec{p}_1$
    - $\longrightarrow$ 3rd PC: maximizes var. along dirs. orthogonal to $\vec{p}_1$ and $\vec{p}_2$; and so on

PCA: the Connection with the SVD

- Suppose you run an SVD on the data: $\tilde{A} = U\Sigma V^T$
  - the covariance matrix is:
    - $S \triangleq \frac{1}{n}\tilde{A}^T\tilde{A} = \frac{1}{n}V\Sigma^T U^T U\Sigma V^T = \boxed{V \boxed{\frac{\Sigma^T\Sigma}{n}} V^T}$ $\quad \frac{1}{n}\begin{bmatrix} \sigma_1^2 & & & & \\ & \sigma_2^2 & & & \\ & & \sigma_3^2 & & \\ & & & \ddots & \\ & & & & \sigma_m^2 \end{bmatrix}$
    - recall PCA: $S = \boxed{P\boxed{\Lambda}P^T}$

IDENTICAL FORM

diagonal and ≥ 0

- i.e., can use the SVD of Ã for PCA:
  - **just set $\lambda_i \triangleq \frac{\sigma_i^2}{n}$ and $P \triangleq V$ (no need to even form S)!**

Computing SVDs via Eigendecomposition

- Prev. slide: SVD: $S = V \frac{\Sigma^T \Sigma}{n} V^T$; PCA: $S = P \Lambda P^T$
- Q: how to calculate an SVD of a matrix A?
  - using eigendecomposition
- A: just use the above insight (PCA/eigendecomposition)!
  - form $S \triangleq A^T A$, eigendecompose $S = P \Lambda P^T$
  - set $\sigma_i \triangleq \sqrt{\lambda_i}$, $V \triangleq P$

more work, because (we had assumed) n ≥ m

nxn

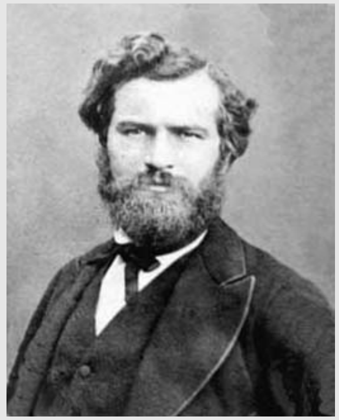
  - what about U?
    - just eigendecompose $\hat{S} \triangleq A A^T = Q \hat{\Lambda} Q^T$; then $U \triangleq Q$
    - can also get V from the **same** eigendecomposition
      - $A = U \Sigma V^T \rightarrow U^T A = \Sigma V^T \rightarrow A^T U = V \Sigma^T \rightarrow$ $\vec{v}_i = \frac{A^T \vec{u}_i}{\sigma_i}$ $i = 1, \cdots, m$
  - set $\sigma_i \triangleq \sqrt{\lambda_i}$

if σ_i = 0, choose v_i arbitrarily to complete orthonormal basis for V

* why didn't we subtract means from A and normalize by n?

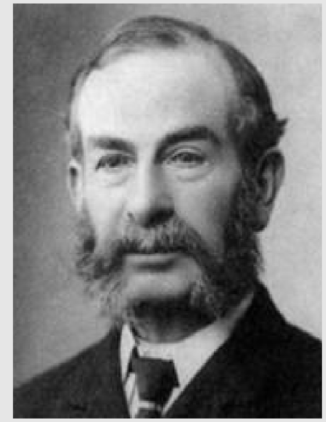
Who Invented the SVD?

- SVD: “**Swiss Army Knife**” of numerical analysis



Camille Jordan
1838-1922

Erhardt Schmidt
1878-1959

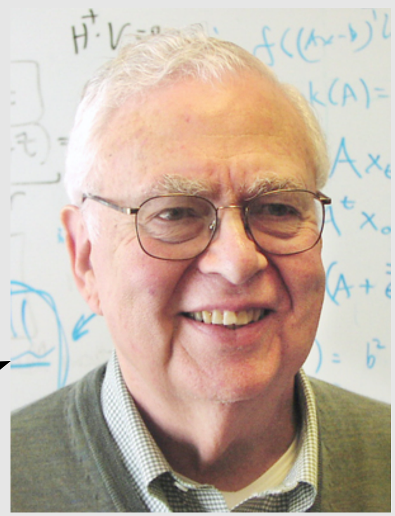


James Joseph
Sylvester 1814-97

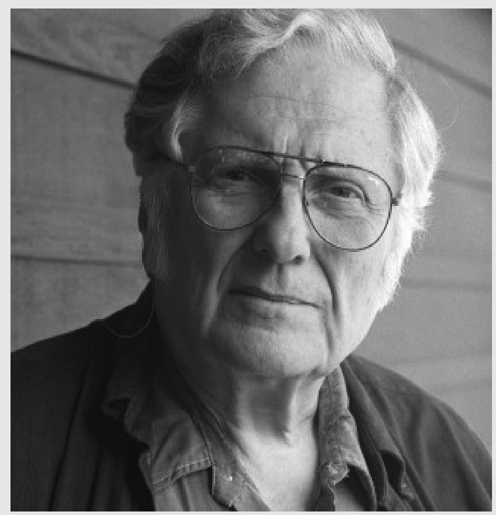
Hermann Weyl
1885-1955

Eugenio Beltrami
1835-1900

proposed the SVD
via eigendecomposition
of $A^T A$ or $A A^T$



Gene Golub
1932-2007



Bill Kahan
UCB EECS

Jim Demmel
UCB EECS

Summary: SVD and PCA

- Singular Value Decomposition (SVD)
  - useful for "low-rank approximations" of matrices
    - image analysis and compression
    - general data analysis, finding important features, clustering
- Covariance, Correlation and PCA
  - visualizing data as scatter plots
  - covariance and correlation matrices of data
  - Principal Component Analysis
    - eigenvecs of covariance matrix: principal components
      - directions along which data varies maximally
        - dropping later PCs can, eg, clean out (small) noise
    - eigenvalues correspond to variances along PCs
    - SVD can be used instead of eigendecomposition
      - eigendecomposition of covariance matrix: performs SVD