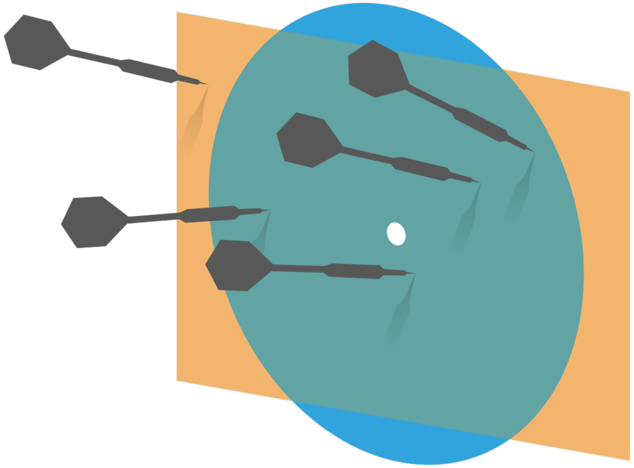
Probability and Statistics for Computer Science



Credit: wikipedia

Principal Component Analysis --- Exploring the data in less dimensions

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Last time

- Review of Bayesian inference
- Visualizing high dimensional data & Summarizing data
- The covariance matrix

Objectives

Principal Component Analysis

Two applications: ① Dimension reduction

② Compression, Reconstruction

Find eigenvectors of Covmat of a data matrix!

see data in those directions!!

Examples: Immune Cell Data

- There are 38816 white blood immune cells from a mouse sample

$N = 38816$

- Each immune cell has 40+ features/ components

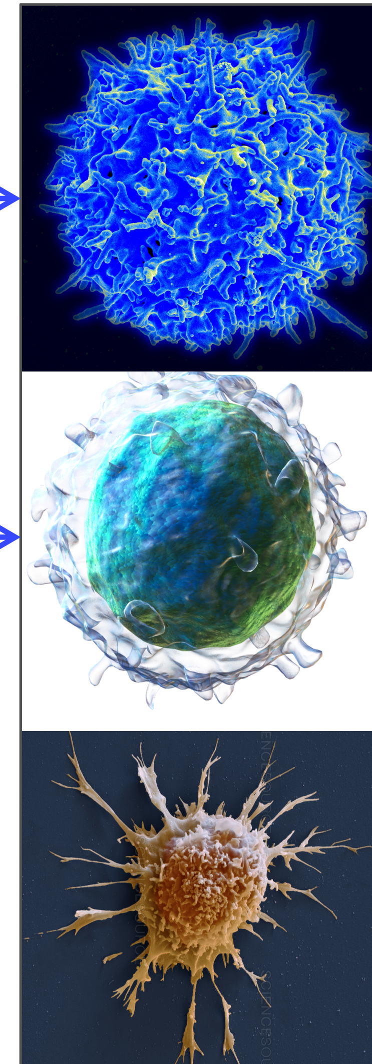
measurements

$d \times N$

- Four features are used as illustration.

choose subset $d = 4$

- There are at least 3 cell types involved



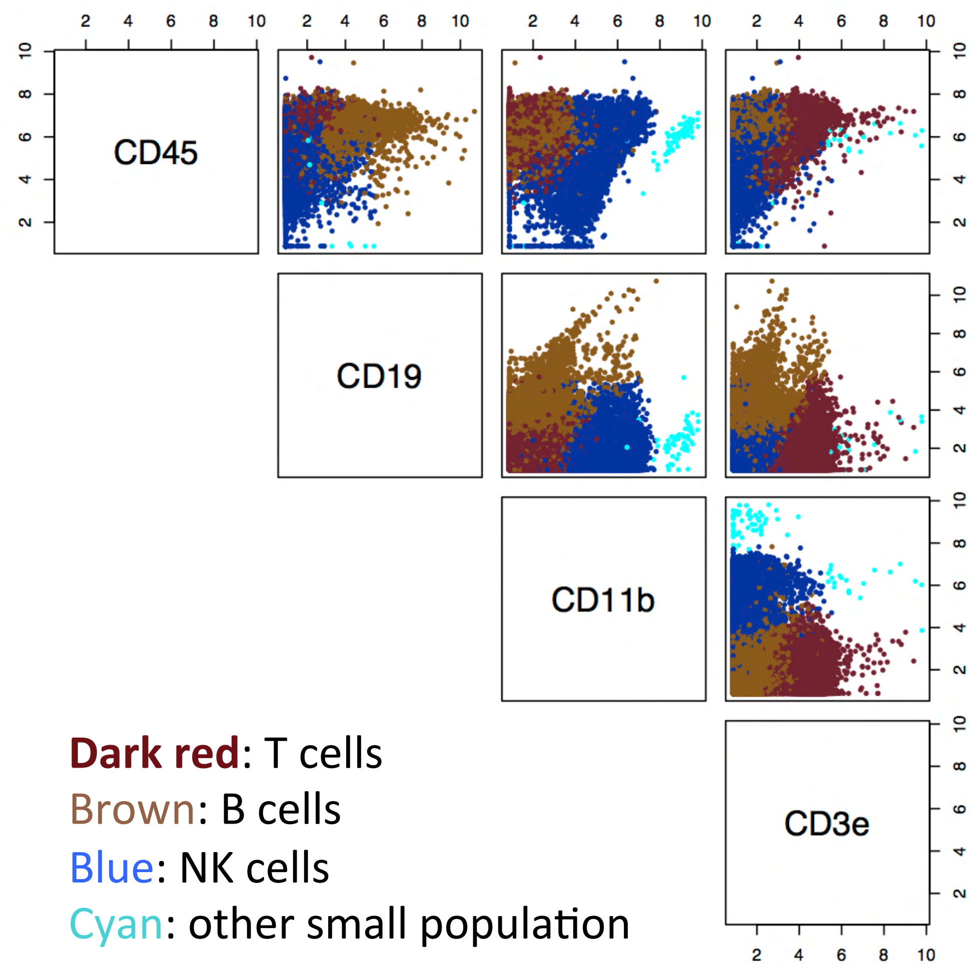
T cells

B cells

Natural killer cells

Scatter matrix of Immune Cells

- There are 38816 white blood immune cells from a mouse sample
- Each immune cell has 40+ features/ components
- Four features are used for the illustration.
- There are at least 3 cell types involved



Dark red: T cells
Brown: B cells
Blue: NK cells
Cyan: other small population

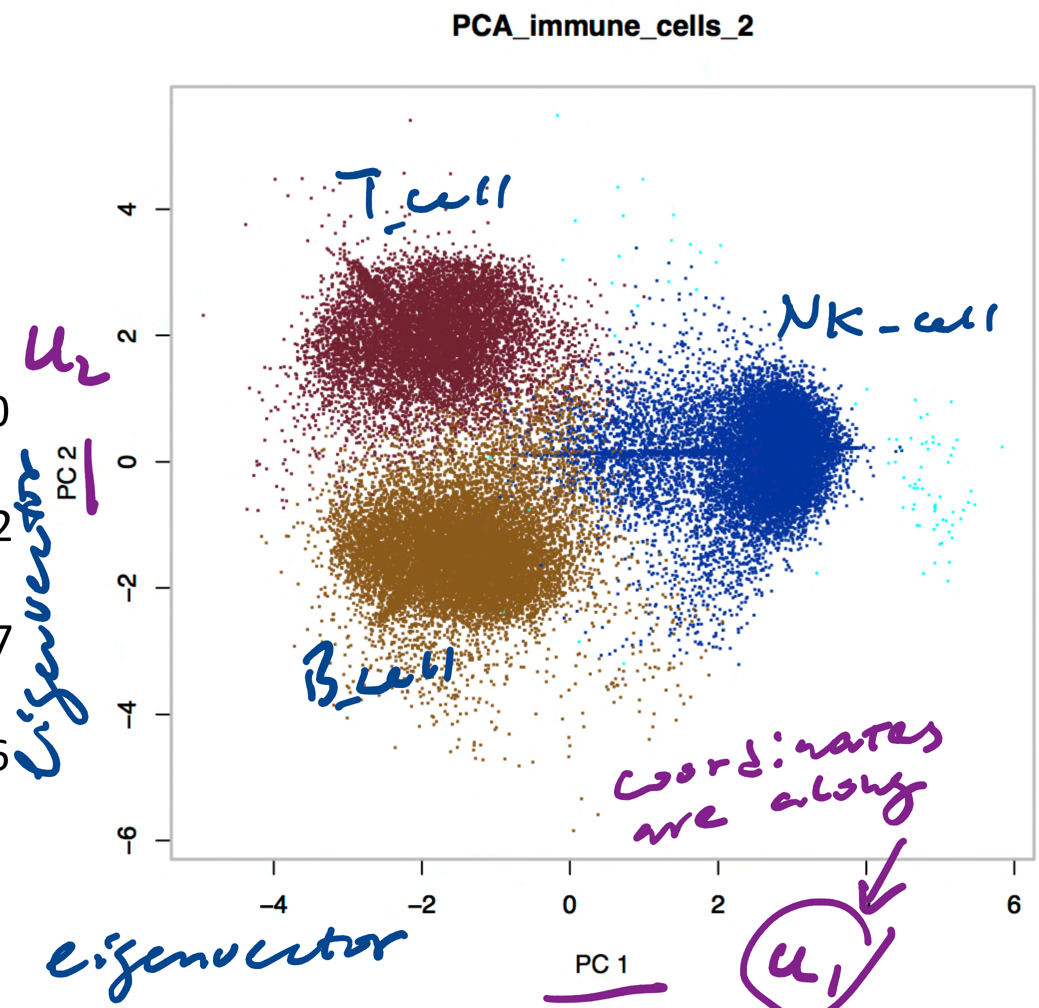
PCA of Immune Cells' Data

```
> res1
$values
[1] 4.7642829 2.1486896 1.3730662
0.4968255

$vectors
          [,1]        [,2]       [,3]       [,4]
[1,]  0.2476698  0.00801294 -0.6822740
0.6878210
[2,]  0.3389872 -0.72010997 -0.3691532
-0.4798492
[3,] -0.8298232  0.01550840 -0.5156117
-0.2128324
[4,]  0.3676152  0.69364033 -0.3638306
-0.5013477
```

Eigenvalues

Eigenvectors



Properties of Covariance matrix

$$cov(\{x\}; j, k) = cov(\{x\}; k, j)$$

Covmat($\{\mathbf{x}\}$) 7×7

- The covariance matrix is **symmetric**!
- And it's **positive semi-definite**, that is all $\lambda_i \geq 0$
- Covariance matrix is diagonalizable

	1	2	3	4	5	6	7
1	*	*	*	*	*	*	*
2	*	*	*	*	*	*	*
3	*	*	*	*	*	*	*
4	*	*	*	*	*	*	*
5	*	*	*	*	*	*	*
6	*	*	*	*	*	*	*
7	*	*	*	*	*	*	*

Properties of Covariance matrix

- If we define $\mathbf{x}_c$ as the mean centered matrix for dataset {x}

$$Covmat(\{x\}) = \frac{X_c X_c^T}{N}$$

- The covariance matrix is a d×d matrix

$\text{Covmat}(\{\mathbf{x}\})$ 7×7

cov(1,2)

	1	2	3	4	5	6	7
1	σ_1^2	*	*	*	*	*	*
2	*	σ_2^2	*	*	*	*	*
3	*	*	σ_3^2	*	*	*	*
4	*	*	*	σ_4^2	*	*	*
5	*	*	*	*	σ_5^2	*	*
6	*	*	*	*	*	σ_6^2	*
7	*	*	*	*	*	*	σ_7^2

d =7

What is the correlation between the 2 components for the data m?

$$Covmat(\boldsymbol{m}) = \begin{bmatrix} 20 & 25 \\ 25 & 40 \end{bmatrix}$$

σ_1^2, σ_2^2

Corr(feat 1, feat 2)

$$\frac{25}{\sqrt{\sigma_1^2}\sqrt{\sigma_2^2}}$$

25 → cov(1, 2)

Example: covariance matrix of a data set

(I)

Mean centering

$$A_0 = \begin{bmatrix} 5 & 4 & 3 & 2 & 1 \\ -1 & 1 & 0 & 1 & -1 \end{bmatrix}$$

mean $\begin{bmatrix} 3 \\ 0 \end{bmatrix}$

$$A_1 = \begin{bmatrix} 2 & 1 & 0 & -1 & -2 \\ -1 & 1 & 0 & 1 & -1 \end{bmatrix}$$

(II) $A_2 = A_1 A_1^T$

Inner product of each pairs:

A_2 [1,1] = 10

A_2 [2,2] = 4

A_2 [1,2] = 0

(III)

Divide the matrix with N – the number of data poits

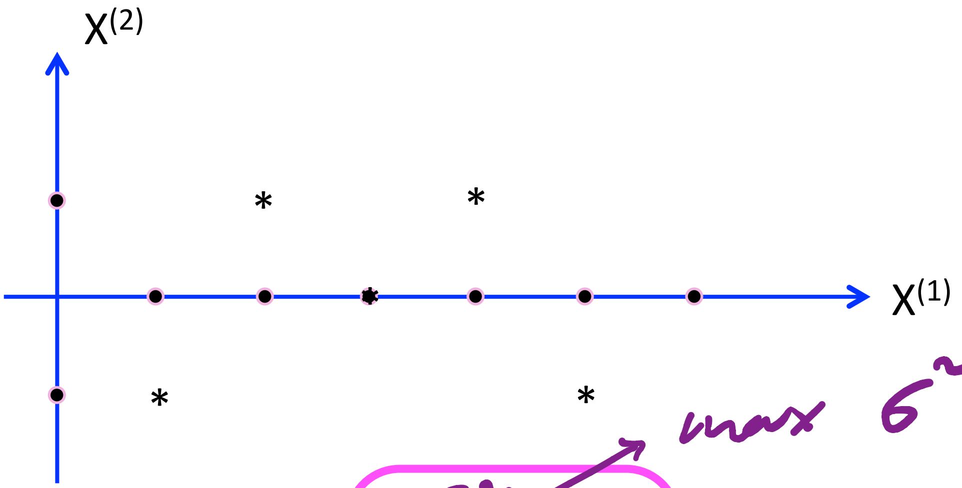
$$\text{Covmat}(\{\mathbf{x}\}) = \frac{1}{N} A_2 = \frac{1}{5} \begin{bmatrix} 10 & 0 \\ 0 & 4 \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 0.8 \end{bmatrix}$$

cov(1, 2) = 0

corr(1, 2) = 0

What do the data look like when Covmat({x}) is diagonal?

$$A_0 = \begin{bmatrix} 5 & 4 & 3 & 2 & 1 \\ -1 & 1 & 0 & 1 & -1 \end{bmatrix} \begin{matrix} x^{(1)} \\ x^{(2)} \end{matrix}$$



$$\text{Covmat}(\{\mathbf{x}\}) = \frac{1}{N} A_2 = \frac{1}{5} \begin{bmatrix} 10 & 0 \\ 0 & 4 \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 0.8 \end{bmatrix}$$

σ_1^2 → max σ^2

→ min σ^2

Diagonalization

eigvect1 eigvect2

$$\begin{bmatrix} 1 & 0 \\ 0 & 6 \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 5 \\ 0 & 6 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 6 \end{bmatrix}$$

$\Lambda \qquad X^{-1} \qquad M \qquad X$

$$M = X \Lambda X^{-1}$$

$$\begin{bmatrix} 8 & 0 \\ 0 & 2 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 5 & 3 \\ 3 & 5 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}$$

$\Lambda \qquad U^T \qquad A \qquad U$

$$A = U \Lambda U^T$$

Diagonalization of a symmetric matrix

- If A is an **n×n** symmetric square matrix, the eigenvalues are real.
- If the eigenvalues are also distinct, their eigenvectors are orthogonal
- We can then scale the eigenvectors to unit length, and place them into an orthogonal matrix $U = [\mathbf{u}_1\ \mathbf{u}_2\ \dots\ \mathbf{u}_n]$
- We can write the diagonal matrix $\Lambda = U^T A U$ such that the diagonal entries of Λ are $\lambda_1, \lambda_2 \dots \lambda_n$ in that order.

Diagonalization example

- For

$$A = \begin{bmatrix} 5 & 3 \\ 3 & 5 \end{bmatrix}$$

λ_i ? $|A - \lambda I| = 0$

$$\begin{vmatrix} 5-\lambda & 3 \\ 3 & 5-\lambda \end{vmatrix} = 0 \Rightarrow \begin{cases} \lambda_1 = 2 \\ \lambda_2 = 8 \end{cases}$$

eigenvectors?

$\lambda_1 = 2$ $A v_1 = 2 v_1$

$(A - 2I) v_1 = 0$

$$\begin{bmatrix} 3 & 3 \\ 3 & 3 \end{bmatrix} v_1 = 0 \Rightarrow v_1 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$$\Rightarrow u_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

↑ normalized eigenvector

$\lambda_2 = 8$ $u_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

$$U = [u_1 \;\; u_2] = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$$

$$\Lambda = U^T A U$$

$$\Lambda = ? \begin{bmatrix} 2 & 0 \\ 0 & 8 \end{bmatrix}$$

Diagonalization example

- For

$$A = \begin{bmatrix} 5 & 3 \\ 3 & 5 \end{bmatrix}$$

$U = [u_1 \quad u_2]$

$= ?$

$\Lambda = U^T A U$

λ_i ?

$|A - \lambda I| = 0$

$\begin{vmatrix} 5-\lambda & 3 \\ 3 & 5-\lambda \end{vmatrix} = 0 \Rightarrow \begin{cases} \lambda_1 = 8 \\ \lambda_2 = 2 \end{cases}$

eigenvectors?

$\lambda_1 = 8$

$A v_1 = 8 v_1$

$(A - 8I) v_1 = 0$

$\begin{bmatrix} -3 & 3 \\ 3 & -3 \end{bmatrix} v_1 = 0 \Rightarrow v_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

$\Rightarrow u_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

normalized eigenvector

$\lambda_2 = 2 \quad u_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$

$\Lambda = ? \begin{bmatrix} 8 & 0 \\ 0 & 2 \end{bmatrix}$

Rotation Matrix

Def: $R^T = R^{-1}$

We can prove $U^T = U^{-1}$ if U is formed by normalized eigenvectors.

U^T & U are called orthonormal matrices

$\Rightarrow$ U^T & U are rotation matrices.

If

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

$u_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ $u_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$ $u_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$

Dot Prod.

$u_1^T \cdot u_2 = ?\ 0$

$u_1^T \cdot u_3 = ?\ 0$

$u_2^T \cdot u_3 = ?\ 0$

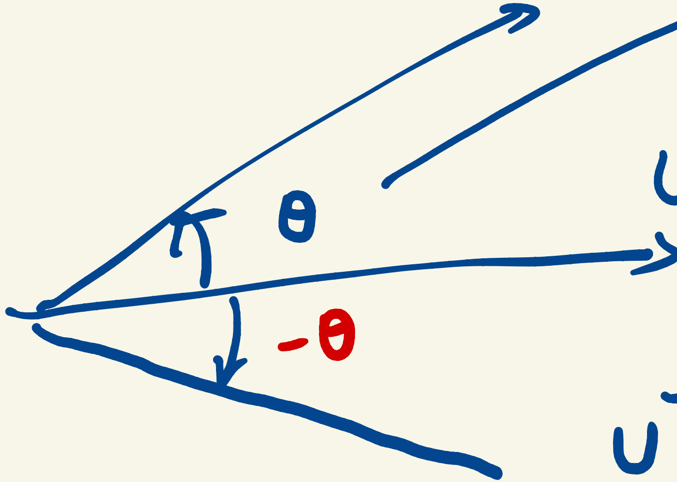
— orthogonal (perpendicular) $\perp$

$||u_1|| = ?\ 1$ $||u_2|| = ?\ 1$ $||u_3|| = ?\ 1$

$\sqrt{\sum_j u_{ij}^2} =$

2D

$U \cdot x$



$U^T x$

$$U = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

$$U^T = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}$$

$$U^T(Ux) = I \cdot x$$

$$U^T = U^{-1} \Rightarrow U^T \cdot U = I$$

Q. Is this true?

Transforming a matrix with orthonormal matrix only rotates the data

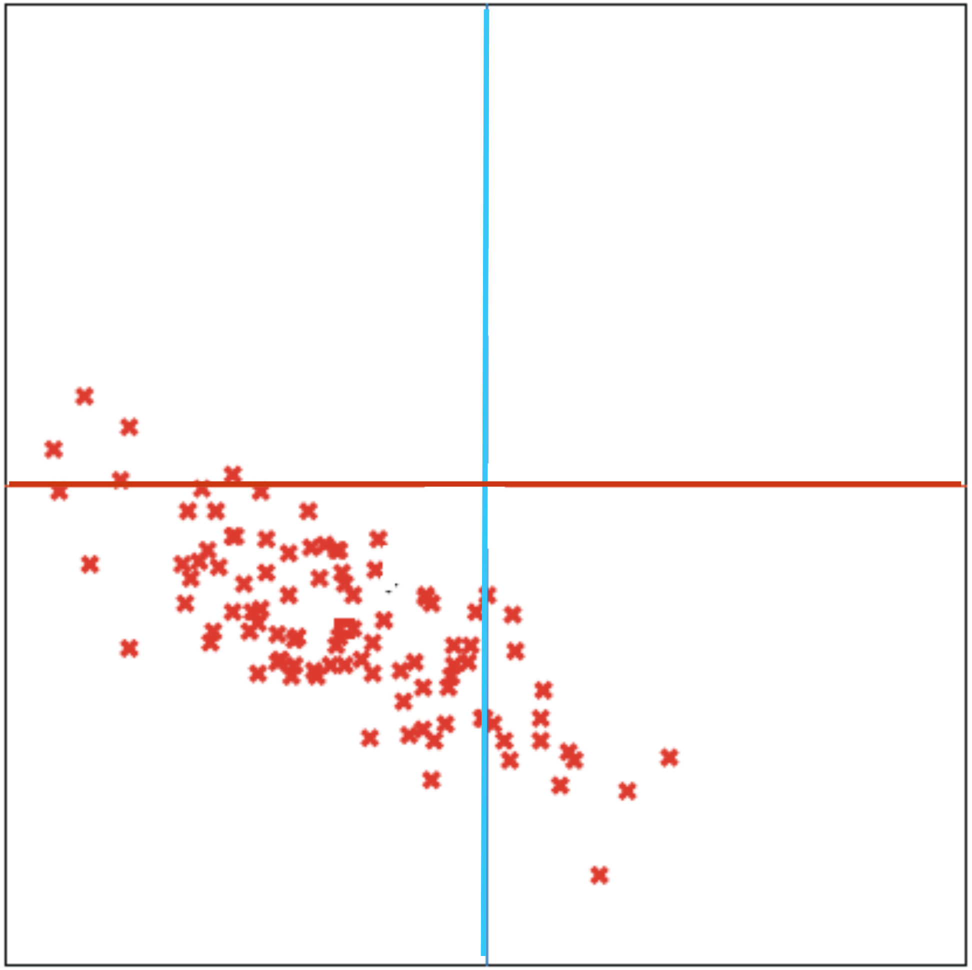
A. Yes

B. No

$U^T x$

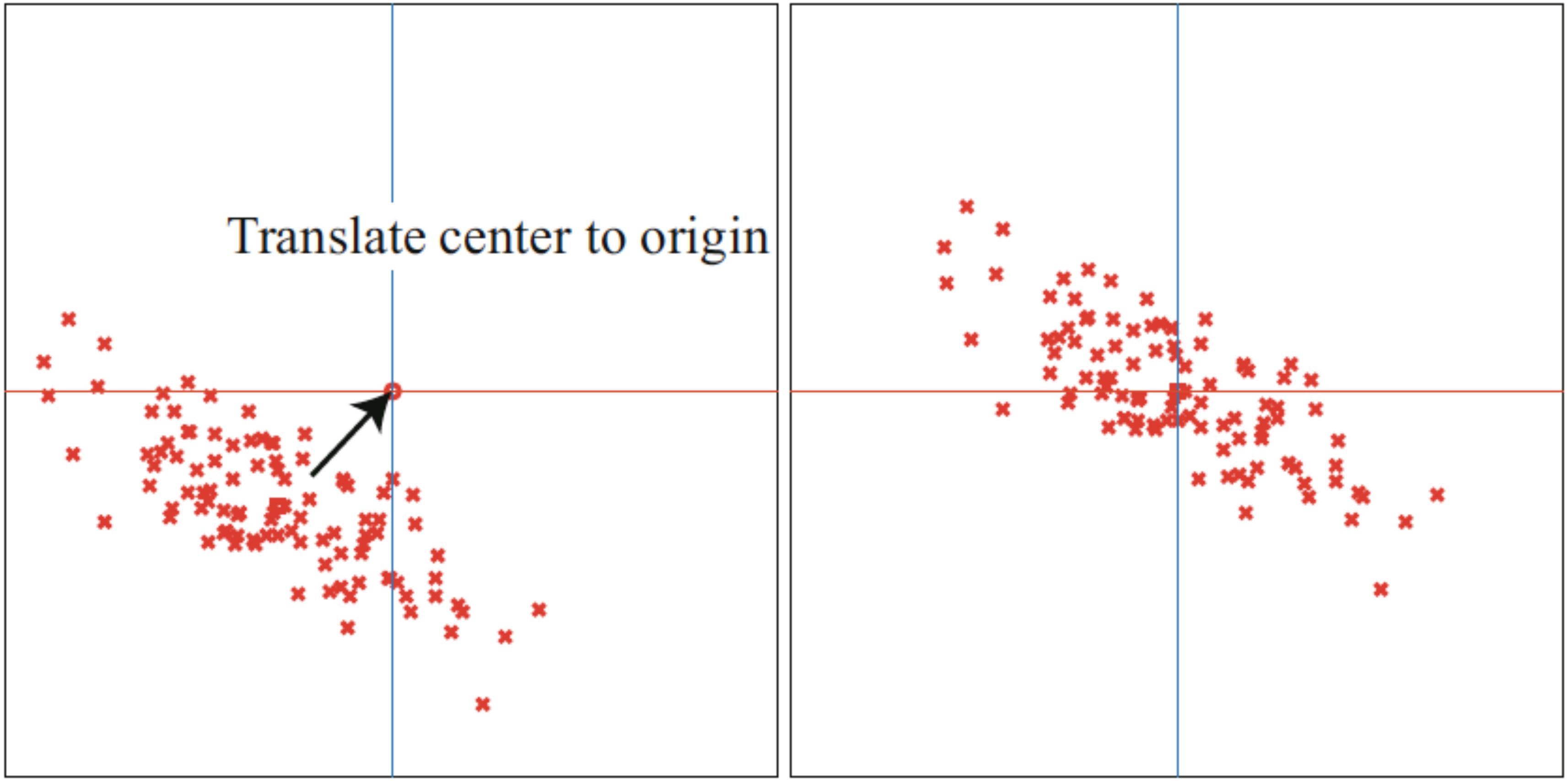
$U x$

Dimension reduction from 2D to 1D



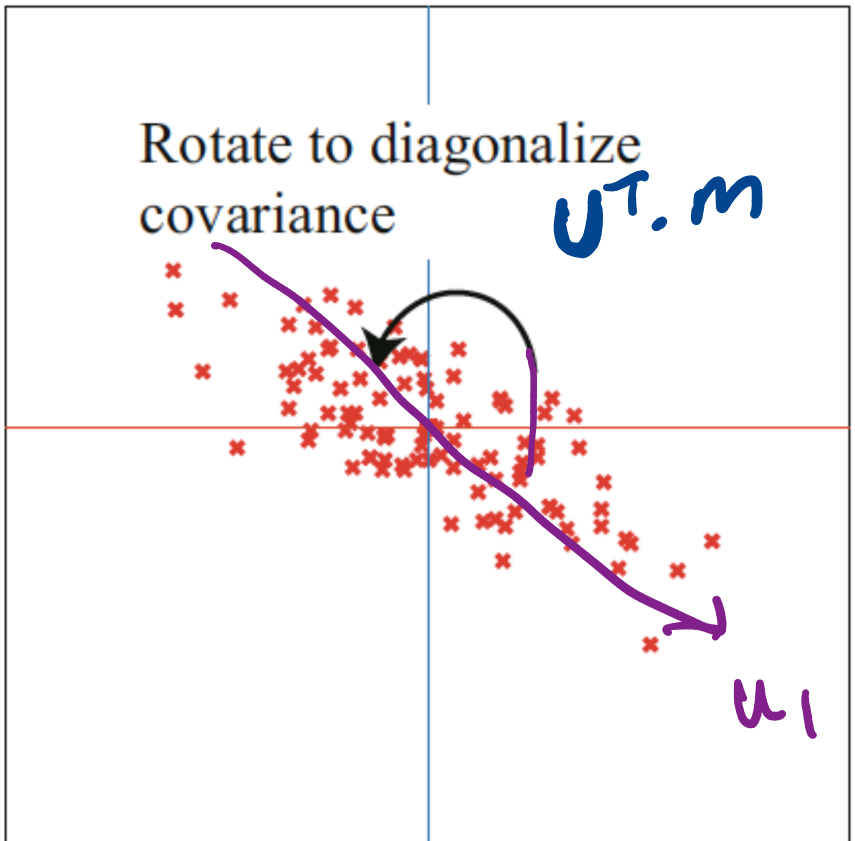
Credit: Prof. Forsyth

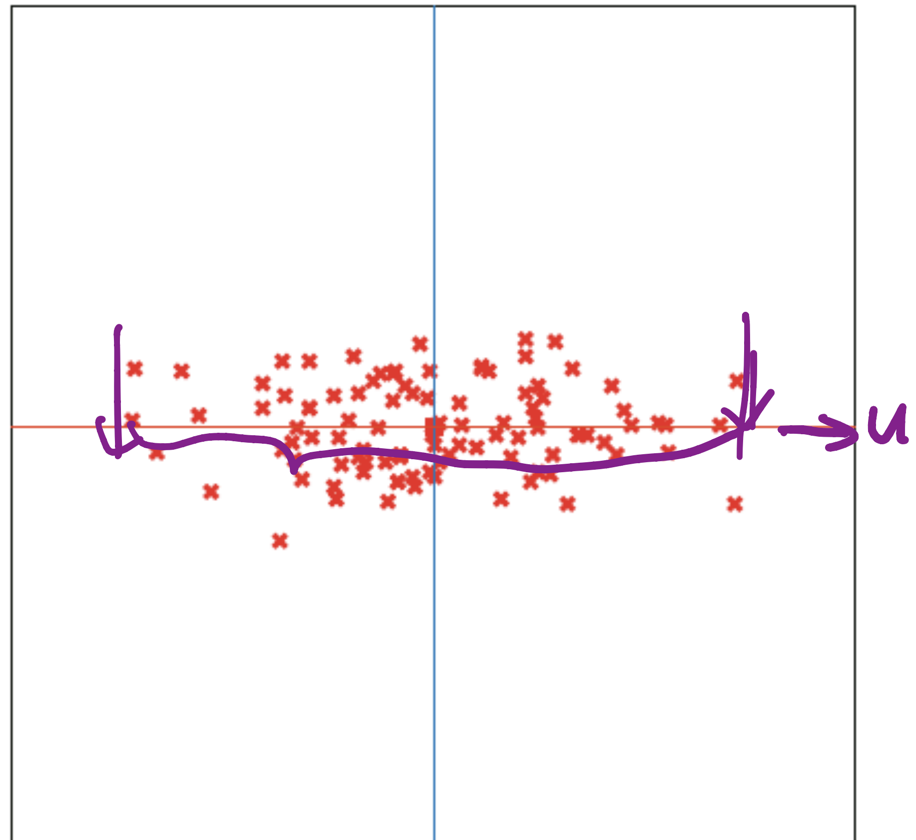
Step 1: subtract the mean



Credit: Prof. Forsyth

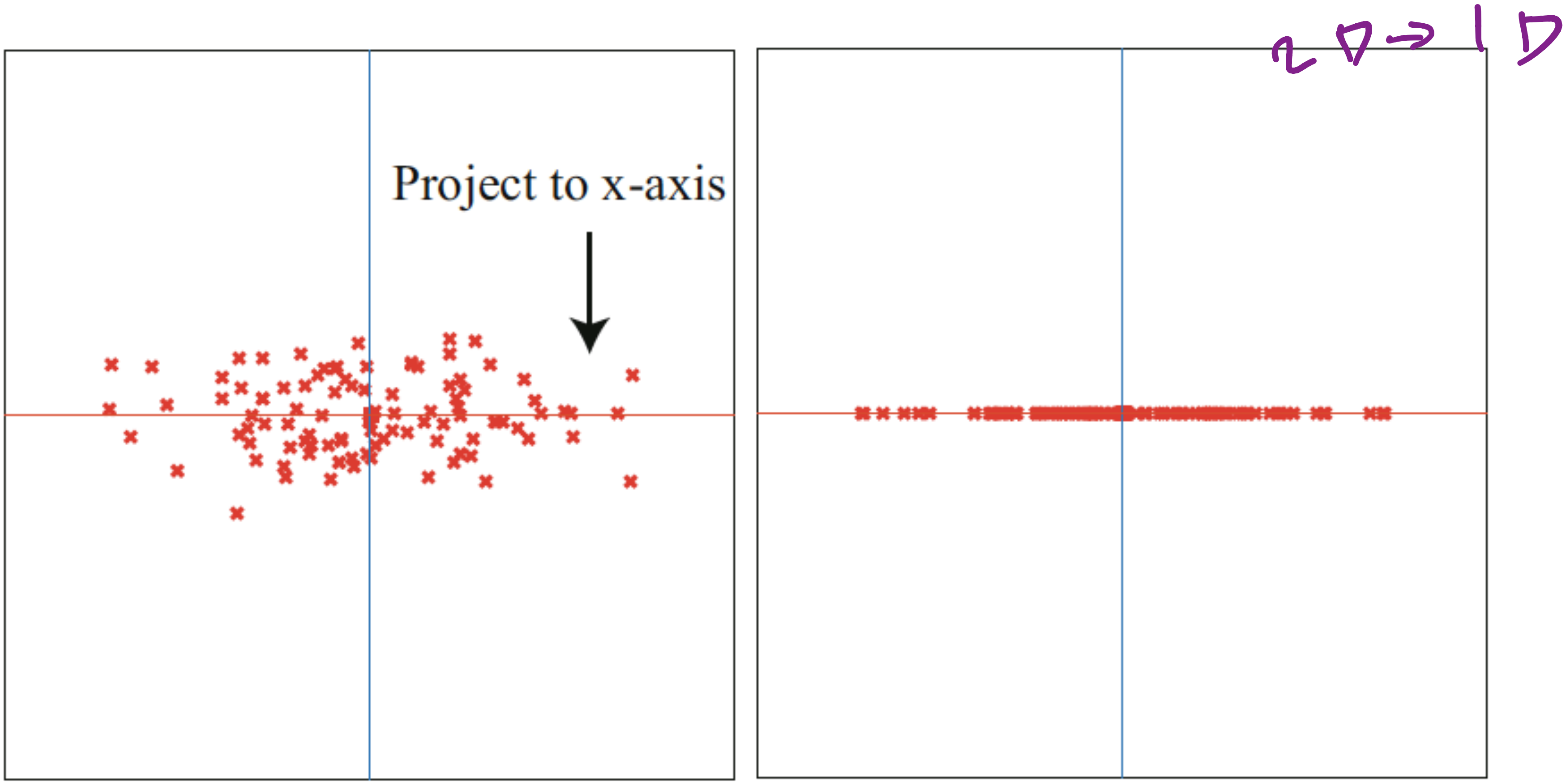
Step 2: Rotate to diagonalize the covariance





Credit: Prof. Forsyth

Step 3: Drop component(s)



Credit: Prof. Forsyth

Principal Components

- The columns of U are the normalized eigenvectors of the Covmat({x}) and are called the **principal components** of the data {x}

Principal components analysis

- We reduce the dimensionality of dataset {**x**} represented by matrix $\boldsymbol{D}_{d\times n}$ from d to s (s < d).
- Step 1. define matrix $\boldsymbol{m}_{d\times n}$ such that $\boldsymbol{m} = \boldsymbol{D} - mean(\boldsymbol{D})$
- Step 2. define matrix $\boldsymbol{r}_{d\times n}$ such that $\boldsymbol{r}_i = \boldsymbol{U}^T \boldsymbol{m}_i$ ↑rotation

  Where $\boldsymbol{U}^T$ satisfies $\boldsymbol{\Lambda} = \boldsymbol{U}^T \; Covmat(\{\boldsymbol{x}\})\boldsymbol{U}$, $\boldsymbol{\Lambda}$ is the diagonalization of $Covmat(\{\boldsymbol{x}\})$ with the eigenvalues sorted in decreasing order, $\boldsymbol{U}$ is the orthonormal eigenvectors' matrix
- Step 3. Define matrix $\boldsymbol{p}_{d\times n}$ such that $\boldsymbol{p}$ is $\boldsymbol{r}$ with the last d-s components of $\boldsymbol{r}$ made zero.

What happened to the mean?

- Step 1.

$$mean(\boldsymbol{m}) = mean(\boldsymbol{D} - mean(\boldsymbol{D})) = 0$$

- Step 2.

$$mean(\boldsymbol{r}) = \boldsymbol{U}^T mean(\boldsymbol{m}) = \boldsymbol{U}^T 0 = 0$$

- Step 3.

$$mean(\boldsymbol{p_i}) = mean(\boldsymbol{r}_i) = 0 \;\; while\ i \in 1 : s$$

$$mean(\boldsymbol{p}_i) = 0 \quad while\ i \in s + 1 : d$$

What happened to the covariances?

- Step 1.

$$Covmat(\boldsymbol{m}) = Covmat(\boldsymbol{D}) = Covmat(\{\boldsymbol{x}\})$$

- Step 2.

$r = U^T m$

$$Covmat(\boldsymbol{r}) = \boldsymbol{U}^T Covmat(\boldsymbol{m})\boldsymbol{U} = \boldsymbol{\Lambda}$$

the property for $Covmat(\{Ax\}) = A\, Covmat(\{x\})\, A^T$

- Step 3. $Covmat(\boldsymbol{p})$ is $\boldsymbol{\Lambda}$ with the last/smallest d-s diagonal terms turned to 0.

Sample covariance matrix

- In many statistical programs, the sample covariance matrix is defined to be

$$Covmat(\boldsymbol{m}) = \frac{\boldsymbol{m_c}\boldsymbol{m_c}^T}{N-1}$$

- Similar to what happens to the unbiased standard deviation

PCA an example

- Step 1.

$$D = \begin{bmatrix} 3 & -4 & 7 & 1 & -4 & -3 \\ 7 & -6 & 8 & -1 & -1 & -7 \end{bmatrix} \Rightarrow mean(\boldsymbol{D}) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\boldsymbol{m} = \begin{bmatrix} 3 & -4 & 7 & 1 & -4 & -3 \\ 7 & -6 & 8 & -1 & -1 & -7 \end{bmatrix}$$

- Step 2.
- Step 3.

PCA an example

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$$\boldsymbol{m} = \begin{bmatrix} 3 & -4 & 7 & 1 & -4 & -3 \\ 7 & -6 & 8 & -1 & -1 & -7 \end{bmatrix}$$

- Step 2.

$$Covmat(\boldsymbol{m}) = \begin{bmatrix} 20 & 25 \\ 25 & 40 \end{bmatrix} \Rightarrow \lambda_1 \simeq 57; \quad \lambda_2 \simeq 3$$

$$\Rightarrow \boldsymbol{U} = \begin{bmatrix} 0.5606288 & -0.8280672 \\ 0.8280672 & 0.5606288 \end{bmatrix} \qquad \boldsymbol{U^T} = \begin{bmatrix} 0.5606288 & 0.8280672 \\ -0.8280672 & 0.5606288 \end{bmatrix}$$

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PCA an example

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$$\Rightarrow \boldsymbol{r} = \boldsymbol{U}^T \boldsymbol{m} = \begin{bmatrix} 7.478 & -7.211 & 10.549 & -0.267 & -3.071 & -7.478 \\ 1.440 & -0.052 & -1.311 & -1.389 & 2.752 & -1.440 \end{bmatrix}$$

- Step 3.

PCA an example

- Step 1.

$$D = \begin{bmatrix} 3 & -4 & 7 & 1 & -4 & -3 \\ 7 & -6 & 8 & -1 & -1 & -7 \end{bmatrix} \Rightarrow mean(\boldsymbol{D}) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

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- Step 2.

$$Covmat(\boldsymbol{m}) = \begin{bmatrix} 20 & 25 \\ 25 & 40 \end{bmatrix} \Rightarrow \lambda_1 \simeq 57; \quad \lambda_2 \simeq 3$$

u_1 u_2

$$\Rightarrow \boldsymbol{U} = \begin{bmatrix} 0.5606288 & -0.8280672 \\ 0.8280672 & 0.5606288 \end{bmatrix} \qquad \boldsymbol{U^T} = \begin{bmatrix} 0.5606288 & 0.8280672 \\ -0.8280672 & 0.5606288 \end{bmatrix}$$

$$\Rightarrow \boldsymbol{r} = \boldsymbol{U}^T \boldsymbol{m} = \begin{bmatrix} 7.478 & -7.211 & 10.549 & -0.267 & -3.071 & -7.478 \\ 1.440 & -0.052 & -1.311 & -1.389 & 2.752 & -1.440 \end{bmatrix}$$

- Step 3.

$$\Rightarrow \boldsymbol{p} = \begin{bmatrix} 7.478 & -7.211 & 10.549 & -0.267 & -3.071 & -7.478 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

→ new coordinates along PC1

What is this matrix for the previous example?

$$\boldsymbol{U}^T Covmat(\boldsymbol{m})\boldsymbol{U} = ?$$

Λ

λ_1

$$= \begin{bmatrix} 57 & 0 \\ 0 & 3 \end{bmatrix}$$

λ_2

The Mean square error of the projection

- The mean square error is the sum of the smallest d-s eigenvalues in $\mathbf{\Lambda}$

$$\frac{1}{N-1}\sum_i \|r_i - p_i\|^2 = \frac{1}{N-1}\sum_i \sum_{j=s+1}^{d} (r_i^{(j)})^2$$

The Mean square error of the projection

- The mean square error is the sum of the smallest d-s eigenvalues in $\mathbf{\Lambda}$

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$$\frac{1}{N-1}\sum_i \|r_i - p_i\|^2 = \frac{1}{N-1}\sum_i \sum_{j=s+1}^{d} (r_i^{(j)})^2 \quad = \sum_{j=s+1}^{d} \sum_i \frac{1}{N-1} (r_i^{(j)})^2$$

$$= \sum_{j=s+1}^{d} var(r_i^{(j)})$$

The Mean square error of the projection

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$$\frac{1}{N-1}\sum_i \|r_i - p_i\|^2 = \frac{1}{N-1}\sum_i \sum_{j=s+1}^{d} (r_i^{(j)})^2 = \sum_{j=s+1}^{d} \sum_i \frac{1}{N-1}(r_i^{(j)})^2$$

$$= \sum_{j=s+1}^{d} var(r_i^{(j)})$$

$$= \sum_{j=s+1}^{d} \lambda_j$$

PCA of Immune Cells' Data

> res1
$values Eigenvalues
[1] 4.7642829 2.1486896 1.3730662 0.4968255

Eigenvectors
$vectors

```
          [,1]       [,2]       [,3]       [,4]
[1,]  0.2476698  0.00801294 -0.6822740  0.6878210
[2,]  0.3389872 -0.72010997 -0.3691532 -0.4798492
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```
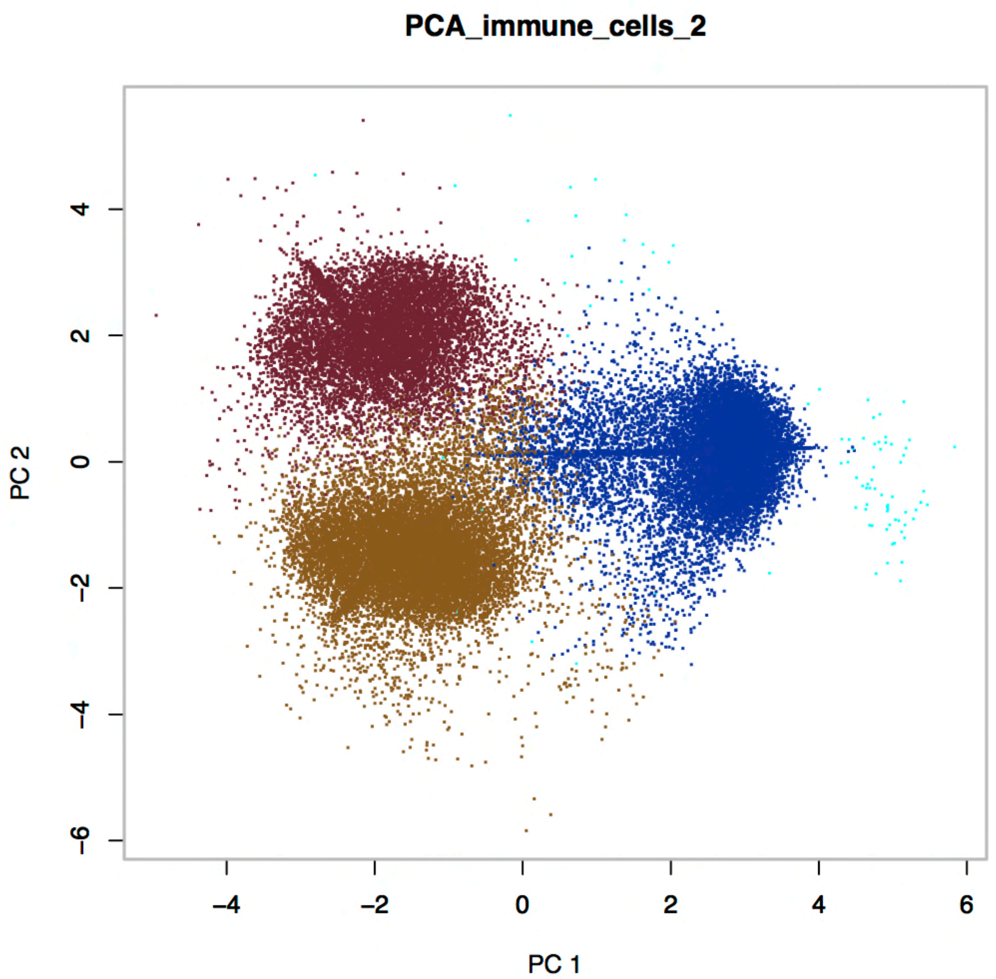



What is the percentage of variance that PC1 covers?

Given the eigenvalues: 4.7642829 2.1486896 1.3730662 0.4968255, what is the percentage that PC1 covers?

A. 54%
B. 16%
C. 25%

$$\doteq \frac{4.764}{4.764+2.1487+1.373+0.4968}$$

Notebook on PCA

https://courses.engr.illinois.edu/cs361/sp2019/notebooks/L18.html

Reconstructing the data

- Given the projected data $\boldsymbol{p}_{d \times n}$ and mean({x}), we can approximately reconstruct the original data

$$\widehat{\boldsymbol{D}} = \boldsymbol{U}\boldsymbol{p} + mean(\{\boldsymbol{x}\})$$

↑ rotation back

- Each reconstructed data item $\widehat{\boldsymbol{D}_i}$ is a linear combination of the columns of $\boldsymbol{U}$ weighted by $\boldsymbol{p}_i$

- The columns of $\boldsymbol{U}$ are the normalized eigenvectors of the Covmat({x}) and are called the **principal components** of the data {x}

End-to-end mean square error

- Each $\boldsymbol{x}_i$ becomes $\boldsymbol{r}_i$ by translation and rotation
- Each $\boldsymbol{p}_i$ becomes $\widehat{\boldsymbol{x}}_i$ by the opposite rotation and translation
- Therefore the end to end mean square error is:

$$\frac{1}{N-1}\sum_i \|\widehat{\boldsymbol{x}}_i - \boldsymbol{x}_i\|^2 = \frac{1}{N-1}\sum_i \|\boldsymbol{r}_i - \boldsymbol{p}_i\|^2 = \sum_{j=s+1}^{d} \lambda_j$$

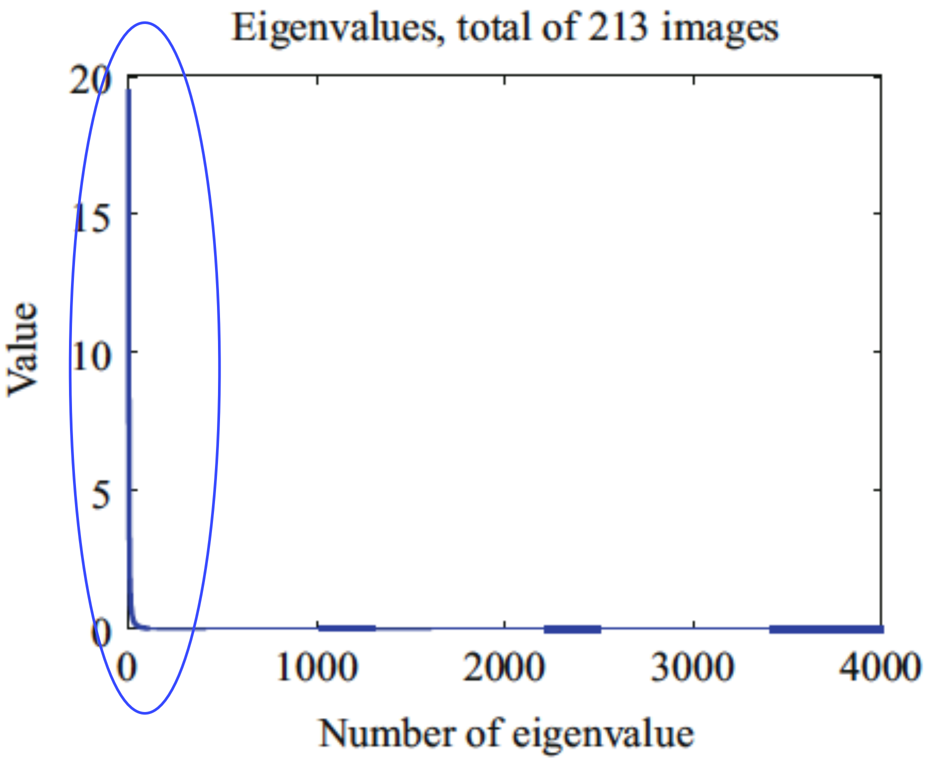
- $\lambda_{s+1}, \ldots, \lambda_d$ are the smallest d-s eigenvalues of the Covmat({x})

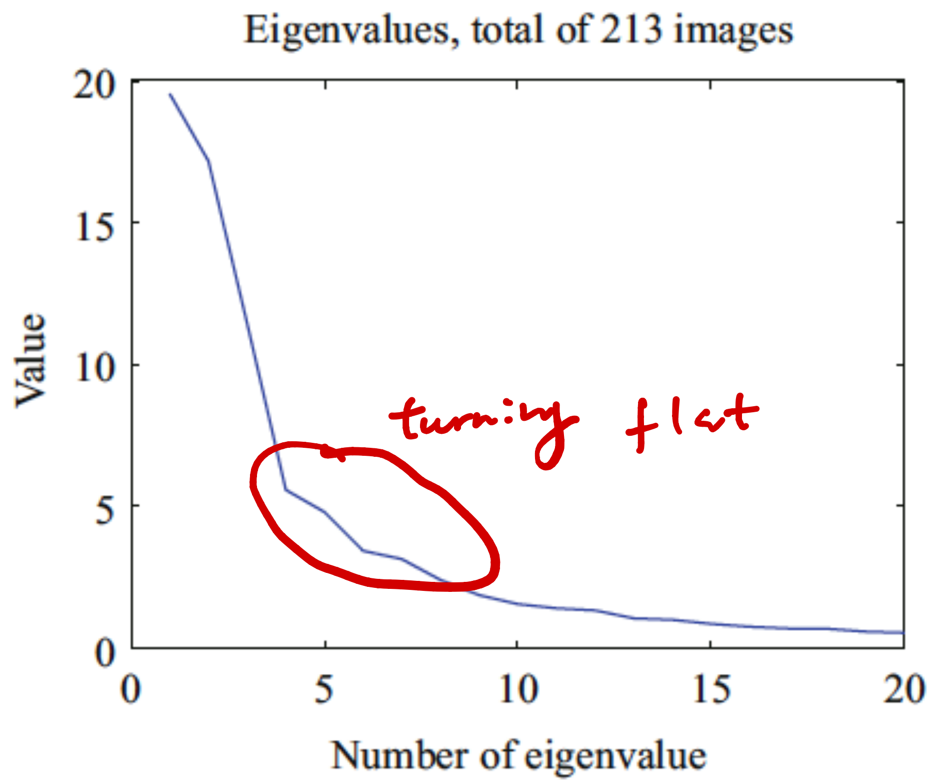
PCA: Human face data

- The dataset consists of 213 images $N = 213$
- Each image is grayscale and has 64 by 64 resolution
- We can treat each image as a vector with dimension d = 4096 $64 \times 64 = 4096$

Credit: Prof. Forsyth

How quickly the eigenvalues decrease?





Credit: Prof. Forsyth

What do the principal components of the images look like?

Mean image

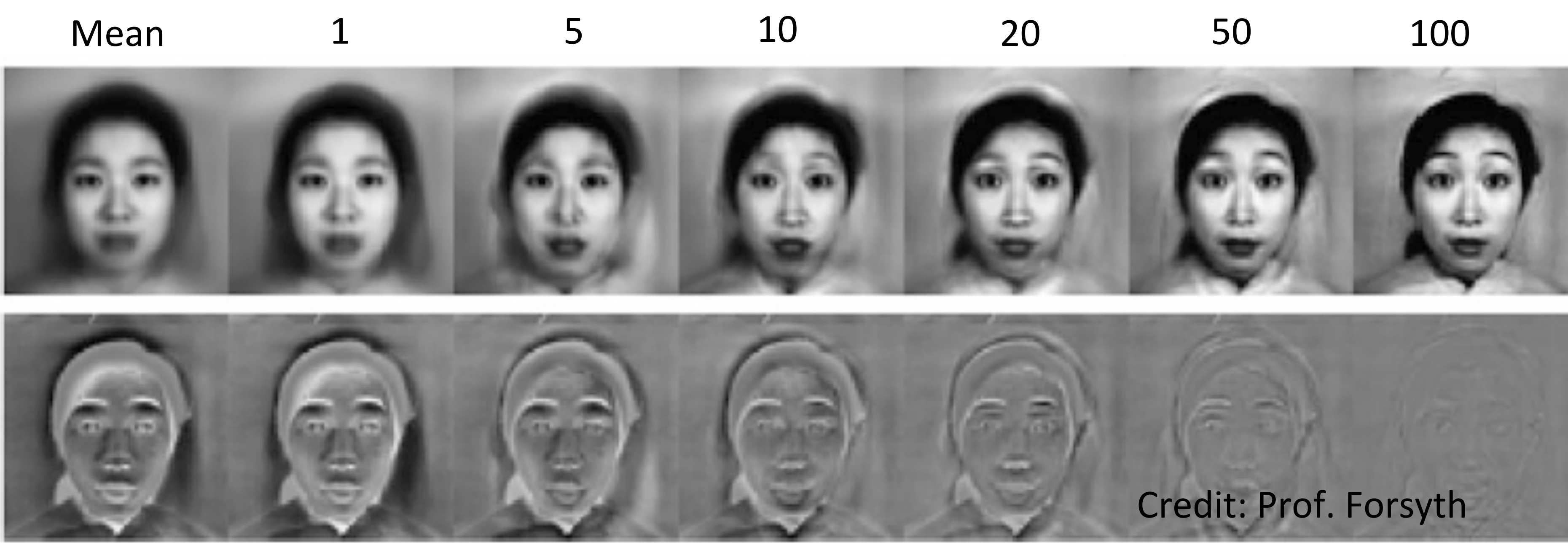
The first 16 principal components arranged into images

Credit: Prof. Forsyth

Reconstruction of the image

The original

1^{st} row show the reconstructions using some number of principal components
2^{nd} row show the corresponding errors



Q. Which are true?

A . PCA allows us to project data to the direction along which the data has the biggest variance
B. PCA allows us to compress data
C. PCA uses linear transformation to show patterns of data
D. PCA allows us to visualize data in lower dimensions
E. All of the above

Assignments

- Read Chapter 10 of the textbook
- Next time: Intro to classification

$$\underset{\|w\|=1}{\operatorname{argmax}} \left\{ \frac{w^T X^T X w}{w^T w} \right\}$$ → Rayleigh Quotient

$= \text{the largest eigenvector } u_1$

$= PC_1$

Additional References

- Robert V. Hogg, Elliot A. Tanis and Dale L. Zimmerman. “Probability and Statistical Inference”
- Morris H. Degroot and Mark J. Schervish "Probability and Statistics”

See you next time

See You!