Dimensionality Reduction (PCA)

Machine Learning

Prof. Sandra Avila
Institute of Computing (IC/Unicamp)

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Why is Dimensionality Reduction useful?

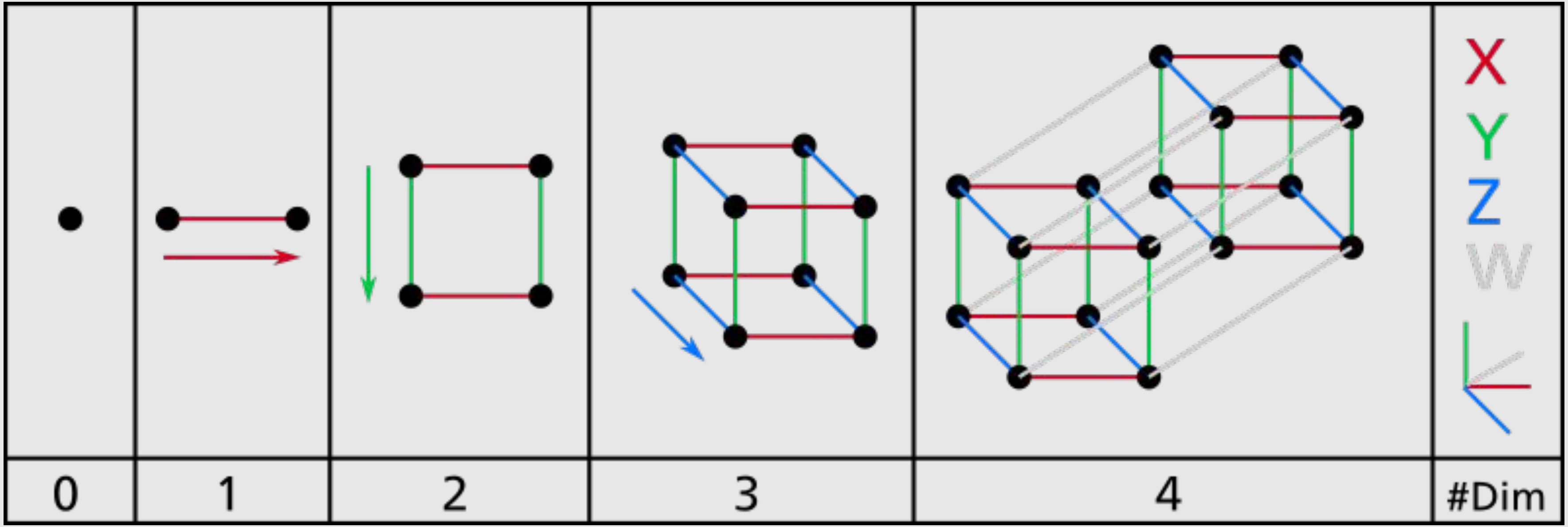
- Data Compression
  - Reduce **time complexity**: less computation required
  - Reduce **space complexity**: less number of features
  - **More interpretable**: it removes noise
- Data Visualization
- To mitigate **“the curse of dimensionality”**

Today's Agenda

- The Curse of Dimensionality
- PCA (Principal Component Analysis)
    - PCA Formulation
    - PCA Algorithm
    - Choosing *k*

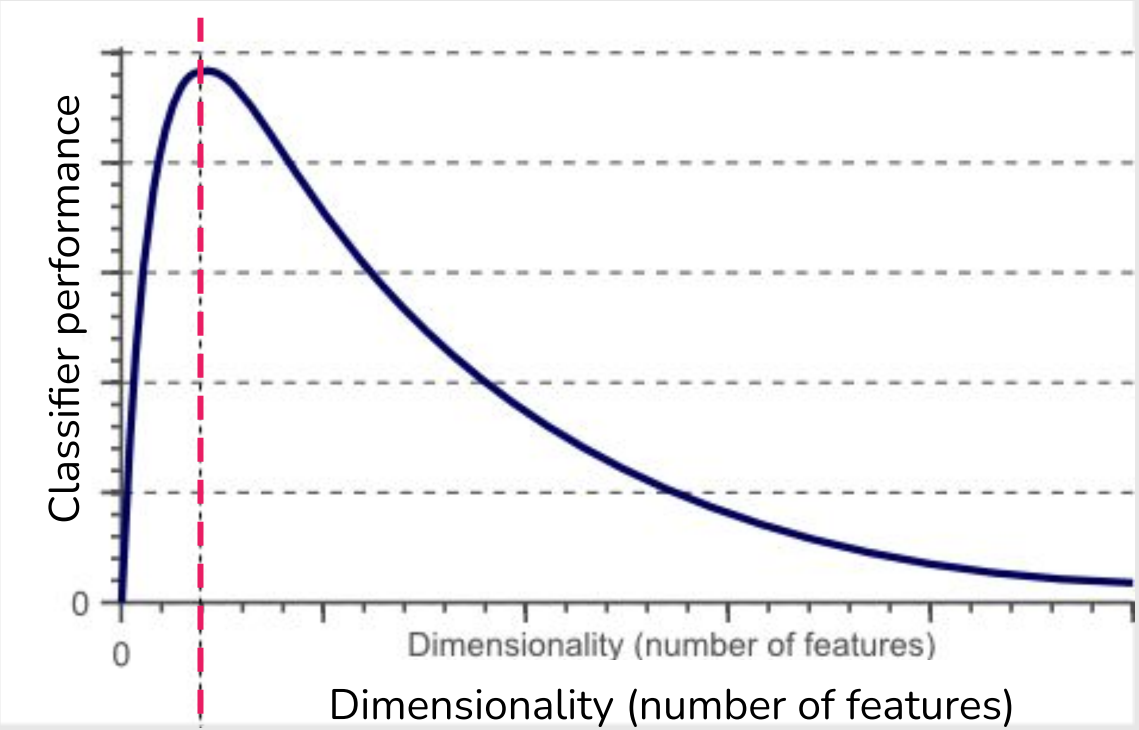
The Curse of Dimensionality

The Curse of Dimensionality



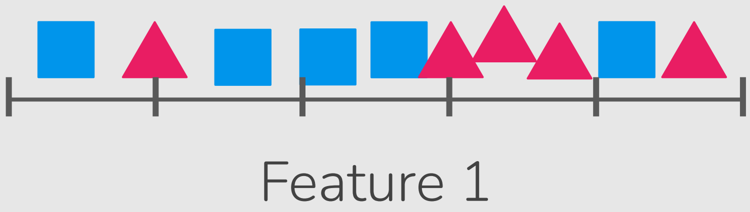
Even a basic 4D hypercube is incredibly hard to picture in our mind.

The Curse of Dimensionality



The Curse of Dimensionality

As the dimensionality of data grows, the density of observations becomes lower and lower and lower.



10 samples
1 dimension: 5 regions

The Curse of Dimensionality

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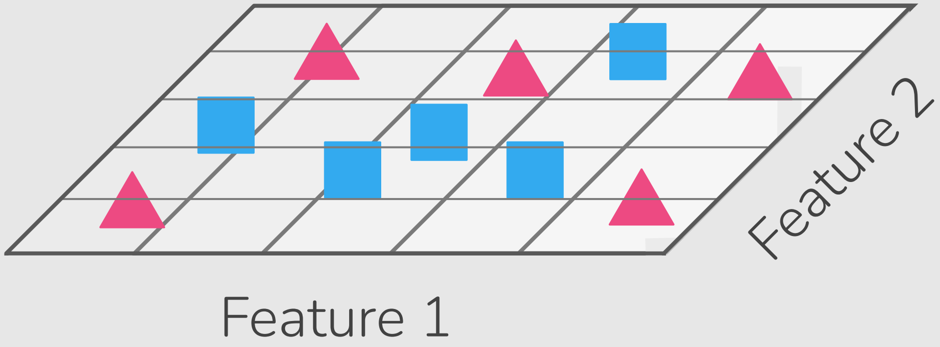
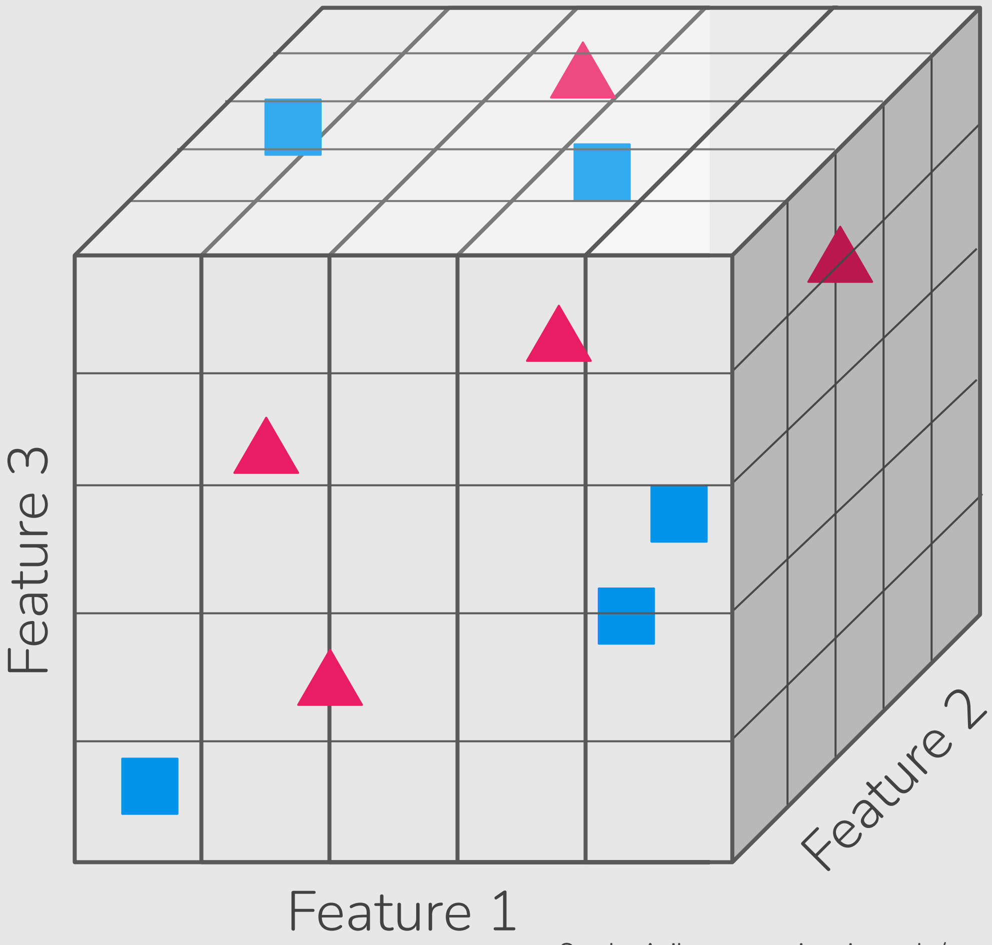
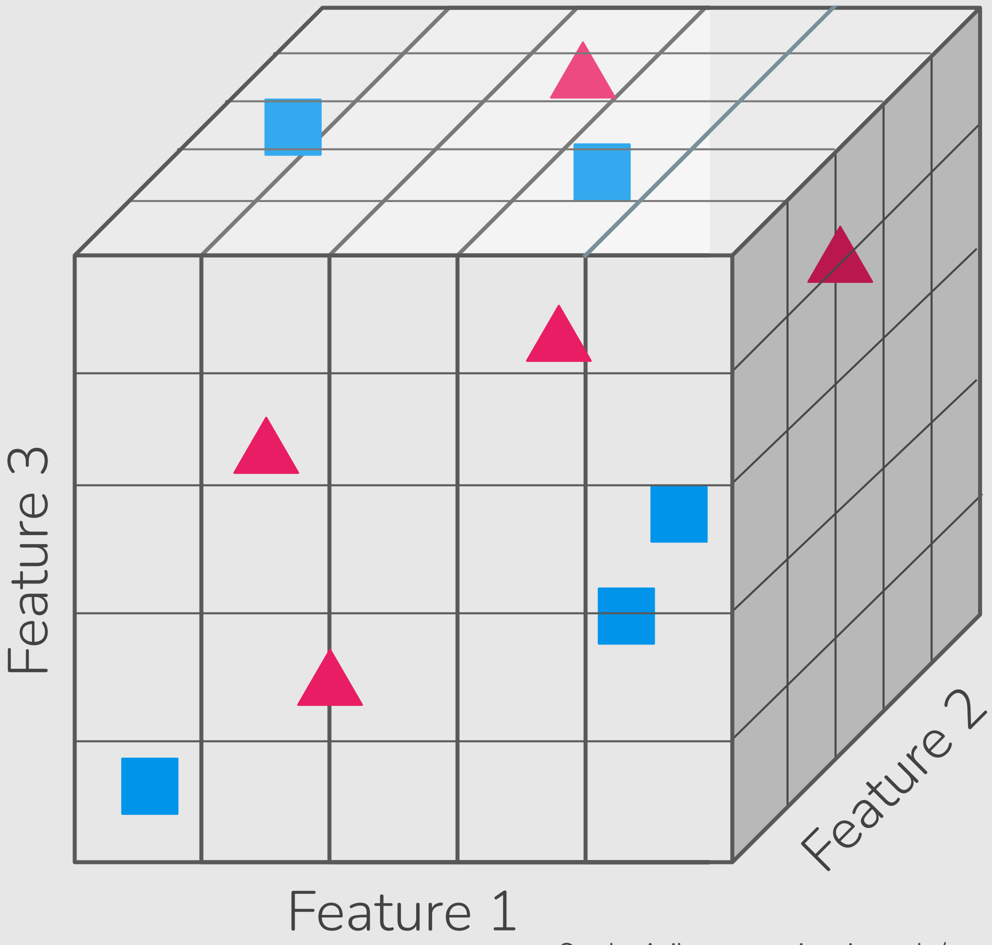


10 samples
2 dimensions: 25 regions



As the dimensionality of data grows, the density of observations becomes lower and lower and lower.

10 samples
3 dimensions: 125 regions



- 1 dimension: the sample density is 10/5 = 2 samples/interval
- 2 dimensions: the sample density is 10/25 = 0.4 samples/interval
- 3 dimensions: the sample density is 10/125 = 0.08 samples/interval

The Curse of Dimensionality: Solution?

- **Increase the size of the training set** to reach a sufficient density of training instances.
- Unfortunately, the number of training instances required to reach a given density grows exponentially with the number of dimensions.

How to reduce dimensionality?

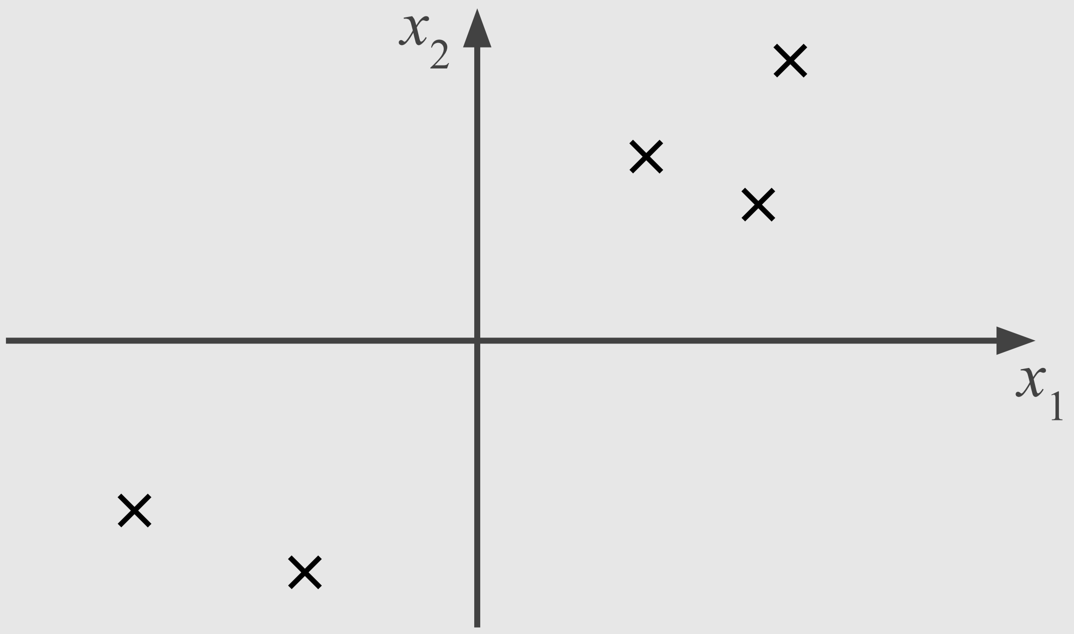
- **Feature Selection:** choosing a subset of all the features (the ones more informative).
    - $\mathbf{x_1}, x_2, \mathbf{x_3}, x_4, \mathbf{x_5}$
- **Feature Extraction:** create a subset of new features by combining the existing ones.
    - $z = f(x_1, x_2, x_3, x_4, x_5)$

PCA: Principal Component Analysis

Principal Component Analysis (PCA)

- The most popular dimensionality reduction algorithm.
- PCA have two steps:
  - It **identifies the hyperplane** that lies closest to the data.
  - It **projects** the data onto it.

Problem Formulation (PCA)



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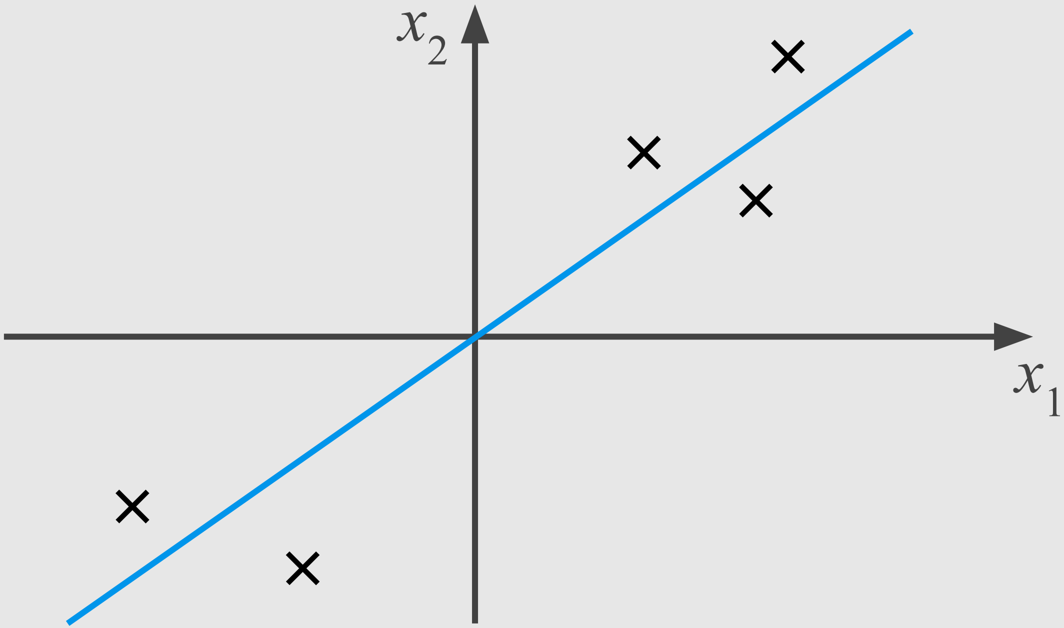

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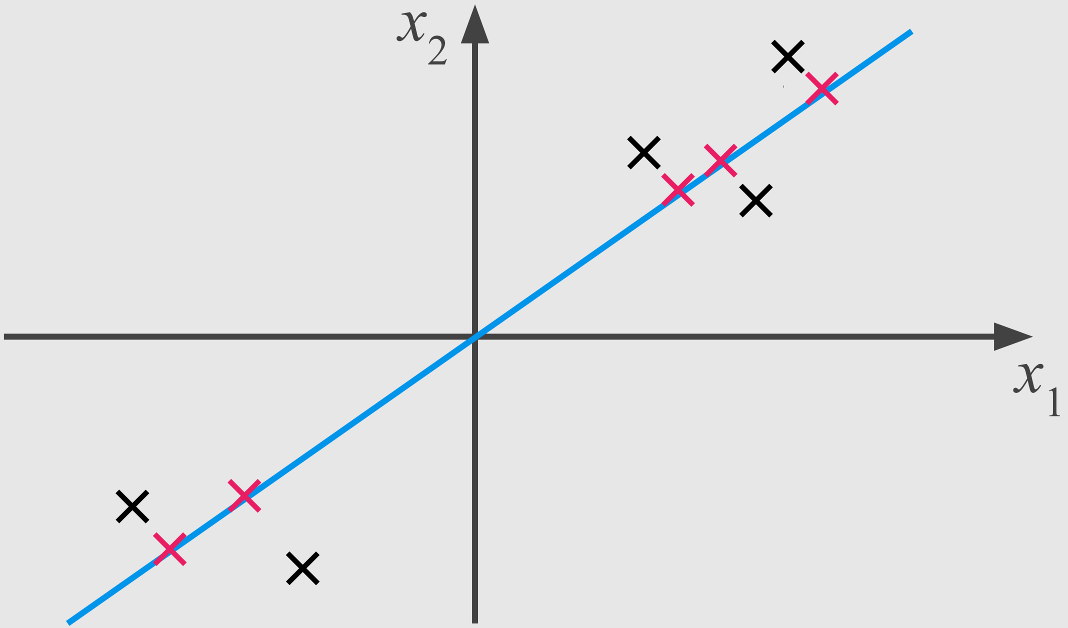

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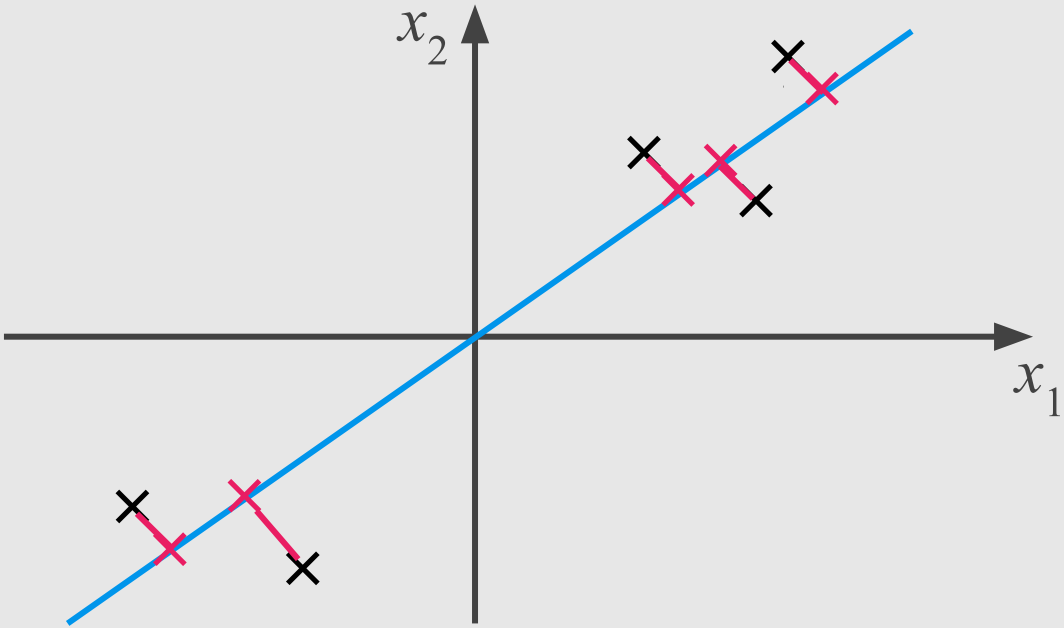

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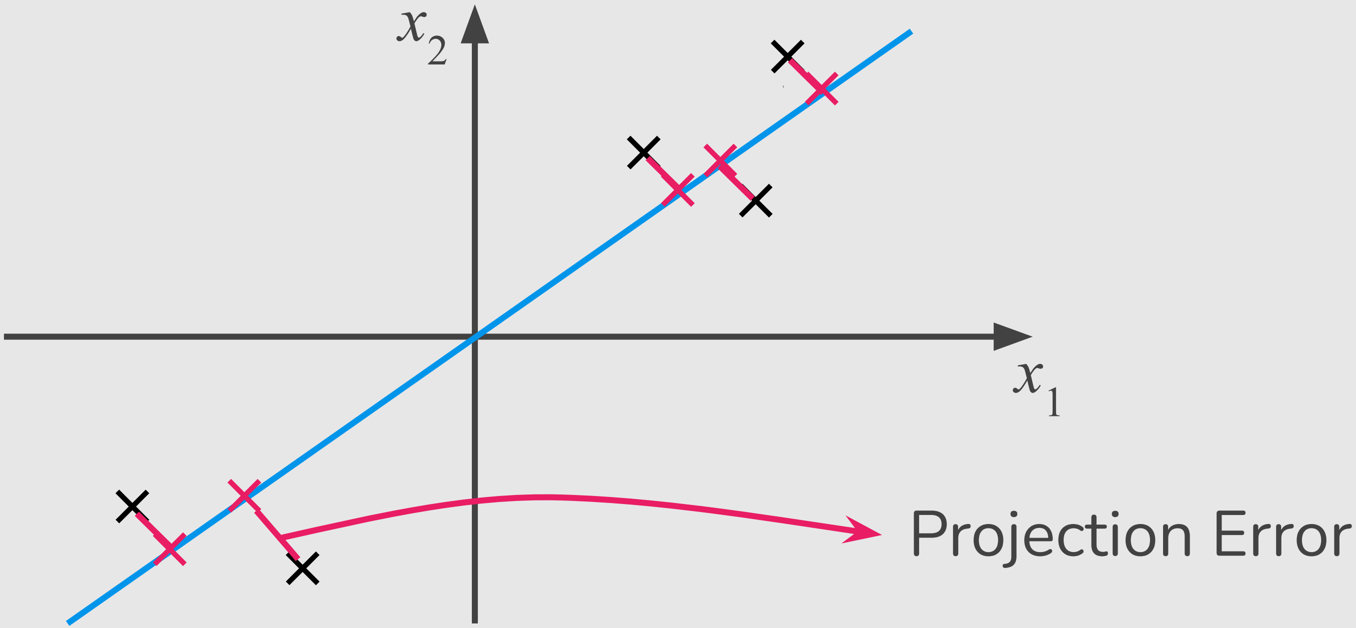

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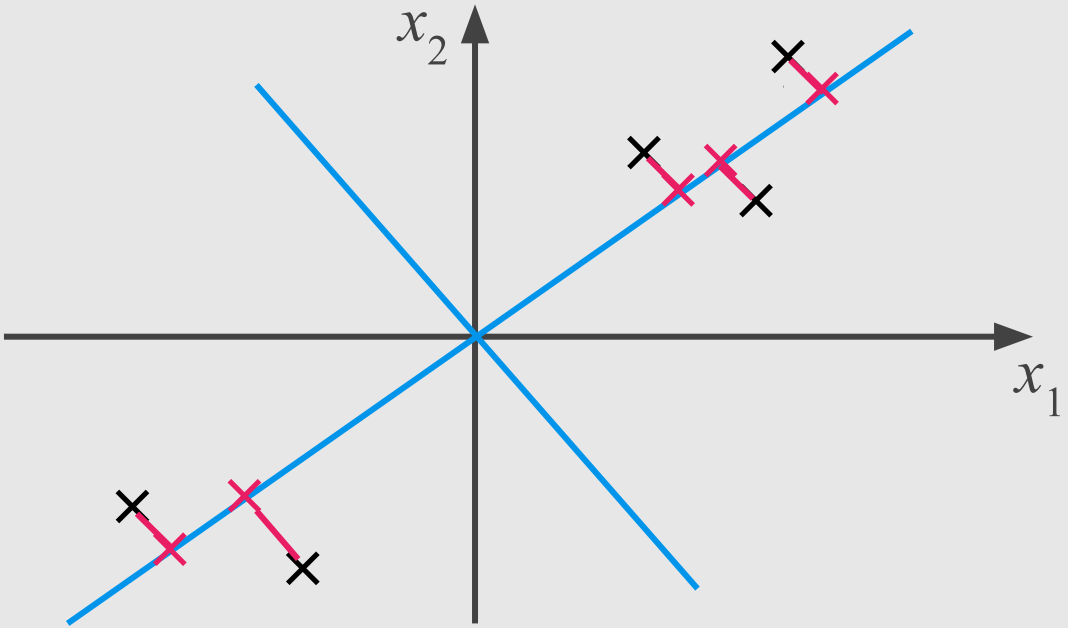

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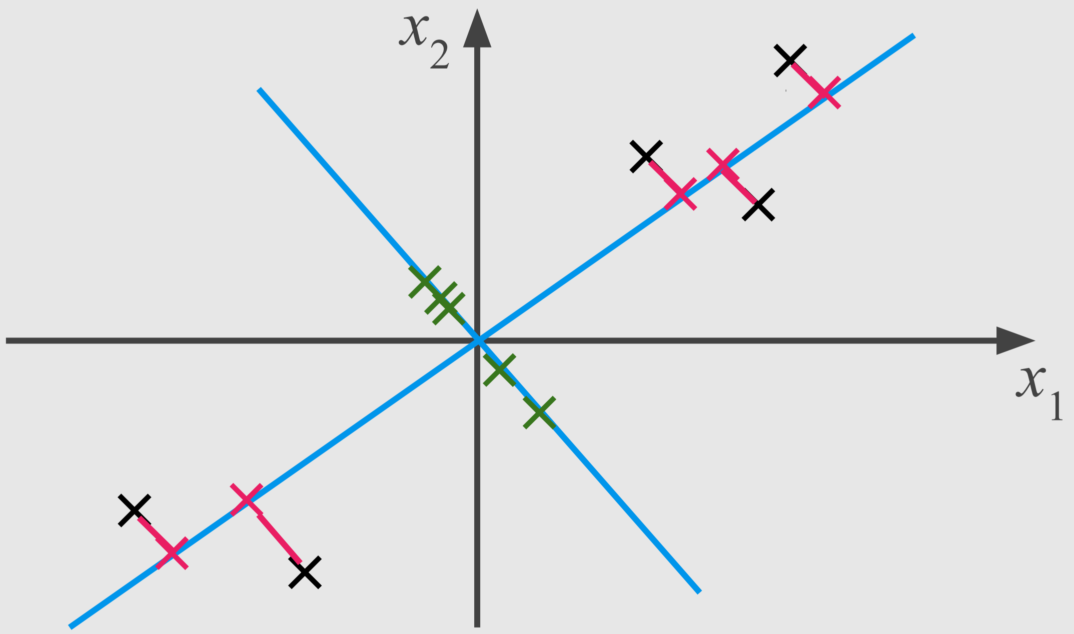

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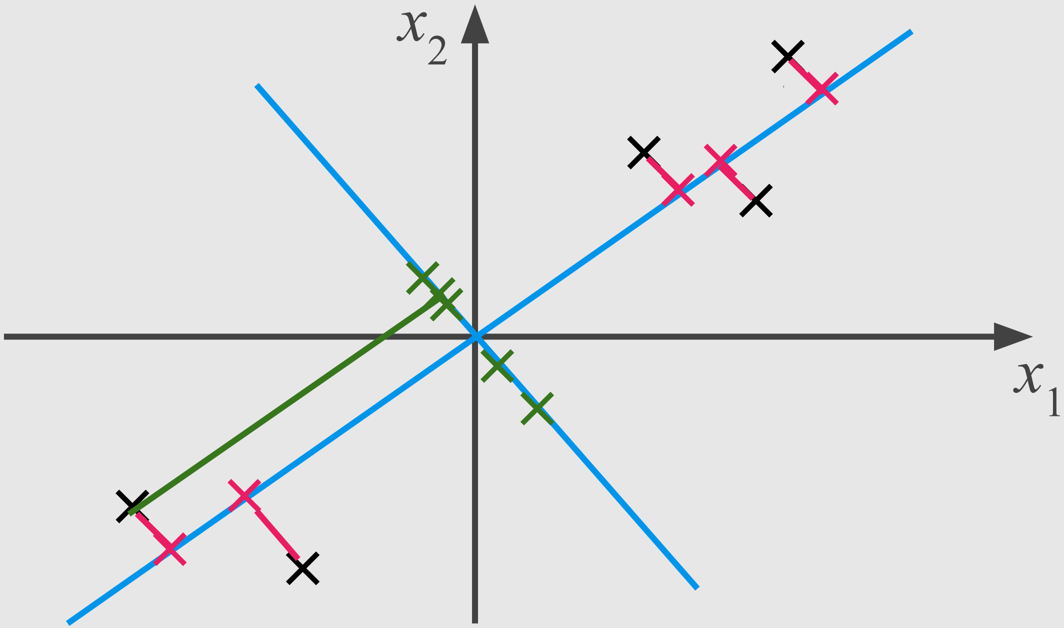

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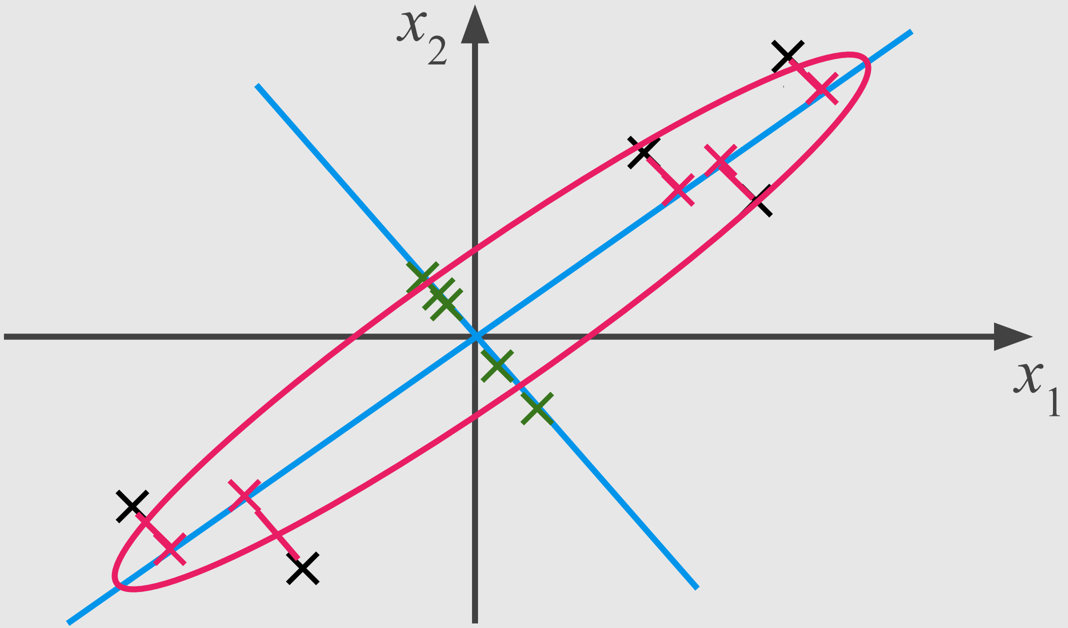

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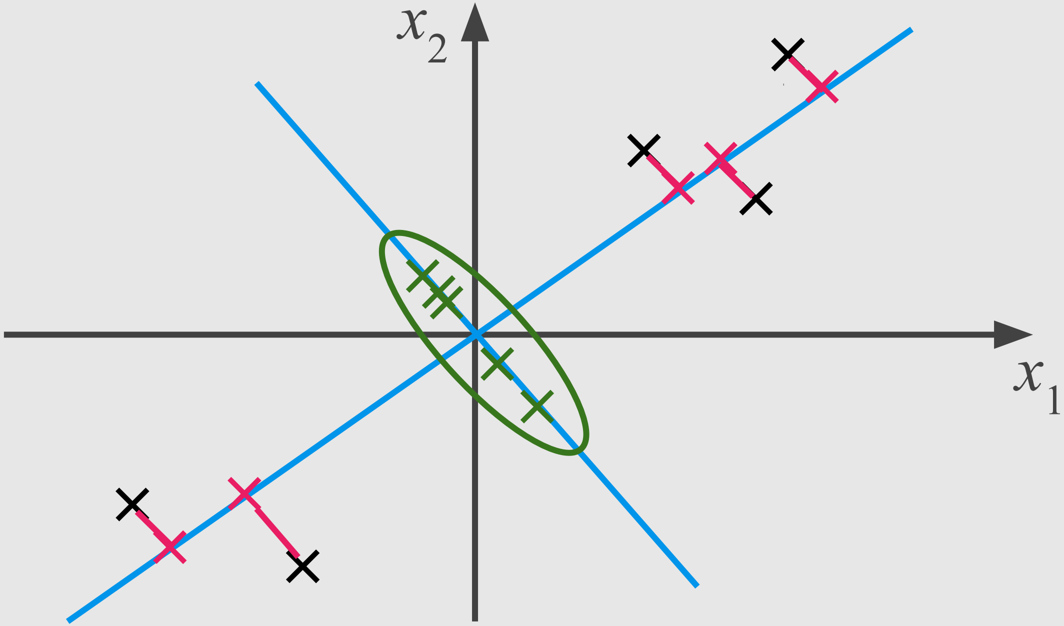
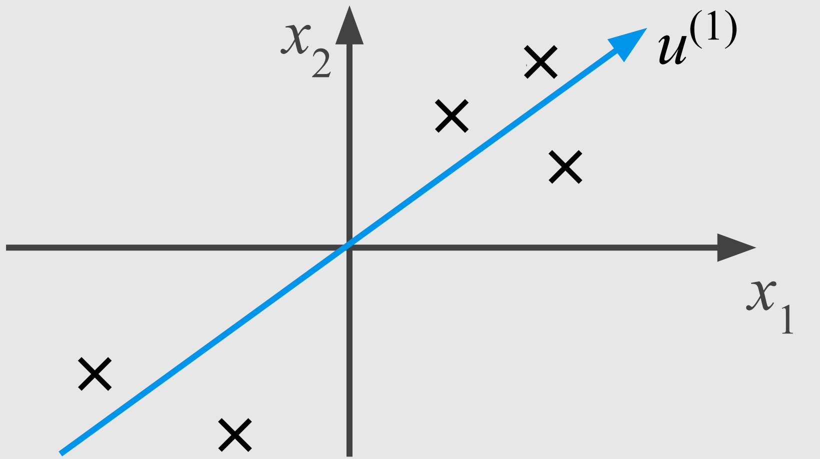


Problem Formulation (PCA)

- Reduce from 2-dimension to 1-dimension: Find a direction (a vector $u^{(1)} \in \mathbb{R}^n$) onto which to project the data so as to minimize the projection error.



Problem Formulation (PCA)

- Reduce from n-dimension to k-dimension: Find k vectors $u^{(1)}, u^{(2)}, \ldots, u^{(k)}$ onto which to project the data, so as to minimize the projection error.

PCA Algorithm
By Eigen Decomposition

PCA in a Nutshell (Eigen Decomposition)

1. Center the data (and normalize)
2. Compute covariance matrix $\mathbf{\Sigma}$
3. Find eigenvectors u and eigenvalues λ
4. Sort eigenvalues and pick first k eigenvectors
5. Project data to k eigenvectors

PCA in a Nutshell (Eigen Decomposition)

1. Center the data (and normalize)
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Data Preprocessing

Training set: $x^{(1)}, x^{(2)}, \ldots, x^{(m)}$

Preprocessing (feature scaling/mean normalization):

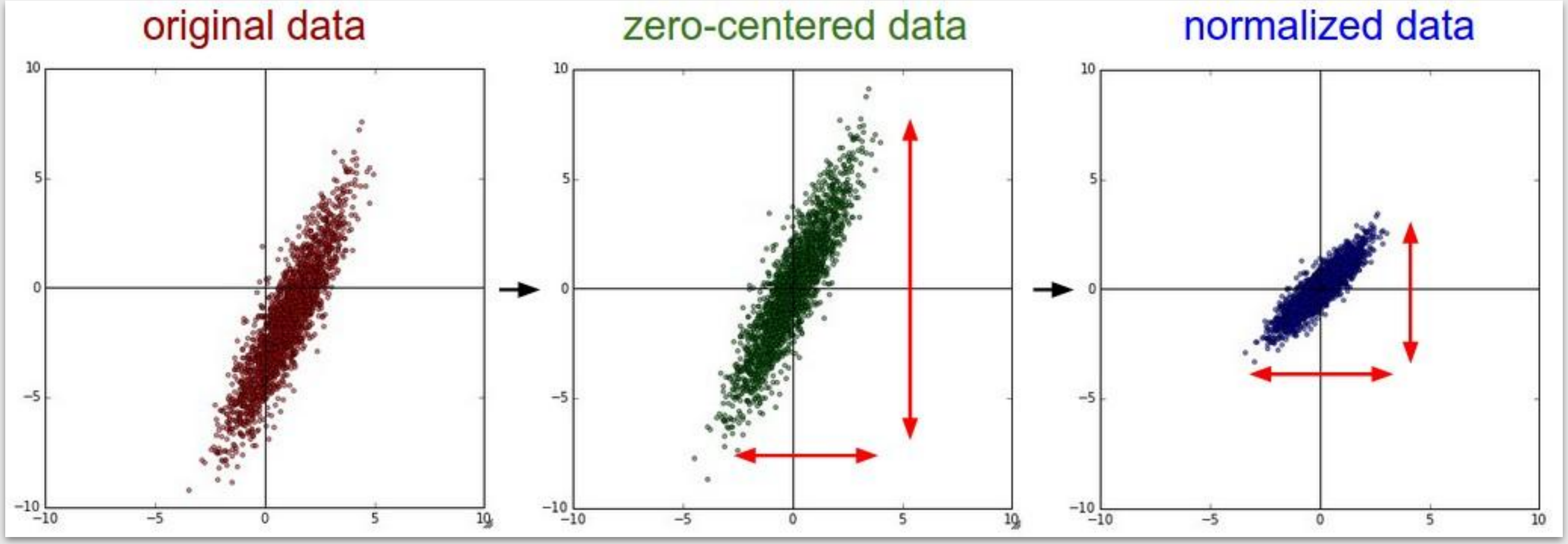
$$\mu_j = \frac{1}{m}\sum_{i=1}^{m} x_j^{(i)}$$

Center the data

Replace each $x_j^{(i)}$ with $x_j - \mu_j$.

If different features on different scales, scale features to have comparable range of values.

Data Preprocessing



Credit: http://cs231n.github.io/neural-networks-2/

PCA in a Nutshell (Eigen Decomposition)

1. Center the data (and normalize)
2. **Compute covariance matrix $\boldsymbol{\Sigma}$**
3. Find eigenvectors u and eigenvalues λ
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PCA Algorithm

Reduce data from n-dimensions to k-dimensions

Compute "covariance matrix":

$$\Sigma = \frac{1}{m} \sum_{i=1}^{n} (x^{(i)})(x^{(i)})^{\mathrm{T}} \Rightarrow n \times n \text{ matrix}$$

PCA Algorithm

Reduce data from n-dimensions to k-dimensions

Compute "covariance matrix":

$$\Sigma = \frac{1}{m} \sum_{i=1}^{n} (x^{(i)})(x^{(i)})^{\mathrm{T}} \Rightarrow n \times n \text{ matrix}$$

Covariance of dimensions x_1 and x_2:

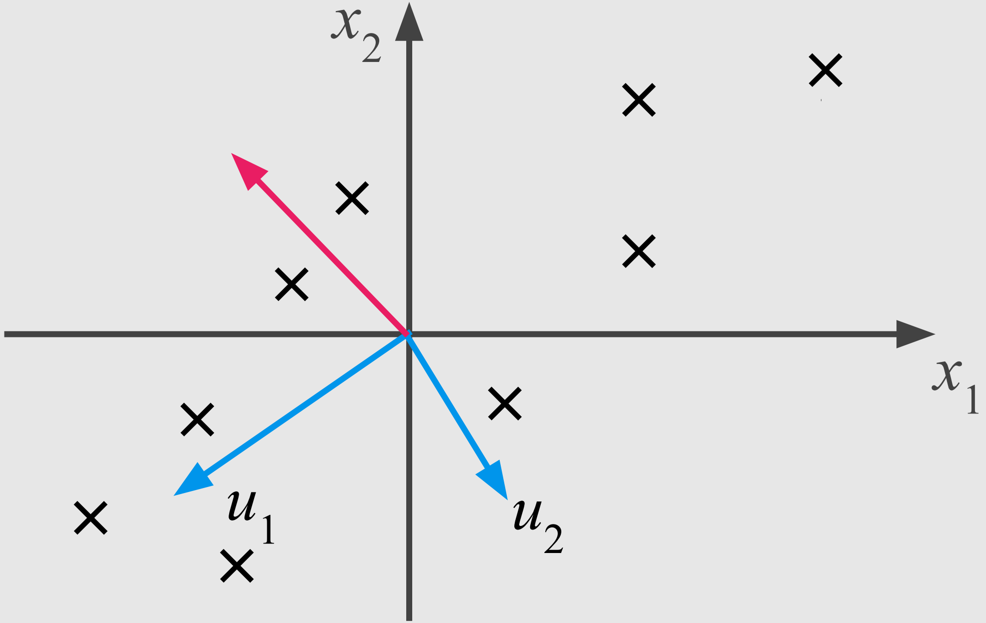
- Do x_1 and x_2 tend to increase together?
- or does x_2 decrease as x_1 increases?

$$\begin{array}{cc} & \begin{array}{cc} x_1 & x_2 \end{array} \\ \begin{array}{c} x_1 \\ x_2 \end{array} & \begin{bmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{bmatrix} \end{array}$$

PCA Algorithm

Multiple a vector by **Σ** :

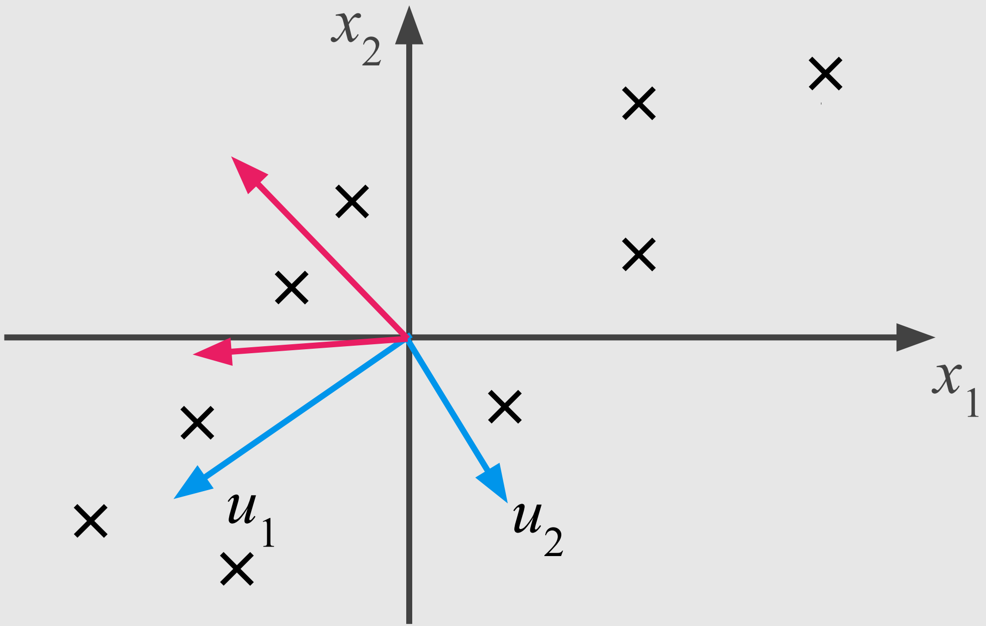
$$\begin{bmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{bmatrix} \times \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$



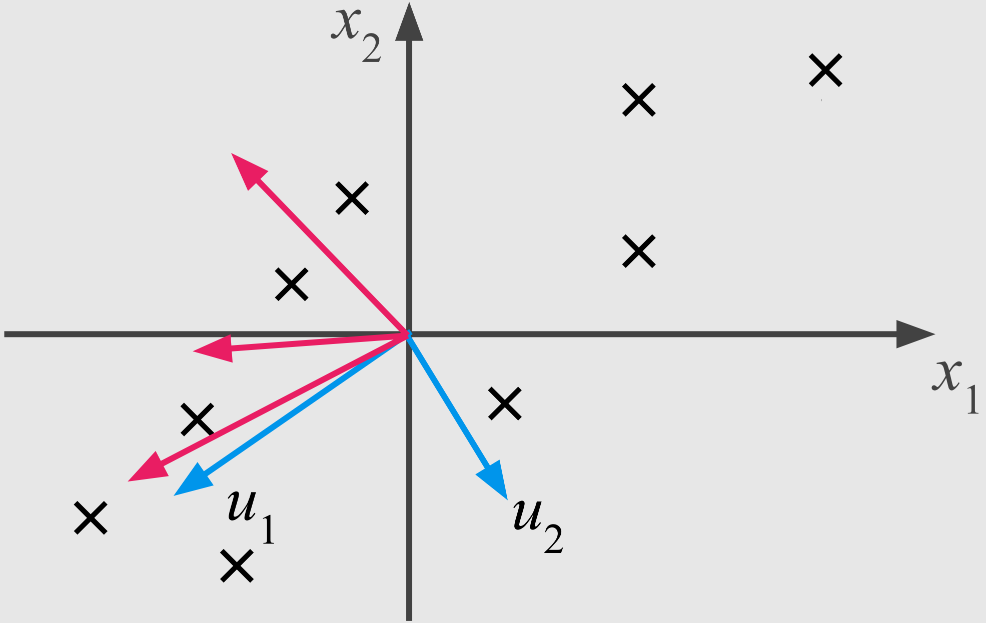
PCA Algorithm

Multiple a vector by $\boldsymbol{\Sigma}$:

$$\begin{bmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{bmatrix} \times \begin{bmatrix} -1 \\ 1 \end{bmatrix} = \begin{bmatrix} -1.2 \\ -0.2 \end{bmatrix}$$



PCA Algorithm



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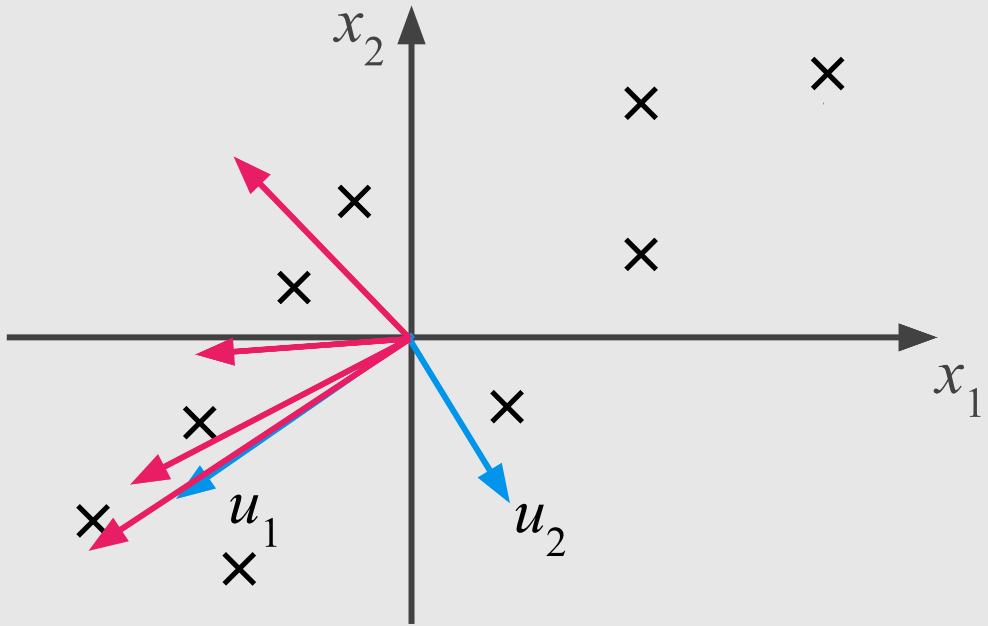
PCA Algorithm



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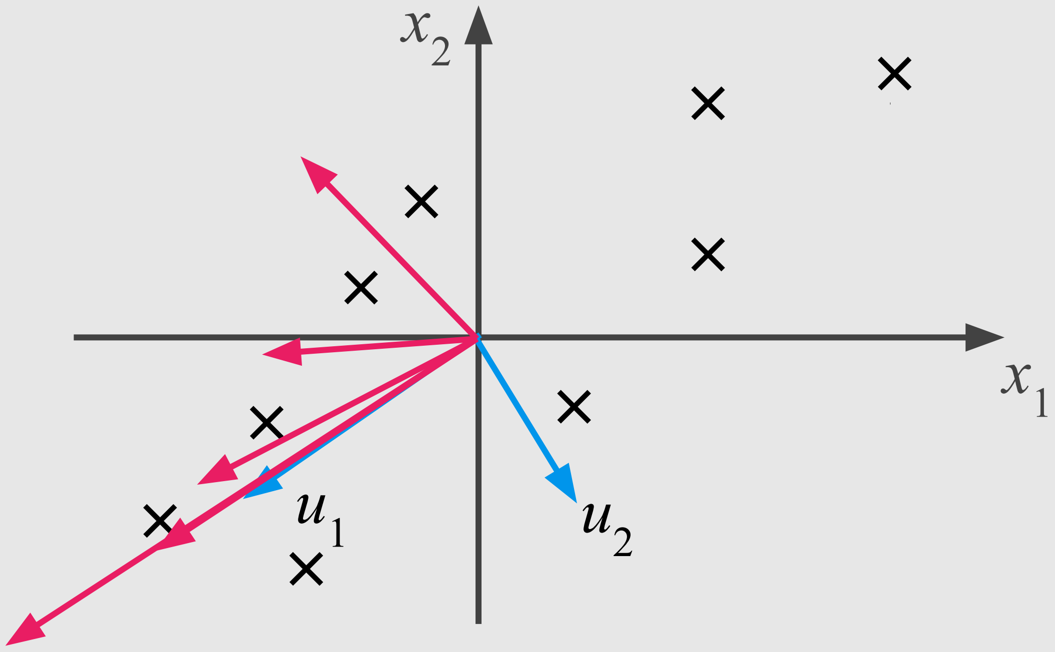
$$\begin{bmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{bmatrix} \times \begin{bmatrix} -2.5 \\ -1.0 \end{bmatrix} = \begin{bmatrix} -6.0 \\ -2.7 \end{bmatrix}$$

PCA Algorithm



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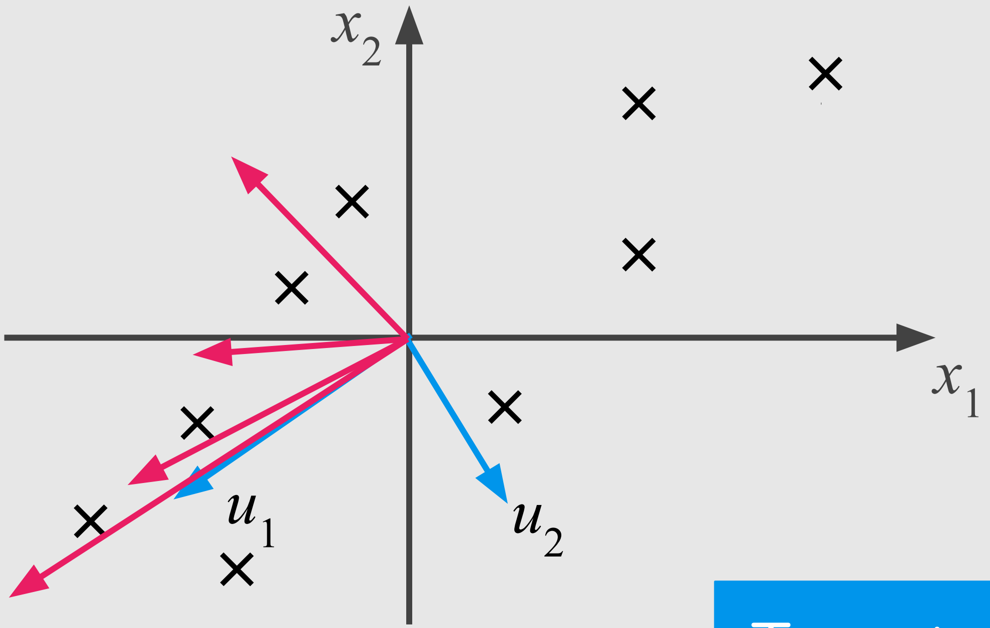
$$\begin{bmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{bmatrix} \times \begin{bmatrix} -6.0 \\ -2.7 \end{bmatrix} = \begin{bmatrix} -14.1 \\ -6.4 \end{bmatrix}$$

PCA Algorithm



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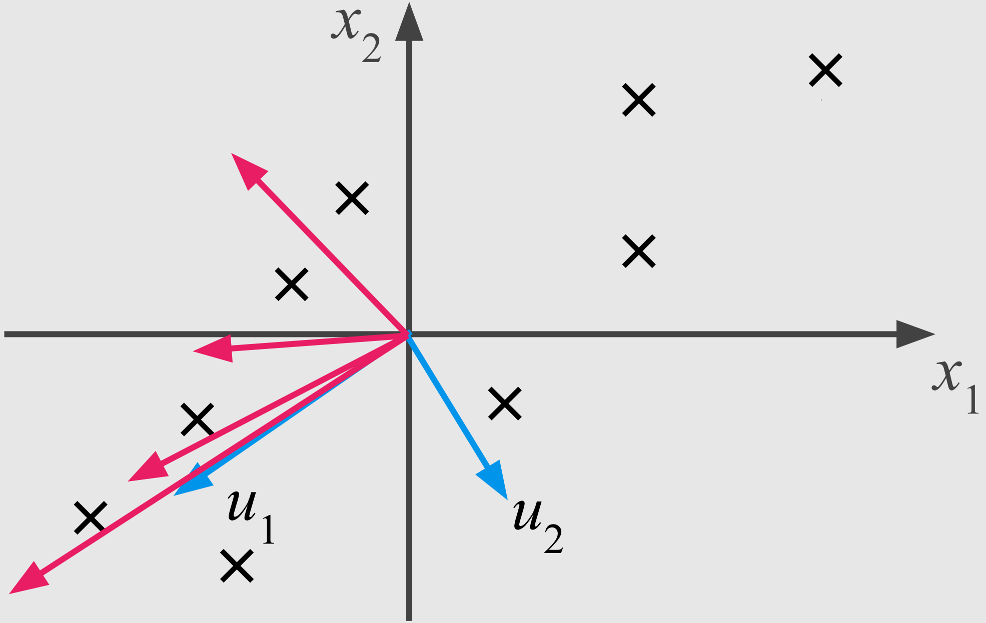
Turns towards direction of variation

PCA Algorithm

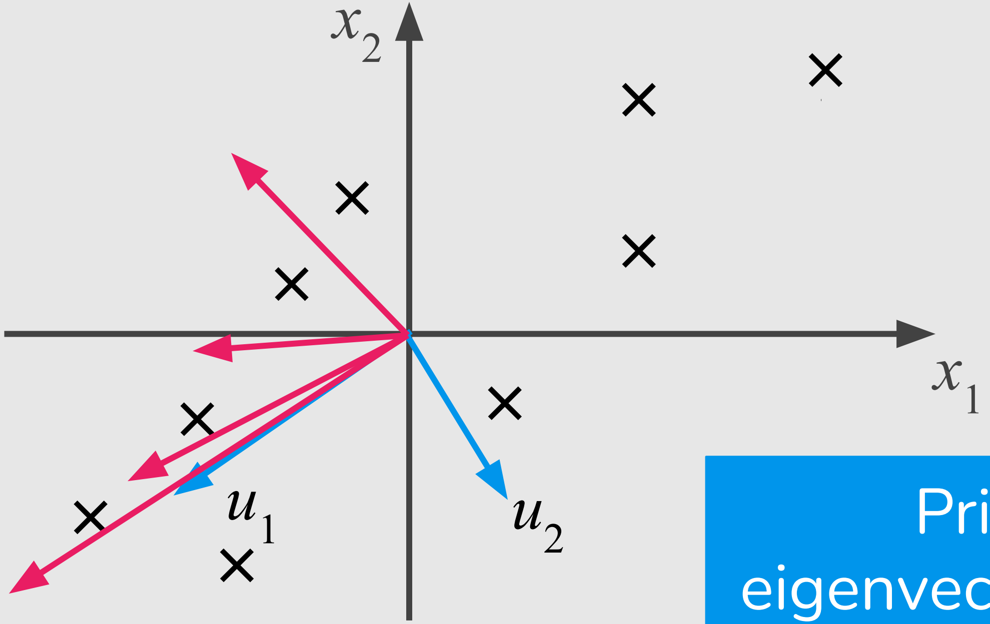


Want vectors u which aren't turned: $\mathbf{\Sigma} u = \lambda u$

u = eigenvectors of $\mathbf{\Sigma}$

λ = eigenvalues

PCA Algorithm



Want vectors u which aren't turned: $\boldsymbol{\Sigma} u = \lambda u$

u = eigenvectors of $\boldsymbol{\Sigma}$

λ = eigenvalues

Principal components = eigenvectors w. largest eigenvalues

PCA in a Nutshell (Eigen Decomposition)

1. Center the data (and normalize)
2. Compute covariance matrix $\mathbf{\Sigma}$
3. **Find eigenvectors $\boldsymbol{u}$ and eigenvalues $\boldsymbol{\lambda}$**
4. Sort eigenvalues and pick first k eigenvectors
5. Project data to k eigenvectors

Finding Principal Components

1. Find eigenvalues by solving: $\det(\mathbf{\Sigma} - \lambda \mathrm{I}) = 0$

$$\det\begin{bmatrix} 2.0-\lambda & 0.8 \\ 0.8 & 0.6-\lambda \end{bmatrix} = (2.0-\lambda)(0.6-\lambda)-(0.8)(0.8) = \lambda^2-2.6\lambda+0.56 = 0$$

$$\{\lambda_1,\lambda_2\} = \{2.36,0.23\}$$

Finding Principal Components

2. Find i^{th} eigenvector by solving: $\mathbf{\Sigma} u_i = \lambda_i u_i$

Finding Principal Components

2. Find i^{th} eigenvector by solving: $\mathbf{\Sigma} u_i = \lambda_i u_i$

$$\begin{bmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{bmatrix} \begin{bmatrix} u_{11} \\ u_{12} \end{bmatrix} = 2.36 \begin{bmatrix} u_{11} \\ u_{12} \end{bmatrix} \Rightarrow \begin{matrix} 2.0u_{11} + 0.8u_{12} = 2.36u_{11} \\ 0.8u_{11} + 0.6u_{12} = 2.36u_{12} \end{matrix} \Rightarrow u_{11} = 2.2u_{12}$$

$$\Downarrow$$

$$\mathrm{u}_1 \sim \begin{bmatrix} 2.2 \\ 1 \end{bmatrix}$$

$$\Downarrow \text{ Want } \|u_1\| = 1$$

$$\begin{bmatrix} 0.91 \\ 0.41 \end{bmatrix}$$

$$\begin{bmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{bmatrix} \begin{bmatrix} u_{21} \\ u_{22} \end{bmatrix} = 0.23 \begin{bmatrix} u_{21} \\ u_{22} \end{bmatrix} \Rightarrow u_2 = \begin{bmatrix} -0.41 \\ 0.91 \end{bmatrix}$$

3. 1^{st} PC: $\begin{bmatrix} 0.91 \\ 0.41 \end{bmatrix}$ and 2^{nd} PC: $\begin{bmatrix} -0.41 \\ 0.91 \end{bmatrix}$

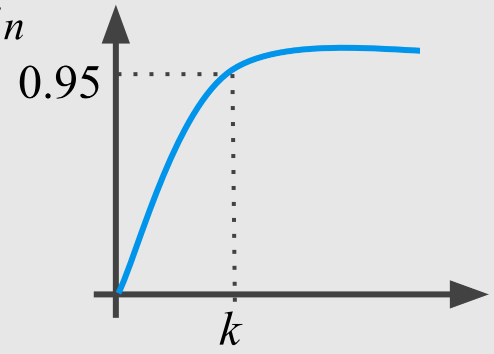
PCA in a Nutshell (Eigen Decomposition)

1. Center the data (and normalize)
2. Compute covariance matrix $\mathbf{\Sigma}$
3. Find eigenvectors u and eigenvalues λ
4. **Sort eigenvalues and pick first k eigenvectors**
5. Project data to k eigenvectors

How many PCs?

- Have eigenvectors $u_1, u_2, \ldots, u_n$, want $k < n$
- eigenvalue λ_i = variance along u_i
- Pick u_i that explain the most variance:
  - Sort eigenvectors s.t. $\lambda_1 > \lambda_2 > \lambda_3 > \ldots > \lambda_n$
  - Pick first k eigenvectors which explain 95% of total variance
    - Typical threshold: 90%, 95%, 99%

$$\frac{\sum_{i=1}^{k} \lambda_i}{\sum_{i=1}^{n} \lambda_i} \leq 1$$



PCA in a Nutshell (Eigen Decomposition)

1. Center the data (and normalize)
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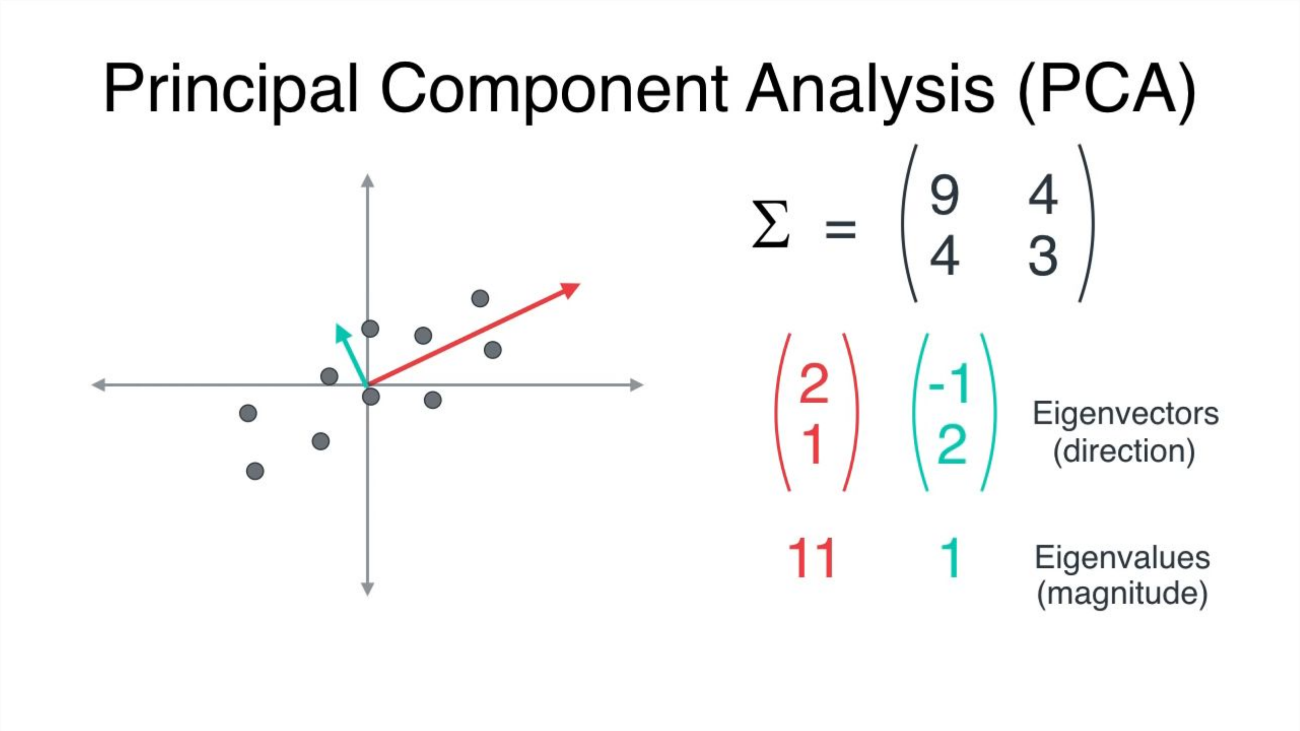
3. Find eigenvectors u and eigenvalues λ
4. Sort eigenvalues and pick first k eigenvectors
5. **Project data to k eigenvectors**

Principal Component Analysis (1 video, 26 min), Luis Serrano

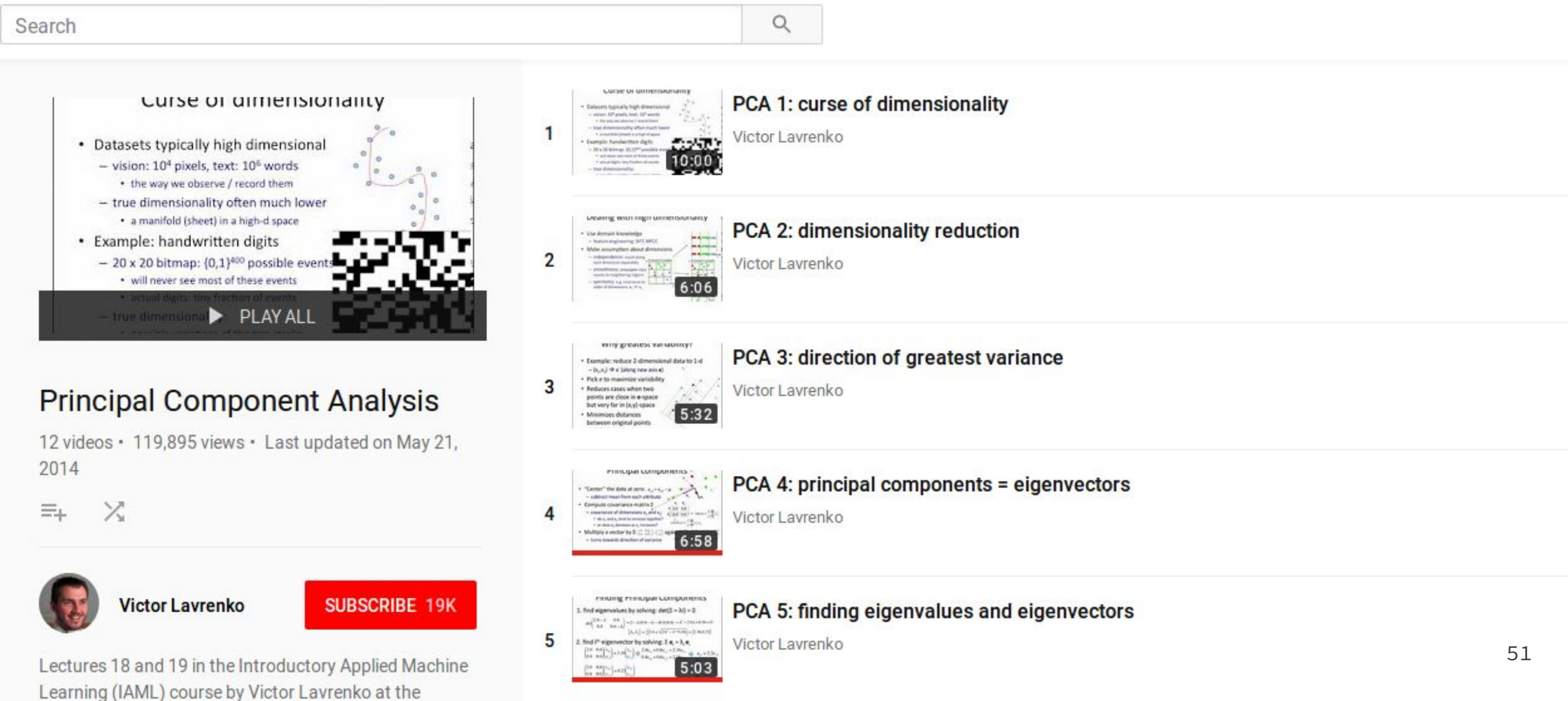
https://youtu.be/g-Hb26agBFg



Principal Component Analysis (PCA)

Principal Component Analysis (12 videos, 3-15 min)

https://www.youtube.com/playlist?list=PLBv09BD7ez_5_yapAg86Od6JeeypkS4YM



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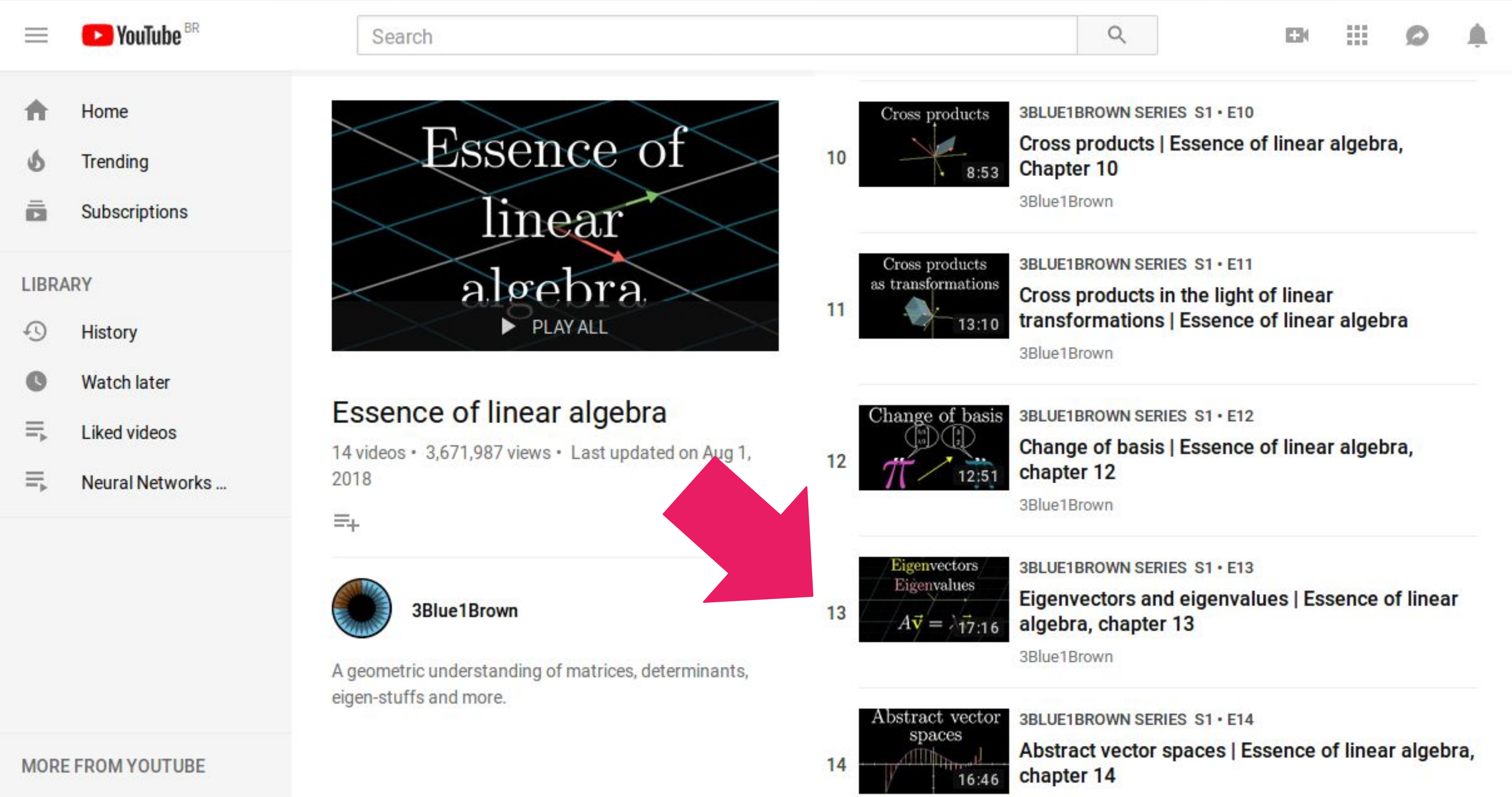

References

Machine Learning Books

- Hands-On Machine Learning with Scikit-Learn and TensorFlow, Chap. 8 “Dimensionality Reduction”
- Pattern Recognition and Machine Learning, Chap. 12 “Continuous Latent Variables”
- Pattern Classification, Chap. 10 “Unsupervised Learning and Clustering”

Machine Learning Courses

- https://www.coursera.org/learn/machine-learning, Week 8