Recall from last time ...

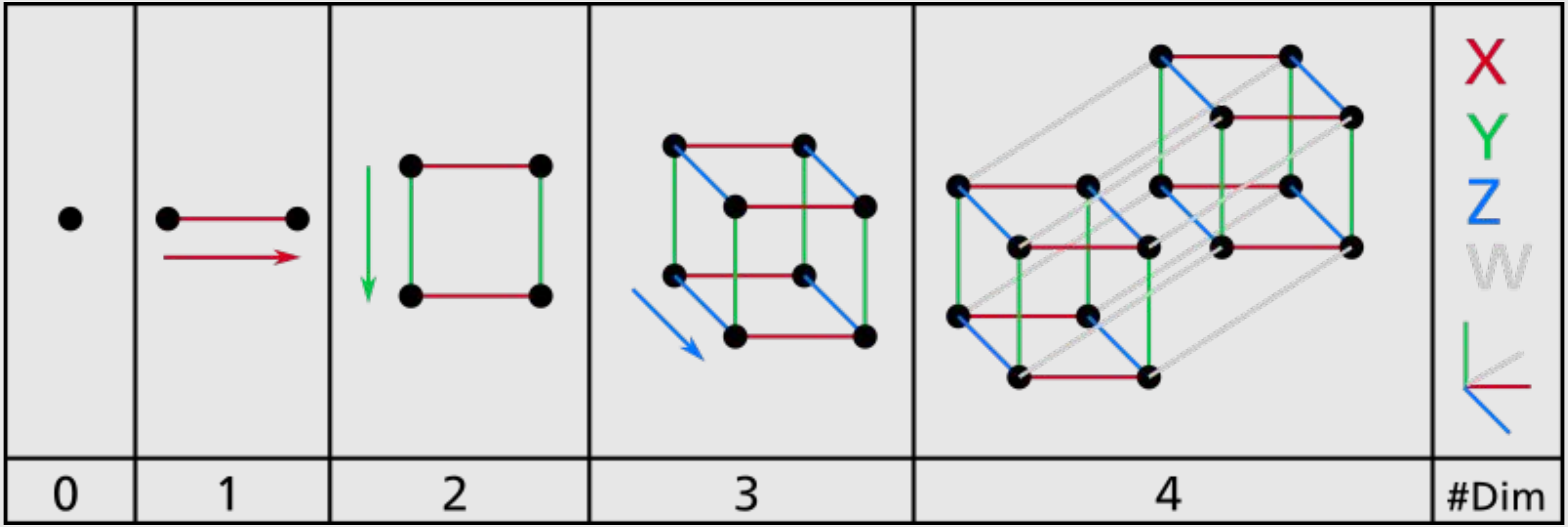
Why is Dimensionality Reduction useful?

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”**

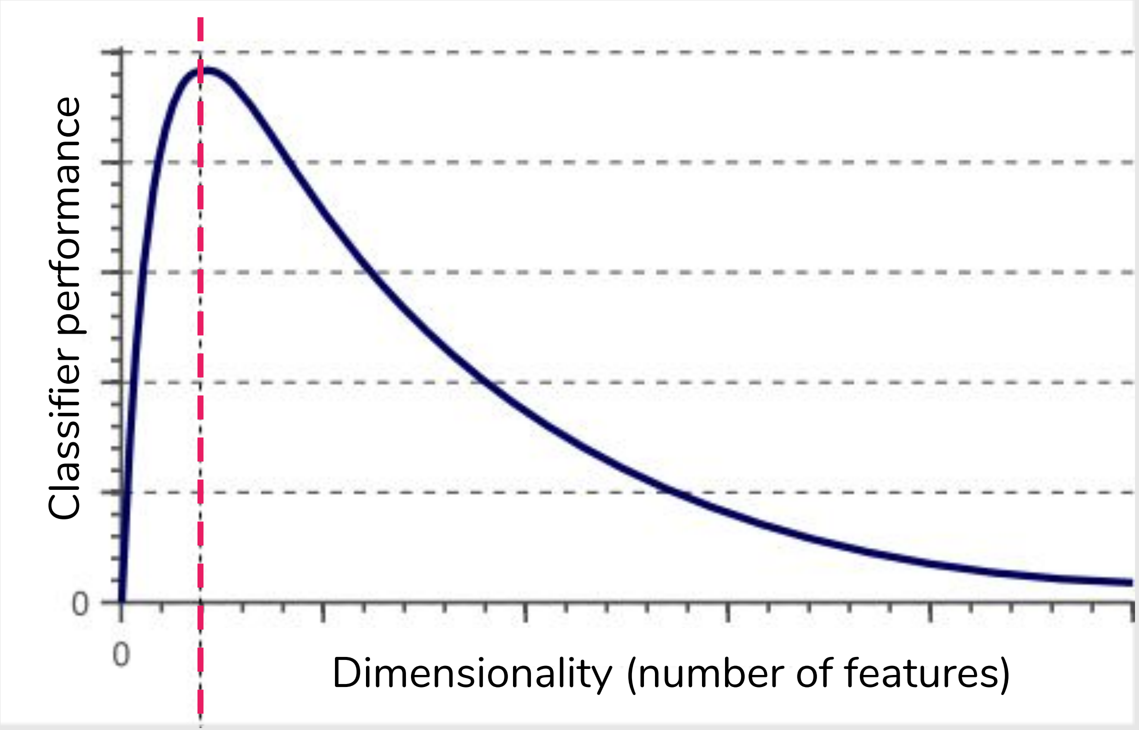
The Curse of Dimensionality

The Curse of Dimensionality



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

The Curse of Dimensionality



Optimal number of features

How to reduce dimensionality?

How to reduce dimensionality?

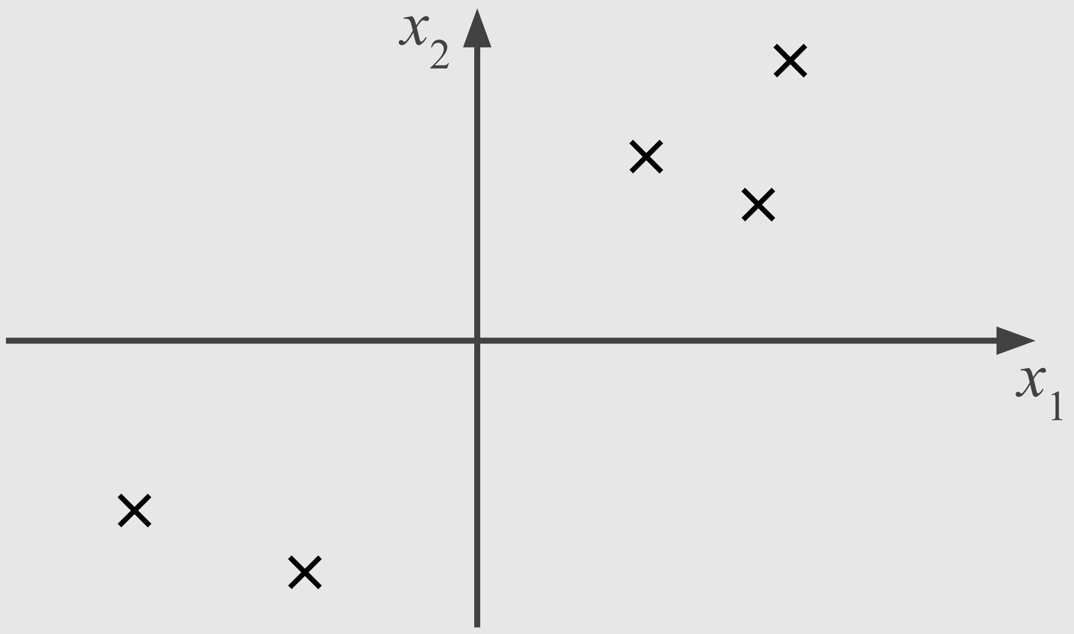
- **Feature Selection:** choosing a subset of all the features (the ones more informative).
  - $\mathbf{x_1}, x_2, \mathbf{x_3}, x_4, \mathbf{x_5}$
- **Feature Extraction:** create a subset of new features by combining the existing ones.
  - $z = f(x_1, x_2, x_3, x_4, x_5)$

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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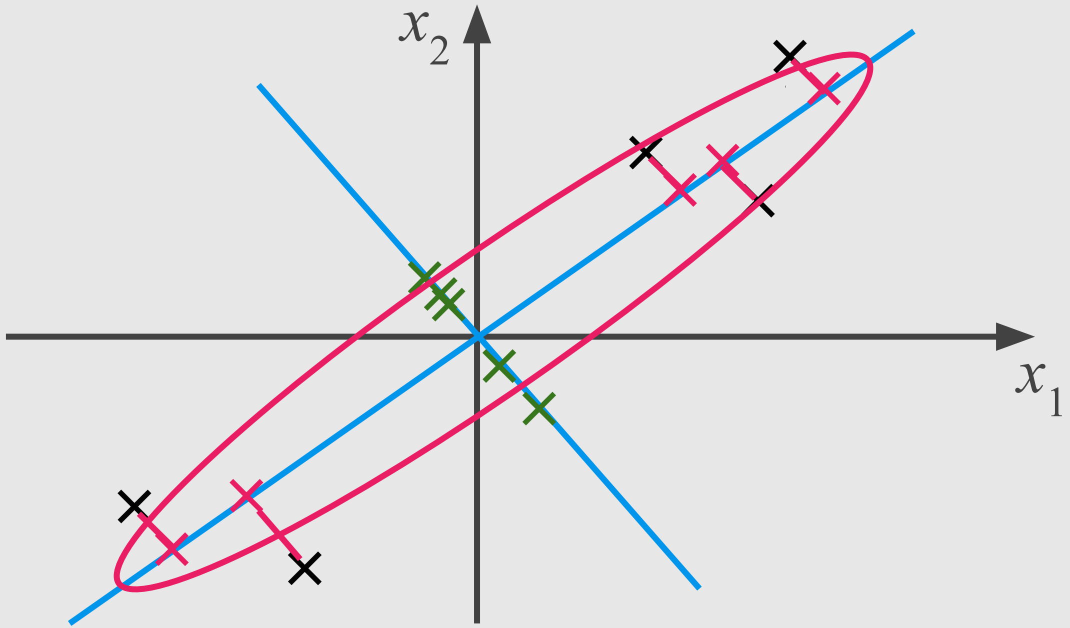
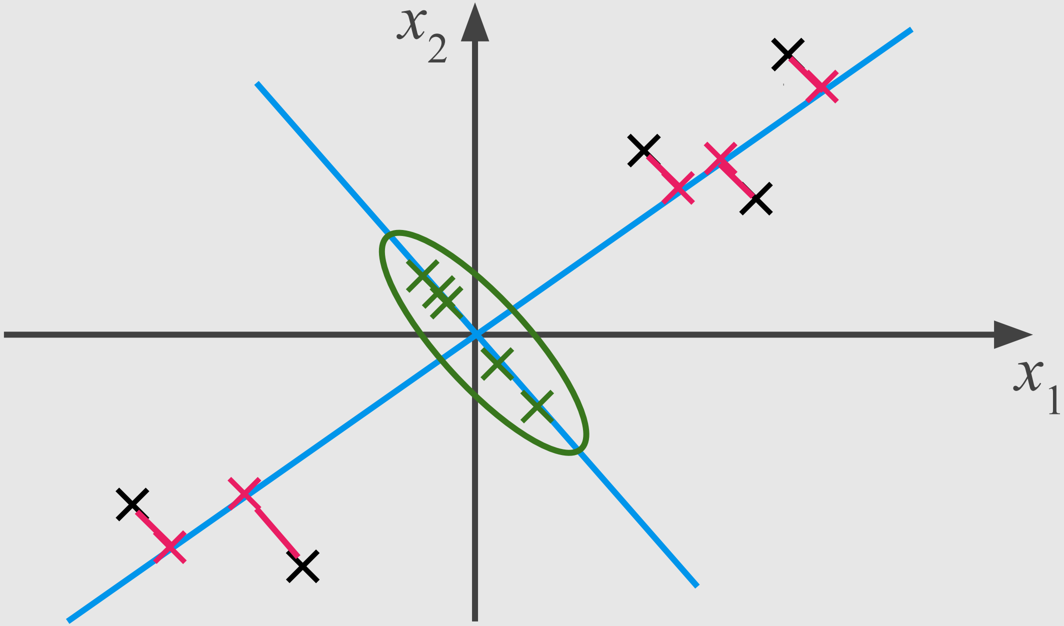
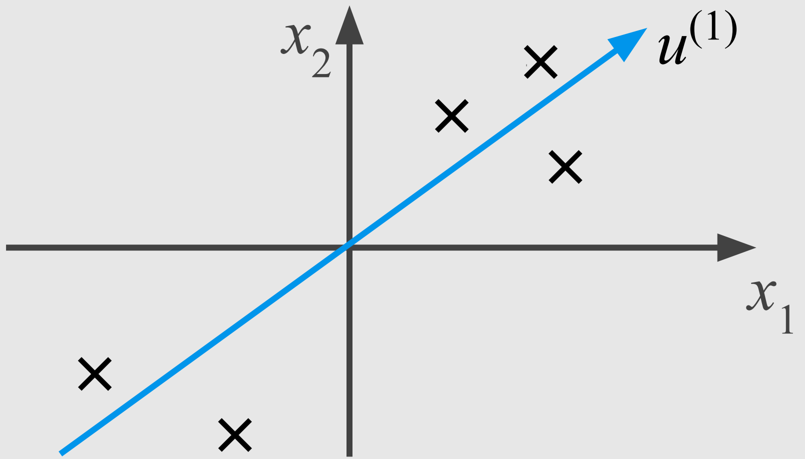


Problem Formulation (PCA)



Problem Formulation (PCA)

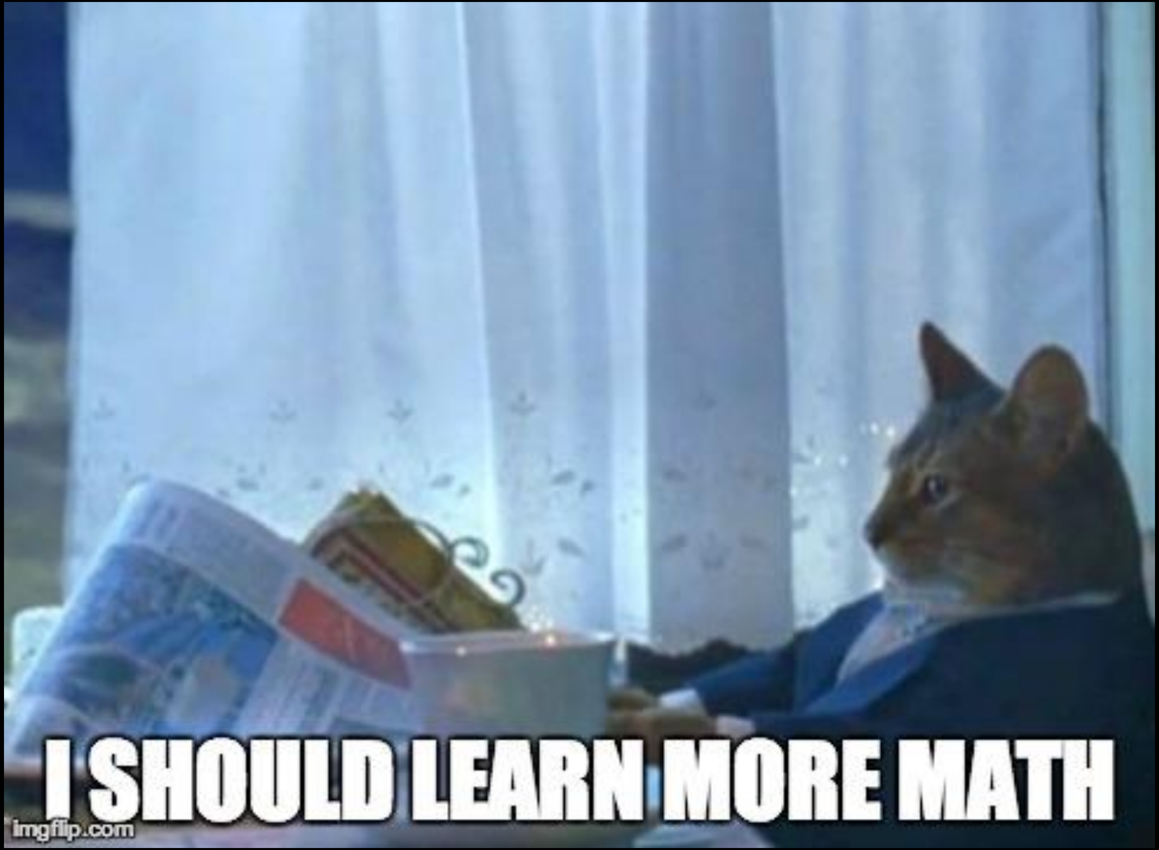
- Reduce from 2-dimension to 1-dimension: Find a direction (a vector $u^{(1)} \in \mathbb{R}^n$) onto which to project the data so as to minimize the projection error.



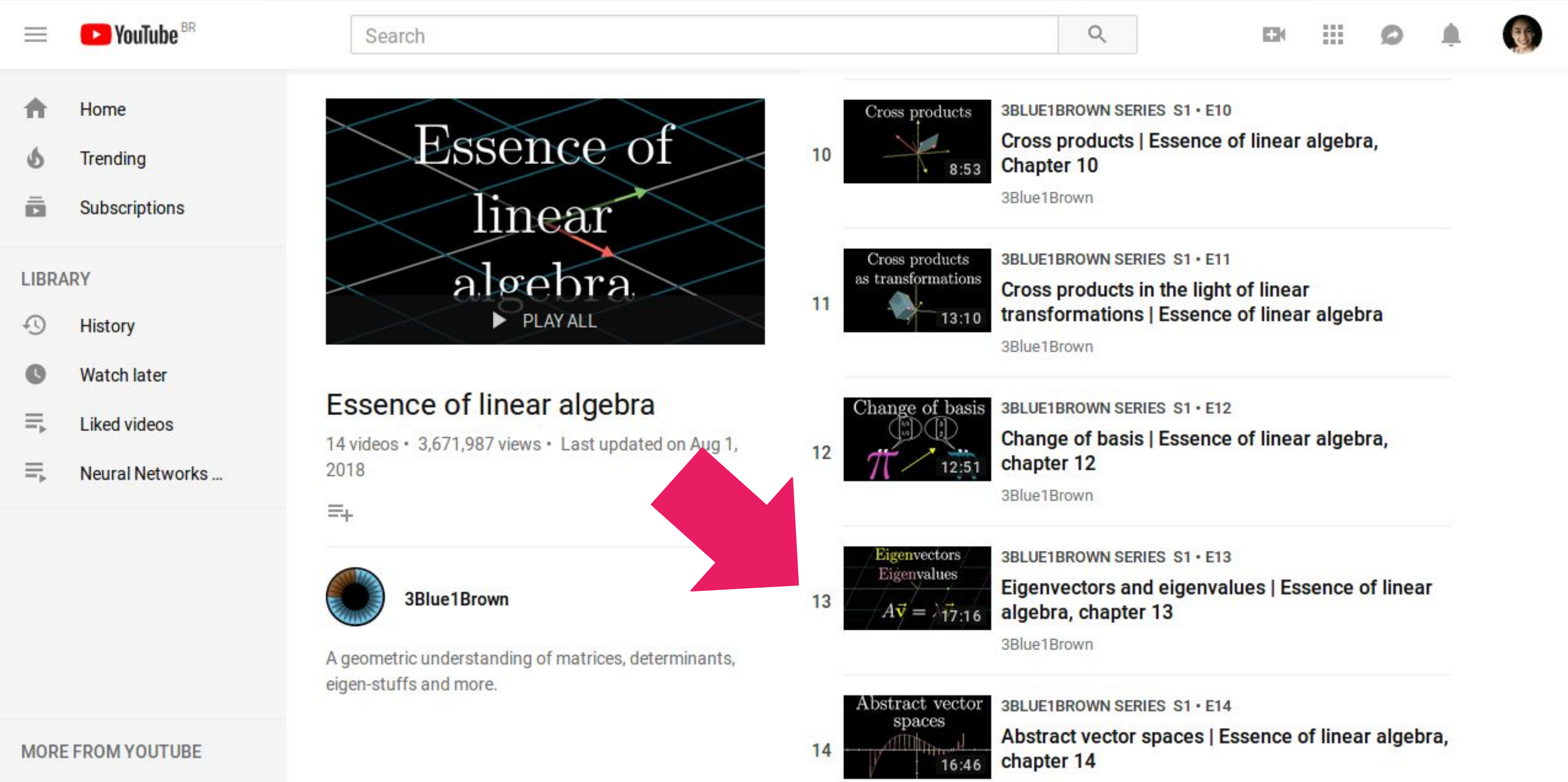
Problem Formulation (PCA)

- 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 Singular Value Decomposition


I SHOULD LEARN MORE MATH
imgflip.com

https://www.youtube.com/playlist?list=PLZHQObOWTQDPD3MizzM2xVFitgF8hE_ab



Data Preprocessing

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

Preprocessing (feature scaling/mean normalization):

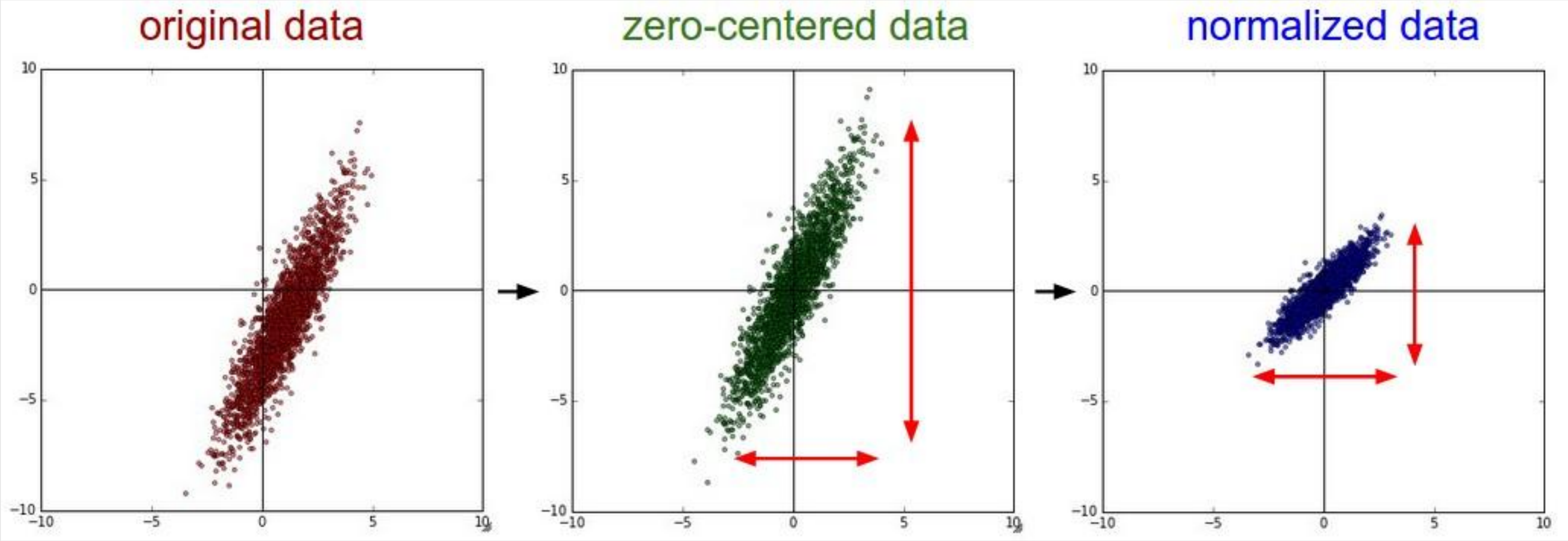
$$\mu_j = \frac{1}{m} \sum_{i=1}^{m} x_j^{(i)}$$

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 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":

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Compute "eigenvectors" of matrix $\mathbf{\Sigma}$:

$[\mathrm{U}, \mathrm{S}, \mathrm{V}] =$ svd(sigma) $\Rightarrow$ Singular Value Decomposition

PCA Algorithm

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eigenvalues

PCA Algorithm

From [U, S, V] = svd(sigma), we get:

$$U = \begin{bmatrix} | & & | \\ u^{(1)} & \cdots & u^{(n)} \\ | & & | \end{bmatrix} \in \mathbb{R}^{n \times n}$$

PCA Algorithm

From [U, S, V] = svd(sigma), we get:

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PCA Algorithm

After mean normalization and optionally feature scaling:

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

$[\mathrm{U}, \mathrm{S}, \mathrm{V}] =$ svd(sigma)

$$z = (\mathrm{U}_{\mathrm{reduce}})^{\mathrm{T}} \times x$$

Choosing the Number of Principal Components

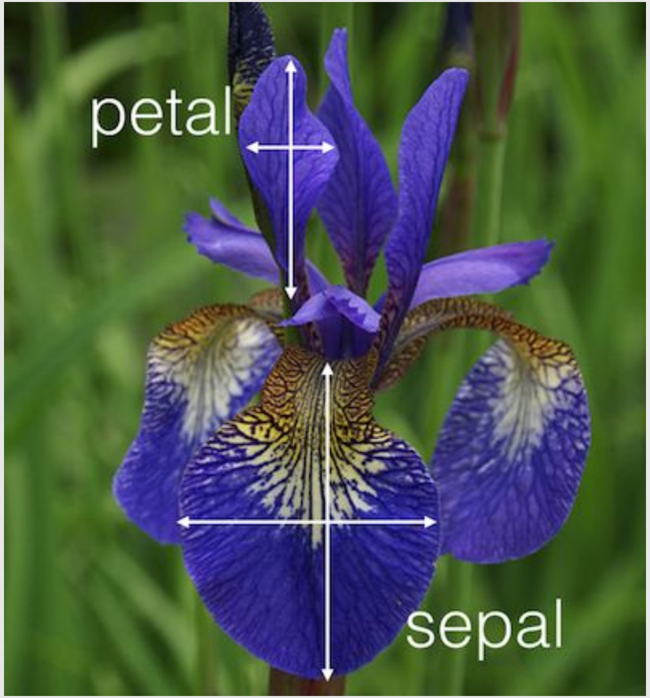
Choosing k (#Principal Components)

eigenvalues

[U, S, V] = svd(sigma)

$$\frac{\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)}-x_{approx}^{(i)}\|^2}{\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)}\|^2} \Rightarrow 1-\frac{\sum_{i=1}^{k} s_{ii}}{\sum_{i=1}^{n} s_{ii}}$$

Using PCA (Iris Dataset)



150 iris flowers from three different species.

The three classes in the Iris dataset:

1. Iris-setosa (n=50)
2. Iris-versicolor (n=50)
3. Iris-virginica (n=50)

The four features of the Iris dataset:

1. sepal length in cm
2. sepal width in cm
3. petal length in cm
4. petal width in cm

PCA Algorithm
By Eigen Decomposition

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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Reduce data from n-dimensions to k-dimensions

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Covariance of dimensions x_1 and x_2:

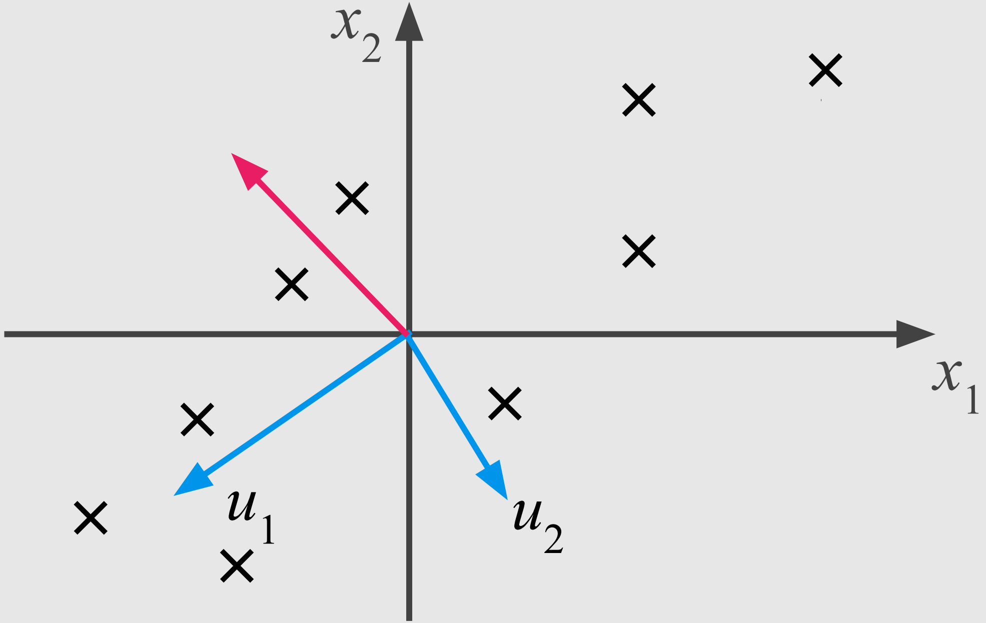
- Do x_1 and x_2 tend to increase together?
- or does x_2 decrease as x_1 increases?

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

PCA Algorithm

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

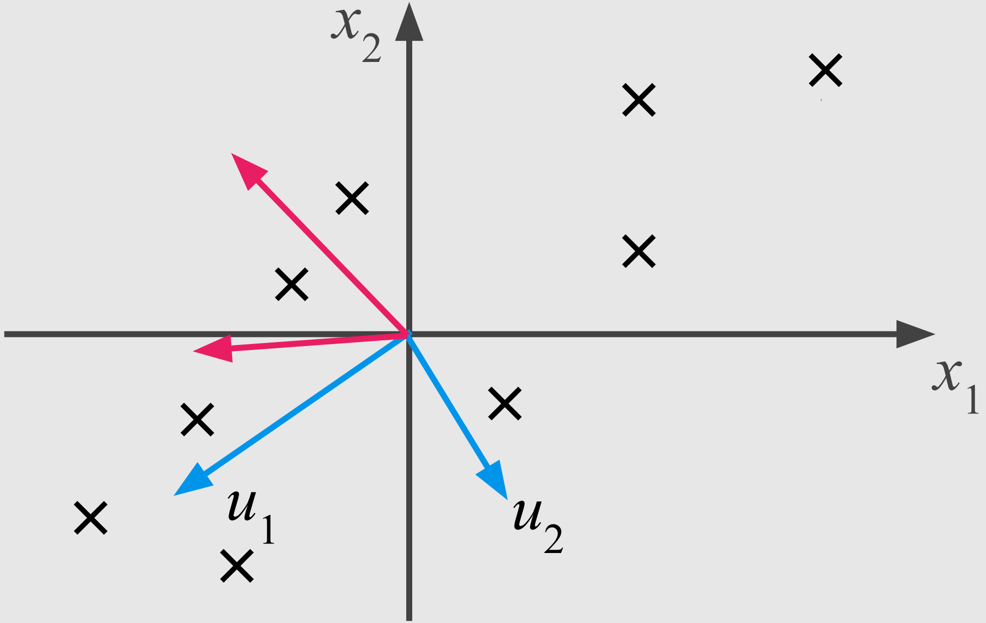
$$\begin{bmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{bmatrix} \times \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$



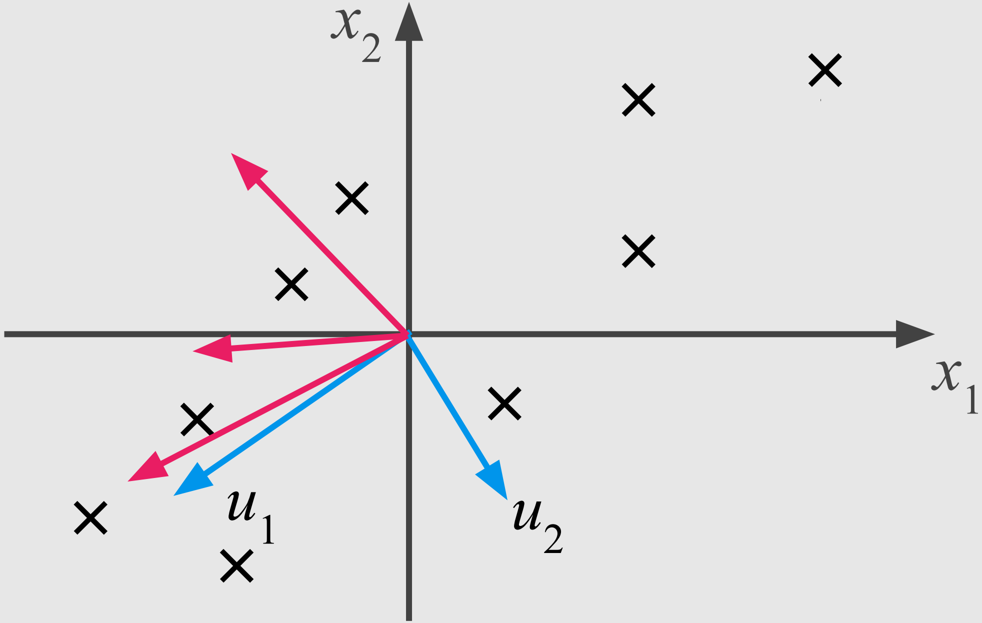
PCA Algorithm

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

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



PCA Algorithm



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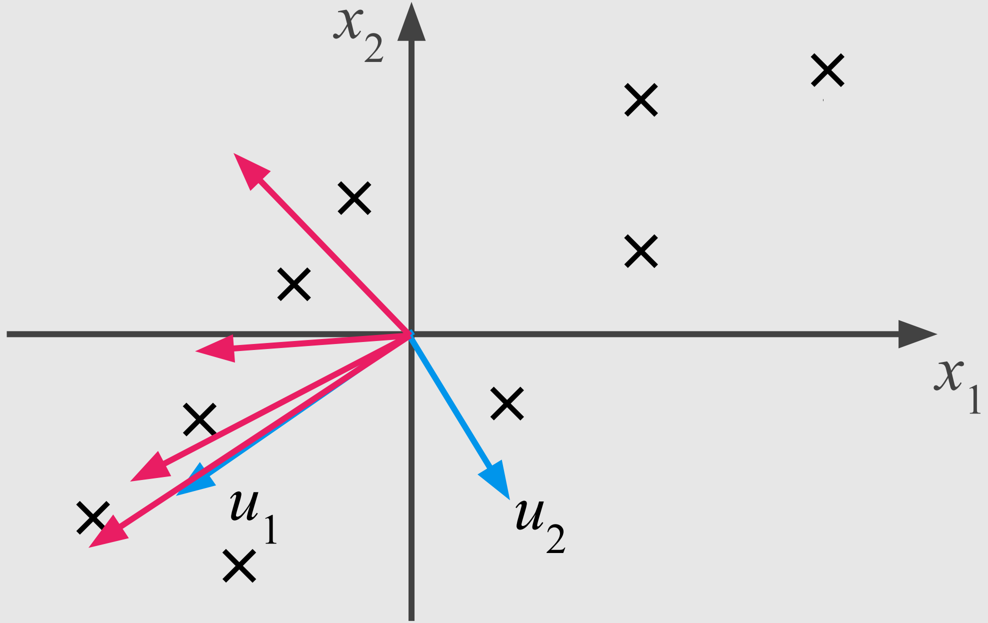
PCA Algorithm



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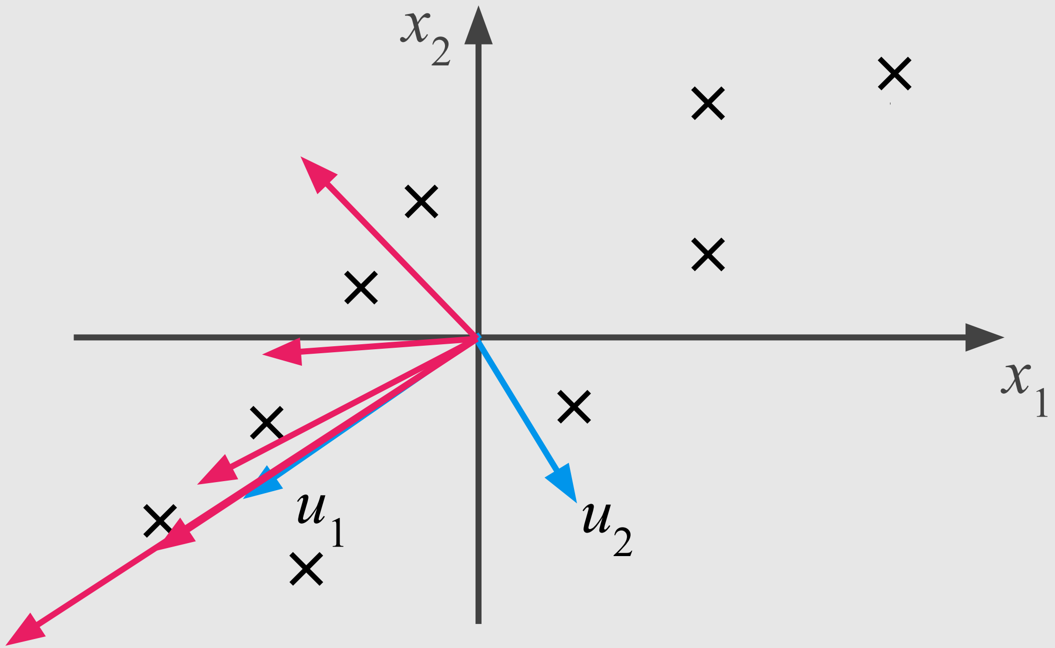
$$\begin{bmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{bmatrix} \times \begin{bmatrix} -2.5 \\ -1.0 \end{bmatrix} = \begin{bmatrix} -6.0 \\ -2.7 \end{bmatrix}$$

PCA Algorithm



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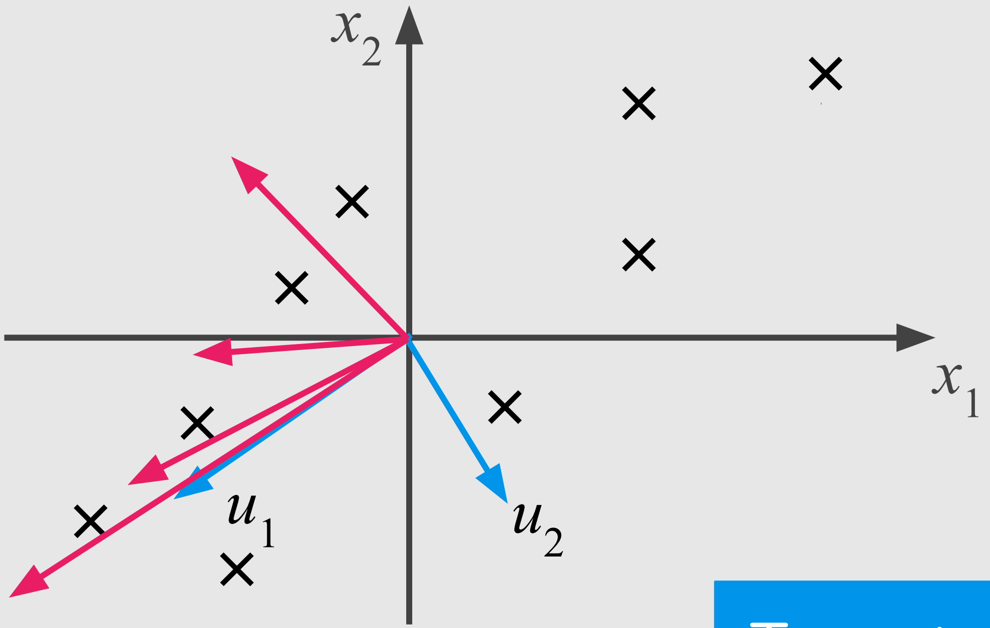
$$\begin{bmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{bmatrix} \times \begin{bmatrix} -6.0 \\ -2.7 \end{bmatrix} = \begin{bmatrix} -14.1 \\ -6.4 \end{bmatrix}$$

PCA Algorithm



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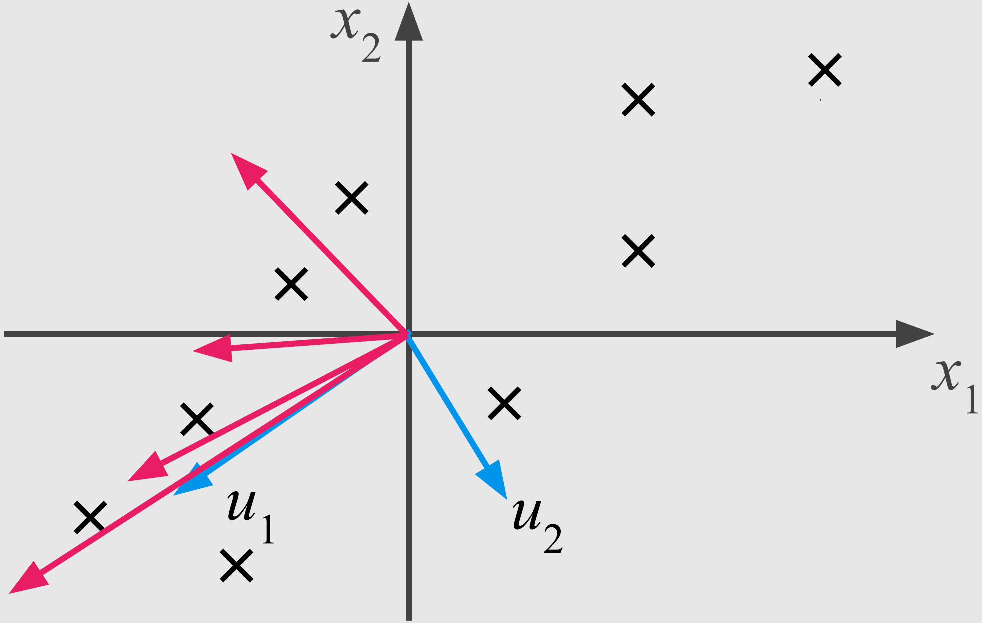
Turns towards direction of variation

PCA Algorithm

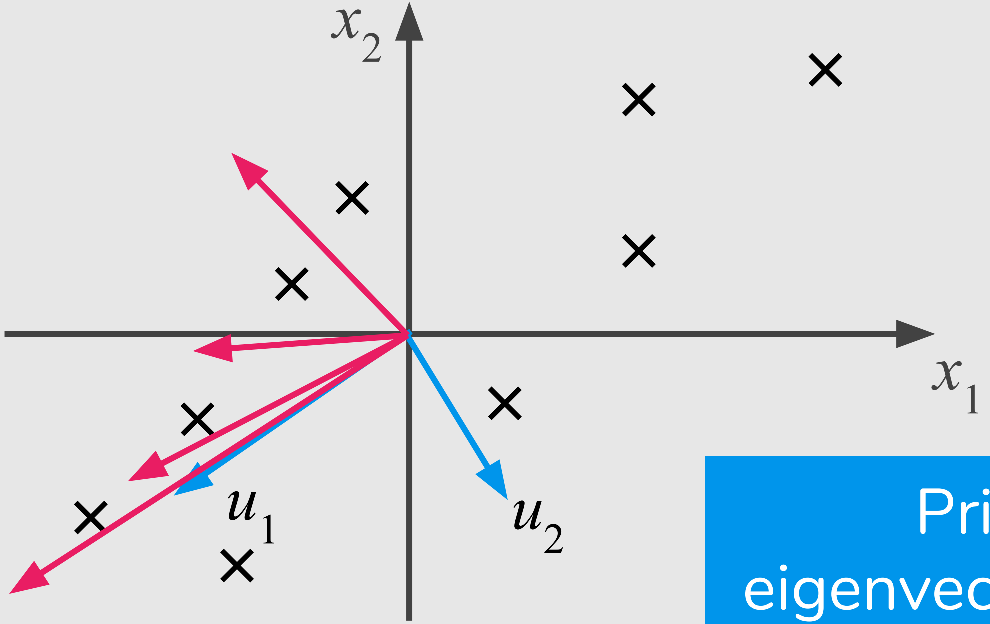


Want vectors u which aren't turned: $\mathbf{\Sigma} u = \lambda u$

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

λ = eigenvalues

PCA Algorithm



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

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λ = eigenvalues

Principal components = eigenvectors w. largest eigenvalues

PCA in a Nutshell (Eigen Decomposition)

1. Center the data (and normalize)
2. Compute covariance matrix $\boldsymbol{\Sigma}$
3. **Find eigenvectors $\boldsymbol{u}$ and eigenvalues $\boldsymbol{\lambda}$**
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Finding Principal Components

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

$$\det\begin{bmatrix} 2.0-\lambda & 0.8 \\ 0.8 & 0.6-\lambda \end{bmatrix} =$$

Finding Principal Components

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

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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: $\boldsymbol{\Sigma} u_i = \lambda_i u_i$

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Finding Principal Components

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$$\Downarrow$$

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

Finding Principal Components

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$$u_{11} = 2.2u_{12}$$

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

Want $\|u_1\|=1$

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

Finding Principal Components

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

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$\Downarrow$ Want $\|u_1\|=1$

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

Finding Principal Components

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

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

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How many PCs?

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  - Pick first k eigenvectors which explain 95% of total variance

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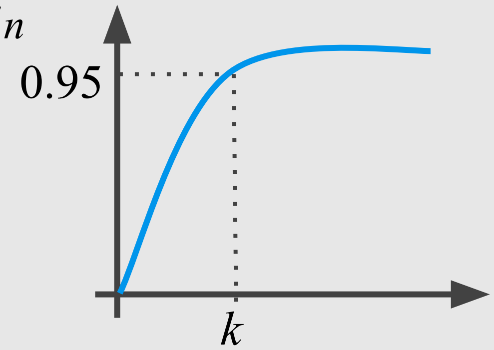
$$\frac{\sum_{i=1}^{k} \lambda_i}{\sum_{i=1}^{n} \lambda_i} \leq 1$$



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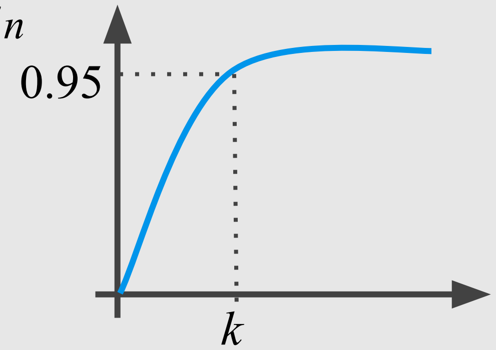
  - Pick first k eigenvectors which explain 95% of total variance
    - Typical threshold: 90%, 95%, 99%

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



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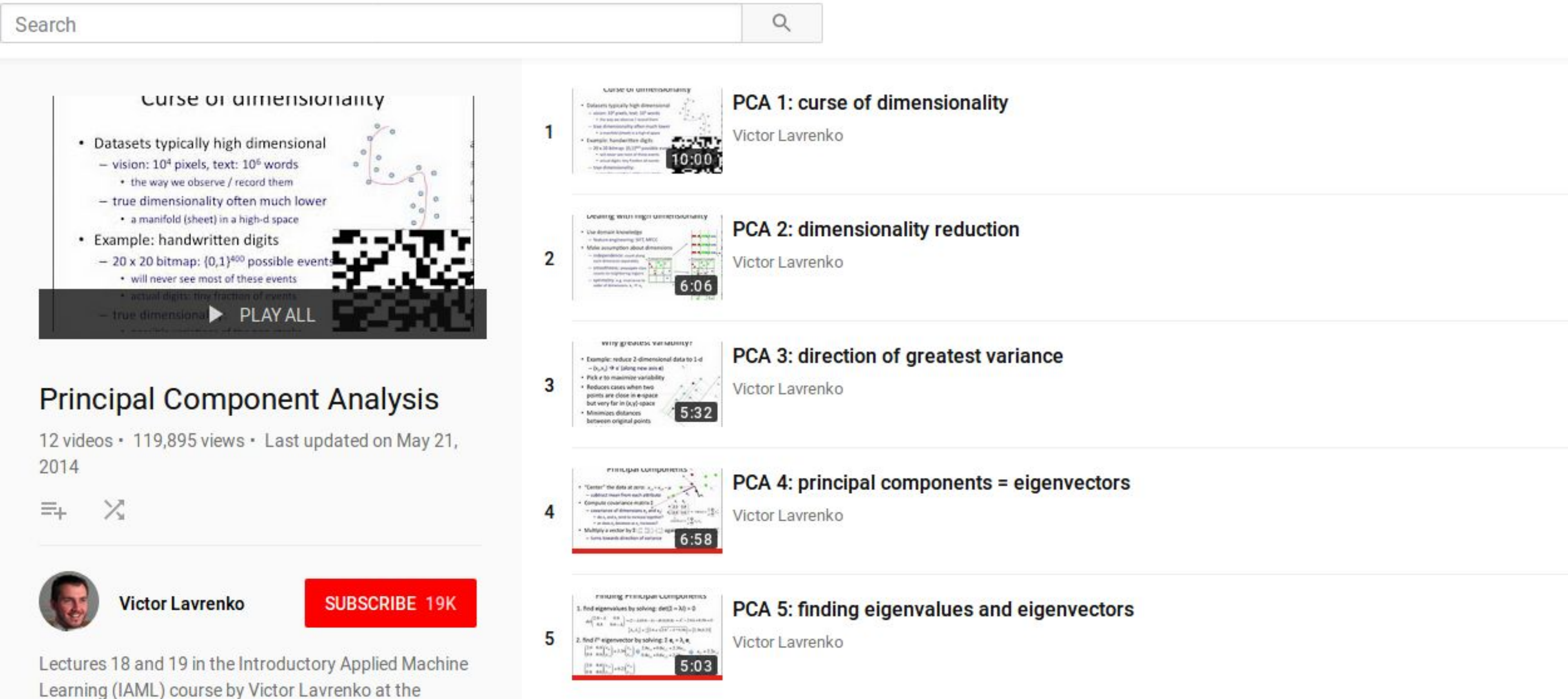
5. **Project data to k eigenvectors**

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

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



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

Linear Discriminant Analysis

Machine Learning and Pattern Recognition

Prof. Sandra Avila

Institute of Computing (IC/Unicamp)

MC886/MO444, September 27, 2018

Today's Agenda

- Linear Discriminant Analysis
  - PCA vs LDA
  - LDA: Simple Example
  - LDA Algorithm
  - LDA Step by Step

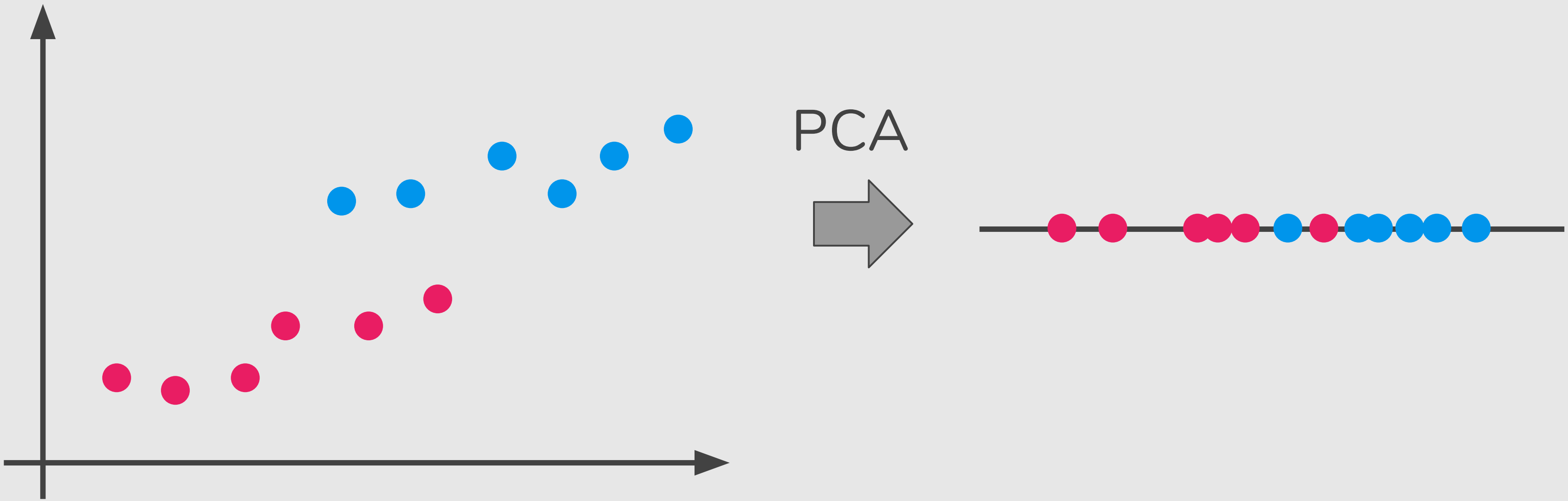
Linear Discriminant Analysis

Linear Discriminant Analysis (LDA)

- LDA pick a new dimension that gives:
  - Maximum separation between means of projected classes
  - Minimum variance within each projected class
- Solution: eigenvectors based on between-class and within-class covariance matrix

LDA: Simple Example

Reducing 2D to 1D



LDA: Simple Example

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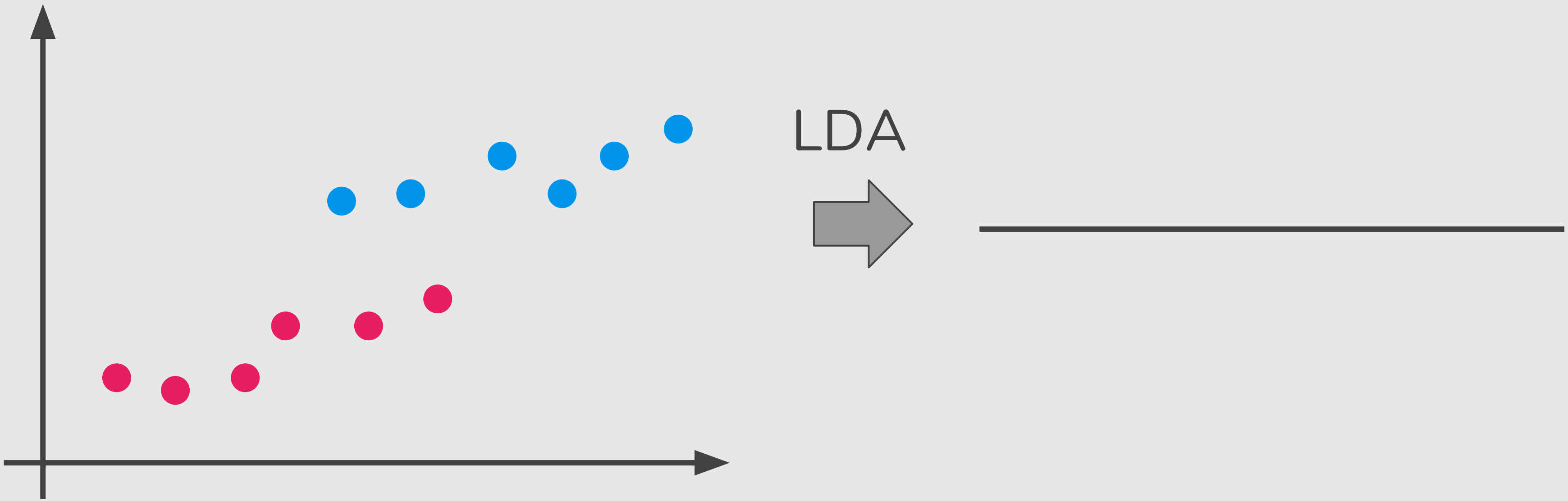
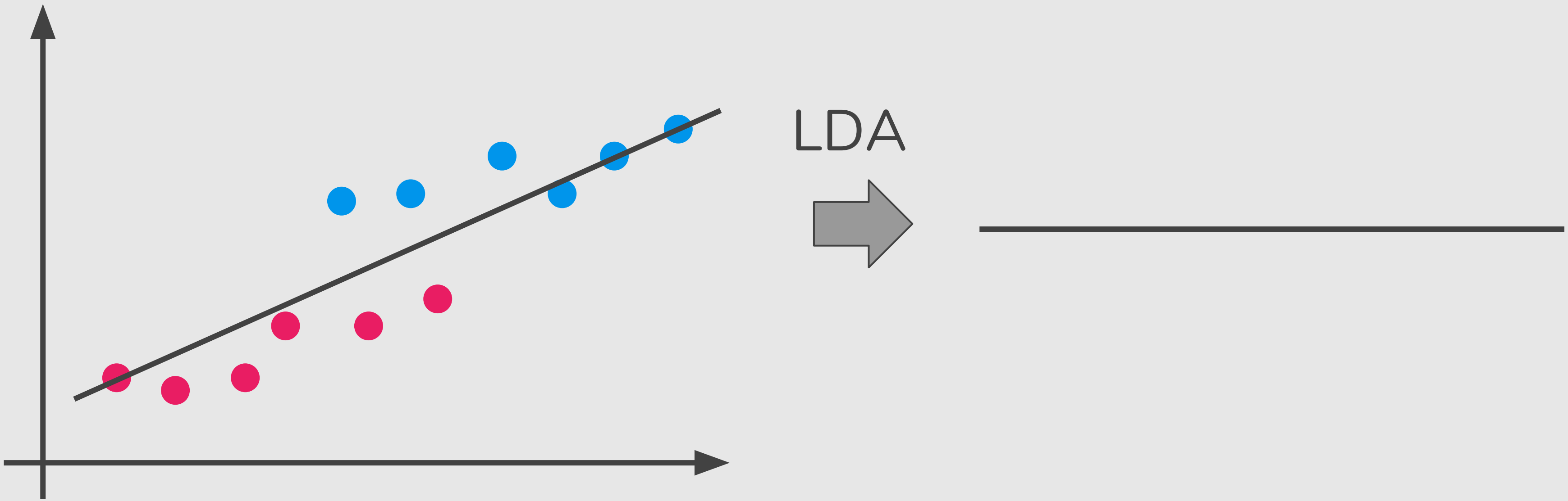


LDA: Simple Example

Reducing 2D to 1D



LDA: Simple Example

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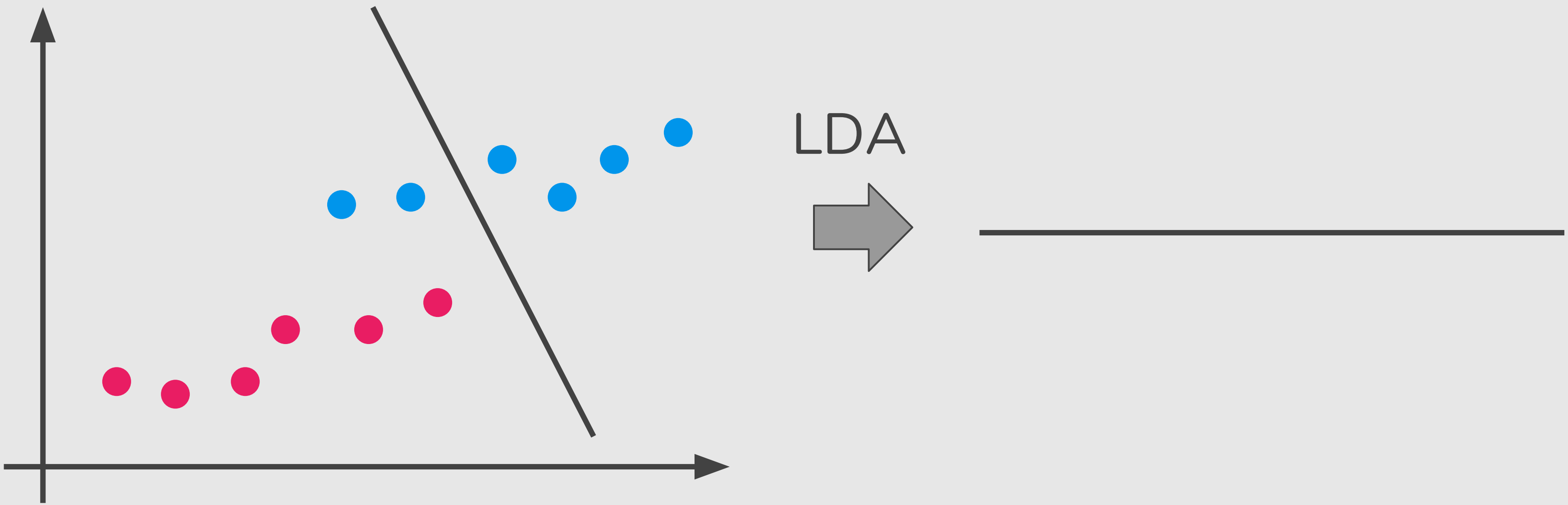
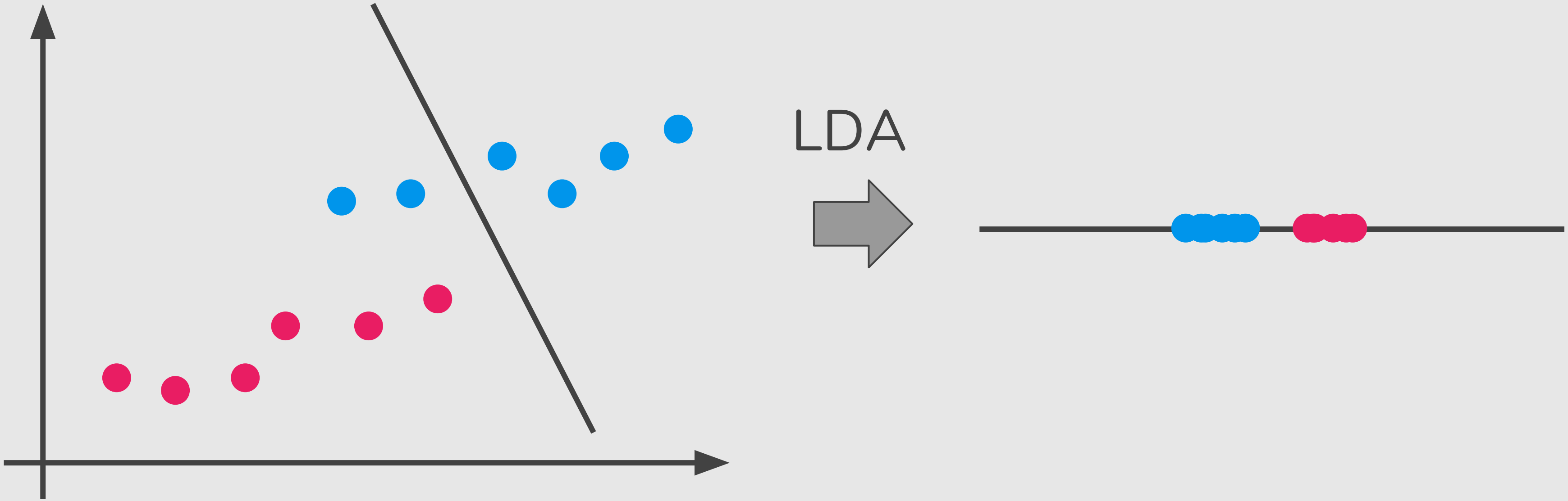


LDA: Simple Example

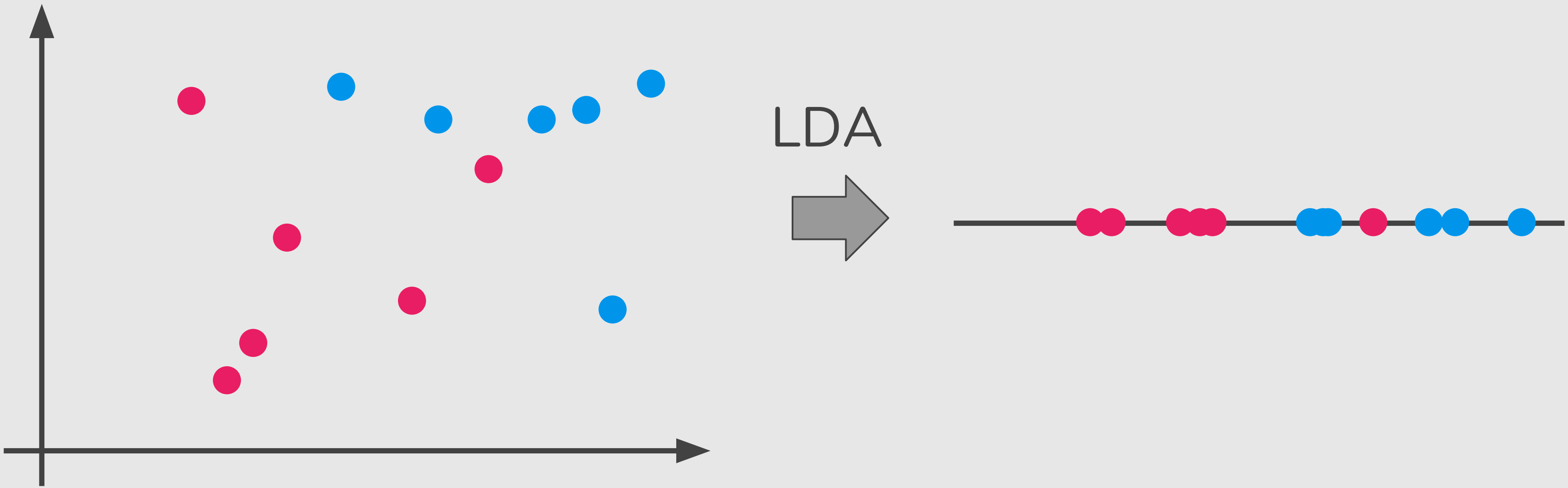
Reducing 2D to 1D



How LDA create a new axis?

How LDA create a new axis?

Reducing 2D to 1D



How LDA create a new axis?

The new axis is created according two criteria:

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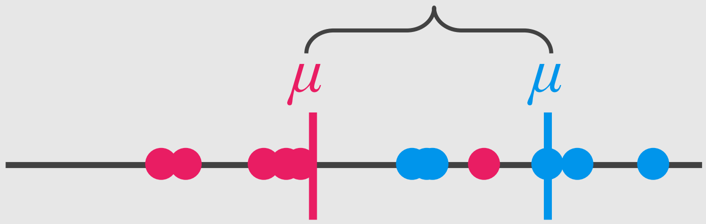
1. Maximize the distance between the means:



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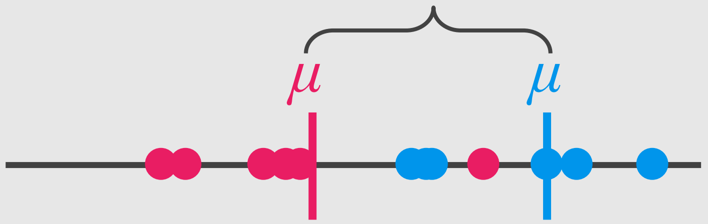

2. Minimize the variation (which LDA calls scatter) within each class.

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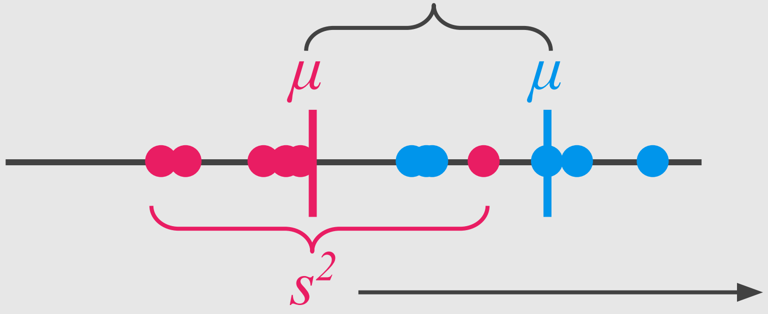

This is the scatter around the pink dots.

2. Minimize the variation (which LDA calls scatter) within each class.

How LDA create a new axis?

The new axis is created according two criteria:

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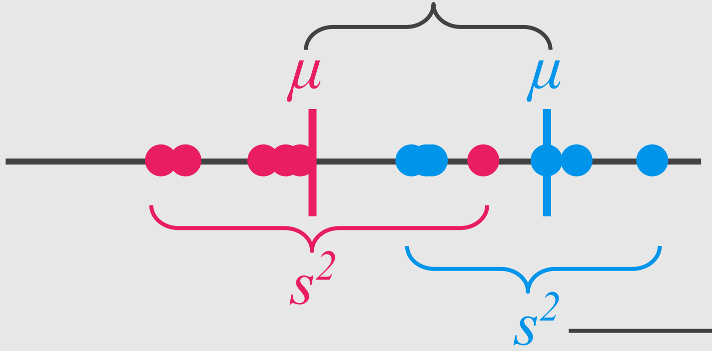

This is the scatter around the blue dots.

2. Minimize the variation (which LDA calls scatter) within each class.

How LDA create a new axis?

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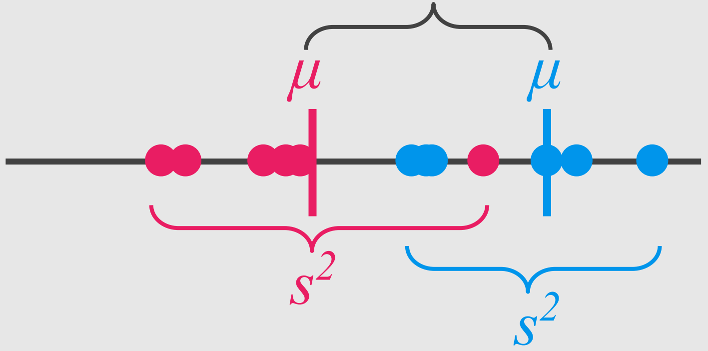

$$\frac{(\mu - \mu)^2}{s^2 + s^2}$$

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How LDA create a new axis?

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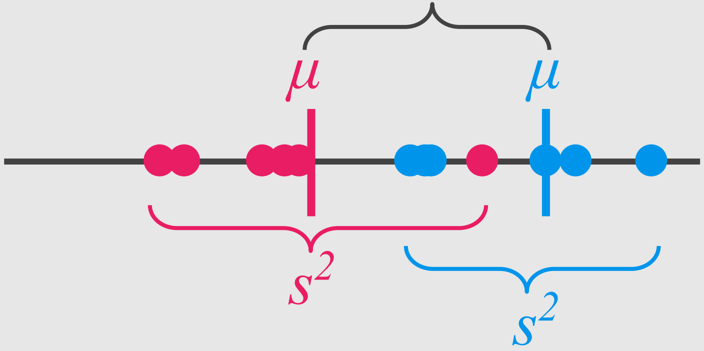

2. Minimize the variation (which LDA calls scatter) within each class.

$$\frac{(\mu - \mu)^2}{s^2 + s^2}$$

→ Ideally large

→ Ideally small

How LDA create a new axis?

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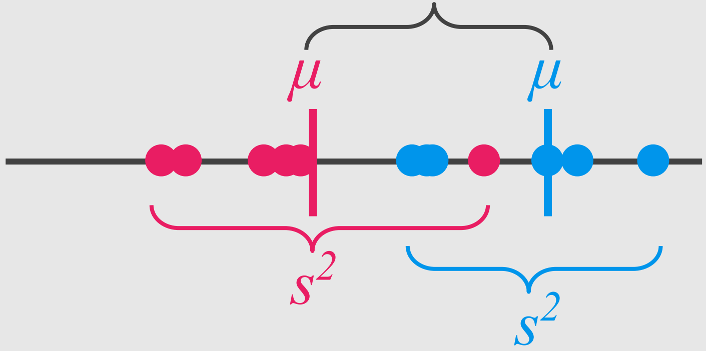
1. Maximize the distance between the means:



2. Minimize the variation (which LDA calls scatter) within each class.

Let's call $(\mu - \mu)$ d for distance.

$$\frac{(\mu - \mu)^2}{s^2 + s^2}$$

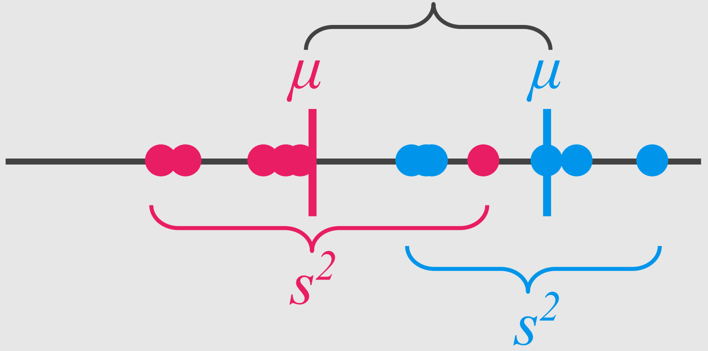
$(\mu - \mu)^2 \longrightarrow$ Ideally large

$s^2 + s^2 \longrightarrow$ Ideally small

How LDA create a new axis?

The new axis is created according two criteria:

1. Maximize the distance between the means:



2. Minimize the variation (which LDA calls scatter) within each class.

Let's call $(\mu - \mu)$ d for distance.

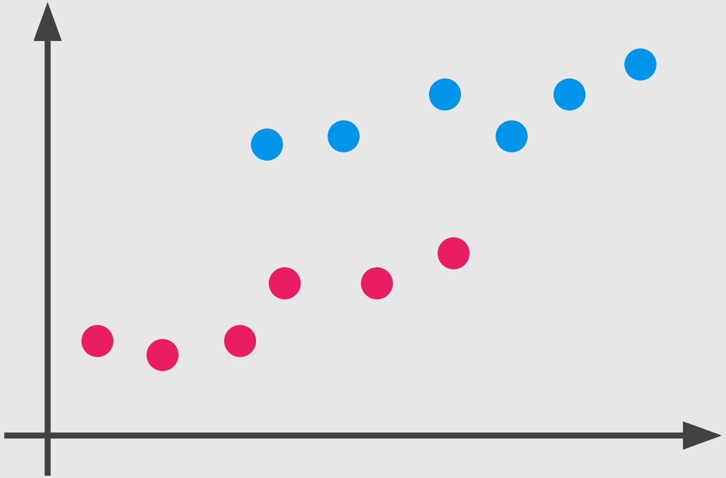
$$\frac{d^2}{s^2 + s^2}$$

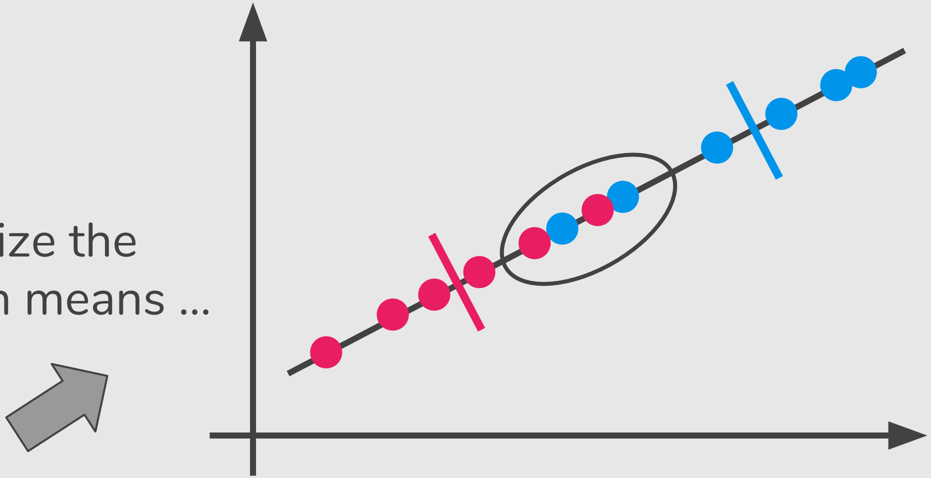
$\longrightarrow$ Ideally large

$\longrightarrow$ Ideally small

Why both distance and scatter are important?

If we only maximize the distance between means ...





Why both distance and scatter are important?

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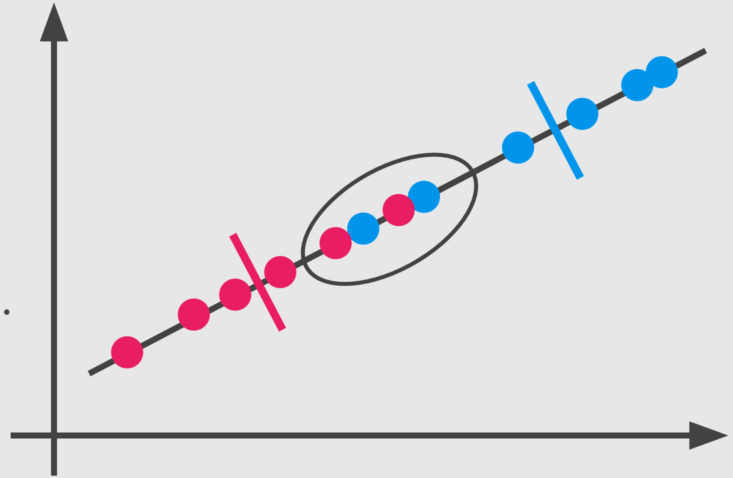
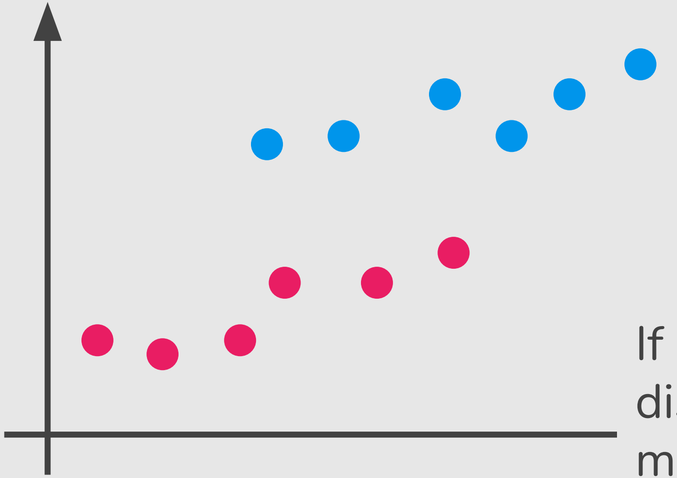
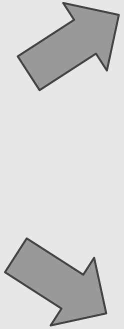
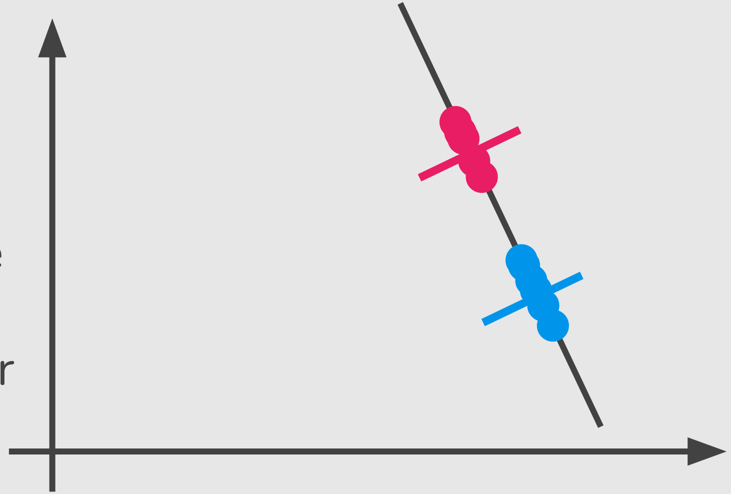


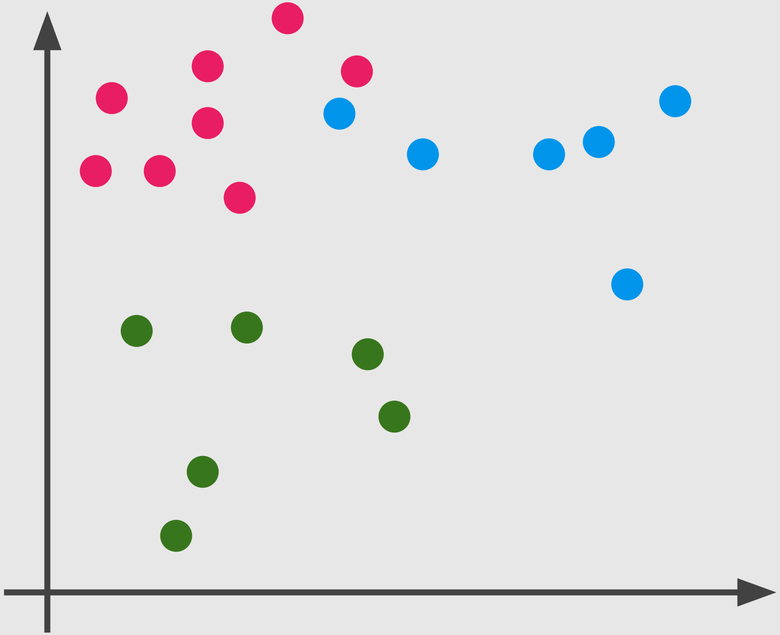




If we optimize the distance between means and scatter



What if we have 3 classes?



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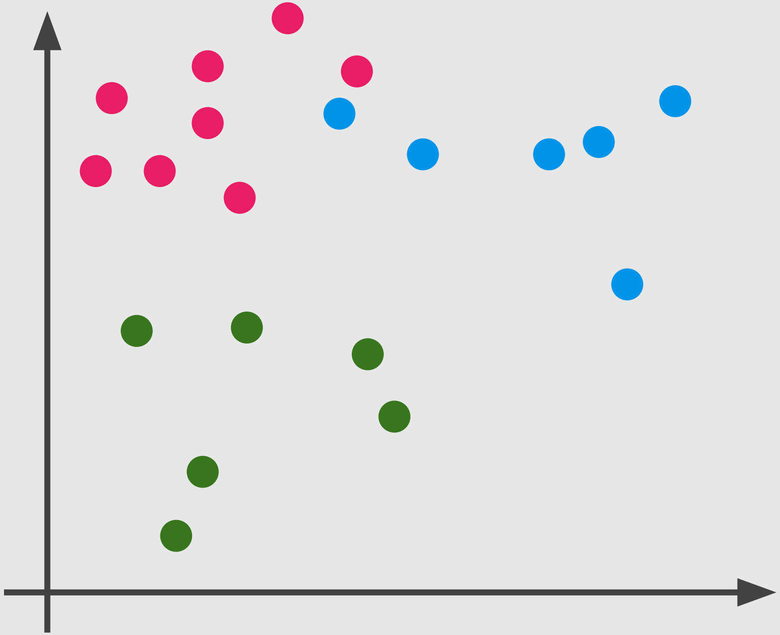
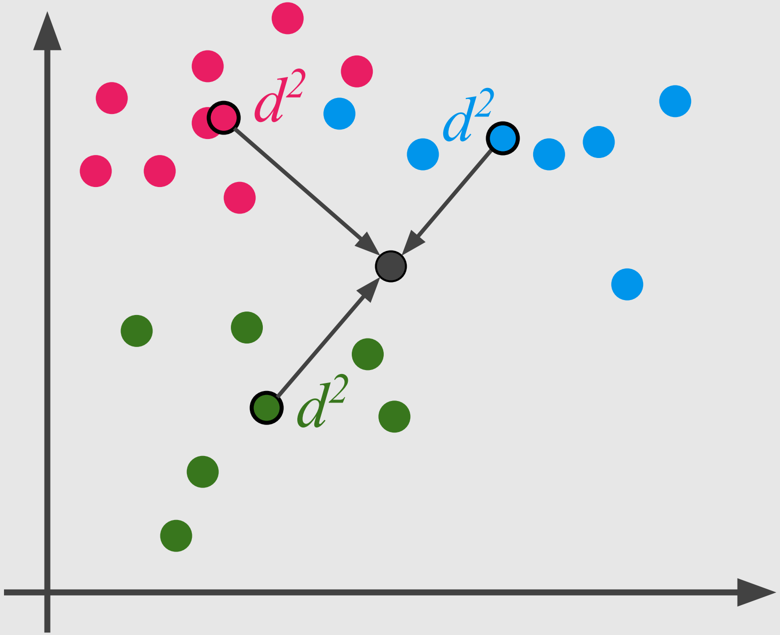


How we measure the distance among the means?

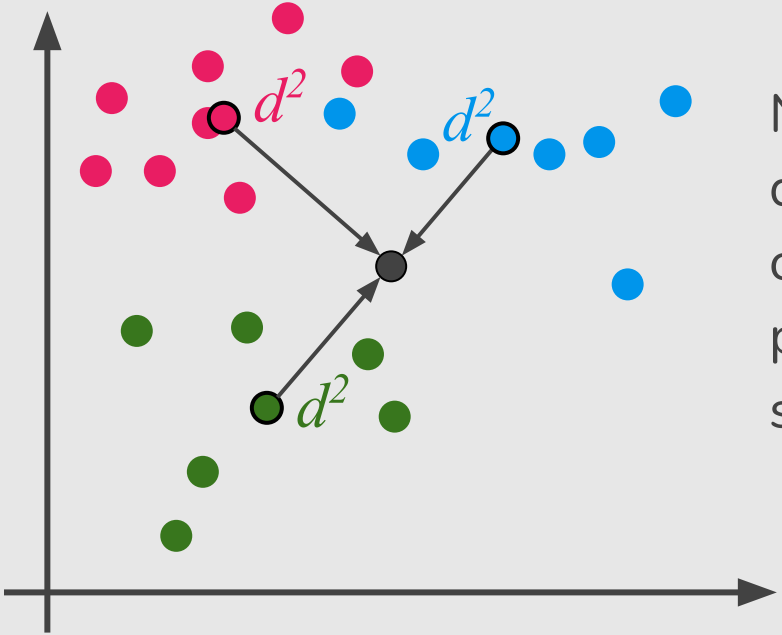
What if we have 3 classes?

What if we have 3 classes?



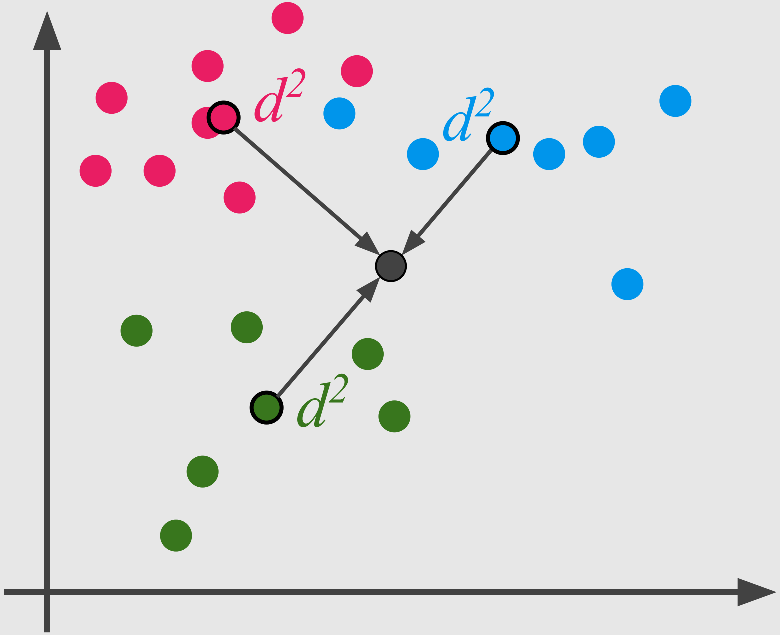
Then measure the distance between a point that is central in each class and the main central point.

What if we have 3 classes?



Now maximize the distance between each class and the central point while minimize the scatter for each class.

What if we have 3 classes?

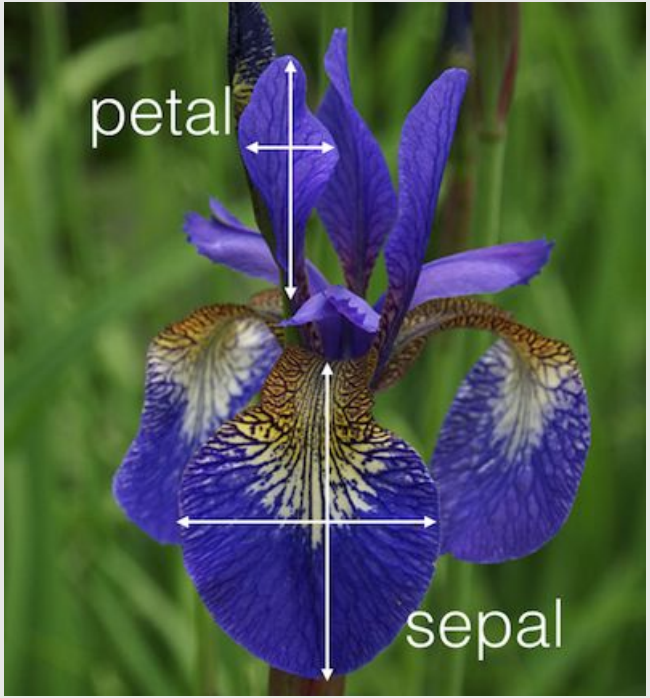


$$\frac{d^2 + d^2 + d^2}{s^2 + s^2 + s^2}$$

LDA in a Nutshell (Eigen Decomposition)

1. Compute the d-dimensional mean vectors for the different classes.
2. Compute the scatter matrices (between-class S_B and within-class S_W).
3. Compute the eigenvectors ($u_1, u_2, \ldots, u_d$) and eigenvalues ($\lambda_1, \lambda_2, \ldots, \lambda_d$) for the scatter matrices $S_W^{-1} S_B$.
4. Sort the eigenvectors by decreasing eigenvalues and choose k eigenvectors.
5. Use this $d \times k$ eigenvector matrix to transform the samples onto the new subspace.

LDA Step by Step



http://sebastianraschka.com/Articles/2014_python_lda.html

150 iris flowers from three different species.

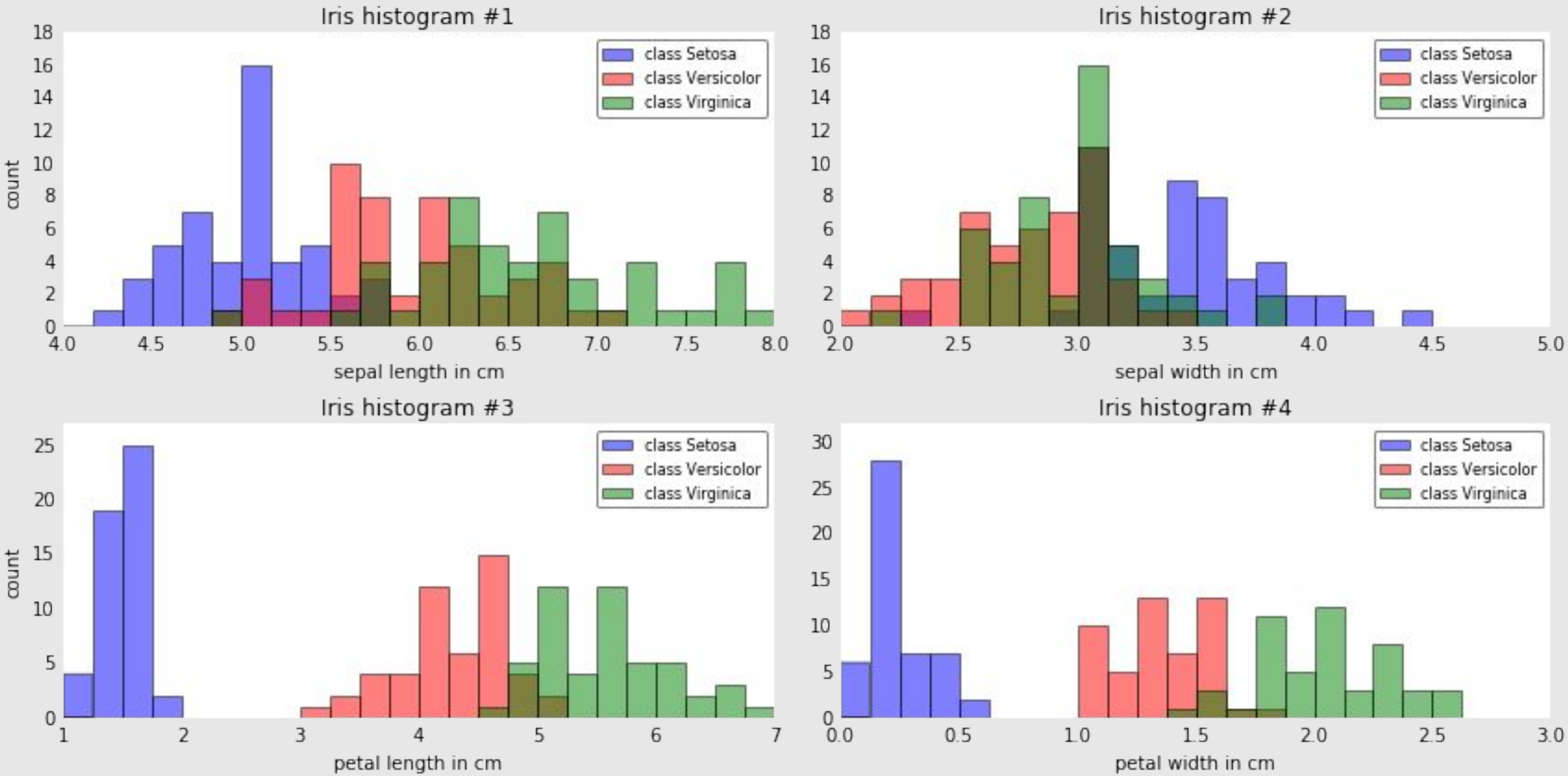
The three classes in the Iris dataset:

1. Iris-setosa (n=50)
2. Iris-versicolor (n=50)
3. Iris-virginica (n=50)

The four features of the Iris dataset:

1. sepal length in cm
2. sepal width in cm
3. petal length in cm
4. petal width in cm

LDA Step by Step



LDA Step by Step

1. Compute the d-dimensional mean vectors for the different classes.

LDA Step by Step

1. Compute the d-dimensional mean vectors for the different classes.

$$\mu_1 : [\ 5.01 \quad 3.42 \quad 1.46 \quad 0.24\ ]$$

$$\mu_2 : [\ 5.94 \quad 2.77 \quad 4.26 \quad 1.33\ ]$$

$$\mu_3 : [\ 6.59 \quad 2.97 \quad 5.55 \quad 2.03\ ]$$

LDA Step by Step

2. Compute the **scatter matrices** (between-class S_B and within-class S_W)

   Within-class scatter matrix S_W:

$$S_W = \sum_{i=1}^{c} S_i \text{ , where } S_i = \sum_{x \in D_i}^{n} (x - \mu_i)(x - \mu_i)^T$$

LDA Step by Step

2. Compute the **scatter matrices** (between-class S_B and within-class S_W)

   Within-class scatter matrix S_W:

$$\begin{bmatrix} 38.96 & 13.68 & 24.61 & 5.66 \\ 13.68 & 7.04 & 8.12 & 4.91 \\ 24.61 & 8.12 & 27.22 & 6.25 \\ 5.66 & 4.91 & 6.25 & 6.18 \end{bmatrix}$$

LDA Step by Step

2. Compute the **scatter matrices** (between-class S_B and within-class S_W)

   Between-class scatter matrix S_B:

$$S_B = \sum_{i=1}^{c} N_i (\mu_i - \mu)(\mu_i - \mu)^{\mathrm{T}}$$

   where μ is the overall mean, and μ_i and N_i are the sample mean and sizes of the respective classes.

LDA Step by Step

2. Compute the **scatter matrices** (between-class S_B and within-class S_W)

   Between-class scatter matrix S_B:

$$\begin{bmatrix} 63.21 & -19.53 & 165.16 & 71.36 \\ -19.53 & 10.98 & -56.05 & -22.49 \\ 65.16 & -56.05 & 436.64 & 186.91 \\ 71.36 & -22.49 & 186.91 & 80.60 \end{bmatrix}$$

LDA Step by Step

3. Compute the eigenvectors $(u_1, u_2, \ldots, u_d)$ and eigenvalues $(\lambda_1, \lambda_2, \ldots, \lambda_d)$ for the scatter matrices $S_W^{-1} S_B$.

u_1: $\begin{pmatrix} -0.205 \\ -0.387 \\ 0.546 \\ 0.714 \end{pmatrix}$ u_2: $\begin{pmatrix} -0.009 \\ -0.589 \\ 0.254 \\ -0.767 \end{pmatrix}$ u_3: $\begin{pmatrix} 0.179 \\ -0.318 \\ -0.366 \\ 0.601 \end{pmatrix}$ u_4: $\begin{pmatrix} 0.179 \\ -0.318 \\ -0.366 \\ 0.601 \end{pmatrix}$

λ_1: 3.23e+01 λ_2: 2.78e-01 λ_3: -4.02e-17 λ_4: -4.02e-17

LDA Step by Step

4. Sort the eigenvectors by decreasing eigenvalues and choose k eigenvectors.

   Eigenvalues in decreasing order:

   32.27
   0.27
   5.71e-15
   5.71e-15

LDA Step by Step

4. Sort the eigenvectors by decreasing eigenvalues and choose k eigenvectors.

Eigenvalues in decreasing order:

32.27
0.27
5.71e-15
5.71e-15

Variance explained:

λ_1: 99.15%
λ_2: 0.85%
λ_3: 0.00%
λ_4: 0.00%

LDA Step by Step

4. Sort the eigenvectors by decreasing eigenvalues and choose k eigenvectors.

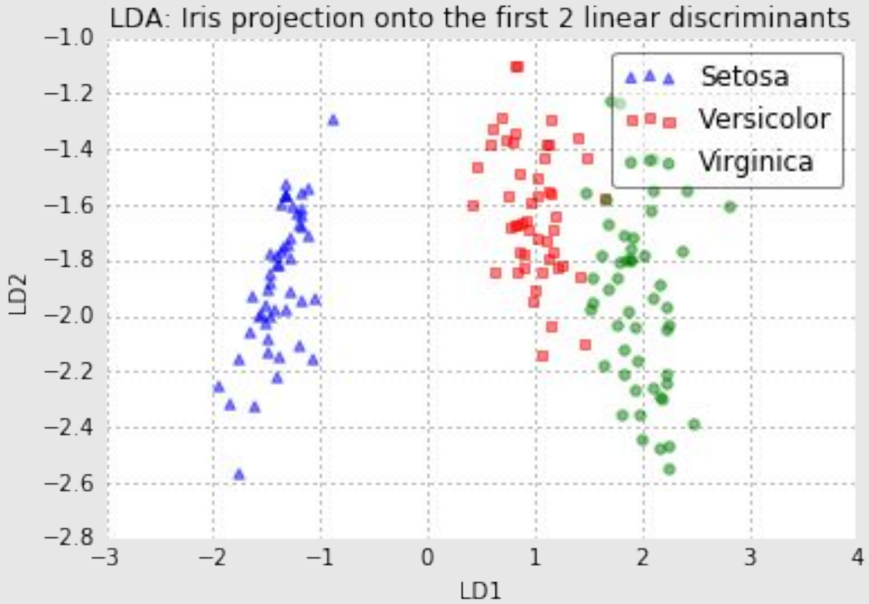
u_1: $\begin{pmatrix} -0.205 \\ -0.387 \\ 0.546 \\ 0.714 \end{pmatrix}$ λ_1: 3.23e+01

u_2: $\begin{pmatrix} -0.009 \\ -0.589 \\ 0.254 \\ -0.767 \end{pmatrix}$ λ_2: 2.78e-01

$$\Rightarrow \begin{pmatrix} -0.205 & -0.009 \\ -0.387 & -0.589 \\ 0.546 & 0.254 \\ 0.714 & -0.767 \end{pmatrix}$$

LDA Step by Step

5. Use this $d \times k$ eigenvector matrix to transform the samples onto the new subspace.



LDA Step by Step

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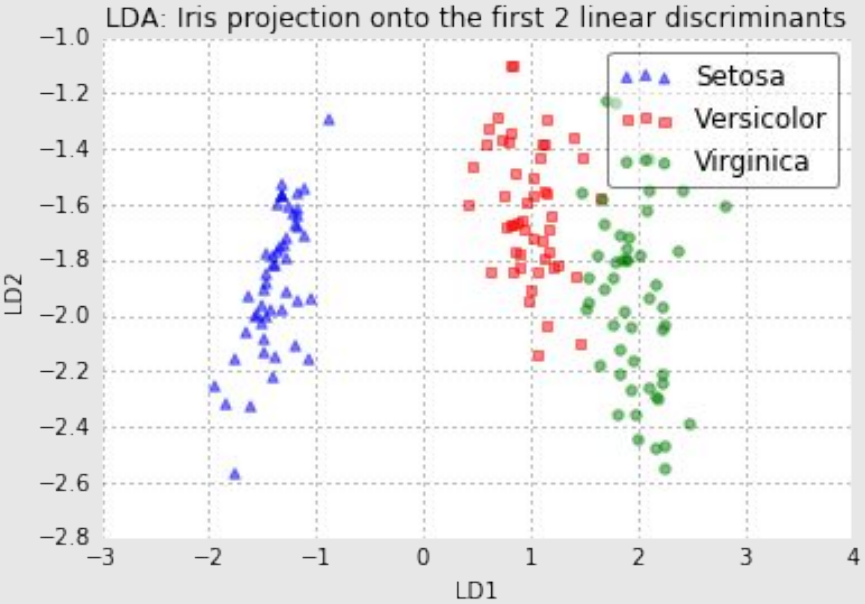

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