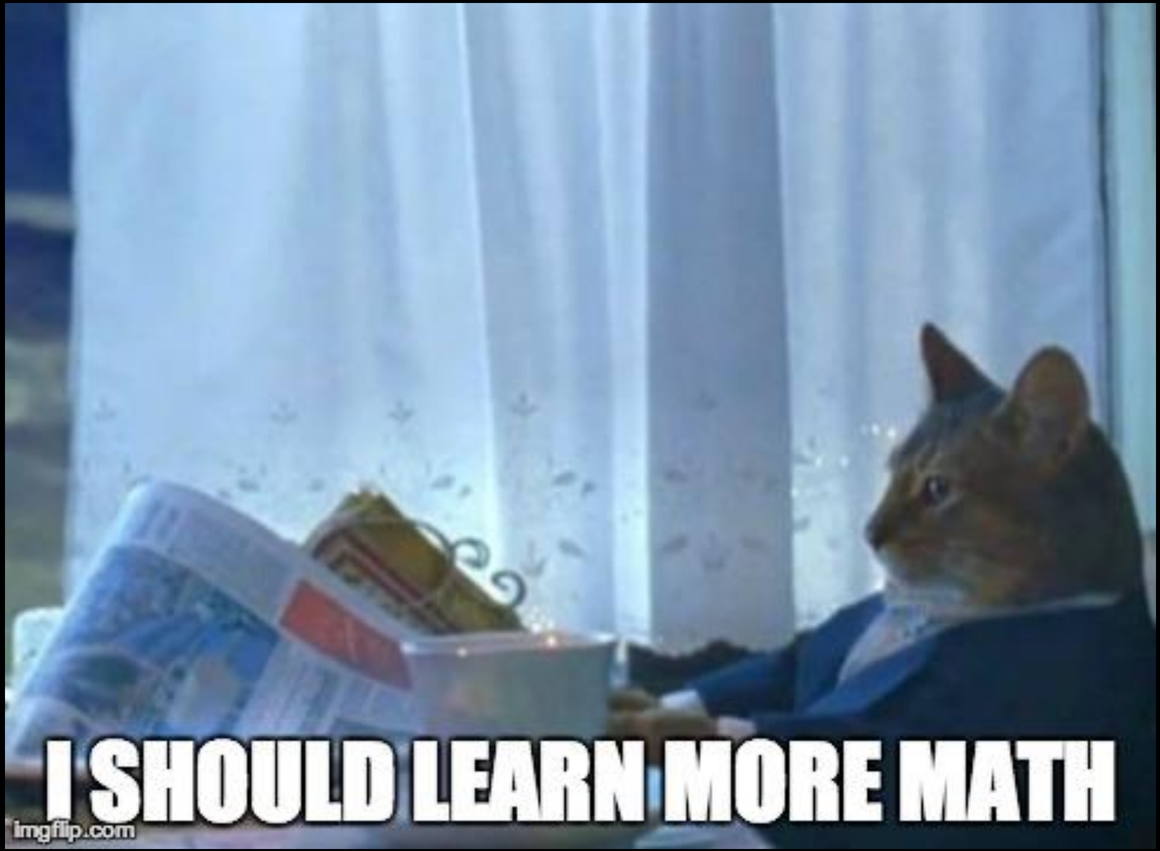
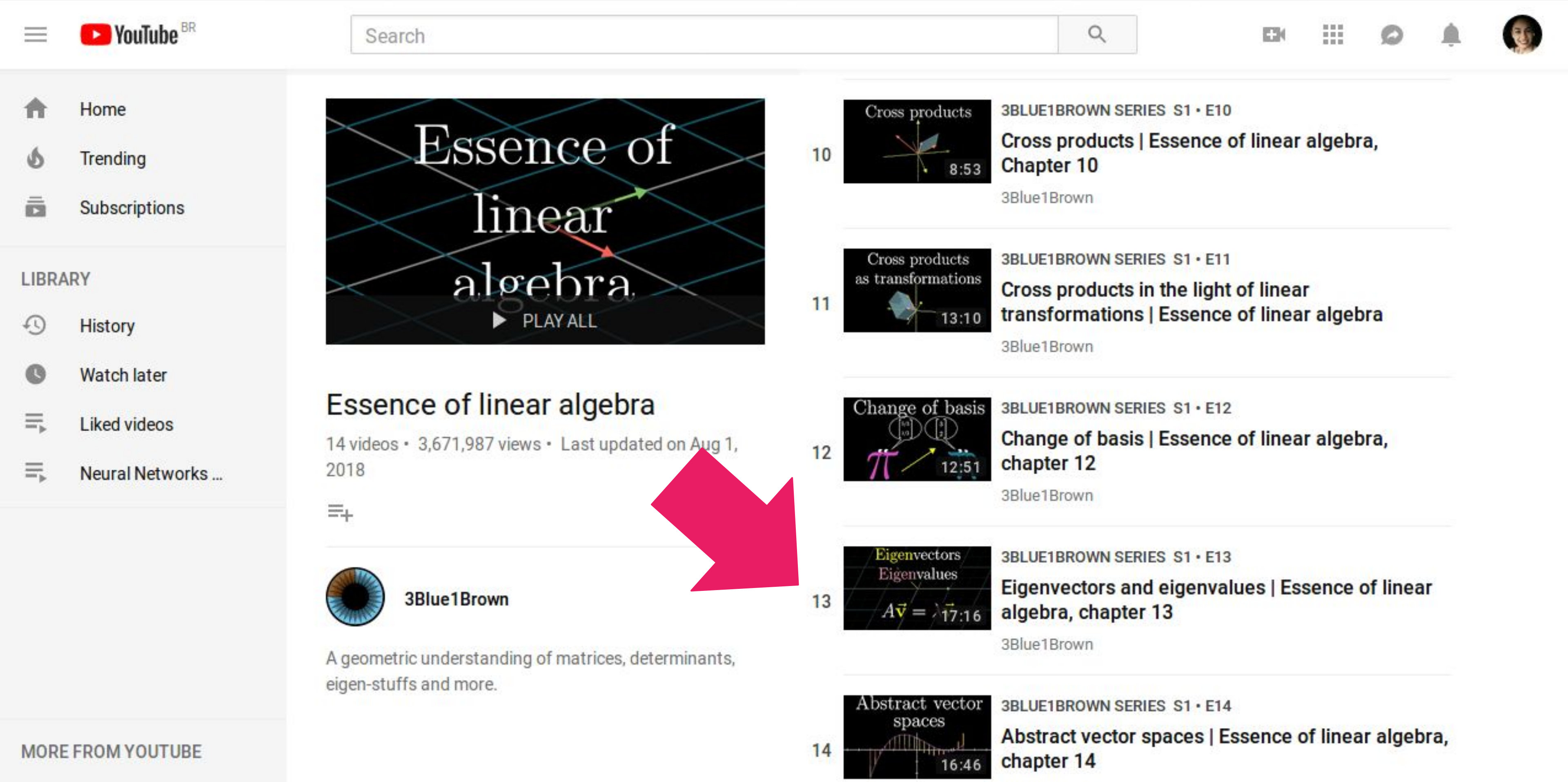

I SHOULD LEARN MORE MATH
imgflip.com

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



PCA Algorithm
By Singular Value Decomposition

Data Preprocessing

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

Preprocessing (feature scaling/mean normalization):

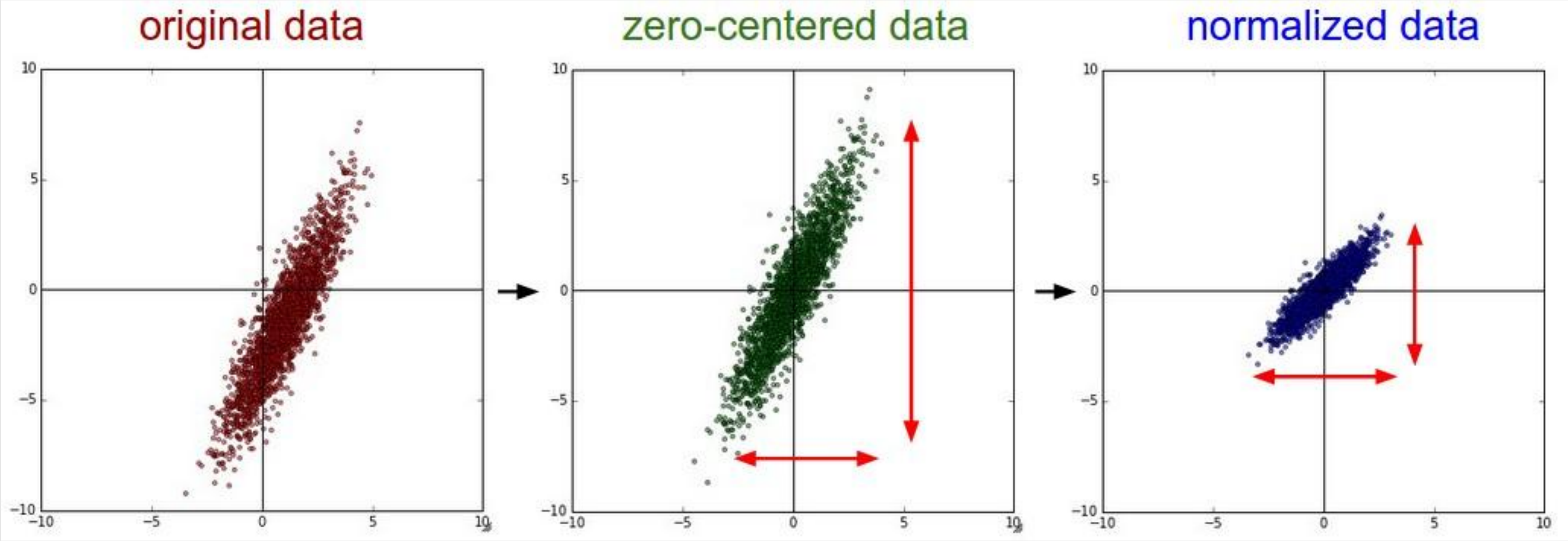
$$\mu_j = \frac{1}{m} \sum_{i=1}^{m} x_j^{(i)}$$

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

Center the data

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":

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

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

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

PCA Algorithm

Reduce data from n-dimensions to k-dimensions

Compute "covariance matrix":

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

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

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

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:

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

$$\underbrace{u^{(1)} \cdots u^{(k)}}_{k}$$

PCA Algorithm

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

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

$$x \in \mathbb{R}^n \rightarrow z \in \mathbb{R}^k$$

$$z = \underbrace{\begin{bmatrix} | & & | \\ u^{(1)} & \cdots & u^{(k)} \\ | & & | \end{bmatrix}^{\mathrm{T}}}_{k \times n} \underbrace{x}_{n \times 1}$$

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)

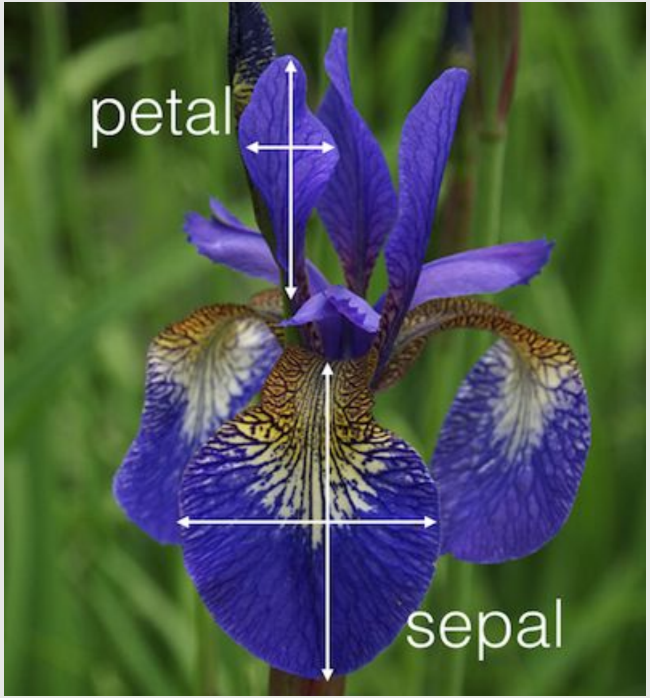
$$z = (\mathrm{U}_{\mathrm{reduce}})^{\mathrm{T}} \times x$$

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

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

reasoning for complex data

Linear Discriminant Analysis

Machine Learning

Prof. Sandra Avila

Institute of Computing (IC/Unicamp)

MC886, October 2, 2019

Today's Agenda

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

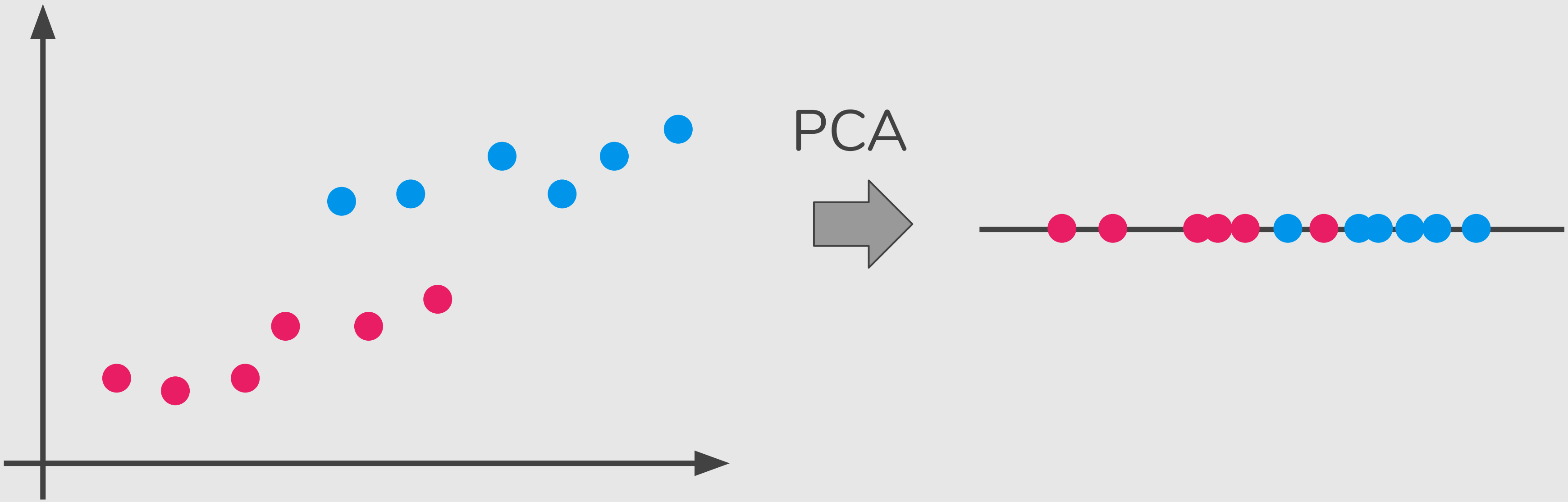
Linear Discriminant Analysis

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

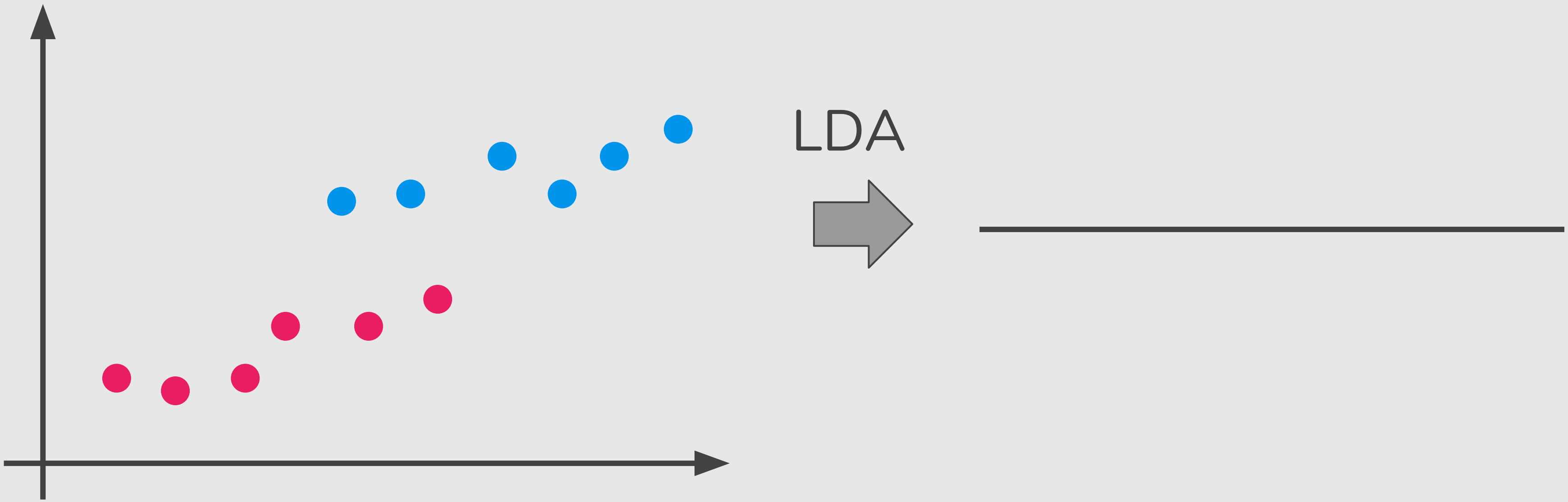
LDA: Simple Example

Reducing 2D to 1D



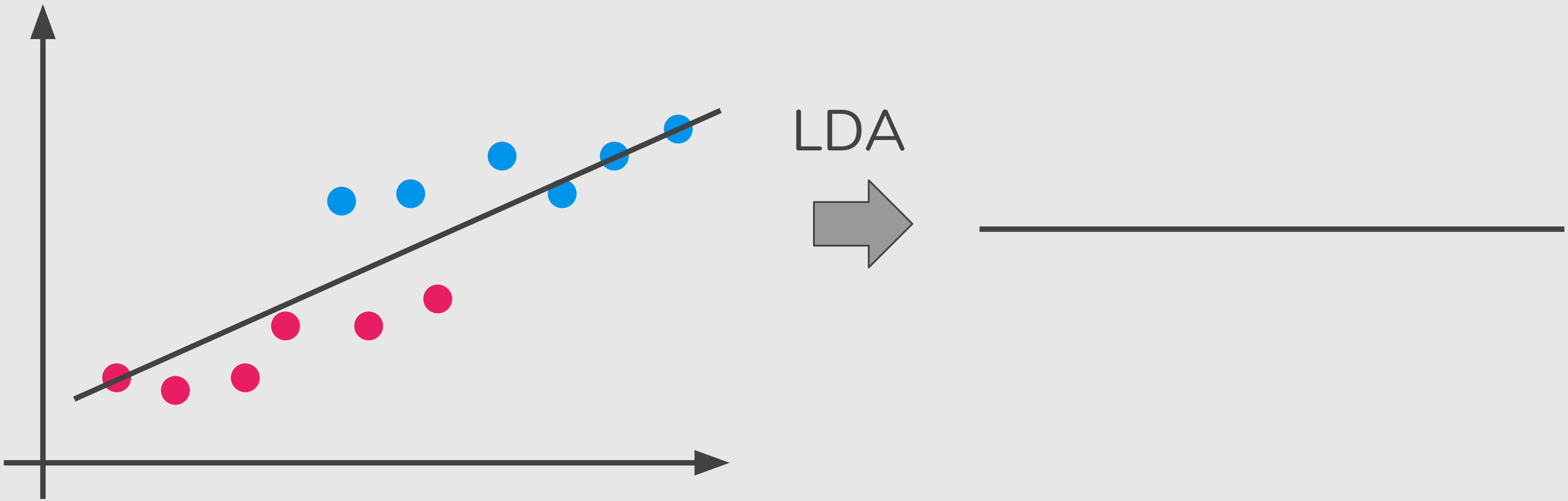
LDA: Simple Example

Reducing 2D to 1D



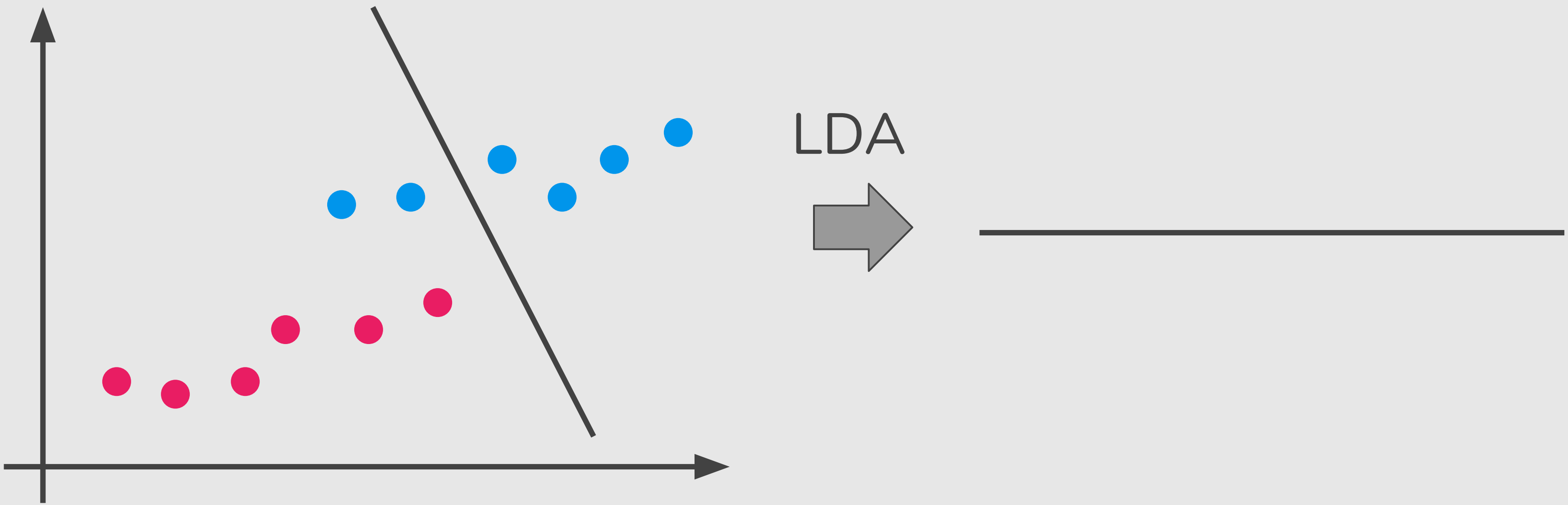
LDA: Simple Example

Reducing 2D to 1D



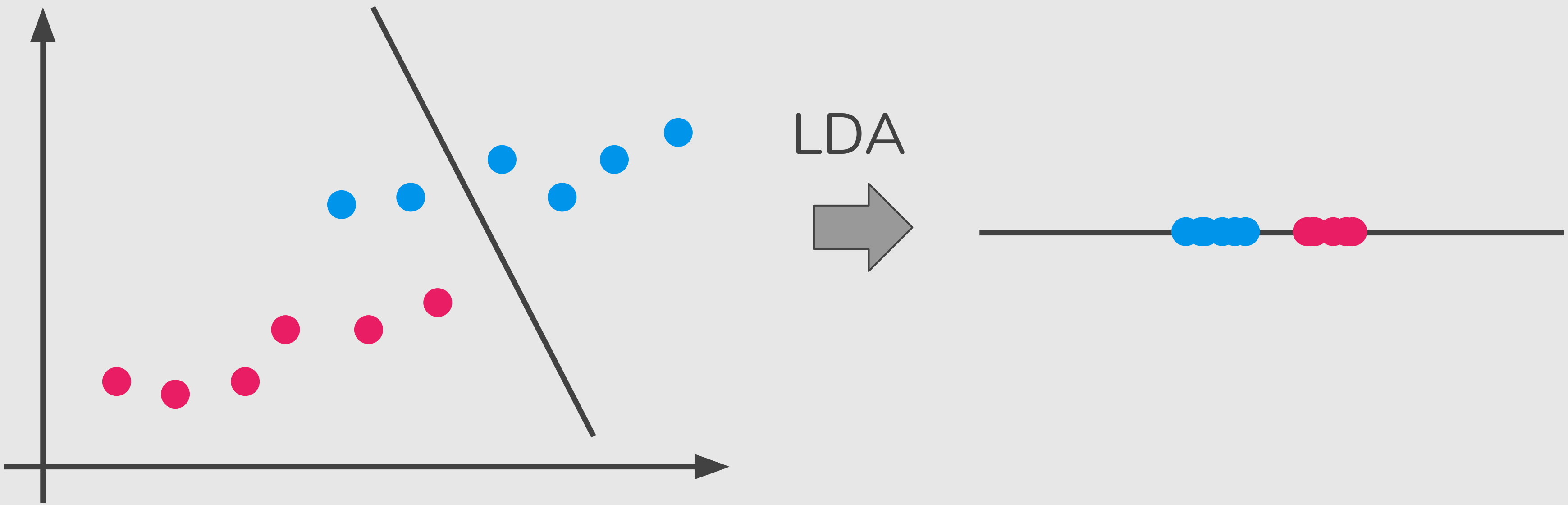
LDA: Simple Example

Reducing 2D to 1D



LDA: Simple Example

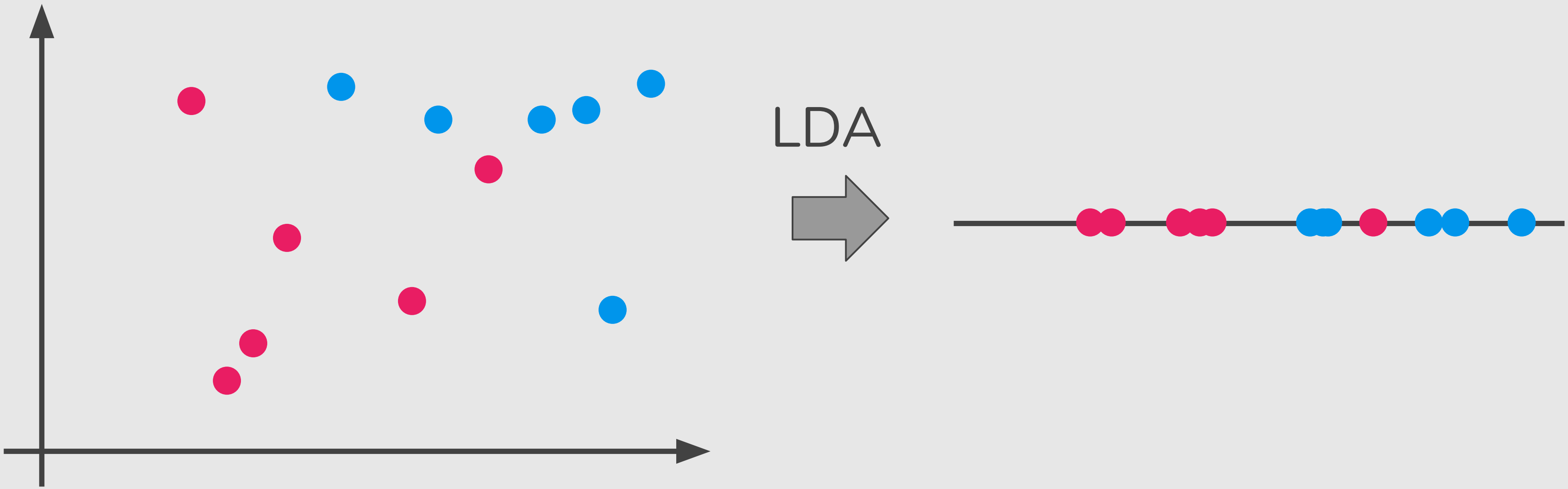
Reducing 2D to 1D



How LDA create a new axis?

How LDA create a new axis?

Reducing 2D to 1D



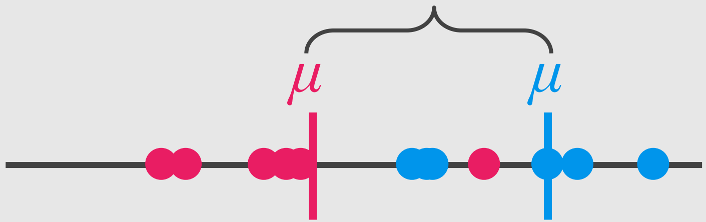
How LDA create a new axis?

The new axis is created according two criteria:

How LDA create a new axis?

The new axis is created according two criteria:

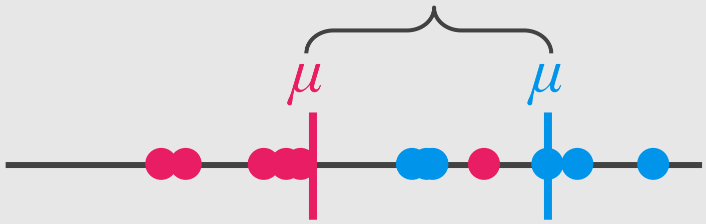
1. Maximize the distance between the means:



How LDA create a new axis?

The new axis is created according two criteria:

1. Maximize the distance between the means:

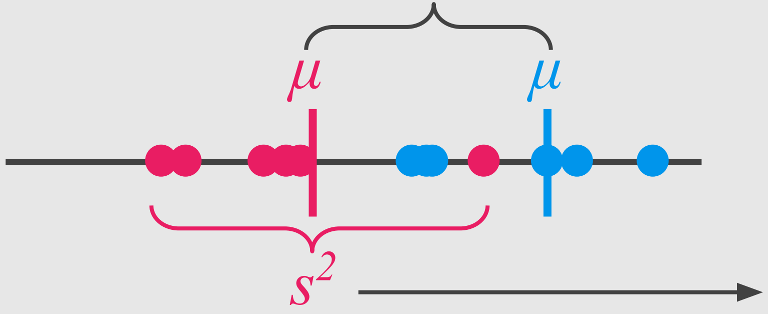


2. Minimize the variation (which LDA calls scatter) within each class.

How LDA create a new axis?

The new axis is created according two criteria:

1. Maximize the distance between the means:



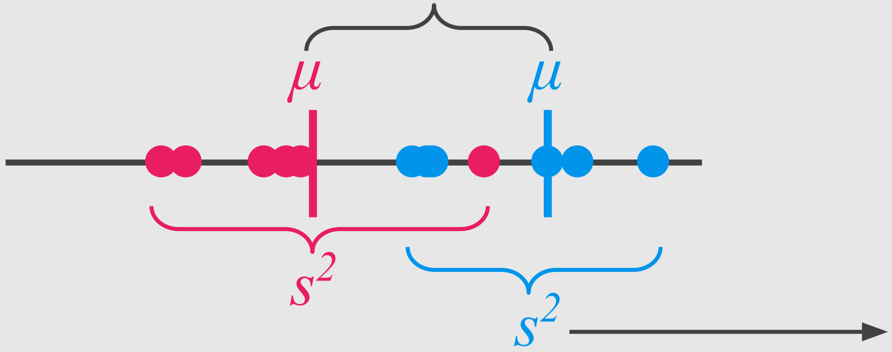
This is the scatter around the pink dots.

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:

1. Maximize the distance between the means:



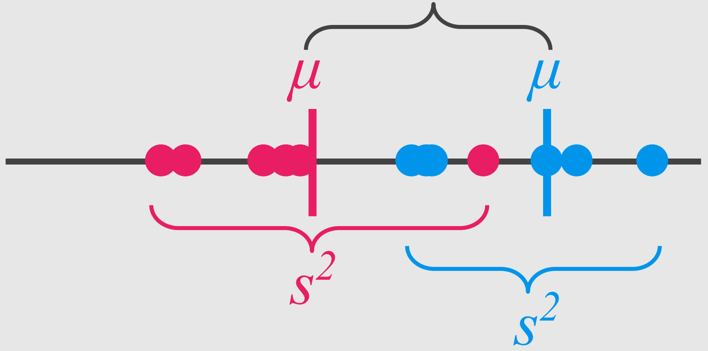
This is the scatter around the blue dots.

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

How LDA create a new axis?

The new axis is created according two criteria:

1. Maximize the distance between the means:



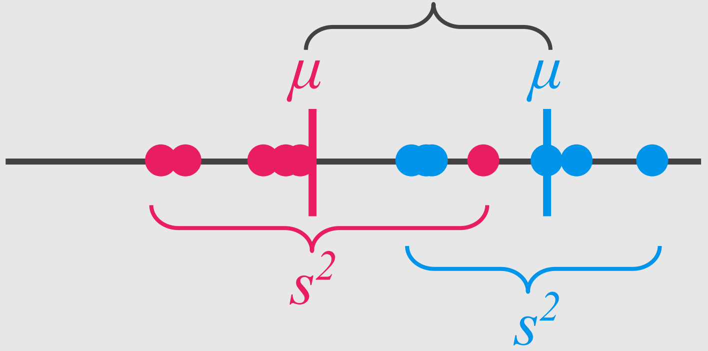
$$\frac{(\mu - \mu)^2}{s^2 + s^2}$$

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:

1. Maximize the distance between the means:



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

$\longrightarrow$ Ideally large

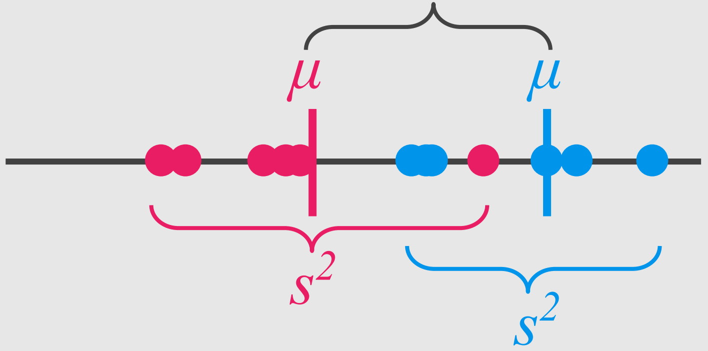
$\longrightarrow$ Ideally small

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:

1. Maximize the distance between the means:



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

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

→ Ideally large

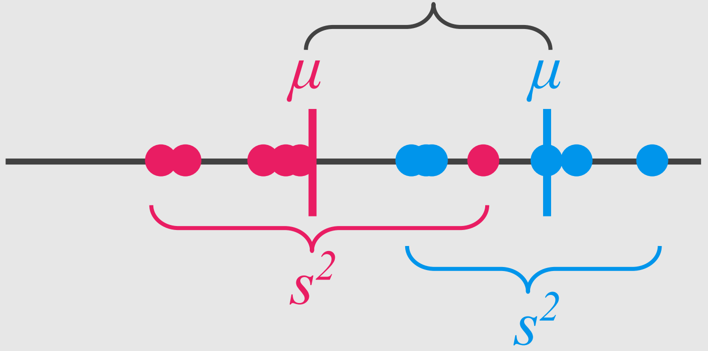
→ Ideally small

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:

1. Maximize the distance between the means:



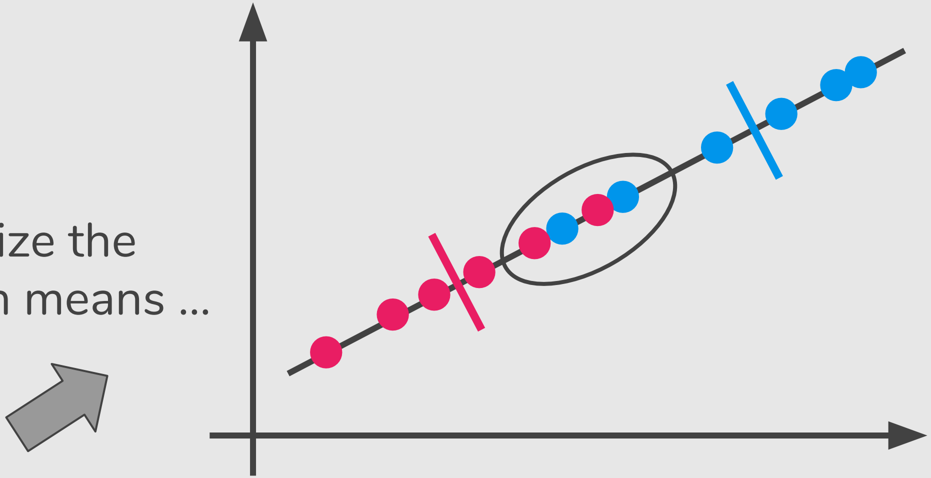
Let’s call $(\mu - \mu)$ d for distance.

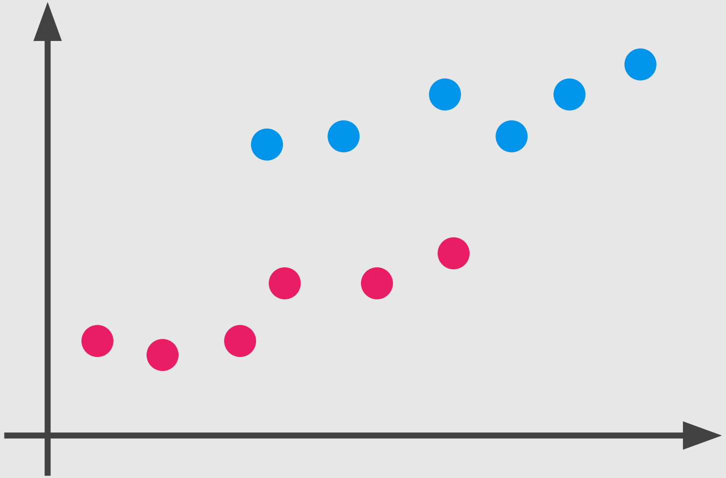
$$\frac{d^2}{s^2 + s^2} \quad \begin{array}{l} \longrightarrow \text{Ideally large} \\ \longrightarrow \text{Ideally small} \end{array}$$

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

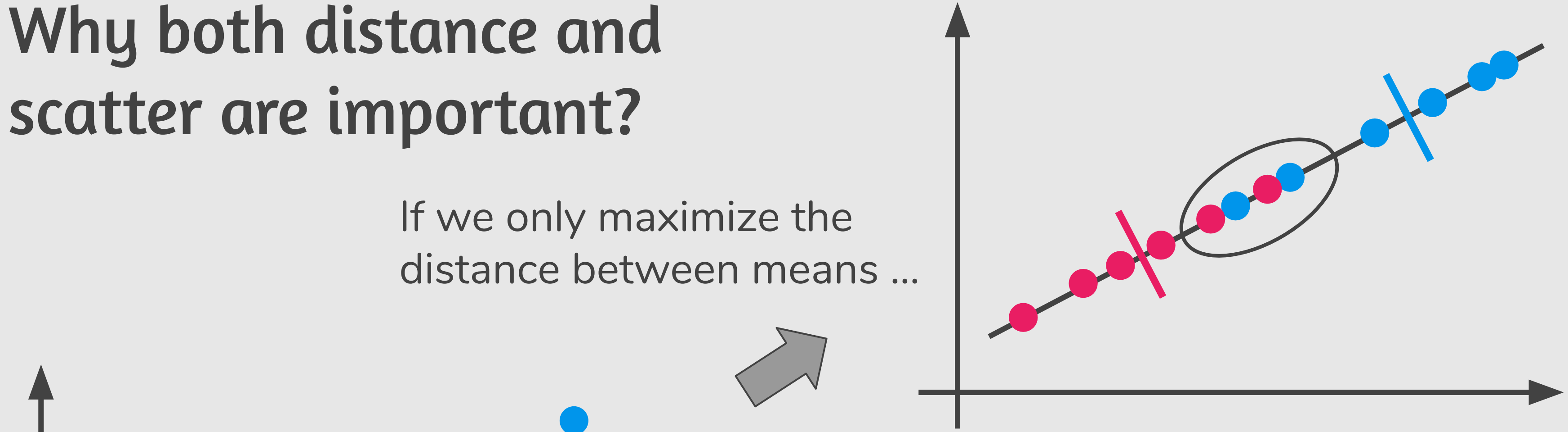
Why both distance and scatter are important?

If we only maximize the distance between means ...

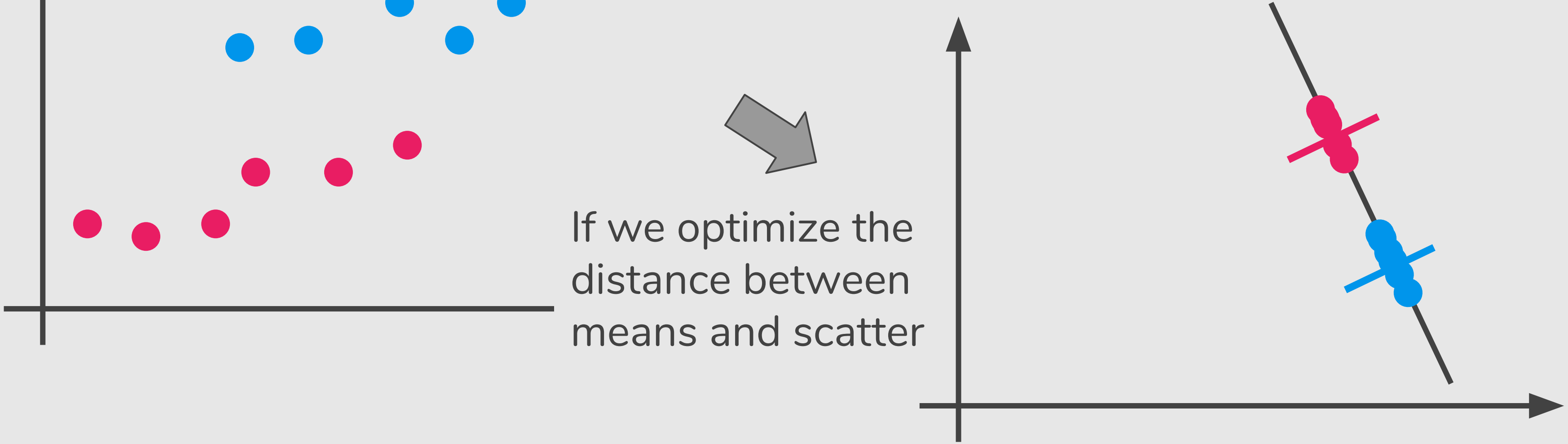




Why both distance and scatter are important?

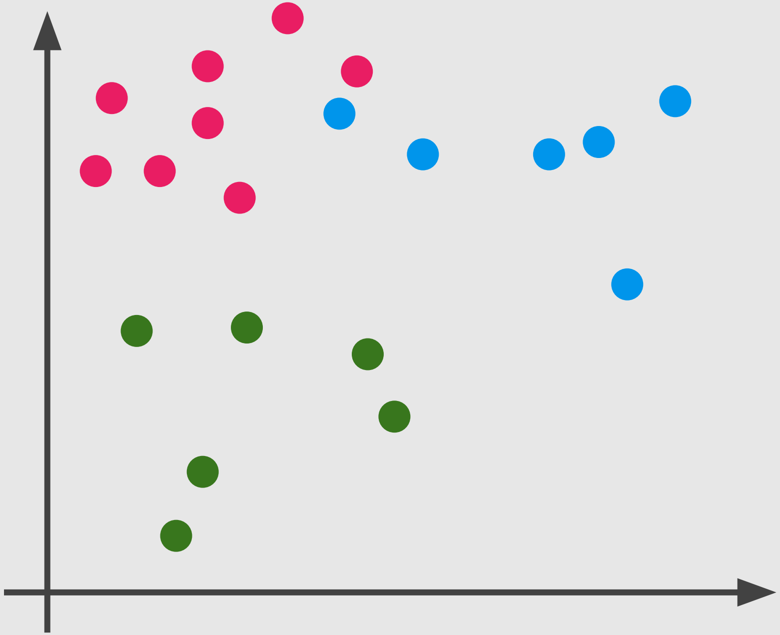


If we only maximize the distance between means ...

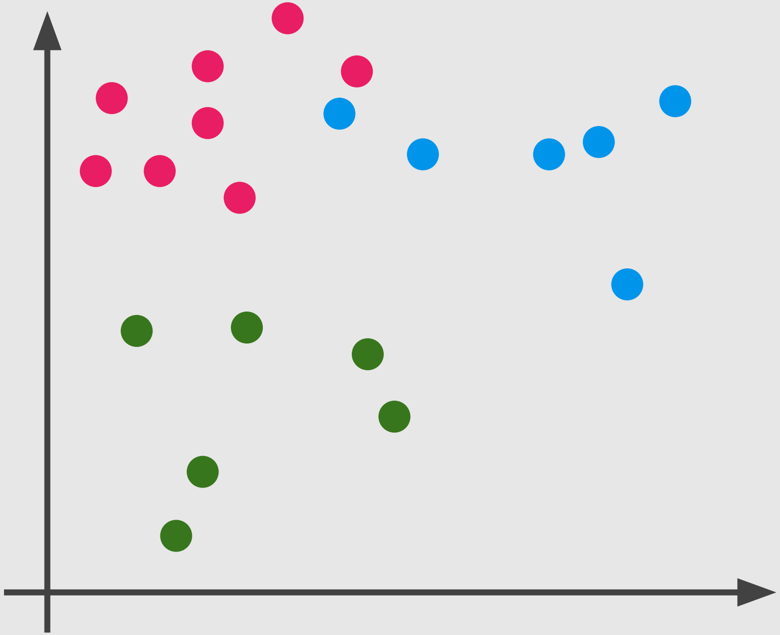


If we optimize the distance between means and scatter

What if we have 3 classes?



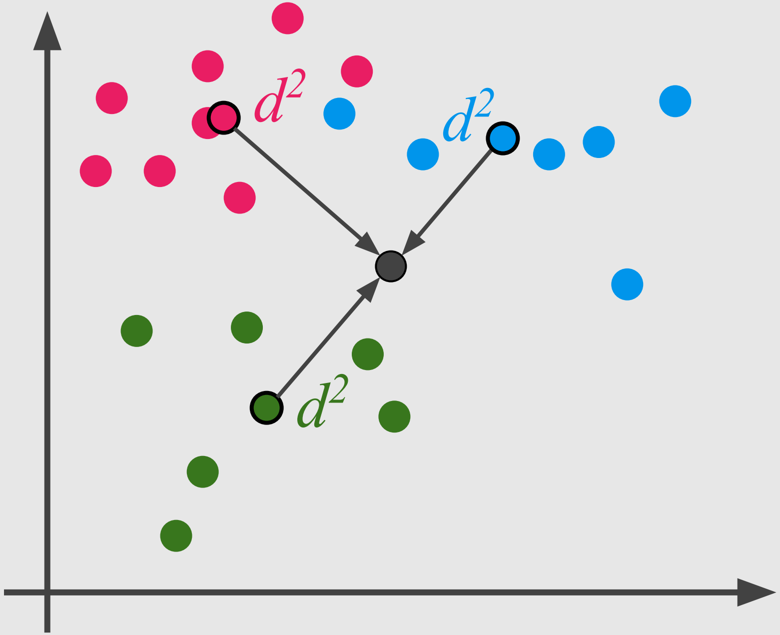
What if we have 3 classes?



How we measure the distance among the means?

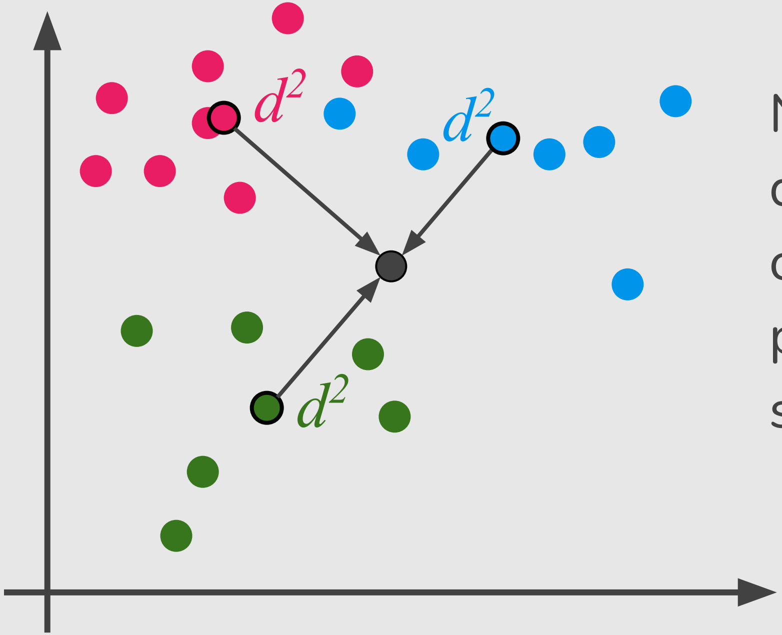
What if we have 3 classes?

What if we have 3 classes?



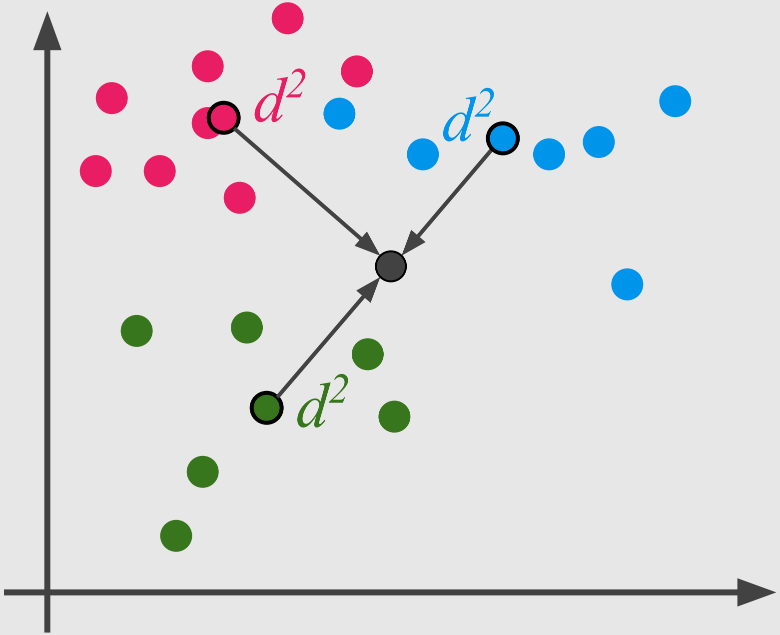
Then measure the distance between a point that is central in each class and the main central point.

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?



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

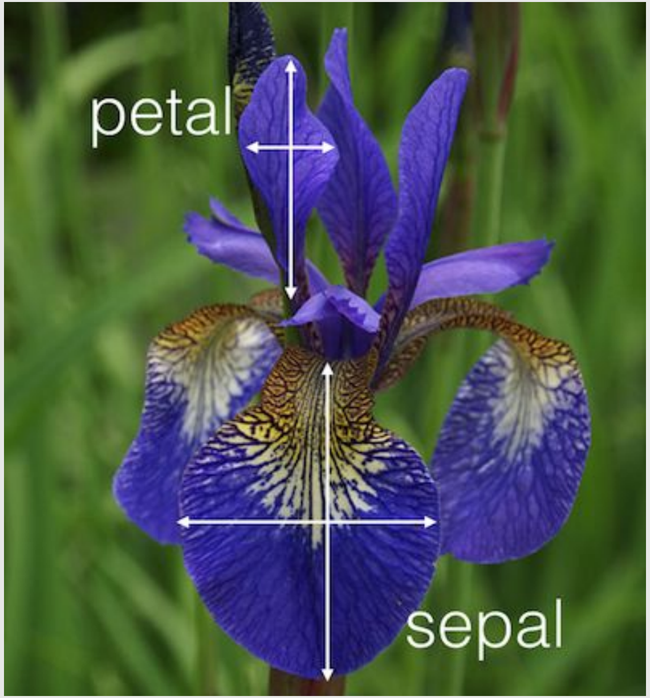
Today's Agenda

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

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.

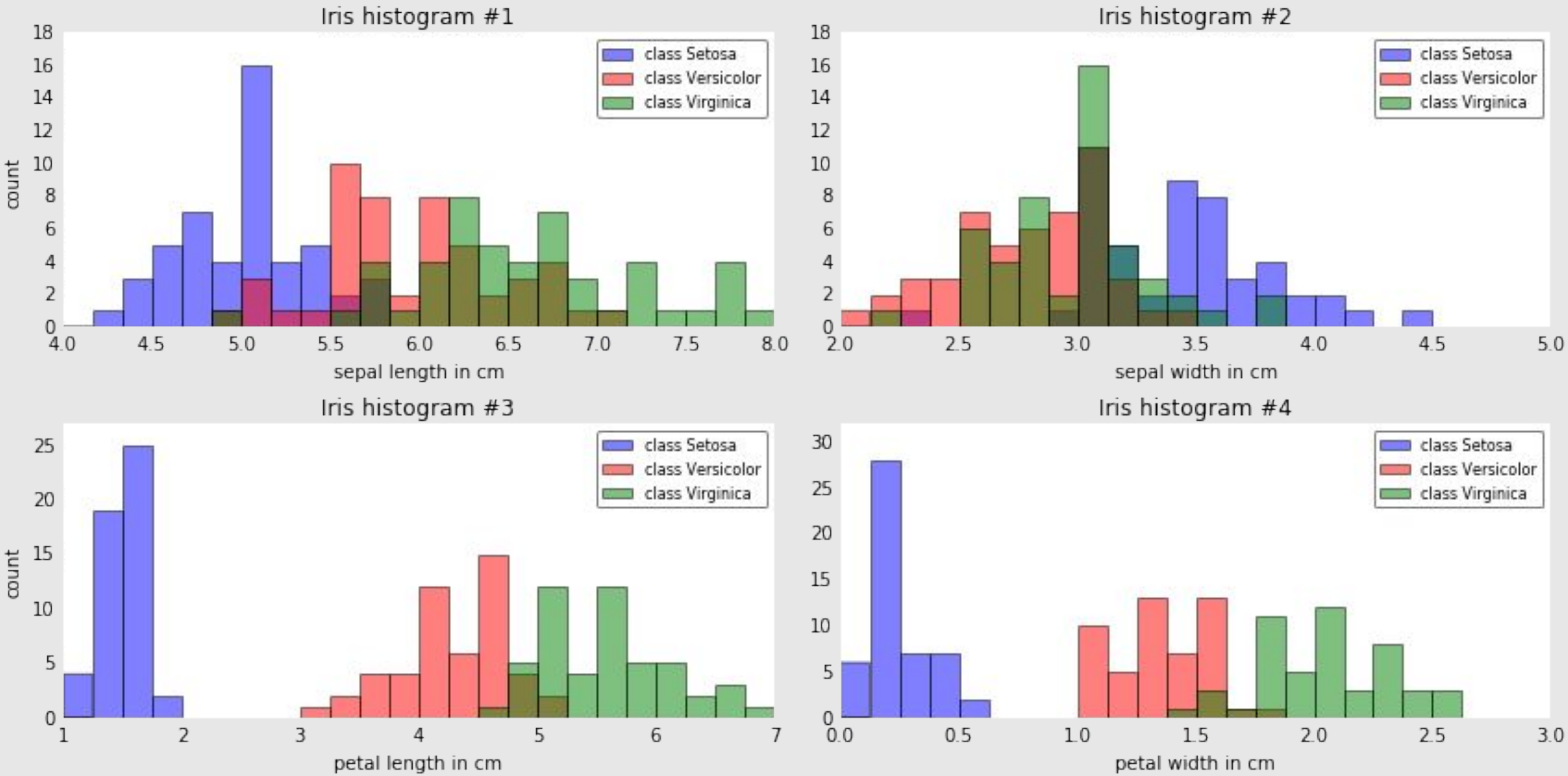
The three classes in the Iris dataset:

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.

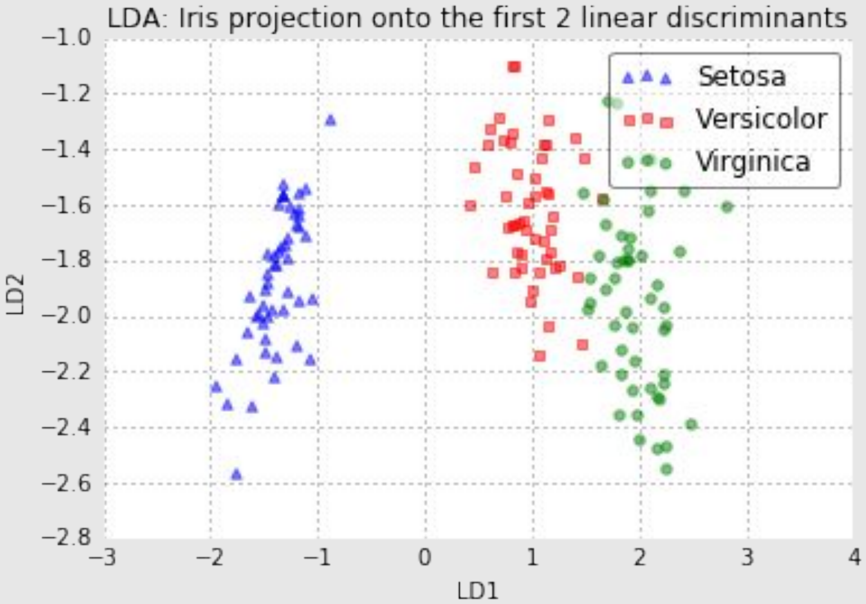
u_1: $\begin{bmatrix} -0.205 \\ -0.387 \\ 0.546 \\ 0.714 \end{bmatrix}$ λ_1: 3.23e+01

u_2: $\begin{bmatrix} -0.009 \\ -0.589 \\ 0.254 \\ -0.767 \end{bmatrix}$ 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

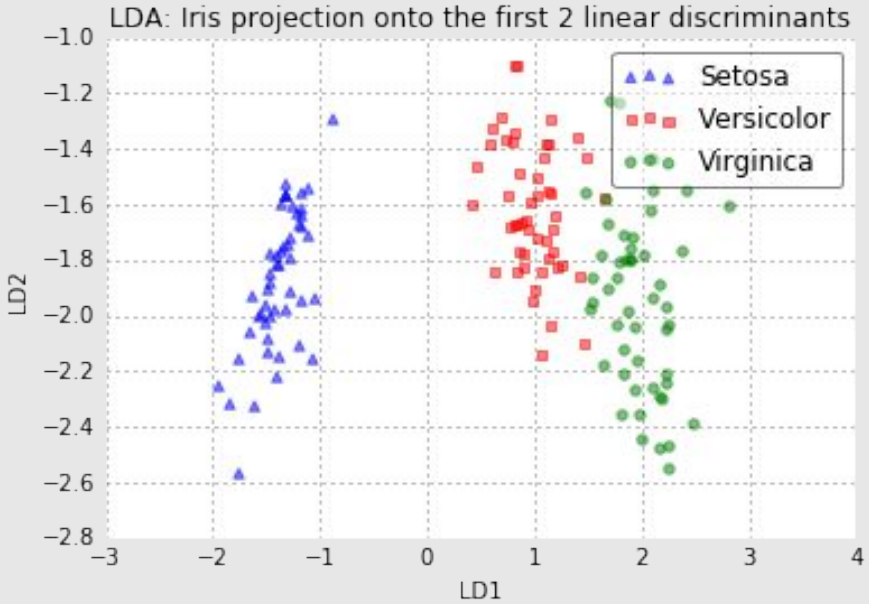
5. Use this $d \times k$ eigenvector matrix to transform the samples onto the new subspace.



LDA Step by Step

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

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



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”