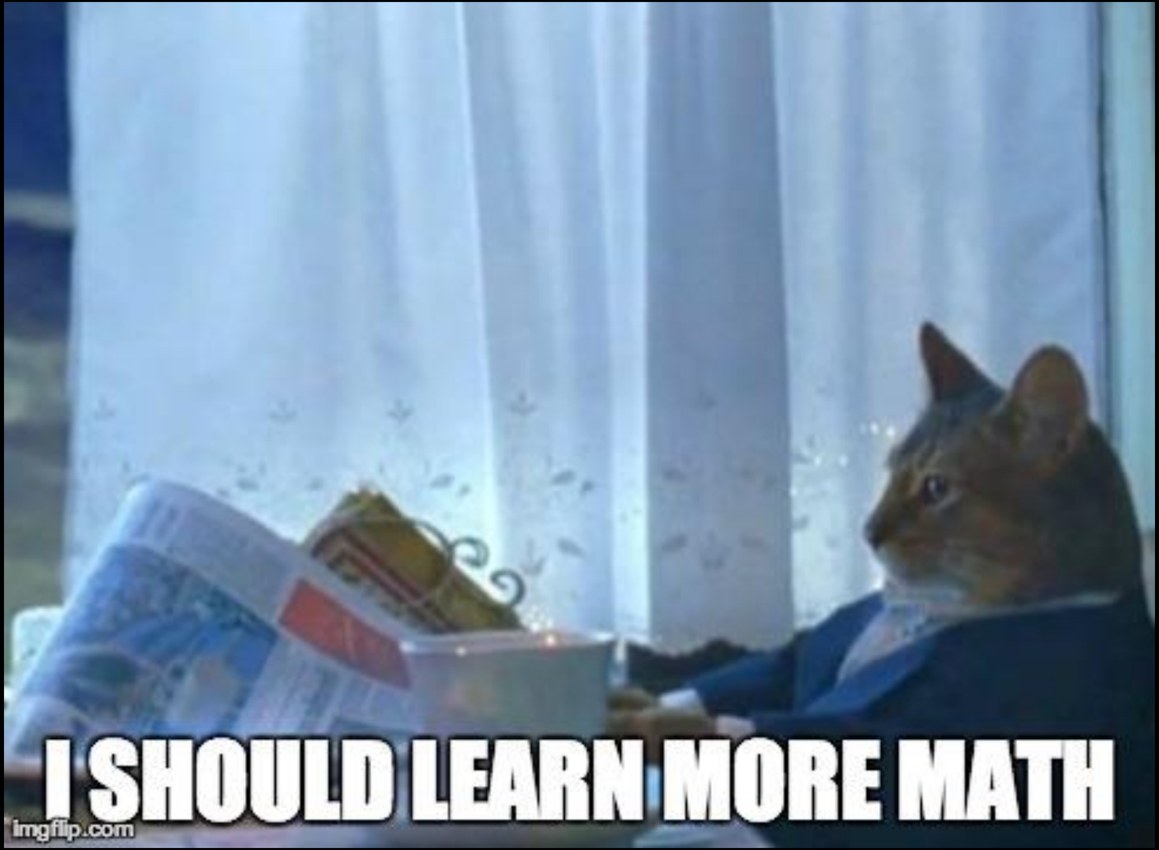

I SHOULD LEARN MORE MATH
imgflip.com

Maior Dúvida da Aula

1. Eu consegui visualizar a projeção dos pontos em duas dimensões (traçando a linha paralela), mas durante toda a aula eu não consegui imaginar isso sendo feito em uma terceira dimensão. Teria como mostrar isso?
2. Como podemos interpretar as features “transformadas” pelo PCA?
3. Na aula foi mencionado que a redução dos dados pode gerar novos dados não mais representativos. Neste caso, como checar se o dado reduzido ainda é representativo?
4. É possível fazer o retorno das componentes principais para as variáveis originais (as mais importantes) para obter maior interpretabilidade do modelo com essas variáveis, individualmente?
5. É possível no método do PCA termos um caso de autovalores degenerados (dois ou mais autovalores com o mesmo valor)? E se sim, têm algum significado?

6. Como saber a porcentagem para manter % da variância? E quando saber se o pca é bom o suficiente para o seu problema?
7. Imagino que não seja possível resolver uma equação polinomial de grau elevado (levando em conta casos de alta dimensionalidade) por uso de fórmulas já conhecidas (como bháskara por exemplo), nesse caso como faremos para resolver essas equações computacionalmente encontrando os autovalores?
8. Olhando para os primeiros k vetores, eu não entendi se a gente escolhe ou é algo aleatório/definido? E como escolheríamos o melhor, caso fosse nossa escolha, a partir de testes?
9. Tal qual a normalização, é válido dizer que, desde que executado da maneira correta - isto é, mantendo um percentual relevante de variância das features -, o PCA também "não faz mal" aos modelos?

Dimensionality Reduction (PCA)

Machine Learning

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

MC886/MO444, October 20, 2022

PCA Algorithm

By Singular Value Decomposition

Data Preprocessing

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

Preprocessing (feature scaling/mean normalization):

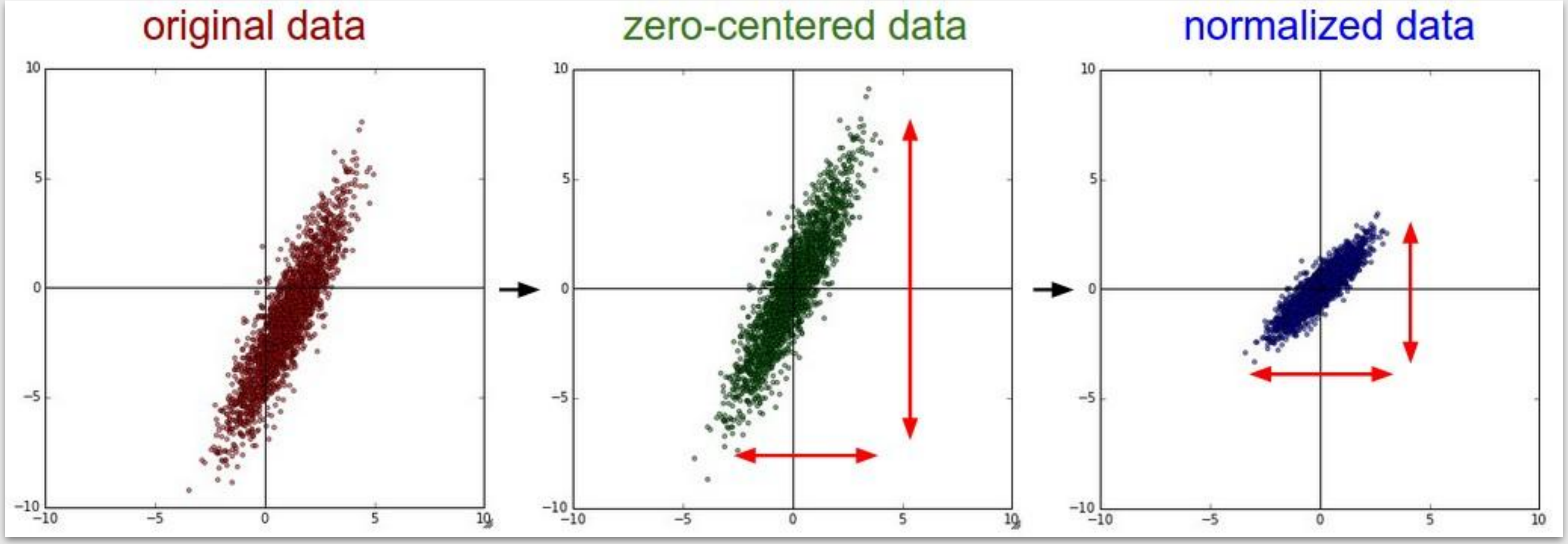
$$\mu_j = \frac{1}{m} \sum_{i=1}^{m} x_j^{(i)}$$

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":

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

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 $\mathbf{\Sigma}$:

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

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:

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

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

PCA Algorithm

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

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

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

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

PCA Algorithm

After mean normalization and optionally feature scaling:

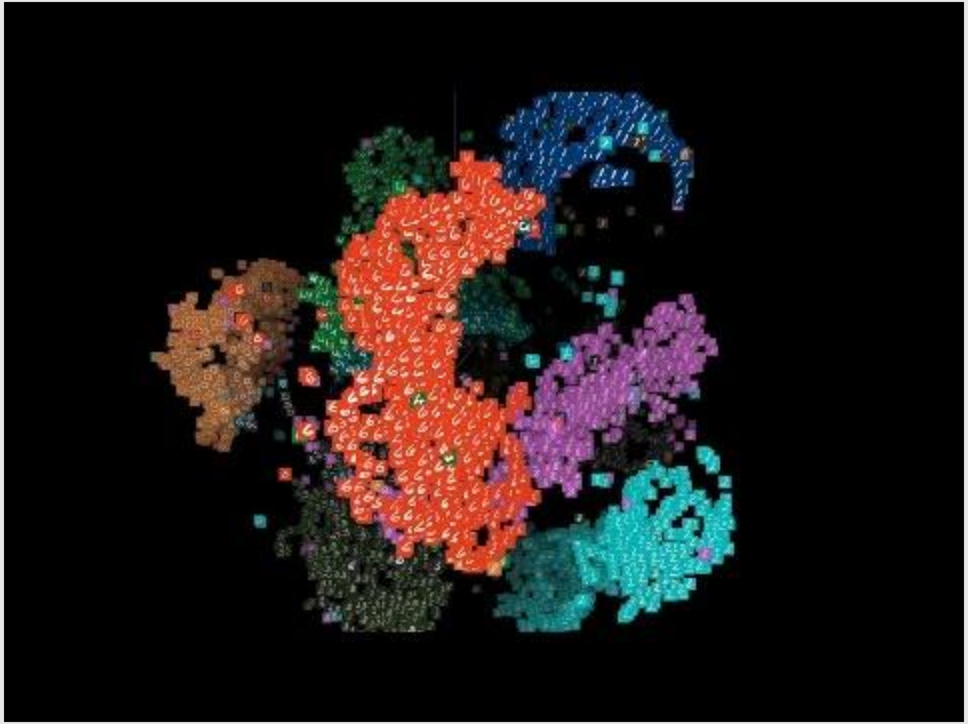
$$\Sigma = \frac{1}{m} \sum_{i=1}^{n} (x^{(i)})(x^{(i)})^{\mathrm{T}}$$

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

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

t-SNE A.I. Experiments: Visualizing High-Dimensional Space

https://youtu.be/wvsE8jm1GzE



Linear Discriminant Analysis

Machine Learning

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

MC886/MO444, October 20, 2022

Today's Agenda

- Linear Discriminant Analysis
  - PCA vs LDA
  - LDA: Simple Example
  - LDA Algorithm
  - LDA Step by Step (Iris Dataset)

Linear Discriminant Analysis

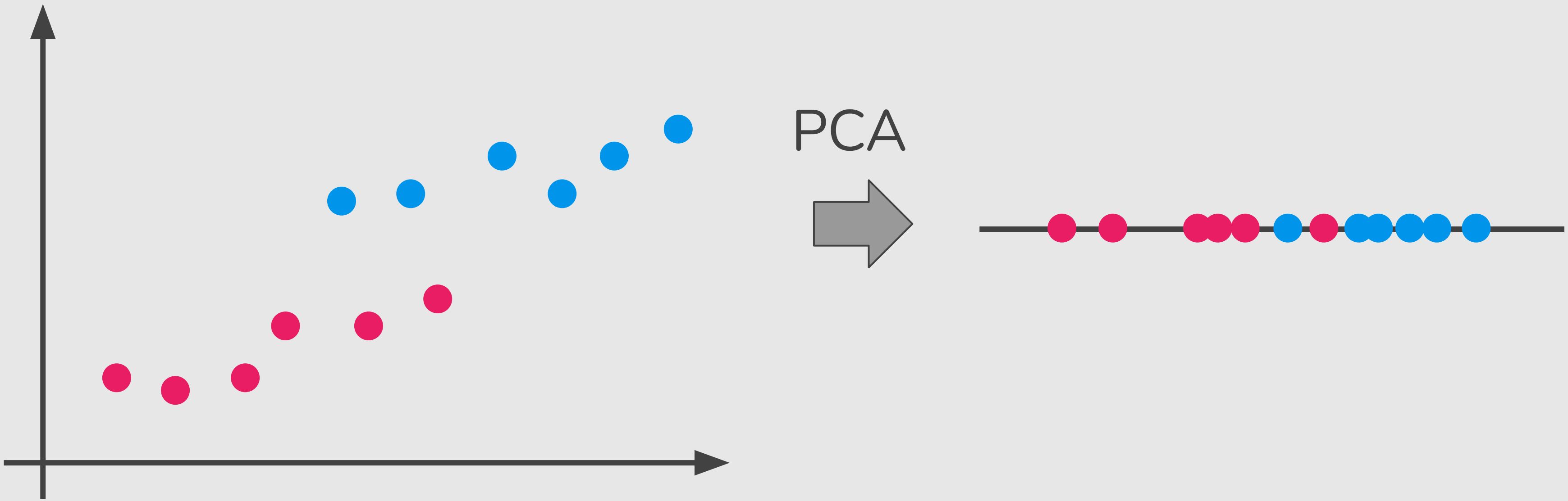
Linear Discriminant Analysis (LDA)

- 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

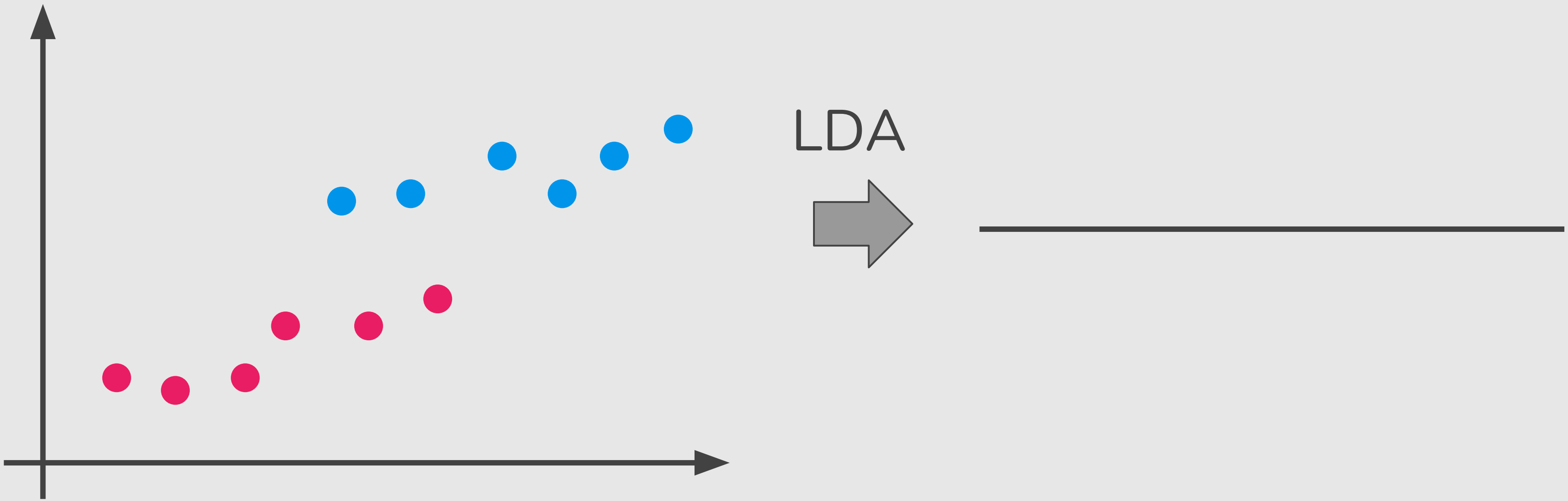
LDA: Simple Example

Reducing 2D to 1D



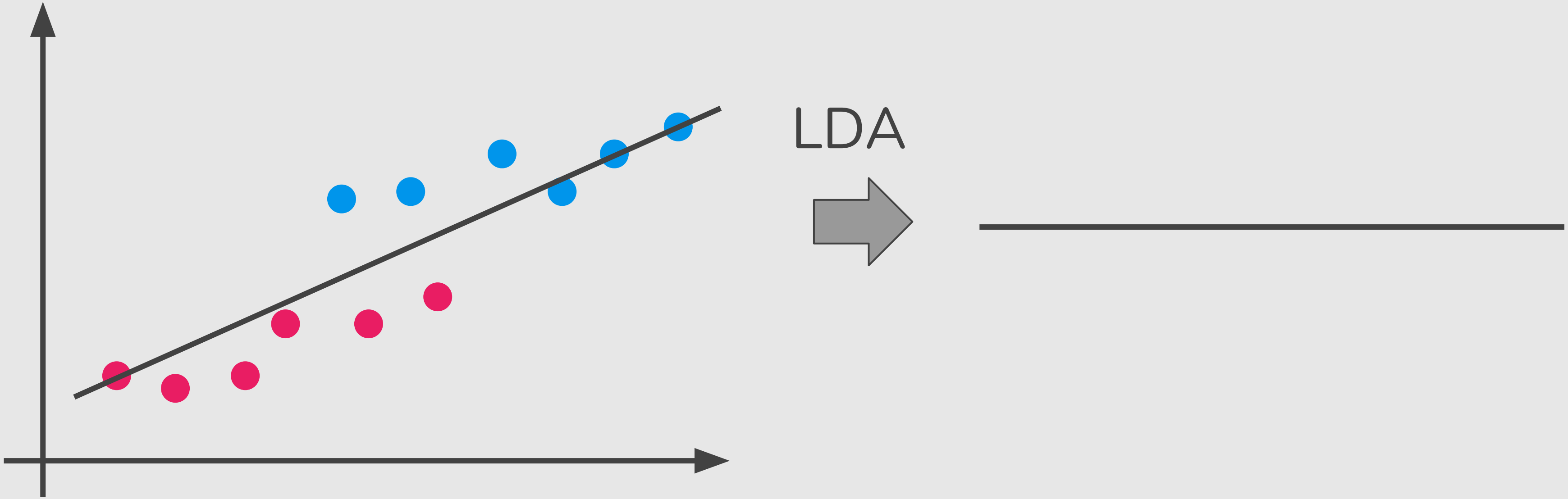
LDA: Simple Example

Reducing 2D to 1D



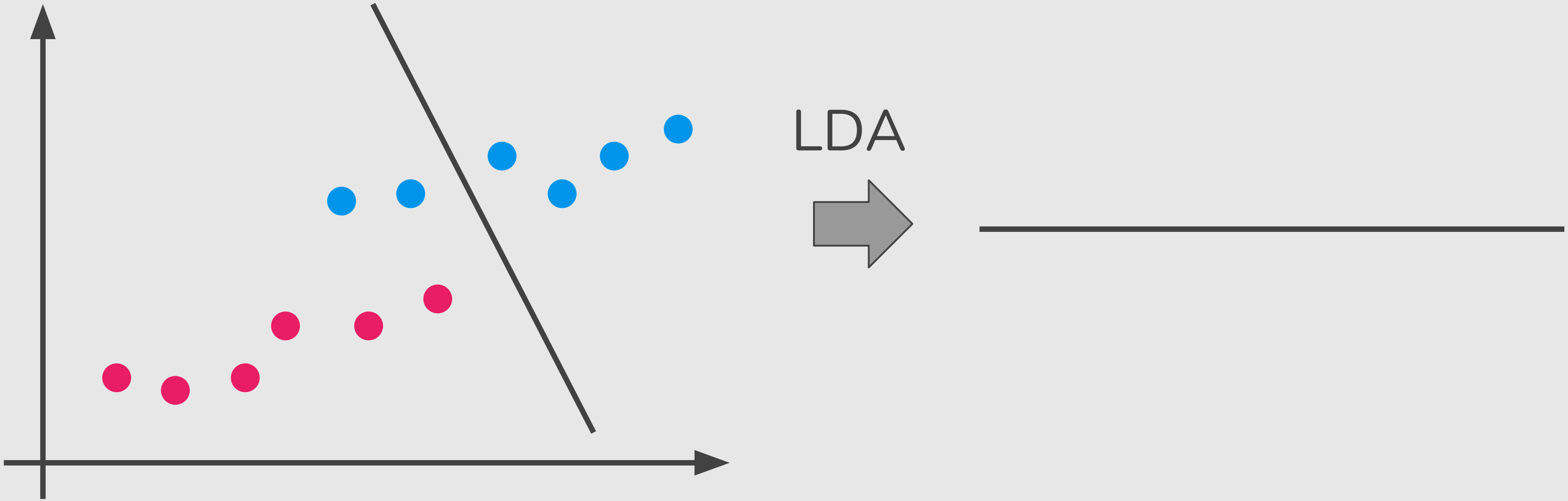
LDA: Simple Example

Reducing 2D to 1D



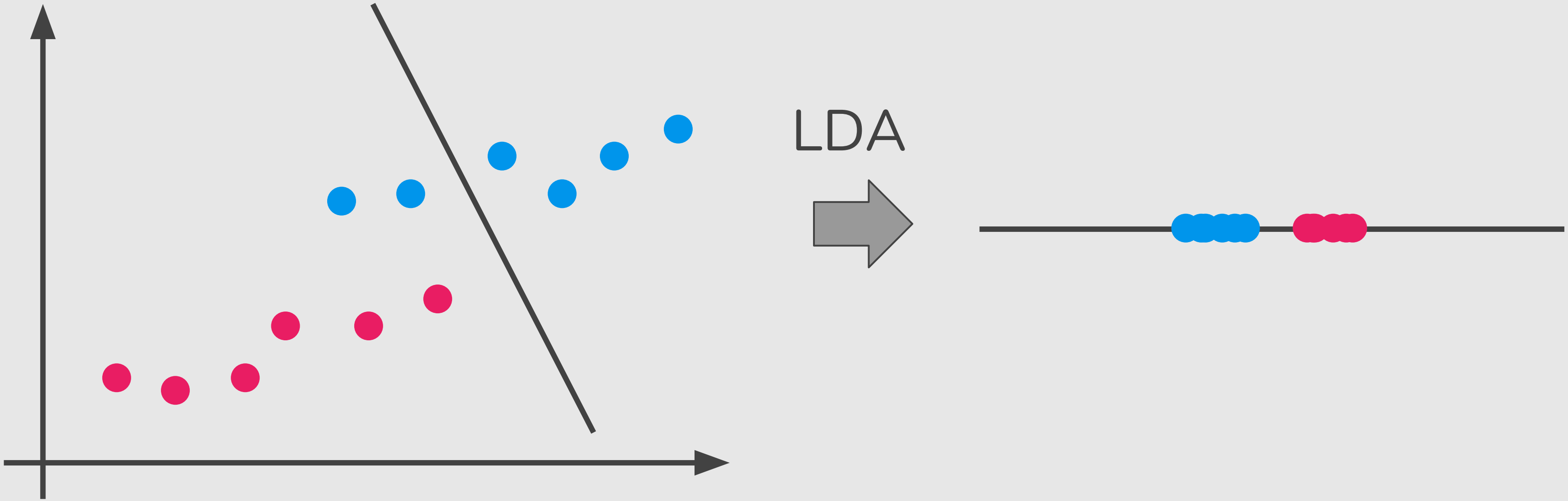
LDA: Simple Example

Reducing 2D to 1D



LDA: Simple Example

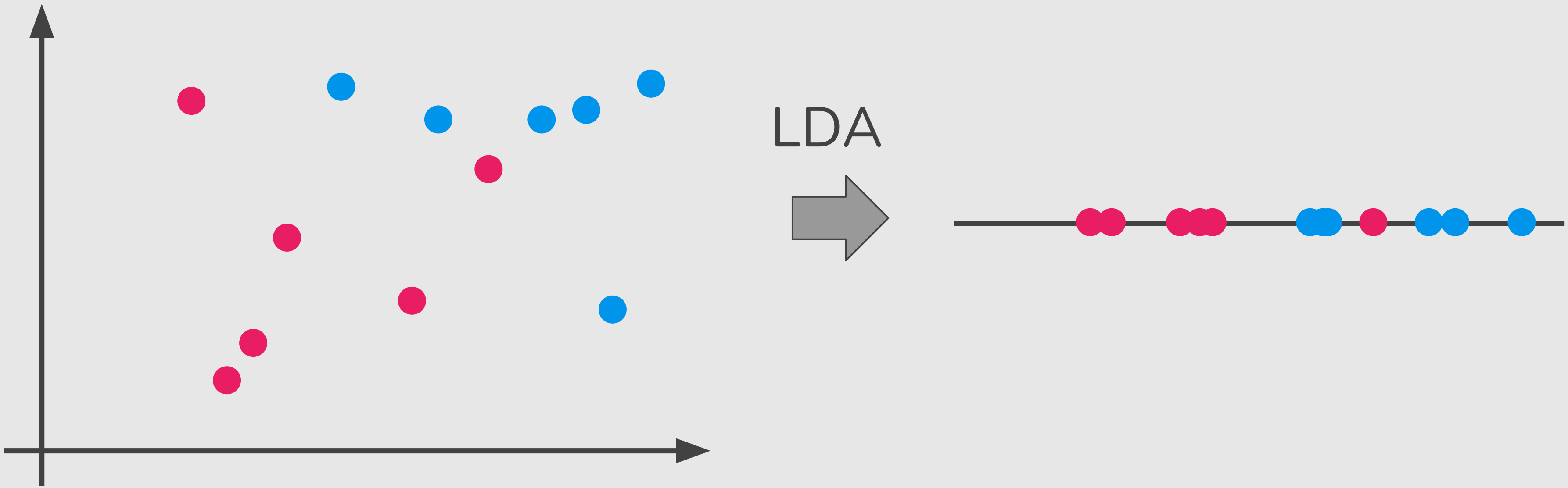
Reducing 2D to 1D



How LDA create a new axis?

How LDA create a new axis?

Reducing 2D to 1D



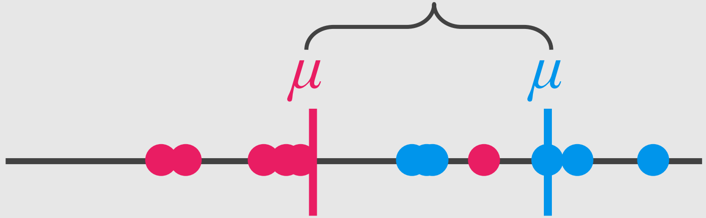
How LDA create a new axis?

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:



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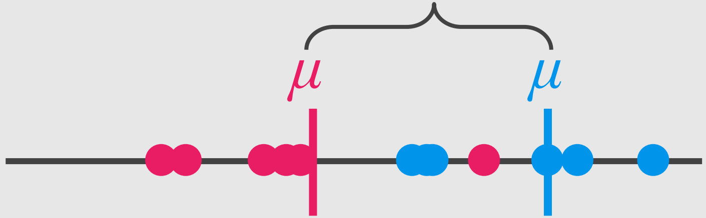

2. Minimize the variation (which LDA calls scatter) within each class.

How LDA create a new axis?

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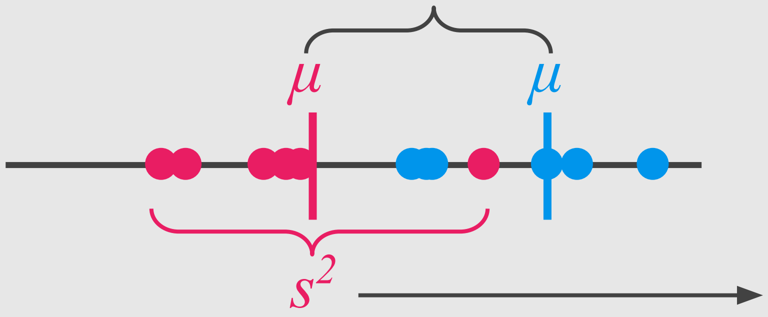


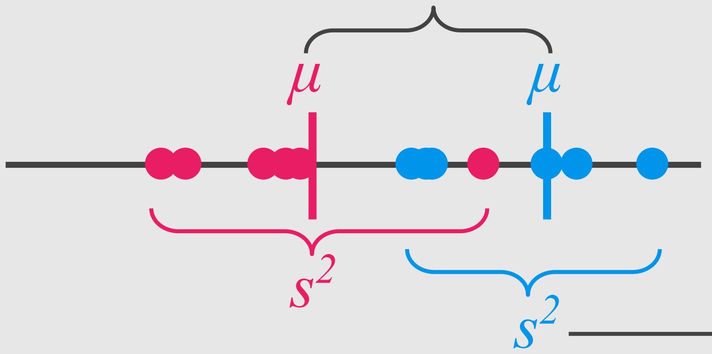
This is the scatter around the pink dots.

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:

1. Maximize the distance between the means:



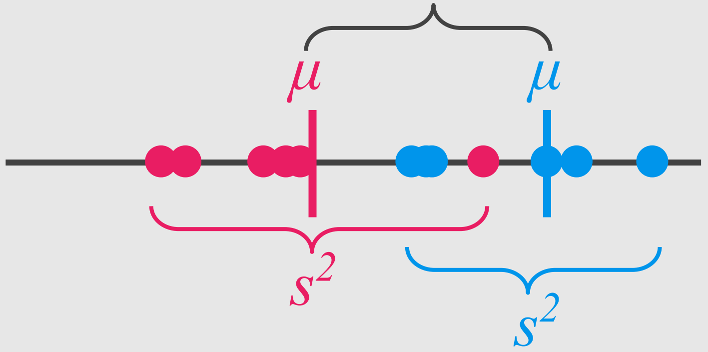
This is the scatter around the blue dots.

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:



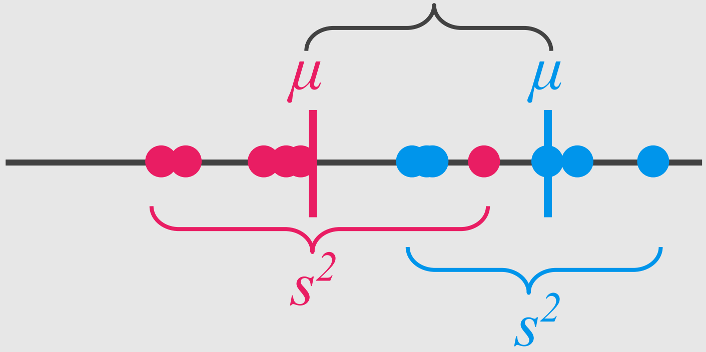
$$\frac{(\mu - \mu)^2}{s^2 + s^2}$$

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:



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

$(\mu - \mu)^2$ → Ideally large

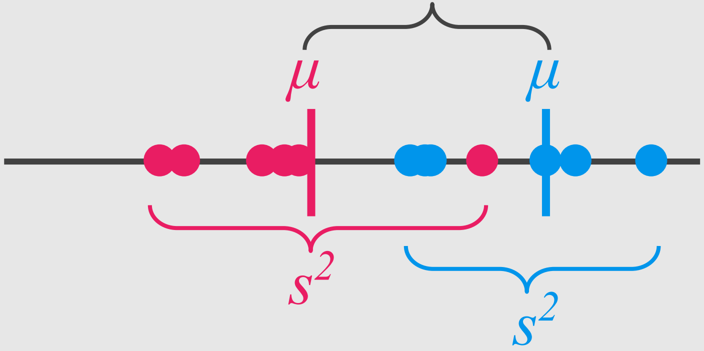
$s^2 + s^2$ → Ideally small

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.

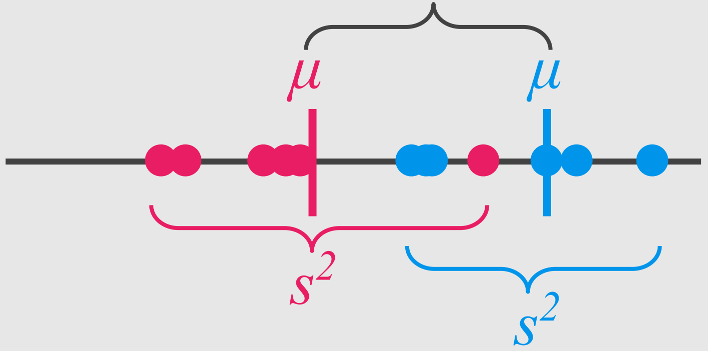
$$\frac{(\mu - \mu)^2}{s^2 + s^2} \quad \begin{array}{l} \longrightarrow \text{Ideally large} \\ \longrightarrow \text{Ideally small} \end{array}$$

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

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.

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

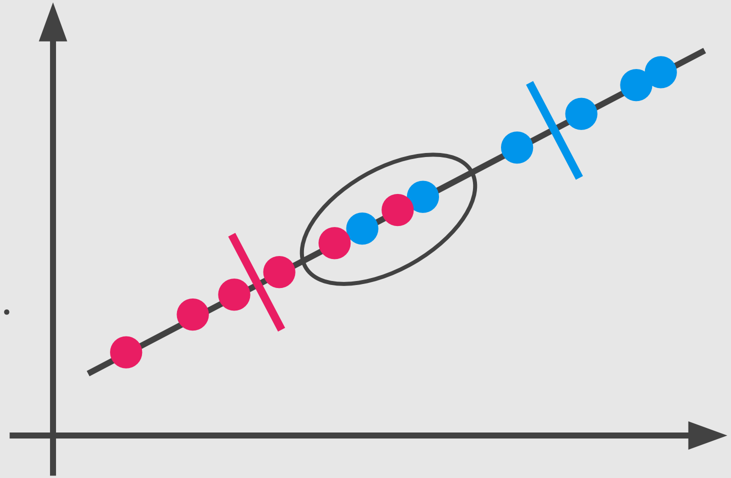
d^2 → Ideally large

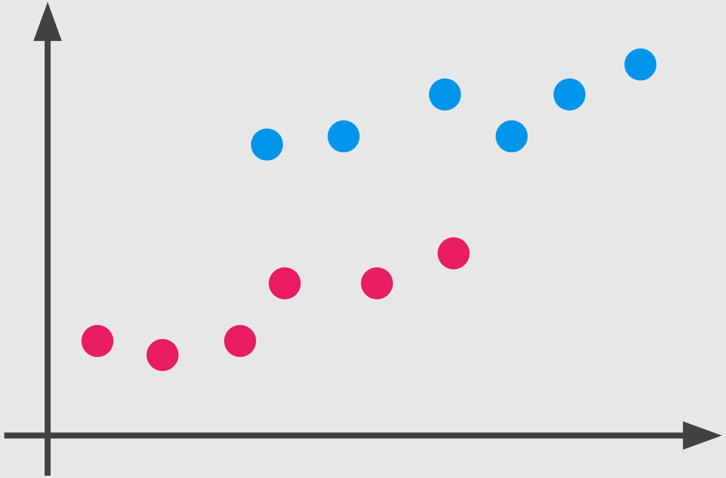
$s^2 + s^2$ → Ideally small

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 ...





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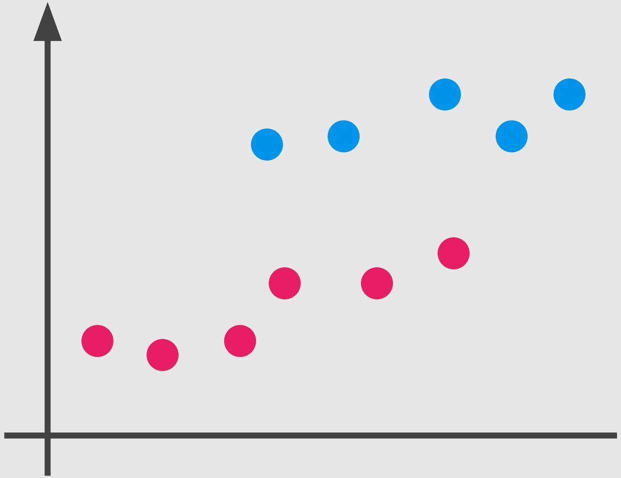
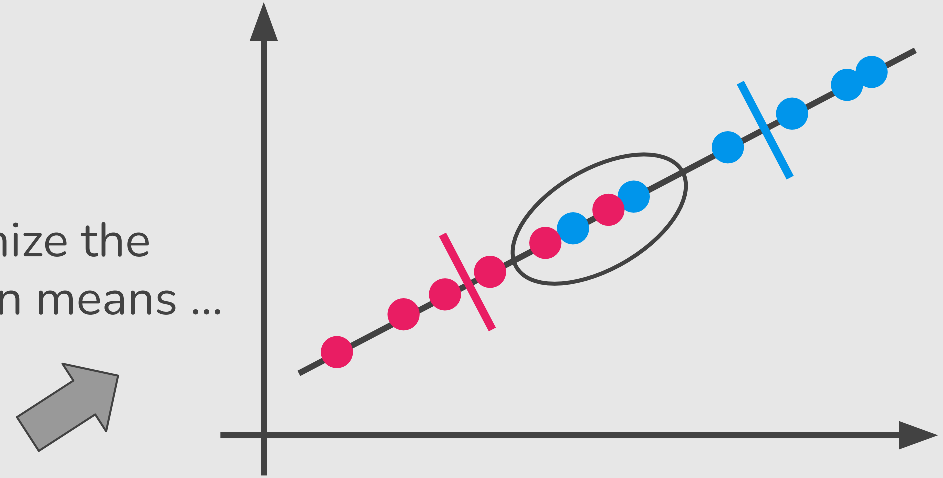
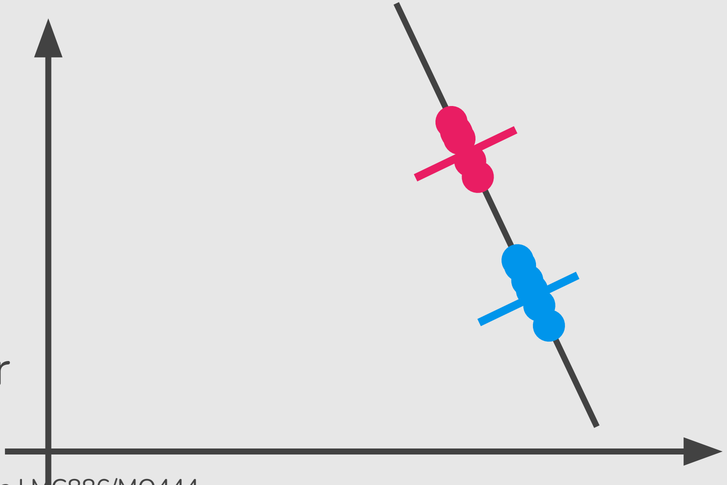
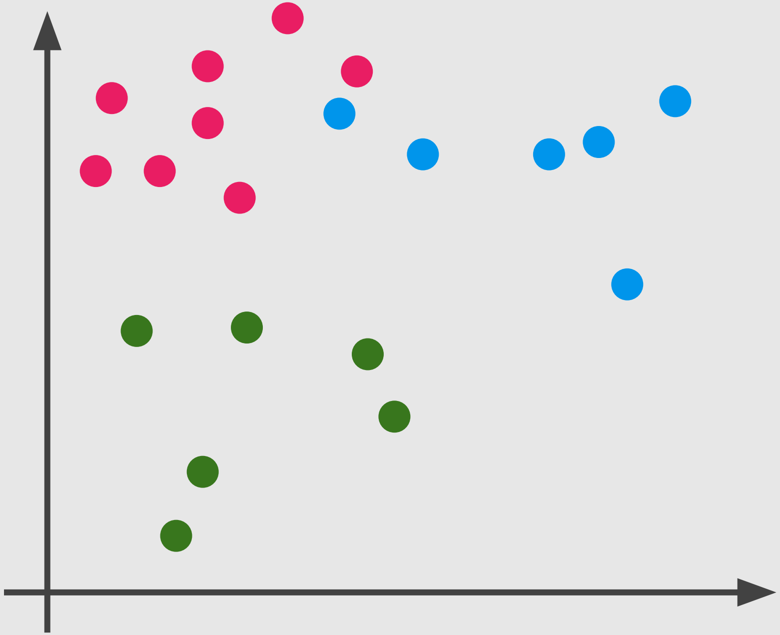




If we optimize the distance between means and scatter



What if we have 3 classes?



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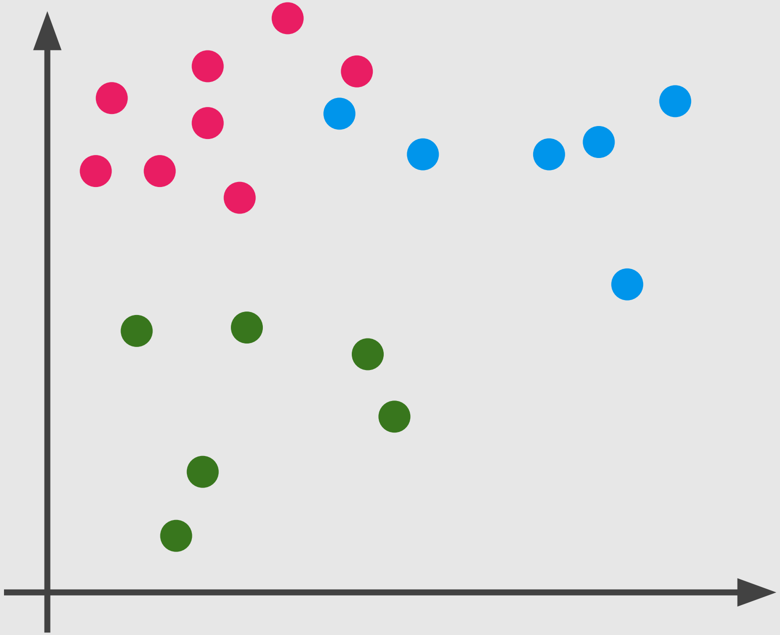
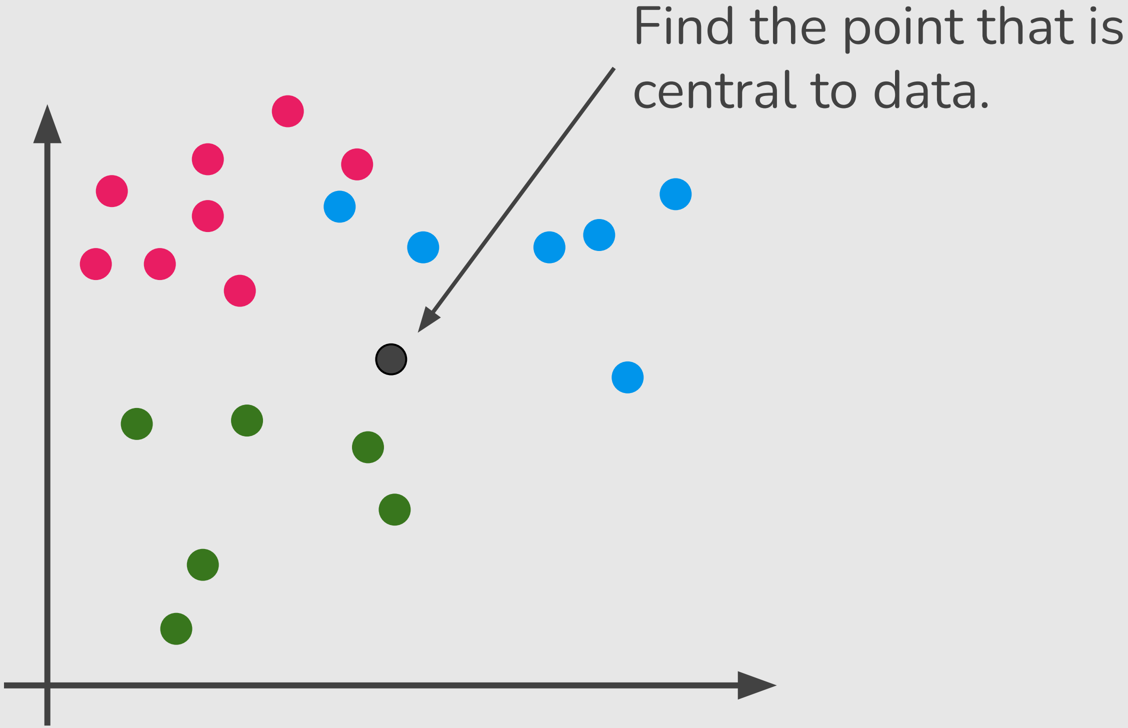
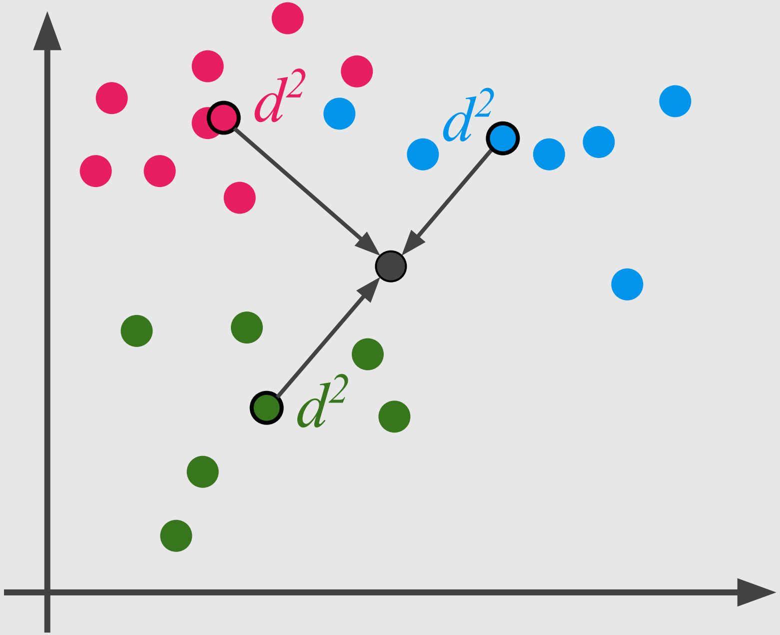


How we measure the distance among the means?

What if we have 3 classes?

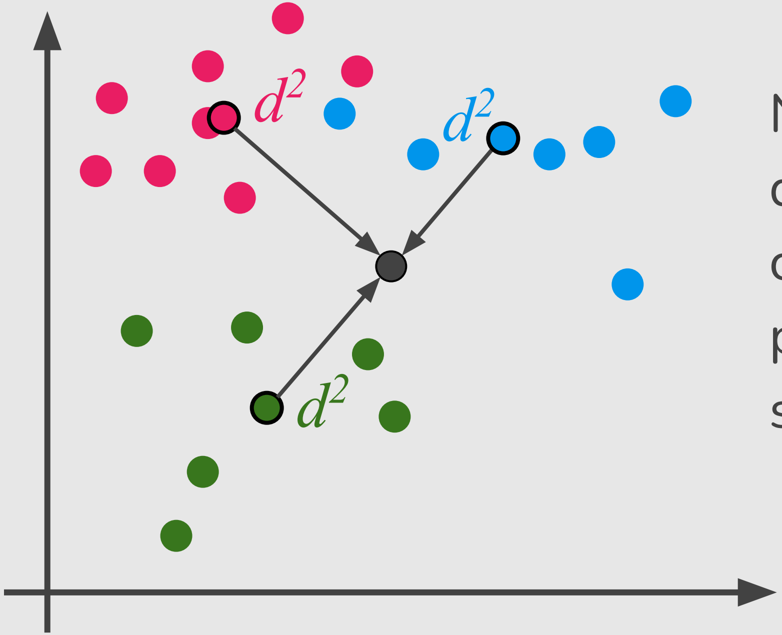


What if we have 3 classes?



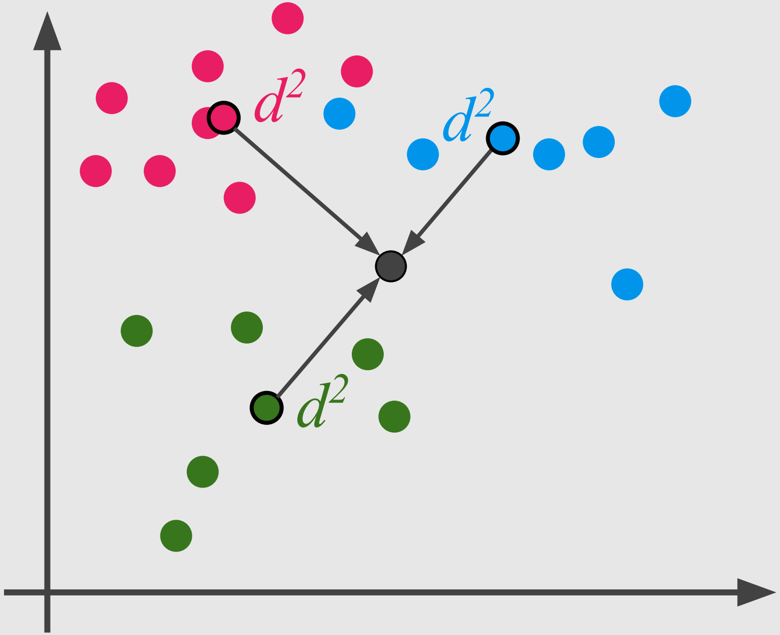
Then measure the distance between a point that is central in each class and the main central point.

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 Algorithm

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

Last Class

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 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.

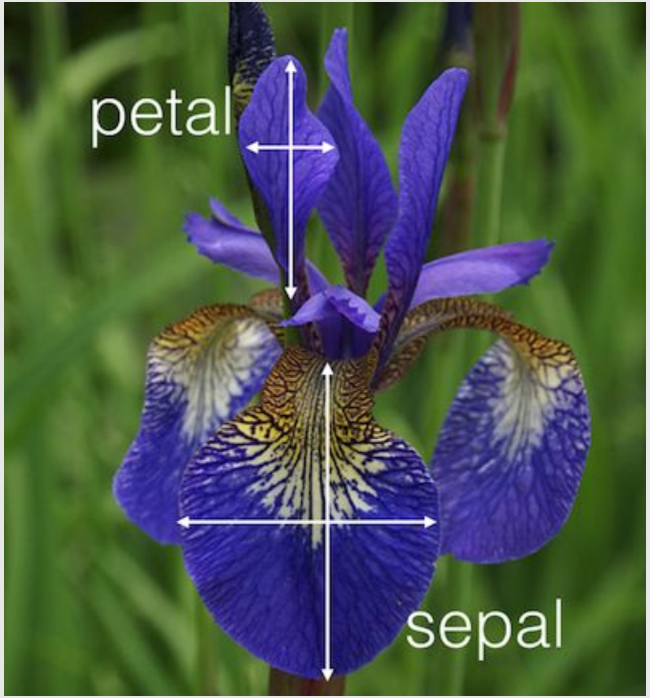
A Tutorial on Data Reduction (LDA)

http://www.sci.utah.edu/~shireen/pdfs/tutorials/Elhabian_LDA09.pdf (slides: 9 to 16)

5. ...ne new subspace.

LDA Step by Step

LDA Step by Step



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

150 iris flowers from three different species.

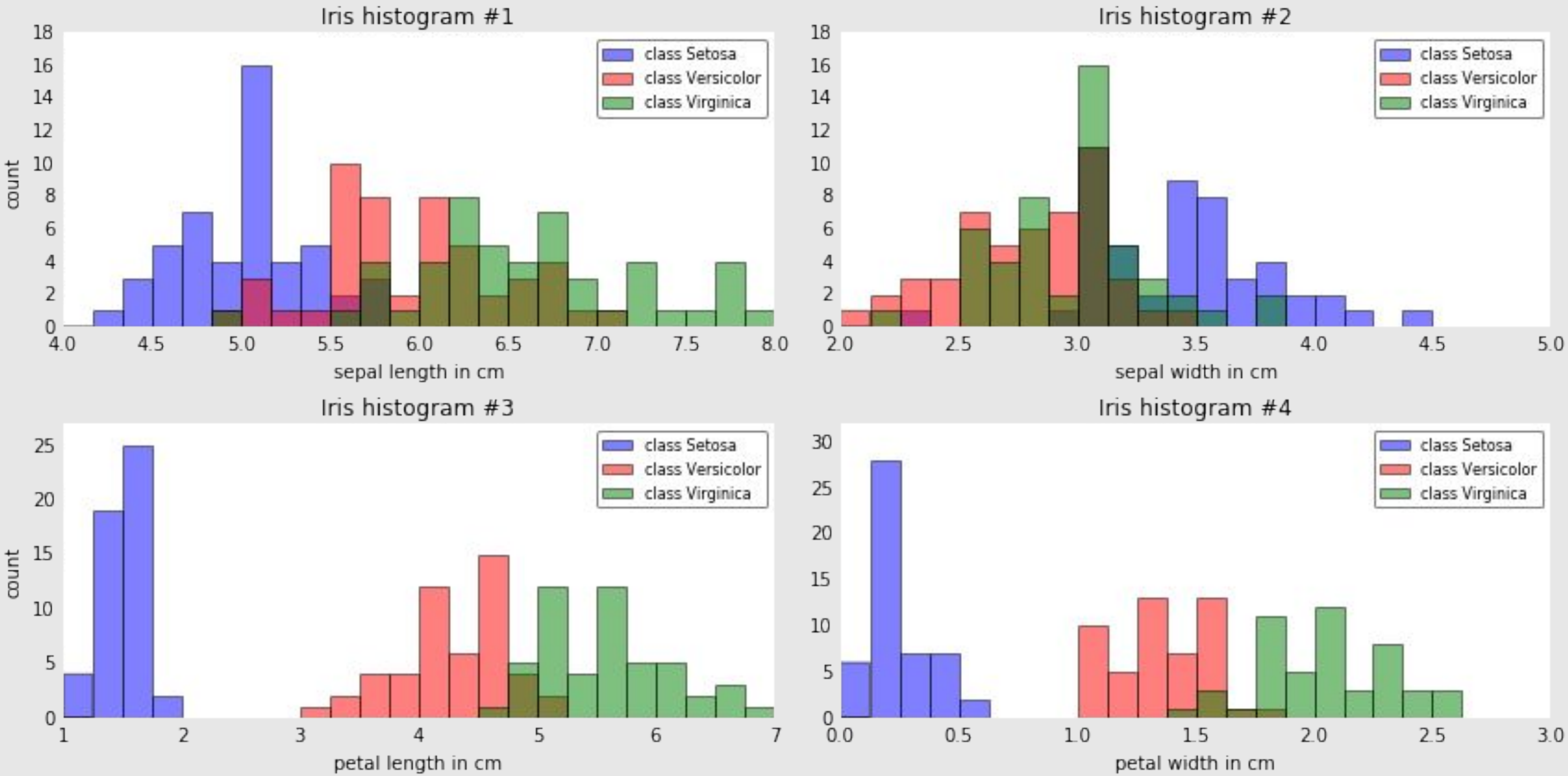
The three classes in the Iris dataset:

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.

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

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

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

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: 32.27 λ_2: 0.27 λ_3: 5.71e-15 λ_4: 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

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.

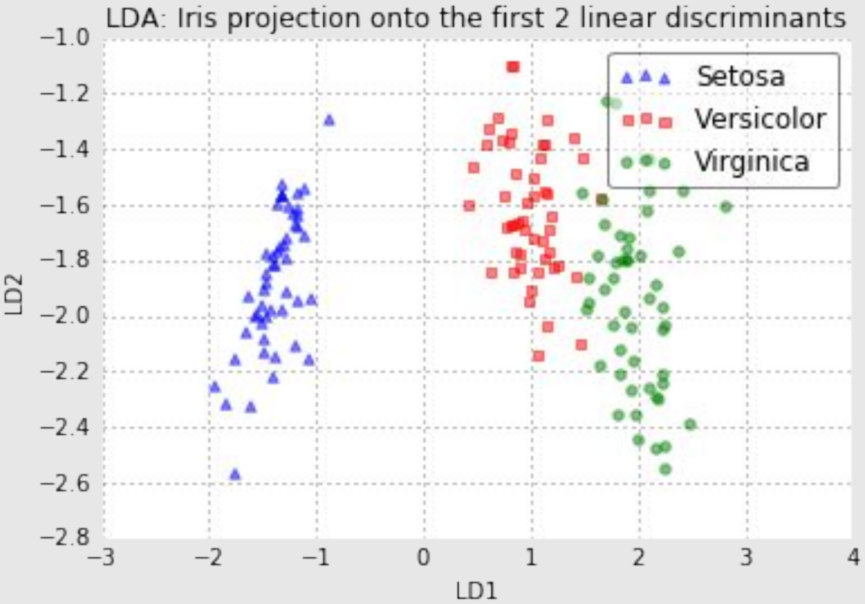
$$u_1: \begin{pmatrix} -0.205 \\ -0.387 \\ 0.546 \\ 0.714 \end{pmatrix} \quad u_2: \begin{pmatrix} -0.009 \\ -0.589 \\ 0.254 \\ -0.767 \end{pmatrix} \Rightarrow \begin{pmatrix} -0.205 & -0.009 \\ -0.387 & -0.589 \\ 0.546 & 0.254 \\ 0.714 & -0.767 \end{pmatrix}$$

λ_1: 3.27 $\quad$ λ_2: 0.27

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”