Lecture 3.1 Supervised learning: Bayesian and linear classifiers



Departament de Ciències Matemàtiques i Informàtica

11752 Aprendizaje Automático
11752 Machine Learning
Máster Universitario
en Sistemas Inteligentes

Alberto ORTIZ RODRÍGUEZ

Contents

- Introduction
- Bayesian classification
- Estimation of probability density functions
- Linear discriminant functions and the perceptron algorithm

Introduction

Supervised classification

It is about classifying a new sample in the correct class, having initially designed a classifier from the data available in a training set, in which, in particular, the samples are labeled with the class to which they belong.

Contents

- Introduction
- Bayesian classification
- Estimation of probability density functions
- Linear discriminant functions and the perceptron algorithm

- The goal is to classify a new sample in the most likely class
 - Given a **classification task** in M classes, $\omega_1, \omega_2, \dots, \omega_M$, and a **new sample** x, we deal with:

$$p(\omega_i|x), i = 1, 2, ..., M$$
 (probabilities a posteriori)

- The classifier decides the most likely class based on the maximum of the probabilities a posteriori:
 - Bayesian classification rule

$$\underline{\text{if}}\ p(\omega_i|x) > p(\omega_j|x), \forall j \neq i, \underline{\text{then}}\ x \text{ is labelled as class } i$$

- Review of probability theory:
 - Probability function: $p:\Omega \to [0,1]$

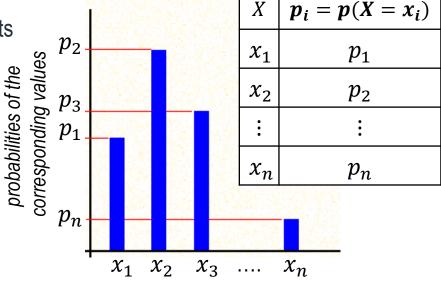
$$v \to p(v)$$

• p assigns a value to each possible event v on the basis of how often that event

occurs

Ω can be stated as the set of events corresponding to a certain discrete random variable X taking certain values, so that

$$p(A_i) = p(X = x_i)$$



values taken by the random variable

• of particular relevance:

$$p(\Omega) = \sum_{i=1}^{n} p(A_i) = 1$$

Review of probability theory:

Law of total probability

Given M events A_i , i = 1, ..., M, such that $\sum_{i=1}^{M} p(A_i) = 1$, for any random event:

$$p(B) = \sum_{i=1}^{M} p(B|A_i)p(A_i)$$

where the probability of B conditioned to the occurrence of event A_i is defined as:

$$p(B|A_i) = \frac{p(B \cap A_i)}{p(A_i)}$$

Bayes Rule

From the definition of conditional probability, given two events A and B: p(B|A)p(A) = p(A|B)p(B)

** All this is verified under exactly the same conditions by substituting probabilities by probability density functions (**pdf** 's)

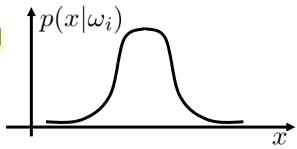
- Bayesian classification: **two-class case** (ω_1, ω_2)
 - Given the **probabilities** a **priori** of both classes $p(\omega_1)$ and $p(\omega_2)$
 - If you do not know $p(\omega_1)$ and $p(\omega_2)$, you can estimate them if necessary:

$$p(\omega_1) \approx \frac{n_1}{n_1 + n_2}, \quad p(\omega_2) \approx \frac{n_2}{n_1 + n_2}$$

and the pdf (probability density functions) of each class

$$p(x|\omega_i), i=1,2$$

 If they are unknown, they have to be estimated from the available training data (we will deal with this topic later)



using Bayes' rule, it follows that:

$$p(\omega_i|x) = \frac{p(x|\omega_i)p(\omega_i)}{p(x)} = \frac{p(x|\omega_i)p(\omega_i)}{\sum_{j=1}^2 p(x|\omega_i)p(\omega_i)}$$
total probability

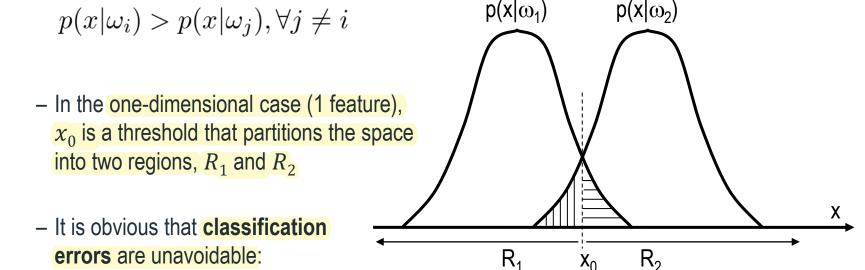
• Bayesian classification: **two-class case** (ω_1 , ω_2)

$$p(\omega_i|x) = \frac{p(x|\omega_i)p(\omega_i)}{p(x)}$$

$$p(\omega_i|x) > p(\omega_j|x), \forall j \neq i$$

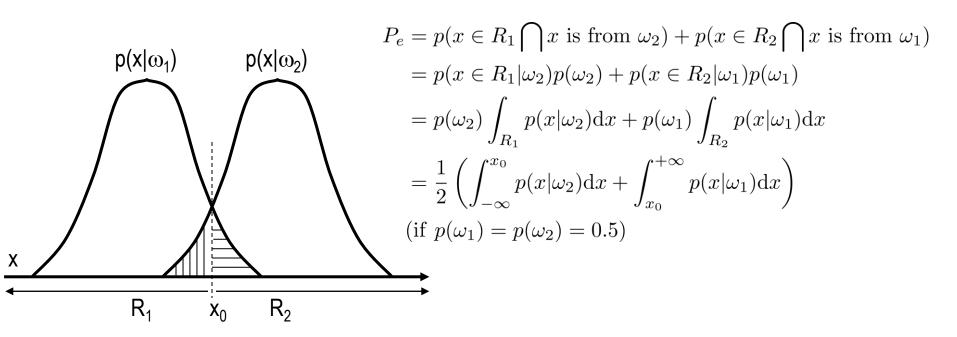
$$p(\omega_i|x) > p(\omega_j|x), \forall j \neq i$$

- If the probabilities a priori are equal $(p(\omega_i) = 1/M = 0.5)$, then the classification rule becomes dependent only on the **pdf**s of the classes:



• Sample x can be inside region R_2 and belong to the class ω_1 (same for R_1 and ω_2)

- Bayesian classification: **two-class case** (ω_1 , ω_2)
 - In the one-dimensional case, the probability of making a classification error is given by:



THEOREM

The Bayesian classifier minimizes the likelihood of classification error

That is to say, if we move x_0 left or right we will increase P_e

• Bayesian classification: **two-class case** (ω_1 , ω_2)

Proof (optimality of the Bayesian classifier)

On the one hand:

$$P_{e} = p(x \in R_{2} \cap \omega_{1}) + p(x \in R_{1} \cap \omega_{2}) = p(x \in R_{2} | \omega_{1}) p(\omega_{1}) + p(x \in R_{1} | \omega_{2}) p(\omega_{2})$$

$$= p(\omega_{1}) \int_{R_{2}} p(x | \omega_{1}) dx + p(\omega_{2}) \int_{R_{1}} p(x | \omega_{2}) dx$$

$$= \int_{R_{2}} p(\omega_{1} | x) p(x) dx + \int_{R_{1}} p(\omega_{2} | x) p(x) dx$$

On the other hand:
$$\int_{\Omega} p(x|\omega_1) \mathrm{d}x = 1 \Rightarrow \int_{\Omega} \frac{p(\omega_1|x)p(x)}{p(\omega_1)} \mathrm{d}x = 1$$

$$\Rightarrow \int_{R_1} p(\omega_1|x)p(x) \mathrm{d}x + \int_{R_2} p(\omega_1|x)p(x) \mathrm{d}x = p(\omega_1)$$
 Therefore:

Therefore:

$$P_e = p(\omega_1) - \int_{R_1} (p(\omega_1|x) - p(\omega_2|x))p(x)dx$$

$$\Rightarrow P_e \text{ is minimum if } R_1 \text{ is defined such that, inside } R_1, \ p(\omega_1|x) > p(\omega_2|x)$$

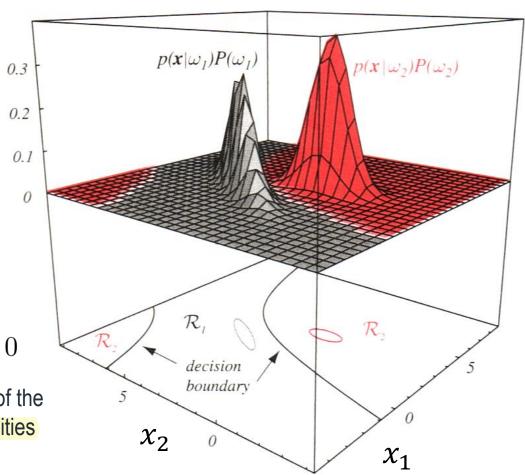
• Bayesian classification:

two-class case (ω_1, ω_2) and 2 features x_1 and x_2

- Minimize the probability
 of error is equivalent to
 partition the space of
 features into M regions
 (as many as classes)
- If the regions R_i and R_j
 are contiguous, then
 they are separated by a
 decision curve that
 is described by the equation:

$$p(\omega_i|x) - p(\omega_j|x) = 0$$

 Corresponds to the points of the space in which the probabilities a posteriori coincide



Bayesian Classification

- **Example** Let us consider a problem of 2 equiprobable classes $(p(\omega_1) = p(\omega_2) = 0.5)$ such that the pdfs are Gaussians of variance 0.5 and means 0 and 1 respectively:

$$p(x|\omega_1) = \frac{1}{\sqrt{\pi}}e^{-x^2}, \quad p(x|\omega_2) = \frac{1}{\sqrt{\pi}}e^{-(x-1)^2} \left(N(\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{(x-\mu)^2}{2\sigma^2}}\right)$$

Calculate the optimal threshold x_0 for minimum error probability.

$$x_0: p(\omega_1|x_0) = p(\omega_2|x_0)$$

$$x_0: p(x_0|\omega_1)p(\omega_1) = p(x_0|\omega_2)p(\omega_2)$$

$$x_0: e^{-x_0^2} = e^{-(x_0-1)^2} \Rightarrow x_0^2 = (x_0-1)^2 = x_0^2 - 2x_0 + 1 \Rightarrow x_0 = 0.5$$

- Bayesian classification for normal distributions
 - In the one-dimensional case:

$$p(x|\omega) = \frac{1}{\sqrt{2\pi}\sigma_{\omega}} e^{-\frac{(x-\mu_{\omega})^2}{2\sigma_{\omega}^2}}$$

— We assume that the pdf of the classes obey the Gaussian L-dimensional distribution:

$$p(x|\omega) = \frac{1}{\sqrt{(2\pi)^L |\Sigma_{\omega}|}} e^{-\frac{1}{2}(x-\mu_{\omega})^T \Sigma_{\omega}^{-1}(x-\mu_{\omega})}$$

• For class ω:

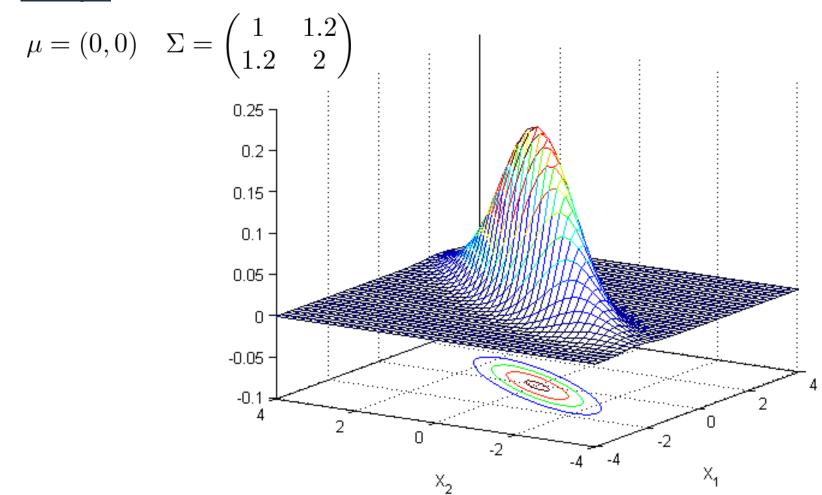
$$\mu_{\omega} = (\mu_{1}, \dots, \mu_{s}, \dots, \mu_{L}) \qquad , \qquad \mu_{s} = \frac{1}{N} \sum_{i=1}^{N} x_{si}$$

$$\Sigma_{\omega} = \begin{bmatrix} \sigma_{1}^{2} & \sigma_{12} & \dots & \sigma_{1L} \\ \sigma_{12} & \sigma_{2}^{2} & \dots & \sigma_{2L} \\ \vdots & \vdots & & \vdots \\ \sigma_{L1} & \sigma_{L2} & \dots & \sigma_{L}^{2} \end{bmatrix} \qquad , \qquad \sigma_{st} = \frac{1}{N-1} \sum_{i=1}^{N} (x_{si} - \mu_{s})(x_{ti} - \mu_{t})$$

$$= \frac{1}{N-1} \sum_{i=1}^{N} (x - \mu_{\omega})(x - \mu_{\omega})^{T}$$

 This distribution models properly many cases and is treatable mathematically and computationally, hence its popularity

- Bayesian classification for normal distributions
 - Example



- Bayesian classifier for normal distributions
 - The goal is to derive the **Bayesian classifier** for the case

$$p(x|\omega_i) = \frac{1}{\sqrt{(2\pi)^L |\Sigma_i|}} e^{-\frac{1}{2}(x-\mu_i)^T \Sigma_i^{-1}(x-\mu_i)}, i = 1, ..., M$$

• Due to the exponential form of the pdf, it is preferable to work with the following discrimination functions $g_i(x)$, which involve the monotonous function $\ln(\cdot)$:

$$g_i(x) = \ln(p(x|\omega_i)p(\omega_i)) = \ln p(x|\omega_i) + \ln p(\omega_i)$$

$$g_i(x) = c_i - \frac{1}{2}(x - \mu_i)^T \Sigma_i^{-1}(x - \mu_i) + \ln p(\omega_i)$$

$$c_i = -\frac{L}{2}\ln 2\pi - \frac{1}{2}\ln |\Sigma_i|$$

Finally:

$$g_i(x) = -\frac{1}{2}x^T \Sigma_i^{-1} x + \frac{1}{2}x^T \Sigma_i^{-1} \mu_i + \frac{1}{2}\mu_i^T \Sigma_i^{-1} x - \frac{1}{2}\mu_i^T \Sigma_i^{-1} \mu_i + \ln p(\omega_i) + c_i$$

- Bayesian classifier for normal distributions
 - Case of 2 uncorrelated characteristics

$$L = 2, \quad x = (x_1, x_2)^T, \quad \Sigma_i = \begin{pmatrix} \sigma_{i1}^2 & 0 \\ 0 & \sigma_{i2}^2 \end{pmatrix}$$

$$g_i(x) = -\frac{1}{2}x^T \Sigma_i^{-1} x + \frac{1}{2}x^T \Sigma_i^{-1} \mu_i + \frac{1}{2}\mu_i^T \Sigma_i^{-1} x - \frac{1}{2}\mu_i^T \Sigma_i^{-1} \mu_i$$

$$+ \ln p(\omega_i) + c_i$$

$$\Rightarrow g_i(x) = -\frac{1}{2} \left(\frac{x_1^2}{\sigma_{i1}^2} + \frac{x_2^2}{\sigma_{i2}^2} \right) + \left(\frac{\mu_{i1}x_1}{\sigma_{i1}^2} + \frac{\mu_{i2}x_2}{\sigma_{i2}^2} \right) - \frac{1}{2} \left(\frac{\mu_{i1}^2}{\sigma_{i1}^2} + \frac{\mu_{i2}^2}{\sigma_{i2}^2} \right)$$

$$+ \ln p(\omega_i) + c_i$$

$$= a_i x_1^2 + b_i x_2^2 + c_i x_1 + d_i x_2 + e_i$$

• The decision rules are now given by the equations $g_i(x) - g_i(x) = 0$

QUADRATIC CLASSIFIER

- L = 2: ellipses, parabola, hyperbole, etc. conics, rule = 2D curve
- L = 3: ellipsoids, paraboloids, hyperboloids, etc. quadrics, rule = 3D surface
- L > 3: hiperquadrics

$$\Rightarrow g_i(x) > g_j(x) \Rightarrow p(\omega_i|x) > p(\omega_j|x) \Rightarrow x \to \omega_i$$

Bayesian classifier for normal distributions

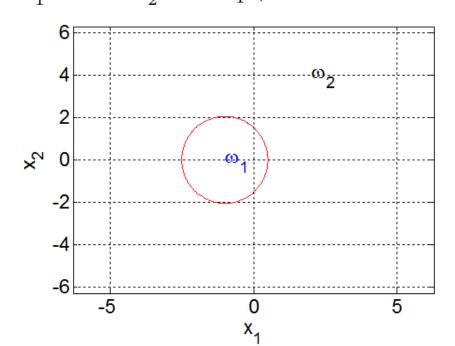
- **Example** (equiprobable classes)

$$\mu_1 = (0,0)^T, \mu_2 = (1,0)^T, \Sigma_1 = \begin{pmatrix} 0.10 & 0.00 \\ 0.00 & 0.15 \end{pmatrix}, \Sigma_2 = \begin{pmatrix} 0.20 & 0.00 \\ 0.00 & 0.25 \end{pmatrix}$$

$$g_1(x) = -5.0x_1^2 - 3.3x_2^2 + 0.2620$$

$$g_2(x) = -2.5x_1^2 - 2.0x_2^2 + 5.0x_1 - 2.840$$

$$g_1(x) - g_2(x) = -2.500x_1^2 - 1.333x_2^2 - 5.0x_1 + 3.102 = 0$$



Bayesian classifier for normal distributions

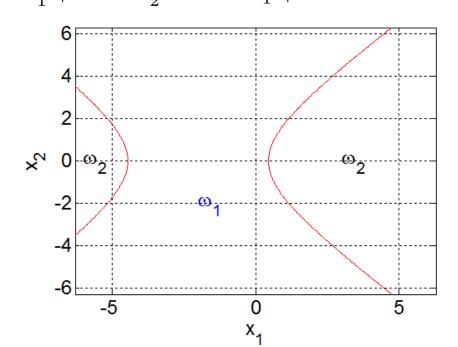
- **Example** (equiprobable classes)

$$\mu_1 = (0,0)^T, \mu_2 = (1,0)^T, \Sigma_1 = \begin{pmatrix} 0.10 & 0.00 \\ 0.00 & 0.15 \end{pmatrix}, \Sigma_2 = \begin{pmatrix} 0.15 & 0.00 \\ 0.00 & 0.10 \end{pmatrix}$$

$$g_1(x) = -5.0x_1^2 - 3.3x_2^2 + 0.2620$$

$$g_2(x) = -3.333x_1^2 - 5.0x_2^2 + 6.667x_1 - 3.071$$

$$g_1(x) - g_2(x) = -1.667x_1^2 + 1.667x_2^2 - 6.667x_1 + 3.333 = 0$$



- Bayesian classifier for normal distributions
 - Classes with the same covariance matrix: decision hyperplanes
 - If the classes have the same covariance matrix ($\Sigma_i = \Sigma$) then the **quadratic term** and **part of the constant term** coincide in all discrimination functions:

$$g_i(x) = -\frac{1}{2}x^T \Sigma^{-1} x + \frac{1}{2}x^T \Sigma^{-1} \mu_i + \frac{1}{2}\mu_i^T \Sigma^{-1} x - \frac{1}{2}\mu_i^T \Sigma^{-1} \mu_i + \ln p(\omega_i) + c$$

• Therefore, they disappear from equations $g_i(x) - g_j(x) = 0$.

This allows us to define more useful discrimination functions:

$$g_i(x) = w_i^T x + w_{i0}$$

$$w_i^T = \mu_i^T \Sigma^{-1}, \quad w_{i0} = \ln p(\omega_i) - \frac{1}{2} \mu_i^T \Sigma^{-1} \mu_i$$

LINEAR • In this way, the discrimination functions are linear (and not quadratic) and the decision rules turn out to be **decision hyperplanes**: (2D) straight lines, (3D) planes, ...

$$\rightarrow g_i(x) > g_j(x) \Rightarrow p(\omega_i|x) > p(\omega_i|x) \Rightarrow x \rightarrow \omega_i$$

• Let us have a look at **two cases of the covariance matrix**: (1) $\Sigma = \sigma^2 I$ and (2) any Σ

- Bayesian classifier for normal distributions
 - Classes with the same covariance matrix: $\Sigma = \sigma^2 I$
 - Then, the discrimination functions take the following form:

$$g_i(x) = \frac{1}{\sigma^2} \mu_i^T x + w_{i0} = \frac{1}{\sigma^2} \mu_i^T x + \ln p(\omega_i) - \frac{1}{2\sigma^2} \mu_i^T \mu_i$$

so that the **decision rules** can be written as:

$$g_{ij}(x) \equiv g_i(x) - g_j(x) = 0$$

$$\Rightarrow \frac{1}{\sigma^2} (\mu_i^T - \mu_j^T) x + \ln p(\omega_i) - \ln p(\omega_j) - \frac{1}{2\sigma^2} (\mu_i^T \mu_i - \mu_j^T \mu_j) = 0$$

$$\Rightarrow (\mu_i - \mu_j)^T x + \sigma^2 \ln \left(\frac{p(\omega_i)}{p(\omega_j)} \right) - \frac{1}{2} (\mu_i - \mu_j)^T (\mu_i + \mu_j) = 0$$

$$\Rightarrow (\mu_i - \mu_j)^T \left[x + \sigma^2 \ln \left(\frac{p(\omega_i)}{p(\omega_j)} \right) \frac{\mu_i - \mu_j}{\|\mu_i - \mu_j\|^2} - \frac{1}{2} (\mu_i + \mu_j) \right] = 0$$

$$\Rightarrow w^T (x - x_0) = 0$$

$$w = \mu_i - \mu_j, x_0 = \frac{1}{2} (\mu_i + \mu_j) - \sigma^2 \ln \left(\frac{p(\omega_i)}{p(\omega_j)} \right) \frac{\mu_i - \mu_j}{\|\mu_i - \mu_j\|^2}$$

- Bayesian classifier for normal distributions
 - Classes with the same covariance matrix: $\Sigma = \sigma^2 I$
 - decision rules:

$$g_{ij}(x) : w^{T}(x - x_{0}) = 0$$

$$w = \mu_{i} - \mu_{j}, x_{0} = \frac{1}{2}(\mu_{i} + \mu_{j}) - \sigma^{2} \ln \left(\frac{p(\omega_{i})}{p(\omega_{j})}\right) \frac{\mu_{i} - \mu_{j}}{\|\mu_{i} - \mu_{j}\|^{2}}$$

two-feature case:

$$g_{ij}(x): w^{T}(x - x_{0}) = 0$$

$$\Rightarrow (\mu_{1,1} - \mu_{2,1})x_{1} + (\mu_{1,2} - \mu_{2,2})x_{2}$$

$$- (\mu_{1,1} - \mu_{2,1})x_{0,1} - (\mu_{1,2} - \mu_{2,2})x_{0,2} = 0$$

$$\Rightarrow Ax_{1} + Bx_{2} + C = 0$$

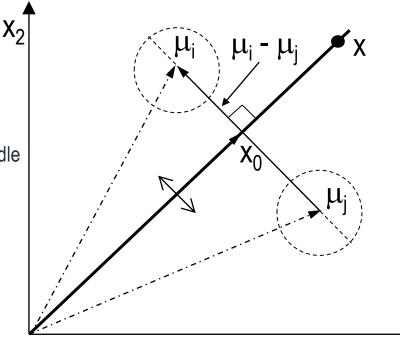
Which is this straight line?

- Bayesian classifier for normal distributions
 - Classes with the same covariance matrix: $\Sigma = \sigma^2 I$
 - decision rules: two-feature case

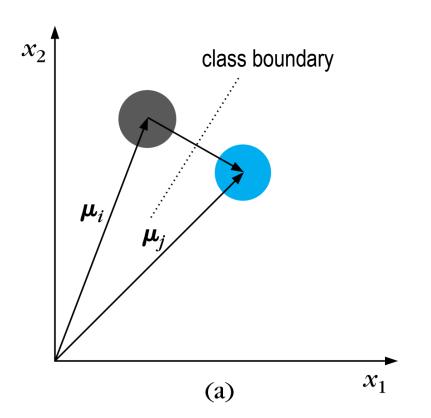
$$g_{ij}(x): w^T(x-x_0) = 0$$

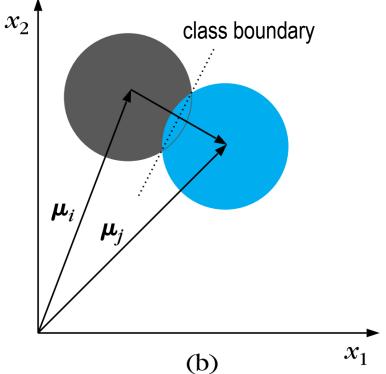
$$w = \mu_i - \mu_j, x_0 = \frac{1}{2}(\mu_i + \mu_j) - \sigma^2 \ln\left(\frac{p(\omega_i)}{p(\omega_j)}\right) \frac{\mu_i - \mu_j}{\|\mu_i - \mu_j\|^2}$$

- any point x such that $x-x_0$ is orthogonal to μ_i μ_j belongs to the straight line
- x₀ is always along the vector μ_i - μ_j
 - if $p(\omega_i) = p(\omega_j)$, x_0 is the middle point between μ_i and μ_i
 - $\begin{array}{ll} & \text{if } p(\omega_i) < p(\omega_j), \ x_0 \\ & \text{moves towards } \mu_i \\ & \text{along vector } \mu_i \mu_j \end{array}$



- Bayesian classifier for normal distributions
 - Classes with the same covariance matrix: $\Sigma = \sigma^2 I$
 - the circles expand to $3\sigma = 98\%$





Bayesian classifier for normal distributions

- Classes with the **same covariance matrix**: any Σ
 - We recover the original linear discrimination functions:

$$g_i(x) = w_i^T x + w_{i0}$$

$$w_i^T = \mu_i^T \Sigma^{-1}, \quad w_{i0} = \ln p(\omega_i) - \frac{1}{2} \mu_i^T \Sigma^{-1} \mu_i$$

• Then:

$$g_{ij}(x) \equiv g_i(x) - g_j(x) = 0$$

$$\Rightarrow (\mu_i - \mu_j)^T \Sigma^{-1} x + \ln \left(\frac{p(\omega_i)}{p(\omega_i)} \right) - \frac{1}{2} (\mu_i - \mu_j)^T \Sigma^{-1} (\mu_i + \mu_j) = 0$$

$$\Rightarrow (\mu_i - \mu_j)^T \Sigma^{-1} \left[x + \ln \left(\frac{p(\omega_i)}{p(\omega_j)} \right) \frac{\mu_i - \mu_j}{(\mu_i - \mu_j)^T \Sigma^{-1} (\mu_i - \mu_j)} - \frac{1}{2} (\mu_i + \mu_j) \right] = 0$$

$$\Rightarrow w^T (x - x_0) = 0$$

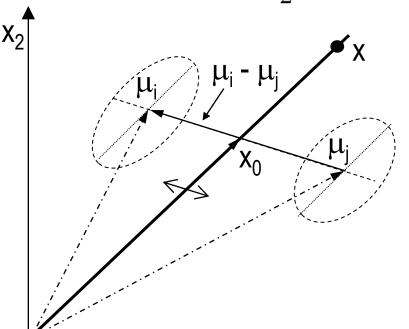
$$w = \Sigma^{-1}(\mu_i - \mu_j), x_0 = \frac{1}{2}(\mu_i + \mu_j) - \ln\left(\frac{p(\omega_i)}{p(\omega_i)}\right) \frac{\mu_i - \mu_j}{(\mu_i - \mu_j)^T \Sigma^{-1}(\mu_i - \mu_j)}$$

Bayesian classifier for normal distributions

– Classes with the same covariance matrix: any $\boldsymbol{\Sigma}$

$$g_{ij}: w^{T}(x - x_0) = 0$$
$$w = \Sigma^{-1}(\mu_i - \mu_j)$$

$$x_0 = \frac{1}{2}(\mu_i + \mu_j) - \ln\left(\frac{p(\omega_i)}{p(\omega_j)}\right) \frac{\mu_i - \mu_j}{(\mu_i - \mu_j)^T \Sigma^{-1} (\mu_i - \mu_j)}$$



- the decision hyperplane is no longer necessarily orthogonal to μ_i μ_i but to $\Sigma^{-1}(\mu_i$ $\mu_i)$
 - $\Sigma^{-1}(\mu_i \mu_j)$ is the result of transforming $(\mu_i \mu_j)$ through the matrix Σ^{-1}
- x_0 it is always on the vector μ_i μ_j
 - if $p(\omega_i) = p(\omega_i)$, x_0 is the average of μ_i y μ_i
 - if $p(\omega_i) < p(\omega_i)$, x_0 moves towards μ_i along $\mu_i \mu_i$

Bayesian classifier for normal distributions

- <u>Example</u> In a two-dimensional classification problem with two equiprobable classes, the classes follow two normal distributions with the following parameters:

$$\mu_1 = (0,0)^T, \mu_2 = (3,3)^T, \Sigma = \Sigma_1 = \Sigma_2 = \begin{pmatrix} 1.1 & 0.3 \\ 0.3 & 1.9 \end{pmatrix}$$

Classify the vector $\mathbf{x} = (1.0, 2.2)^{\mathsf{T}}$ using a Bayesian classifier.

$$g_{12} = w^{T}(x - x_{0})$$

$$w = \Sigma^{-1}(\mu_{1} - \mu_{2})$$

$$x_{0} = \frac{1}{2}(\mu_{1} + \mu_{2}) - \ln\left(\frac{p(\omega_{1})}{p(\omega_{2})}\right) \frac{\mu_{1} - \mu_{2}}{(\mu_{2} - \mu_{2})^{T}\Sigma^{-1}(\mu_{1} - \mu_{2})}$$

$$g_{12} = (-3, -3) \begin{pmatrix} 1.1 & 0.3 \\ 0.3 & 1.9 \end{pmatrix}^{-1} ((1, 2.2)^{T} - (1.5, 1.5)^{T})$$

$$= 0.36 > 0$$

• Therefore, $\mathbf{x} \to \mathbf{\omega}_1$.

Bayesian classifier for normal distributions

So far we have considered two-class cases and derived the boundaries between class pairs through the discrimination functions:

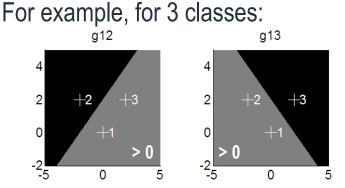
$$g_{ij}(x) = g_i(x) - g_j(x) = 0$$

- For two classes:

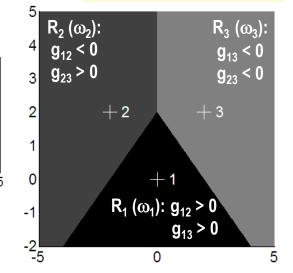
if
$$g_{12}(x) > 0$$
, then $x \to \omega_1$ [if $g_1(x) > g_2(x)$, then $x \to \omega_1$ if $g_{12}(x) < 0$, then $x \to \omega_2$ [if $g_1(x) < g_2(x)$, then $x \to \omega_2$]

- If there are more classes, we have to determine $g_i \mid g_i > g_j$, $\forall j \neq i$, so we have to use several g_{ij} to decide, since the isolated g_{ij} are not useful to define the borders.

 $\begin{array}{c}
\mu_i \\
\hline
(0,0) \\
(-2,2) \\
(+2,2) \\
\sigma = 1
\end{array}$



to determine R_i we need {g_{ik}, g_{ki}}
 M classes: M-1 pairs



- Bayesian classifier for normal distributions
 - Minimum distance classifiers
 - We can see the above from another point of view
 - We assume **equiprobable classes with the same covariance matrix**. Then:

$$g_{i}(x) = c_{i} - \frac{1}{2}(x - \mu_{i})^{T} \Sigma_{i}^{-1}(x - \mu_{i}) + \ln p(\omega_{i})$$

$$c_{i} = -\frac{L}{2} \ln 2\pi - \frac{1}{2} \ln |\Sigma_{i}|$$

$$\rightarrow g_i(x) = -\frac{1}{2}(x - \mu_i)^T \Sigma^{-1}(x - \mu_i)$$

- We assign **x** to the class for which the probability is greater $\Rightarrow g_i(x) > g_i(x) \forall j \neq i$
 - (1) If $\Sigma = \sigma^2 \mathbf{I}$, $g_i(x)$ is higher the closer it is x to μ_i
 - \Rightarrow assign **x** to the class whose center μ_i is closer (**Euclidean distance**)
 - (2) For generic Σ , we have to assign \mathbf{x} to the class for which the following expression takes a lowest value: $d_m^2 = (x \mu_i)^T \Sigma^{-1} (x \mu_i)$
 - $d_m =$ Mahalanobis distance (considers the scattering present in the features)

Bayesian classifier for normal distributions

Example In a two-dimensional classification problem into two equiprobable classes the classes have two normal distributions with the following parameters:

$$\mu_1 = (0,0)^T, \mu_2 = (3,3)^T, \Sigma = \Sigma_1 = \Sigma_2 = \begin{pmatrix} 1.1 & 0.3 \\ 0.3 & 1.9 \end{pmatrix}$$

Classify the vector $\mathbf{x} = (1.0, 2.2)^{\mathsf{T}}$ using a Bayesian classifier.

$$d_m^2(x, \mu_1) = (x - \mu_1)^T \Sigma^{-1}(x - \mu_1)$$

$$= (1.0, 2.2) \begin{pmatrix} 0.95 & -0.15 \\ -0.15 & 0.55 \end{pmatrix} \begin{pmatrix} 1.0 \\ 2.2 \end{pmatrix} = 2.952$$

$$d_m^2(x, \mu_2) = (x - \mu_2)^T \Sigma^{-1}(x - \mu_2)$$

$$= (-2.0, -0.8) \begin{pmatrix} 0.95 & -0.15 \\ -0.15 & 0.55 \end{pmatrix} \begin{pmatrix} -2.0 \\ -0.8 \end{pmatrix} = 3.672$$

- $d_m(x,\mu_1) < d_m(x,\mu_2) \Rightarrow \mathbf{x} \rightarrow \mathbf{\omega}_1$.
- <u>REMARK</u>: the Euclidean distances would be $d_e(x,\mu_1) = 2.417$ and $d_e(x,\mu_2) = 2.154$, so, if we used them, we would assign $x \to \omega_2$.

Contents

- Introduction
- Bayesian classification
- Estimation of probability density functions
- Linear discriminant functions and the perceptron algorithm

- Estimation of probability density functions (pdfs)
 - The Bayesian classifier assumes that we have knowledge on the pdfs of the classes of the problem
 - There are different methods to get this type of information:
 - The expression of the pdf is known but the parameters are unknown
 - → parametric estimation
 - Maximum likelihood estimators
 - others
 - The expression of the pdf is not known → non-parametric estimation
 - Parzen windows method
 - k-nearest neighbours method (KNN)
 - others

- Estimation of probability density functions
 - Maximum likelihood estimators
 - Let us consider an M-class classification problem whose samples are distributed in accordance to $p(x|\omega_i; \theta_i)$, i=1,...,M, where θ_i is the **vector of parameters** for class ω_i
 - It's about estimating θ_i by means of a set of samples $x_1, x_2, ..., x_k$ from class ω_i
 - We assume that the samples of one class do not affect the estimation of parameters for the other classes in order to formulate the problem irrespective of the class
 - ⇒ the estimation is repeated for each class
 - In this way, given the statistically independent samples $x_1, x_2, ..., x_N$ from $p(x_k|\theta)$, we calculate the following joint pdf:

$$p(X;\theta) = p(x_1, x_2, ..., x_N; \theta) = \prod_{k=1}^{N} p(x_k; \theta)$$

• Then, the **maximum likelihood estimator** of θ is given by:

$$\theta_{ML} \mid p(X; \widehat{\theta}_{ML}) = \max\{p(X; \theta)\}\$$

- This represents that θ that better explains samples $x_1, x_2, ..., x_N$

- Estimation of probability density functions
 - Maximum likelihood estimators
 - To simplify the calculations we will go once again to the function ln(⋅) to define the log-likelihood function:

$$L(\theta) \equiv \ln \prod_{k=1}^{N} p(x_k; \theta) = \sum_{k=1}^{N} \ln p(x_k; \theta)$$

Now, you can find the derivative of the log-likelihood and equal to 0:

$$\frac{\partial L(\theta)}{\partial \theta} = \sum_{k=1}^{N} \frac{\partial \ln p(x_k; \theta)}{\partial \theta} = \sum_{k=1}^{N} \frac{1}{p(x_k; \theta)} \frac{\partial p(x_k; \theta)}{\partial \theta} = 0$$

• For sufficiently high N values, the maximum likelihood estimator is asymptotically unbiased, follows a normal distribution and exhibits minimal variance

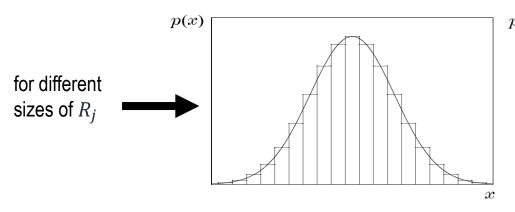
- Estimation of probability density functions
 - Maximum likelihood estimators
 - L-dimensional Gaussian distribution with Σ known

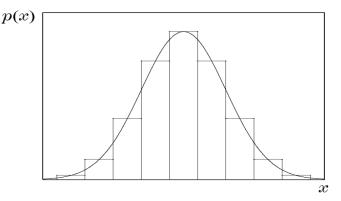
$$\widehat{\mu}_{ML} = \frac{1}{N} \sum_{k=1}^{N} x_k$$

• L-dimensional Gaussian distribution, μ and Σ unknown

$$\widehat{\mu}_{ML} = \frac{1}{N} \sum_{k=1}^{N} x_k, \quad \widehat{\Sigma}_{ML} = \frac{1}{N} \sum_{k=1}^{N} (x_k - \widehat{\mu}_{ML})(x_k - \widehat{\mu}_{ML})^T$$

- Estimation of probability density functions
 - Non-parametric estimation: first approximation
 - It is about estimating a certain pdf p(x) without setting any expression for the pdf
 - Let us assume we have **N** independent samples $x_1, x_2, ..., x_N$ that come from the pdf that we want to estimate
 - To this end, we build a histogram using bins R_i of the same size:





- $-k_{N,Rj}$ = how many of the N samples belong to bin R_i
- $-\{k_{N,Rj}/N\}$ is an aproximation of P_{Rj} = probability that x belongs to R_j :

$$P_{R_j} = p(x \in R_j) = \int_{R_j} p(x') dx'$$

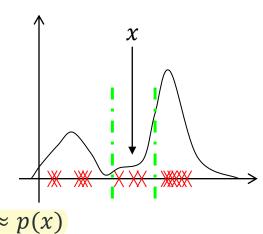
- Non-parametric estimation: first approximation
 - We now define sufficiently small regions R around x, aiming at calculating p(x). In this regard, if p(x) is assumed constant inside R:

$$P_R = \int_R p(x') dx' \approx p(x) \int_R dx' = p(x)V$$

- V is the (hyper)volume occupied by region R (1D length, 2D area, 3D volume, etc.)
- e.g. if R is a (hyper)cube of dimension L and side length $h, V = h^L$

• Therefore:
$$p(x) \approx \frac{P_R}{V} = \frac{k_{N,R}/N}{V} = p_{N,R}(x)$$

- $p_{N,R}(x) \to p(x)$ as $N \to \infty$ if the following holds:
 - $-V \rightarrow 0$ (small regions)
 - $-k_{N,R} \rightarrow \infty$ (sufficient number of samples in each R)
 - $-k_{N,R}/N \rightarrow 0$ (high total number of samples)
- In short: for each x, p(x) is approximated by defining a small R region around x and counting how many x_i fall into R (= $k_{N,R}$); if $k_{N,R}$ $\uparrow \uparrow$ and N $\uparrow \uparrow \uparrow$, then $p_{N,R}(x) \approx p(x)$



- Estimación de funciones de densidad de probabilidad
 - Non-parametric estimation: Parzen windows (Parzen, 1962)
 - Let us consider a region R shaped like a (hyper) L-dimensional cube of side h_N . Then:

 $V_N = (h_N)^L$

Let us consider the following function (box function or kernel):

$$\varphi(u) = \begin{cases} 1 & |u_j| \le \frac{1}{2}, j = 1, ..., L \\ 0 & \text{otherwise} \end{cases}$$

• So, for a certain x:

$$\varphi\left(\frac{x-x_i}{h_N}\right)=1 \text{ if } x_i \in \text{(hyper)cube with volume } V_N \text{ centered at } x$$

• Then, the number of samples that are inside the x-centered (hyper)cube is:

$$k_N(x) = \sum_{i=1}^{N} \varphi\left(\frac{x - x_i}{h_N}\right)$$

- Estimation of probability density functions
 - Non-parametric estimation: Parzen windows
 - At last:

$$p_N(x) = \frac{k_N(x)/N}{V_N} = \frac{1}{N} \sum_{i=1}^N \frac{1}{h_N^L} \varphi\left(\frac{x - x_i}{h_N}\right)$$

• Therefore, given a certain x, to obtain the estimate of p(x): (1D case)

```
def parzen_box_1D(x,X,h):
# x = point where to evaluate the PDF
# X = table of samples
# h = side of the (hyper)cube

N = X.shape[0]; kn = 0
for i in range(N):
   if abs((x - X[i])/h) <= 0.5:
     kn = kn+1
p = (kn/N)/h
return p</pre>
```

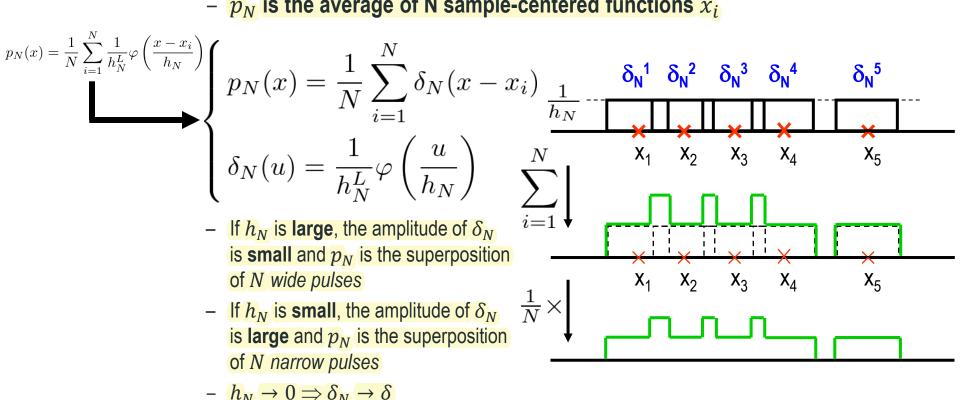
- Estimation of probability density functions
 - Non-parametric estimation: Parzen windows
 - Comments on p_N :
 - $-p_N$ is a legitimate pdf
 - 1. $p_N(x) \geq 0, \forall x \text{ (obvious, it is a sum of 1's)}$
 - 2. $\int p_N(x) dx = 1$

$$\int \frac{1}{N} \sum_{i=1}^{N} \frac{1}{h_N^L} \varphi\left(\frac{x - x_i}{h_N}\right) dx = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{h_N^L} \int \varphi\left(\frac{x - x_i}{h_N}\right) dx =$$

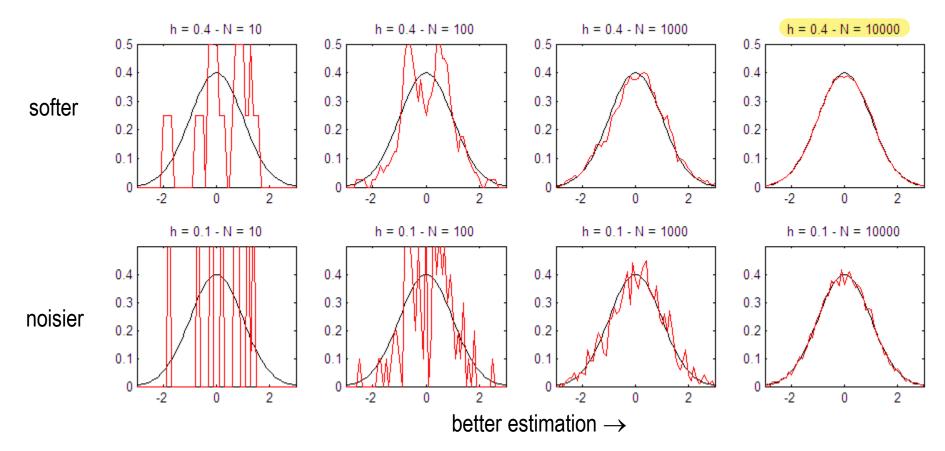
$$= \{u = x - x_i\} = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{h_N^L} \int \varphi\left(\frac{u}{h_N}\right) du =$$

$$= \frac{1}{N} \sum_{i=1}^{N} \frac{1}{h_N^L} \int_{(-h_N/2, \dots, -h_N/2)}^{(+h_N/2, \dots, +h_N/2)} du = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{h_N^L} h_N^L = 1$$

- Estimation of probability density functions
 - Non-parametric estimation: Parzen windows
 - Comments on p_N :
 - p_N is the average of N sample-centered functions x_i



- Estimation of probability density functions
 - Non-parametric estimation: Parzen windows
 - Example: N random values extracted from a distribution N(0,1) rectangular kernel



Estimation of probability density functions

- Non-parametric estimation: Parzen windows
 - As we have already seen in the previous example, when approximating continuous functions $[p(\cdot)]$ by discontinuous step functions $[\varphi(\cdot)]$, the resulting estimate also presents discontinuities
 - To avoid this, it is suggested to use continuous kernels $\varphi(\cdot)$
 - It can be shown that the resulting estimate $p_N(x)$ is a legitimate pdf if:

$$\varphi(u) \ge 0$$
 and $\int \varphi(u) du = 1$

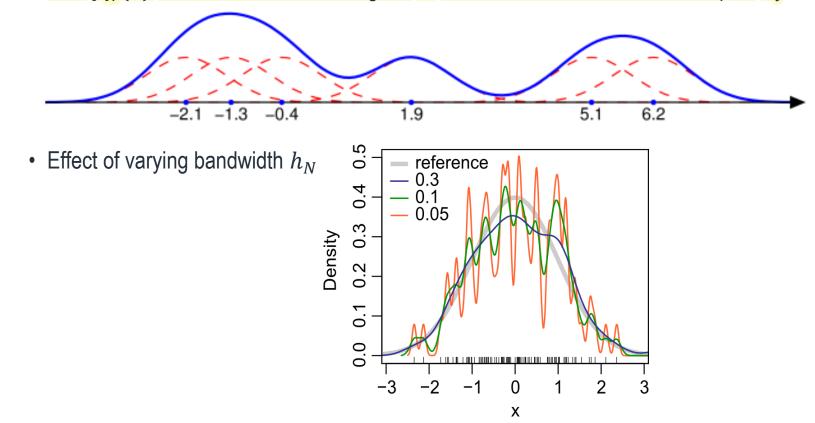
 One of the most commonly used kernels is the Gaussian kernel (mean 0, variance 1):

$$\varphi(u) = \frac{1}{\sqrt{(2\pi)^L}} e^{-\frac{1}{2}u^T u}$$

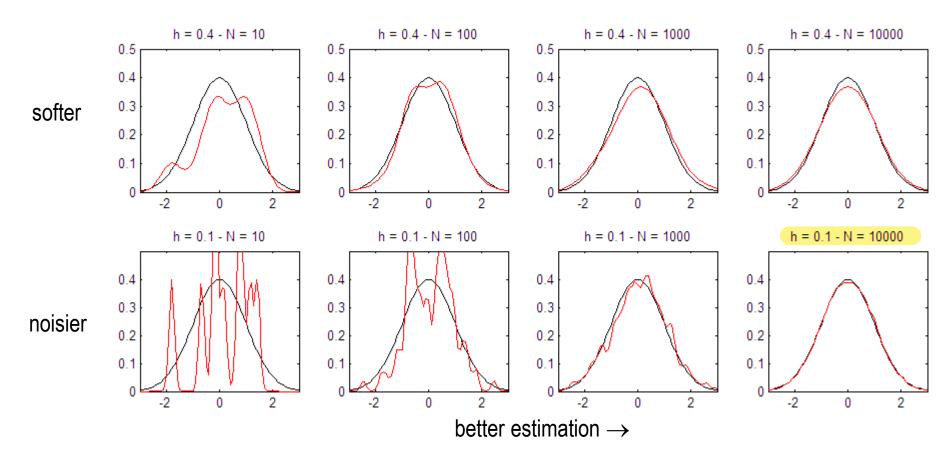
$$p_N(x) = \frac{1}{N} \sum_{i=1}^N \frac{1}{h_N^L} \varphi\left(\frac{x - x_i}{h_N}\right)$$
$$= \frac{1}{N} \frac{1}{h_N^L} \sum_{i=1}^N \frac{1}{\sqrt{(2\pi)^L}} e^{-\frac{1}{2}u_i^T u_i}$$
$$\left(u_i = \frac{x - x_i}{h_N}\right)$$

```
def parzen gauss 1D(x,X,h):
                      # x = point where to evaluate the PDF
# X = data samples
                       \# h = side of the (hyper)cube
                      N = X.shape[0]; kn = 0 for i in range(N):
                                kn += 1/(sqrt(2*pi))*exp(-0.5*((x-X[i])/h)**2)
\left(u_i = \frac{x - x_i}{h_N}\right) \qquad p = \frac{\text{km f } 17}{\text{km/N}} / h
                          return p
```

- Estimation of probability density functions
 - Non-parametric estimation: Parzen windows
 - Now $p_N(x)$ is obtained as the average of N Gaussians centered on the samples x_i



- Estimation of probability density functions
 - Non-parametric estimation: Parzen windows
 - Example: N random values extracted from a distribution N(0,1) Gaussian kernel



- Estimation of probability density functions
 - Non-parametric estimation: k nearest neighbours
 - Given x and a collection of samples $x_1, x_2, ..., x_N$ from a certain pdf p(x), to estimate p(x):
 - **Parzen windows method** first, a search volume is set around x, V_N , and next we determine the number of samples k_N belonging to that volume

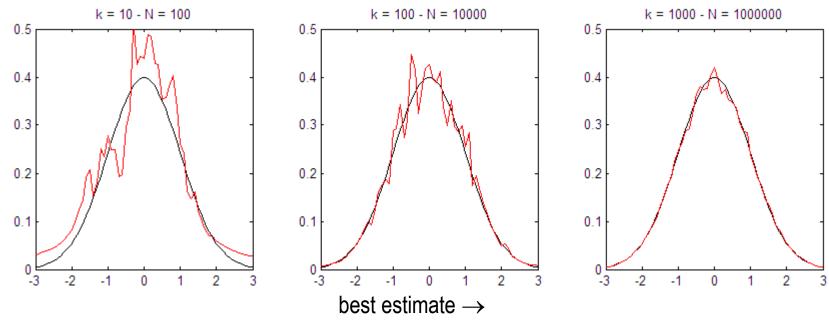
We set
$$V_N$$
 and find $k_N \to p_N(x) = \frac{k_N/N}{V_N}$

- Method of the k nearest neighbors – we first find the k_N samples nearest to x, and next we determine the minimal volume V_{kN} where they are contained in

We set
$$k_N$$
 and find $V_N \to p_N(x) = \frac{k_N/N}{V_{kN}}$ def knn_1D(x, X, k):

```
def knn_1D(x,X,k):
# x = point where to evaluate the PDF
# X = data samples
# k = number of neighbours
N = X.shape[0]; d = []
for i in range(N):
    d.append(abs(x-X[i]))
d.sort()
V = 2 * d[min(N,k)-1]
p = (k/N)/V
return p
```

- Estimation of probability density functions
 - Non-parametric estimation: k nearest neighbours
 - **Example**: N random values sampled from a distribution N(0,1)



- In this case, it has been used: $k_N = \sqrt{N}$
- In the case of Parzen windows, it is suggested to use: $h_N = \frac{h_1}{\sqrt{N}}$

Contents

- Introduction
- Bayesian classification
- Estimation of probability density functions
- Linear discriminant functions and the perceptron algorithm

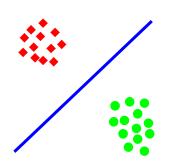
We have already seen that, depending on the pdf's of the classes (Gaussian case), a
Bayesian classifier can derive in a set of linear discrimination functions. For
example, for 2 classes:

$$g_{12}(x) = w^T(x - x_0), \quad g_{12}(x) = \begin{cases} > 0 & x \in \omega_1 \\ < 0 & x \in \omega_2 \end{cases}$$

- simple and computationally very interesting classifier
- In this section, we concentrate again on linear discrimination functions, but from a different perspective: we do not assume any pdf for the classes
 - Therefore, regardless of the pdf of the classes, we expect them to be separable by (hyper)planes (1D – point, 2D – straight, 3D – plane, etc.)
 - In this case it is said that the classes are linearly separable
 - We will see how you can find a (hyper)plane that separates the classes from each other (perceptron algorithm)

Linear discrimination functions

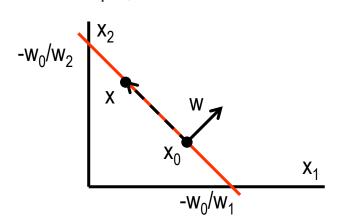
- Goal: find a (hyper)plane that allows us to separate the training samples in 2 classes



$$g_{12}(x) = w^T(x - x_0), \quad g_{12}(x) = \begin{cases} > 0 & x \in \omega_1 \\ < 0 & x \in \omega_2 \end{cases}$$

(hyper)plane:
$$x \mid g_{12}(x) = w^T(x - x_0) = 0$$

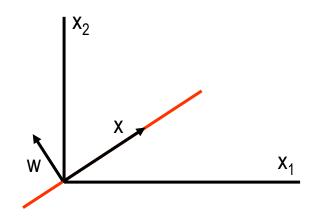
– For example, for L = 2 characteristics:

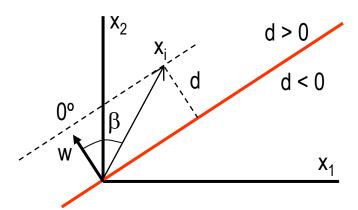


$$\begin{split} &(w_1,w_2)\left[\binom{x_1}{x_2}-\binom{x_{01}}{x_{02}}\right]=0\\ &w_1x_1+w_2x_2-(w_1x_{01}+w_2x_{02})=0\\ &w_1x_1+w_2x_2+w_0=0 \qquad \text{(normal form)} \end{split}$$

$$x_2 = \left(-\frac{w_1}{w_2}\right)x_1 + \left(-\frac{w_0}{w_2}\right)$$
 (slope-intercept form)

 Linear discrimination functions. For now, we will only consider hyperplanes which go through the origin





- This means that \mathbf{x}_0 = $(0,0)^{\mathsf{T}}$ and thus in $w^T(x-x_0)$ $w_0=w^Tx_0=0$ $\mathbf{w}_1x_1+w_2x_2=0$ $\mathbf{w}_1x_1+w_2x_2=0$

- For any point x_i outside the hyperplane we can state:

$$w^{T}x_{i} = ||w|| ||x_{i}|| \cos \beta \neq 0$$

$$\downarrow \qquad ||w|| = 1$$

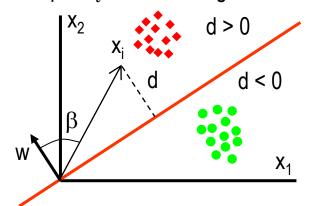
$$||x_{i}|| \cos \beta = d$$

- The sign of d depends on the **relative position** of x_i with regard to the hyperplane:

$$\begin{cases} \beta \in \left[-\frac{\pi}{2}, +\frac{\pi}{2} \right] & w^T x_i = d > 0 \\ |\beta| > \frac{\pi}{2} & w^T x_i = d < 0 \end{cases}$$

- $|d| = |w^T x_i|$ indicates **how far away the sample is** from the (hyper)plane of discrimination

- We assume that the classes ω_1 and ω_2 are **linearly separable**, i.e. the hyperplane exists
- The goal is thus to find a function $g_{12}(x) = w^T x$ such that $g_{12}(x)$ is as follows for each sample x_i of the training set:



$$g_{12}(x_i) = w^T x_i > 0, \forall x_i \in \omega_1$$
$$g_{12}(x_i) = w^T x_i < 0, \forall x_i \in \omega_2$$

- $-g_{12}$ defined in this way is also named as a **discrimination function**, which in this case turns out to be linear, and thus it is a **linear discrimination function**
- To find the hyperplane, we consider the following function (perceptron cost):

$$J(w) = \sum_{x_i \in \mathcal{V}} (\delta_{x_i} w^T x_i)$$

where:
$$-\mathcal{Y}$$
 is the set of samples x_i wrongly classified by w

$$-\delta_{x_i} = -1 \text{ if } x_i \in \omega_1 \text{ y } \delta_{x_i} = +1 \text{ if } x_i \in \omega_2$$

$$-J(w) \geq 0, \forall w \ (x_i \in \omega_1 \text{ but } x_i \to \omega_2, \text{ then } \delta_{x_i} \omega^T x_i = (-1)(<0) > 0)$$

$$-J(w) = 0 \text{ if all samples are well classified } (\mathcal{Y} = \emptyset)$$

$$-J(w) \text{ is piece-wise linear } \Rightarrow \text{minimization is not trivial}$$

• The **perceptron algorithm** (Rosenblatt, 1950s) is able to find, through the next iterative approach, the required hyperplane: (sort of **gradient descent** but not exactly)

$$w(t+1) = w(t) - \rho_t \sum_{x_i \in \mathcal{Y}} \delta_{x_i} x_i$$
$$w(0) = \text{any vector of } \mathbb{R}^L$$

• The algorithm converges if the classes are **linearly separable** and if the sequence of values ρ_t meets certain conditions:

$$\lim_{t \to \infty} \sum_{k=0}^{t} \rho_k = \infty, \quad \lim_{t \to \infty} \sum_{k=0}^{t} \rho_k^2 < \infty$$

- for instance, $\rho_t=c/t$ and $\rho_t=\rho$ (ρ bounded) meet those conditions
- the sequence ρ_t determines the convergence speed

- Variants of the (basic) perceptron algorithm:
 - (1a) To deal with hyperplanes that do not contain the origin, the feature vectors must be augmented in one additional dimension $x_i^* = (x_i, 1)^T$. In this way:

$$w^{T}x + w_{0} = 0 \equiv \underbrace{(w_{1}, w_{2}, \dots, w_{L}, w_{0})}_{w^{T}} \begin{pmatrix} x_{1} \\ x_{2} \\ \vdots \\ x_{L} \\ 1 \end{pmatrix} = (w^{*})^{T}x^{*} = 0$$

- \clubsuit We will use \mathbf{w}^{T} instead of $(\mathbf{w}^{\star})^{\mathsf{T}}$ and \mathbf{x} instead of \mathbf{x}^{\star} to simplify the notation
- (1b) The rule for modifying **w** within every iteration can be generically implemented as follows: L+1

follows:
$$S = (0,0,\ldots,0)^T$$
 for $i=1$ to n_training_samples
$$\text{if } x_i \in \omega_1 \text{ and } w(t)^T x_i < 0 \text{ then } S = S + x_i$$
 if $x_i \in \omega_2 \text{ and } w(t)^T x_i > 0 \text{ then } S = S - x_i$ end for
$$w(t+1) = w(t) + \rho_t S$$

Variants of the (basic) perceptron algorithm:

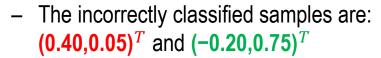
(1) Example 1

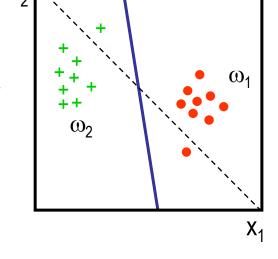
– The dashed line corresponds to:

$$(1, 1, -0.5)x =$$

 $x_1 + x_2 - 0.5 = 0$

where $w(t) = (1,1,-0.5)^T$ is the result of the previous step of the perceptron algorithm using $\rho_t = \rho = 0.7$





The new iteration yields

$$w(t+1) = w(t) - \frac{1}{-\rho_t \sum_{x_i \in \mathcal{V}} \delta_{x_i} x_i}$$

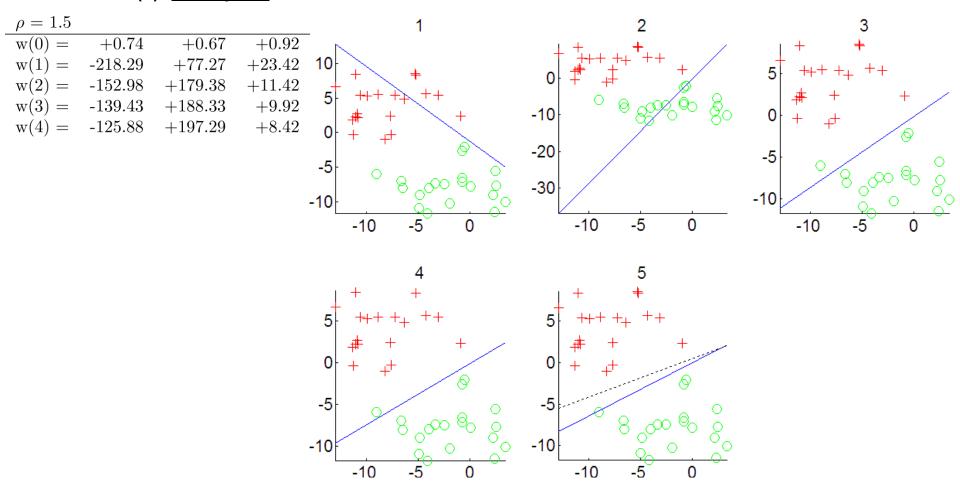
$$\begin{bmatrix} w(t+1) = w(t) - \\ -\rho_t \sum_{x_i \in \mathcal{Y}} \delta_{x_i} x_i \end{bmatrix} w(t+1) = \begin{pmatrix} 1 \\ 1 \\ -0.5 \end{pmatrix} - 0.7(-1) \begin{pmatrix} 0.4 \\ 0.05 \\ 1 \end{pmatrix} - 0.7(+1) \begin{pmatrix} -0.2 \\ 0.75 \\ 1 \end{pmatrix} = \begin{pmatrix} 1.42 \\ 0.51 \\ -0.5 \end{pmatrix}$$

The resulting hyperplane classifies correctly all the samples and the algorithm ends with:

$$1.42x_1 + 0.51x_2 - 0.5 = 0$$

• Variants of the (basic) perceptron algorithm:

(1) **Example 2**



- Variants of the (basic) perceptron algorithm:
 - (1) Implementation

```
S = \text{np.zeros}(3); \text{ ic} = 0 for i in range(N): xs = \text{np.ones}(3) xs[0] = X[i,0]; xs[1] = X[i,1] if np.dot(w,xs) <= 0 and y[i] == 1: S = S + xs; \text{ ic} += 1 elif np.dot(w,xs) > 0 and y[i] == 0: S = S - xs; \text{ ic} += 1 if ic == 0: # Y = empty set break else: w = w + \text{rho} * S
```

return w

N = X.shape[0]w = np.zeros(3)

for t in range(nit):

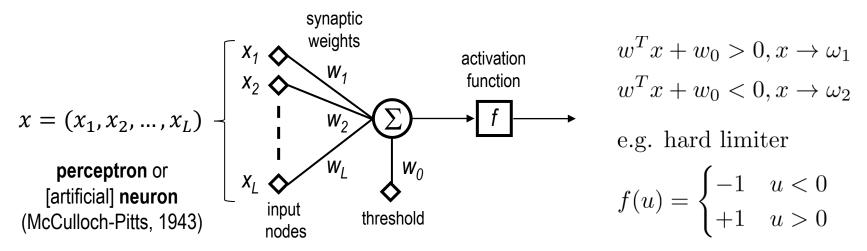
def perceptron 2D(X, y, rho, nit):

w = w / sqrt(w[0] ** 2 + w[1] ** 2)

- Variants of the (basic) perceptron algorithm:
 - (2) The pocket algorithm
 - Stops after a number of iterations (T), providing the best hyperplane which has been found along that number of iterations
 - Partially solves the convergence problem of the original perceptron algorithm when the classes are not linearly separable
 - (1) Initialize w(0) randomly
 - (2) $w_s = w(0)$ $h_s = \text{no. samples correctly classified by } w(0)$
 - (3) **for** t = 0 **to** T(3.1) $w(t+1) = w(t) - \rho_t \sum_{x_i \in \mathcal{Y}} \delta_{x_i} x_i$ (3.2) h = no. samples correctly classified by w(t+1)(3.3) **if** $h > h_s$ **then** $w_s = w(t+1), h_s = h$ **end if**
 - (4) end for

Classification device:

– Once the perceptron algorithm has converged with e.g. $w=(w_1,w_2,...,w_L,w_0)$, then the following structure can implement the classification operation:



 The perceptron can be considered as the basic building element for more complex learning machines, e.g. neural networks

Lecture 3.1 Supervised learning: Bayesian and linear classifiers



Departament de Ciències Matemàtiques i Informàtica 11752 Aprendizaje Automático
11752 Machine Learning
Máster Universitario
en Sistemas Inteligentes

Alberto ORTIZ RODRÍGUEZ