Cognitive Algorithms
Lecture 2

Linear Classification

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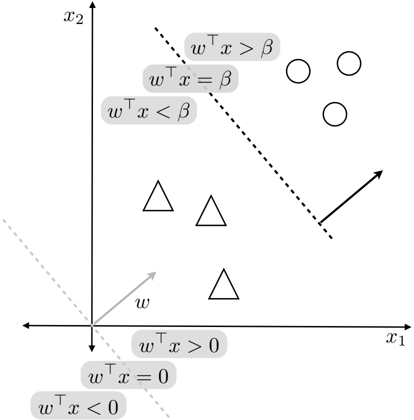
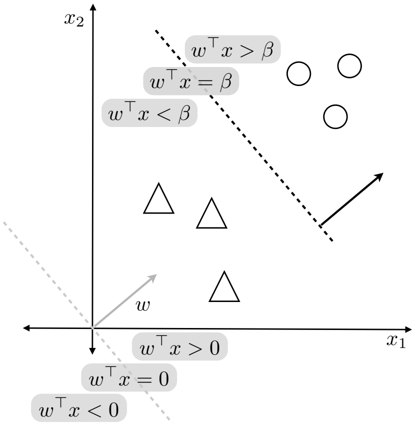
Recap: Linear Classification



Linear decision boundary:

$$\boldsymbol{w}^T \boldsymbol{x} - \beta = 0$$

Recap: Nearest Centroid Classifier



Comparison of distance between data point $\boldsymbol{x} \in \mathbb{R}^d$ to class means $\bar{\boldsymbol{x}}_\Delta, \bar{\boldsymbol{x}}_o \in \mathbb{R}^d$ is equivalent to linear classification with

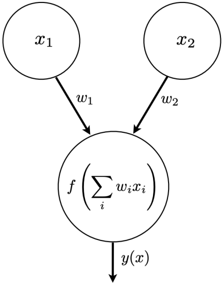
$$\boldsymbol{w} = \bar{\boldsymbol{x}}_o - \bar{\boldsymbol{x}}_\Delta$$

and

$$\beta = \frac{1}{2} \cdot \boldsymbol{w}^\top (\bar{\boldsymbol{x}}_o + \bar{\boldsymbol{x}}_\Delta)$$

Note notation change: $\boldsymbol{w}_o = \bar{\boldsymbol{x}}_o$, $\boldsymbol{w}_\Delta = \bar{\boldsymbol{x}}_\Delta$.

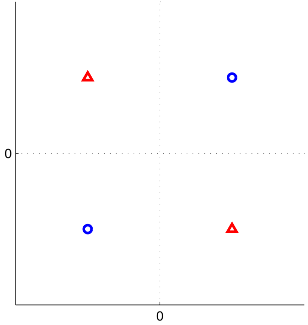
Recap: Perceptron



Problem	Classification
Model	$\hat{y} = f(\boldsymbol{w}^T x)$
Loss function	$-\sum_{m \in \mathcal{M}} \boldsymbol{w}^T \boldsymbol{x}_m y_m$
Optimization	stochastic gradient descent (SGD)

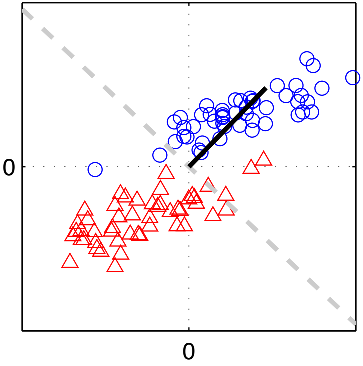
Problems with Nearest Centroid Classification

Not linearly separable data



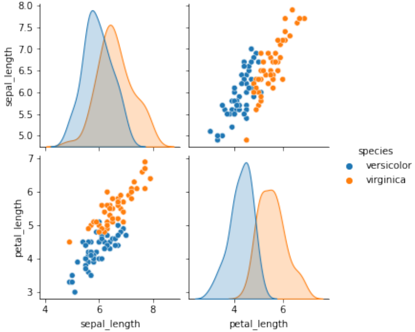
Solution
Non-linear methods (later in this course)

Correlated data



Solution
(Fisher's) Linear Discriminant Analysis

A “real” example



Two features from two species in the *Iris* dataset[1]

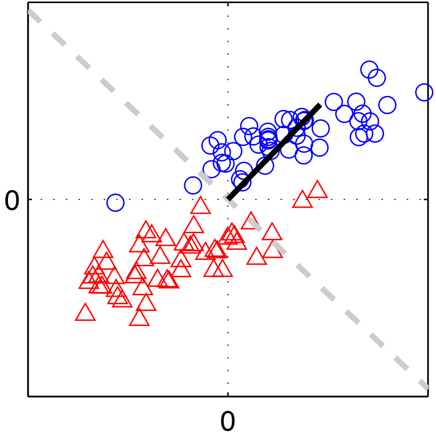
Petal length and sepal length are correlated in each species

[1] https://en.wikipedia.org/wiki/Iris_flower_data_set

What is correlation?

Let's go through some definitions first

→ They will be useful later



Random variables

Denote by Ω the sample space, the set of all possible outcomes of an experiment.
A mapping $X : \Omega \to \mathbb{R}$ which assigns a real value to every elementary event, is called a real-valued random variable.

Example: coin toss $\Rightarrow \Omega = \{\text{head}, \text{tail}\}$

$$X(\omega) = \begin{cases} 0, & \text{if } \omega = \text{tail} \\ 1, & \text{if } \omega = \text{head} \end{cases} \quad \text{for } \omega \in \Omega$$

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- We use random variables to model the world
- In this course, we take a practical approach and introduce concepts when we need them

Probabilities and expected values

If X is a **discrete random variable**, i.e. if X takes on only finitely[2] many values, we can assign probabilities $p_i \in [0, 1]$ to the values x_i of X.
A probability of p_i means that out of very many trials, a fraction of p_i will have value x_i.

The **expected value** of X is given by

$$\mathbb{E}[X] = \sum_i p_i x_i \,.$$

Example: coin toss with $p_0 = p_1 = \frac{1}{2}$, then

$$\mathbb{E}[X] = 0 \cdot p_0 + 1 \cdot p_1 = \frac{1}{2} \,.$$

[2]Strictly speaking, a discrete random variable takes finitely many or countably many values.

Probability distributions and expected values

The probabilities of the values of a **continuous random variable** are described by a **probability density function**, a function $p : X(\Omega) \to \mathbb{R}_+$ with $\int_{X(\Omega)} p(x)\,\mathrm{d}x = 1$.
The probability of observing a value in $[a, b] \subset \mathbb{R}$ is given by

$$\int_a^b p(x)\,\mathrm{d}x\,.$$

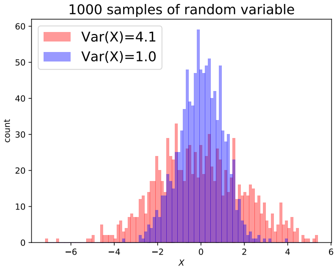
The expected value of X is given by

$$\mathbb{E}[X] = \int_{-\infty}^{\infty} x \cdot p(x)\,\mathrm{d}x\,.$$

Variance

measure of variability of X around its mean

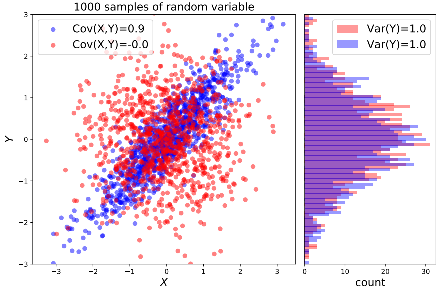
$$\mathrm{Var}(X) = \mathbb{E}[(X - \mathbb{E}[X])^2]$$



Covariance

measure of the joint variability of X and Y

$$\mathrm{Cov}(X, Y) := \mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])]$$



Covariance

$$\mathrm{Cov}(X, Y) := \mathbb{E}[(X - \mathbb{E}(X))(Y - \mathbb{E}(Y))]$$

Correlation

$$\mathrm{Corr}(X, Y) := \frac{\mathrm{Cov}(X, Y)}{\sqrt{\mathrm{Var}(X)}\sqrt{\mathrm{Var}(Y)}} \in [-1, 1] \,.$$

normalized covariance

Covariance

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Correlation

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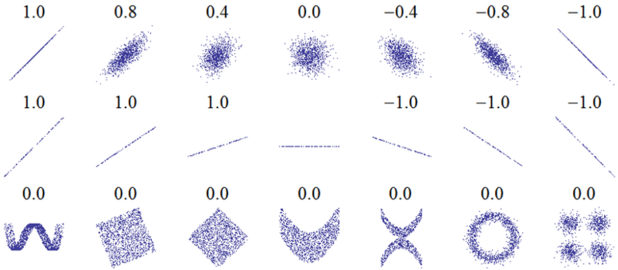
normalized covariance

Indicate the strength of a **linear** relationship



Correlation vs. dependence vs. causation

Consider two random variables X, Y.

- X and Y are called **independent** if $p(X, Y) = p(X) \cdot p(Y)$
- X and Y are called **uncorrelated** if $\mathrm{Corr}(X, Y) = 0$

We might call X and Y **causally related** if X influences Y or vice versa.

Note

- X and Y independent implies X and Y uncorrelated
- X and Y uncorrelated *does not* imply X and Y independent! (example $Y = X^2$ on $[-1, 1]$)
- X and Y dependent does not imply X and Y causally related

Normal distribution

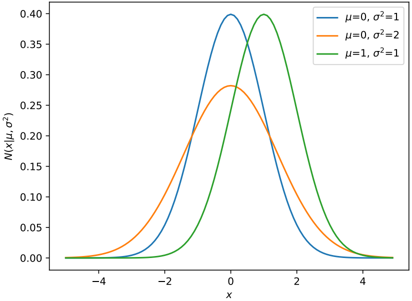
Parameters:

- Mean $\mu \in \mathbb{R}$
- Variance $\sigma^2 \in \mathbb{R}$

The probability density function

$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}\right)$$

defines the **normal distribution** or **Gaussian distribution** with parameters μ, σ^2.



The parameters μ and σ^2 are called 'mean' and 'variance', because the mean $\mathbb{E}[X]$ and variance $\mathbb{E}[(X-\mathbb{E}[X])^2]$ of the distribution are μ and σ^2

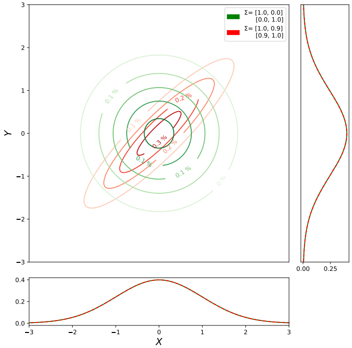
Multivariate normal distribution

For d dimensions:

$$\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}, \Sigma) = (2\pi)^{-\frac{d}{2}} \det(\Sigma)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T \Sigma^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right)$$

Parameters:

- Mean $\boldsymbol{\mu} \in \mathbb{R}^d$
- Covariance matrix $\Sigma \in \mathbb{R}^{d \times d}$



Estimating the covariance matrices

Given n data points $\boldsymbol{x}_i \in \mathbb{R}^D$ in a data matrix $X \in \mathbb{R}^{D\times n}$ the empirical estimate of the **covariance matrix** is defined as

$$\hat{\Sigma} = \frac{1}{n}\,(X - \bar{X})(X - \bar{X})^\top\,,$$

where the estimate of the expected value is given by the mean

$$\bar{\boldsymbol{x}} = \frac{1}{n}\sum_{i=1}^{n}\boldsymbol{x}_i\,,\quad \bar{X} = (\bar{\boldsymbol{x}}, \bar{\boldsymbol{x}}, \dots, \bar{\boldsymbol{x}}) \in \mathbb{R}^{D\times n}$$

The diagonal entries of $\hat{\Sigma}$ are estimates of the variance.

We call $(X - \bar{X})(X - \bar{X})^\top$ the *empirical scatter matrix*

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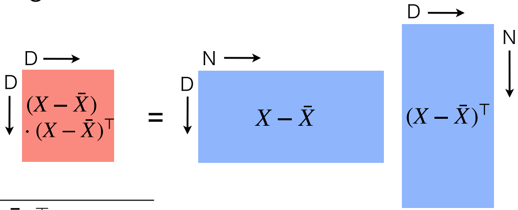
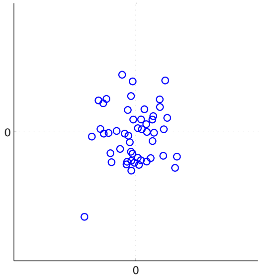


We call $(X - \bar{X})(X - \bar{X})^\top$ the *empirical scatter matrix*

Create correlated data from uncorrelated data

We can generate correlated data using a diagonal scaling matrix D and a rotation R. We assume centered data here (i.e. $\bar{X} = 0$), so $\hat{\Sigma} = \frac{1}{n} X X^\top$

Uncorrelated



$$x \sim \mathcal{N}(0, 1)$$

$$\frac{1}{n} X X^\top = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

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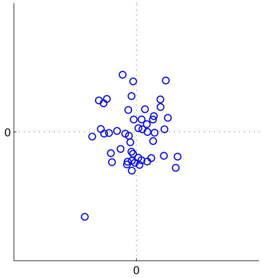

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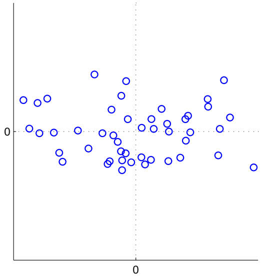
Uncorrelated, scaled



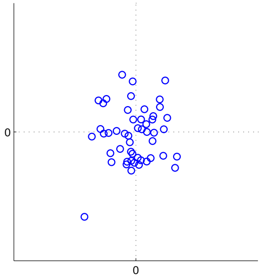
$$\begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix} X$$

$$\frac{1}{n} X X^\top = \begin{bmatrix} 9 & 0 \\ 0 & 1 \end{bmatrix}$$

Create correlated data from uncorrelated data

We can generate correlated data using a diagonal scaling matrix D and a rotation R. We assume centered data here (i.e. $\bar{X} = 0$), so $\hat{\Sigma} = \frac{1}{n} XX^\top$

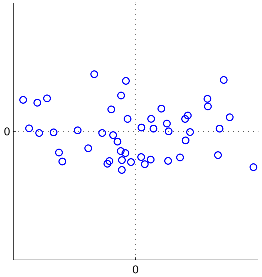
Uncorrelated



$$x \sim \mathcal{N}(0, 1)$$

$$\frac{1}{n} XX^\top = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

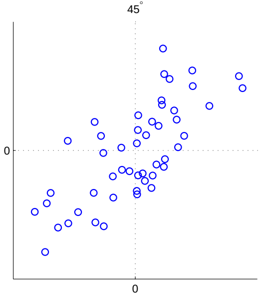
Uncorrelated, scaled



$$\begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix} X$$

$$\frac{1}{n} XX^\top = \begin{bmatrix} 9 & 0 \\ 0 & 1 \end{bmatrix}$$

Scaled, rotated by 45°



$$\begin{bmatrix} cos(\phi) & -sin(\phi) \\ sin(\phi) & cos(\phi) \end{bmatrix} \begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix} X$$

$$\frac{1}{n} XX^\top = \begin{bmatrix} 5 & 4 \\ 4 & 5 \end{bmatrix}$$

Ronald A. Fisher

Ronald A. Fisher (1890 – 1962)

Founder of modern statistics

Interested in Biology

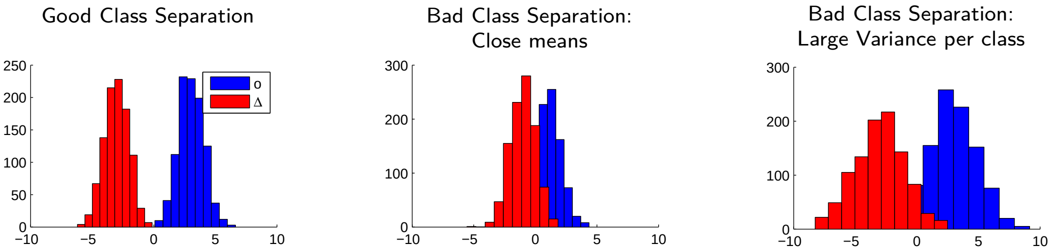
Suggested *Linear Discriminant Analysis* (LDA)

Held some very problematic opinions

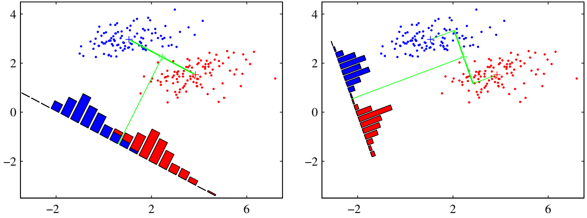
https://priceonomics.com/why-the-father-of-modern-statistics-didnt-believe/, https://statmodeling.stat.columbia.edu/2020/08/01/ra-fisher-and-the-science-of-hatred/

The Fisher Criterion - measure for class separability

Consider one dimensional data and two classes



Linear Discriminant Analysis

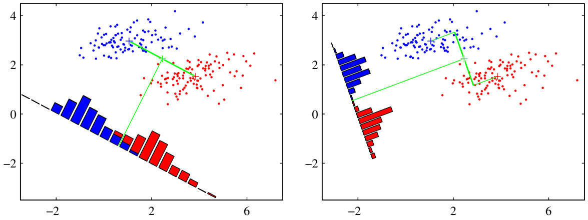


Goal: Find a (normal vector of a linear decision boundary) $\boldsymbol{w} \in \mathbb{R}^d$ that

Maximizes mean class difference, and

Minimizes variance in each class

Linear Discriminant Analysis



Maximize the **Fisher criterion**:

$$J(\boldsymbol{w}) = \frac{\text{between class variance}}{\text{within class variance}} = \frac{(\mu_o - \mu_\Delta)^2}{\sigma_o^2 + \sigma_\Delta^2}$$

where $\boldsymbol{x}_{1o}, \ldots, \boldsymbol{x}_{n_o o} \in \mathbb{R}^d$ and

$\mu_o = \frac{1}{n_o} \sum_{i=1}^{n_o} \boldsymbol{w}^\top \boldsymbol{x}_{io}$ and $\sigma_o^2 = \frac{1}{n_o} \sum_{i=1}^{n_o} (\boldsymbol{w}^\top \boldsymbol{x}_{io} - \mu_o)^2$ and similarly for Δ.

Linear Discriminant Analysis

Rewrite Fisher criterion to separate out $\boldsymbol{w}$-dependence using

$$\bar{\boldsymbol{x}}_o := \frac{1}{n_o}\sum_{i=1}^{n_o}\boldsymbol{x}_{io} \quad \Rightarrow \quad \mu_o = \frac{1}{n_o}\sum_{i=1}^{n_o}\boldsymbol{w}^\top\boldsymbol{x}_{io} = \boldsymbol{w}^\top\bar{\boldsymbol{x}}_o\,, \quad \sigma_o^2 = \frac{1}{n_o}\sum_{i=1}^{n_o}(\boldsymbol{w}^\top\boldsymbol{x}_{io} - \mu_o)^2 = \frac{1}{n_o}\sum_{i=1}^{n_o}(\boldsymbol{w}^\top(\boldsymbol{x}_{io} - \bar{\boldsymbol{x}}_o))^2$$

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Hence,

$$(\mu_o - \mu_\Delta)^2 = (\boldsymbol{w}^\top(\bar{\boldsymbol{x}}_o - \bar{\boldsymbol{x}}_\Delta))^2 = \boldsymbol{w}^\top\underbrace{(\bar{\boldsymbol{x}}_o - \bar{\boldsymbol{x}}_\Delta)(\bar{\boldsymbol{x}}_o - \bar{\boldsymbol{x}}_\Delta)^\top}_{S_B - \text{"between class scatter"}}\boldsymbol{w}\,.$$

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$$\sigma_o^2 + \sigma_\Delta^2 = \frac{1}{n_o}\sum_{i=1}^{n_o}(\boldsymbol{w}^\top(\boldsymbol{x}_{io} - \bar{\boldsymbol{x}}_o))^2 + \frac{1}{n_\Delta}\sum_{j=1}^{n_\Delta}(\boldsymbol{w}^\top(\boldsymbol{x}_{j\Delta} - \bar{\boldsymbol{x}}_\Delta))^2$$

$$= \boldsymbol{w}^\top \underbrace{\left[\frac{1}{n_o}\sum_{i=1}^{n_o}(\boldsymbol{x}_{io} - \bar{\boldsymbol{x}}_o)(\boldsymbol{x}_{io} - \bar{\boldsymbol{x}}_o)^\top + \frac{1}{n_\Delta}\sum_{j=1}^{n_\Delta}(\boldsymbol{x}_{j\Delta} - \bar{\boldsymbol{x}}_\Delta)(\boldsymbol{x}_{j\Delta} - \bar{\boldsymbol{x}}_\Delta)^\top\right]}_{S_W - \text{“within class scatter”}} \boldsymbol{w}\,.$$

Linear Discriminant Analysis

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Hence,

$$(\mu_o - \mu_\Delta)^2 = (\boldsymbol{w}^\top(\bar{\boldsymbol{x}}_o - \bar{\boldsymbol{x}}_\Delta))^2 = \boldsymbol{w}^\top \underbrace{(\bar{\boldsymbol{x}}_o - \bar{\boldsymbol{x}}_\Delta)(\bar{\boldsymbol{x}}_o - \bar{\boldsymbol{x}}_\Delta)^\top}_{S_B - \text{"between class scatter"}} \boldsymbol{w}\,.$$

$$\begin{aligned}\sigma_o^2 + \sigma_\Delta^2 &= \frac{1}{n_o}\sum_{i=1}^{n_o}(\boldsymbol{w}^\top(\boldsymbol{x}_{io} - \bar{\boldsymbol{x}}_o))^2 + \frac{1}{n_\Delta}\sum_{j=1}^{n_\Delta}(\boldsymbol{w}^\top(\boldsymbol{x}_{j\Delta} - \bar{\boldsymbol{x}}_\Delta))^2 \\ &= \boldsymbol{w}^\top \underbrace{\left[\frac{1}{n_o}\sum_{i=1}^{n_o}(\boldsymbol{x}_{io} - \bar{\boldsymbol{x}}_o)(\boldsymbol{x}_{io} - \bar{\boldsymbol{x}}_o)^\top + \frac{1}{n_\Delta}\sum_{j=1}^{n_\Delta}(\boldsymbol{x}_{j\Delta} - \bar{\boldsymbol{x}}_\Delta)(\boldsymbol{x}_{j\Delta} - \bar{\boldsymbol{x}}_\Delta)^\top\right]}_{S_W - \text{"within class scatter"}} \boldsymbol{w}\,.\end{aligned}$$

And therefore ($\boldsymbol{w} \neq 0$),

$$J(\boldsymbol{w}) = \boldsymbol{w}^\top S_B \boldsymbol{w} \big/ \boldsymbol{w}^\top S_W \boldsymbol{w}\,.$$

Linear Discriminant Analysis

The optimal weight vector $\boldsymbol{w}$ is given by

$$\boldsymbol{w} = \underset{\boldsymbol{w}'}{\operatorname{argmax}}\, J(\boldsymbol{w}') = \underset{\boldsymbol{w}'}{\operatorname{argmax}} \frac{\boldsymbol{w}'^\top S_B \boldsymbol{w}'}{\boldsymbol{w}'^\top S_W \boldsymbol{w}'}$$

To optimize the Fisher criterion, we set its derivative (with respect to $\boldsymbol{w}$) to 0

Linear Discriminant Analysis

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To optimize the Fisher criterion, we set its derivative (with respect to $\boldsymbol{w}$) to 0

$$0 = \frac{\partial}{\partial \boldsymbol{w}} J(\boldsymbol{w})\Big|_{\boldsymbol{w}} = \frac{(\boldsymbol{w}^{\top} S_W \boldsymbol{w}) S_B \boldsymbol{w} - (\boldsymbol{w}^{\top} S_B \boldsymbol{w}) S_W \boldsymbol{w}}{(\boldsymbol{w}^{\top} S_W \boldsymbol{w})^2}$$

Linear Discriminant Analysis

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To optimize the Fisher criterion, we set its derivative (with respect to $\boldsymbol{w}$) to 0

$$\begin{aligned}
0 &= \frac{\partial}{\partial \boldsymbol{w}} J(\boldsymbol{w})\Big|_{\boldsymbol{w}} = \frac{(\boldsymbol{w}^{\top} S_W \boldsymbol{w}) S_B \boldsymbol{w} - (\boldsymbol{w}^{\top} S_B \boldsymbol{w}) S_W \boldsymbol{w}}{(\boldsymbol{w}^{\top} S_W \boldsymbol{w})^2} \\
(\boldsymbol{w}^{\top} S_B \boldsymbol{w}) S_W \boldsymbol{w} &= (\boldsymbol{w}^{\top} S_W \boldsymbol{w}) S_B \boldsymbol{w} \\
S_W \boldsymbol{w} &= S_B \boldsymbol{w} \underbrace{\frac{\boldsymbol{w}^{\top} S_W \boldsymbol{w}}{\boldsymbol{w}^{\top} S_B \boldsymbol{w}}}_{scalar \equiv \lambda}
\end{aligned}$$

Linear Discriminant Analysis

$$\boldsymbol{w} = \operatorname*{argmax}_{\boldsymbol{w}'} \frac{\boldsymbol{w}'^{\top} S_B \boldsymbol{w}'}{\boldsymbol{w}'^{\top} S_W \boldsymbol{w}'}$$

$$\rightarrow S_W \boldsymbol{w} = S_B \boldsymbol{w} \lambda$$

Linear Discriminant Analysis

$$\mathbf{w} = \underset{\mathbf{w}'}{\operatorname{argmax}} \frac{\mathbf{w}'^{\top} S_B \mathbf{w}'}{\mathbf{w}'^{\top} S_W \mathbf{w}'}$$

$$\rightarrow S_W \mathbf{w} = S_B \mathbf{w} \lambda$$

Now we plug $S_B = (\bar{\mathbf{x}}_o - \bar{\mathbf{x}}_\Delta)(\bar{\mathbf{x}}_o - \bar{\mathbf{x}}_\Delta)^\top$ in

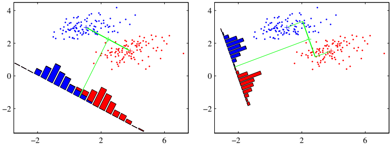
$$S_B \mathbf{w} = (\bar{\mathbf{x}}_o - \bar{\mathbf{x}}_\Delta) \underbrace{(\bar{\mathbf{x}}_o - \bar{\mathbf{x}}_\Delta)^\top \mathbf{w}}_{\text{scalar}}$$

finally, left multiplying with S_W^{-1} yields

$$\mathbf{w} \propto S_W^{-1} (\bar{\mathbf{x}}_o - \bar{\mathbf{x}}_\Delta).$$

($\propto$ denotes proportionality, e.g. $x \propto 2x$)

Interim summary



Goal

Find $\boldsymbol{w} \in \mathbb{R}^d$ that

- maximizes mean class difference
- minimizes variance in each class

Formalization

Maximize the **Fisher criterion**

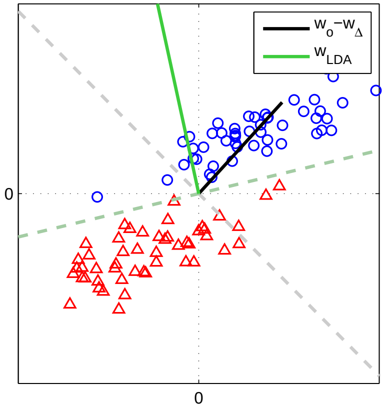
$$J(\boldsymbol{w}) = \frac{\text{between class variance}}{\text{within class variance}} = \frac{(\mu_o - \mu_\Delta)^2}{\sigma_o^2 + \sigma_\Delta^2}$$

Solution

After some calculations...

$$\boldsymbol{w} \propto S_W^{-1}(\bar{\boldsymbol{x}}_o - \bar{\boldsymbol{x}}_\Delta)$$

Linear Discriminant Analysis vs Nearest Centroid Classifier



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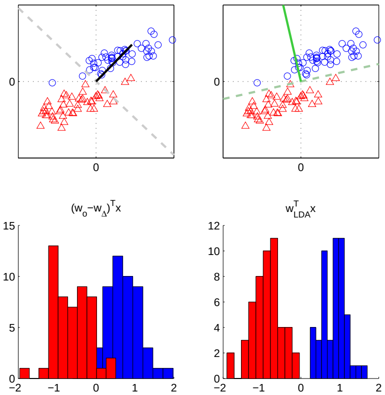

If correlated data are the problem, why don't we decorrelate the data and then apply the nearest-centroid classifier?

How can we decorrelate the data?

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\end{aligned}$$

There is more than one way of whitening (we can multiply $\tilde{X}$ with any orthogonal matrix $OO^T = I$)

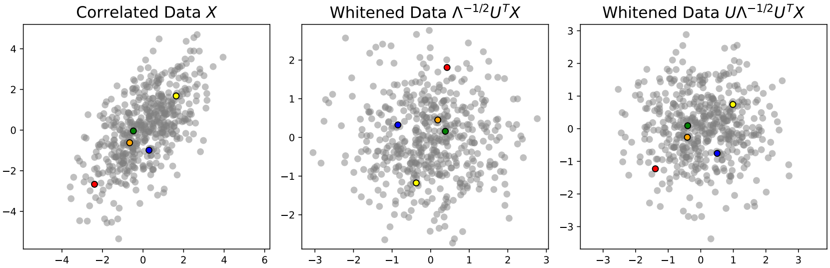
Whitening

Transforms data to data with covariance matrix that is the identity.

$\rightarrow$ Data are decorrelated after whitening

Often used as part of preprocessing

Leads to more numeric stability



Linear Discriminant Analysis

For centered data, we have

$$S = \frac{1}{n_\Delta + n_o} X X^T = S_W + \frac{n_\Delta n_o}{n_\Delta + n_o} S_B$$

Compare Subsection 4.1.5 in PRML[3] and Exercise 4.6 in PRML, a solution of the exercise is available here `https://github.com/zhengqigao/PRML-Solution-Manual`.

Then, for the LDA weight vector $\boldsymbol{w}$:

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The predictions of LDA then are:

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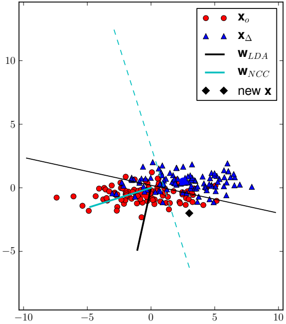
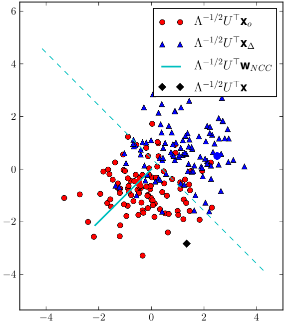


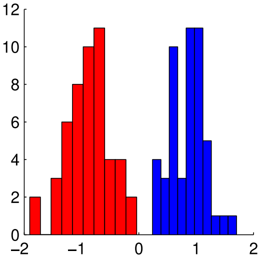


Discriminative and Generative Model

So far:

Find one-dimensional projection via $\boldsymbol{w}$ which best separates the two classes.

How can we build a discriminator, i.e. find a bias?



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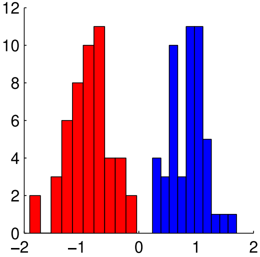

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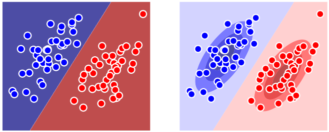
Generative approach:

Let's model how data was generated



Probabilistic modelling

Decision theory: The optimal classifier is Bayes classifier
For a new data point $\boldsymbol{x} \in \mathbb{R}^d$

$$\text{Decide class } \Delta \qquad \text{if } p(\Delta|\boldsymbol{x}) > p(o|\boldsymbol{x}).$$

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Calculate $p(\Delta|\boldsymbol{x})$ with Bayes rule:

$$p(\Delta|\boldsymbol{x}) = \frac{p(\Delta)p(\boldsymbol{x}|\Delta)}{p(\boldsymbol{x})}$$

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Calculate $p(\Delta|\boldsymbol{x})$ with Bayes rule:

$$p(\Delta|\boldsymbol{x}) = \frac{p(\Delta)p(\boldsymbol{x}|\Delta)}{p(\boldsymbol{x})}$$

For the decision, $p(\boldsymbol{x})$ is irrelevant:

$$p(\Delta|\boldsymbol{x}) > p(o|\boldsymbol{x}) \quad \Leftrightarrow \quad p(\Delta)p(\boldsymbol{x}|\Delta) > p(o)p(\boldsymbol{x}|o)\,.$$

Probabilistic modelling

The class probabilities $p(\Delta)$, $p(o)$ can be estimated using

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One solution:

Choose distributions for $p(\boldsymbol{x}|\Delta)$, $p(\boldsymbol{x}|o)$ that are easy to deal with.

$\rightarrow$ Most popular: The Gaussian (or normal) distribution

$$\boldsymbol{x} \in \mathbb{R}^d \text{ in class } \Delta \;\sim \mathcal{N}(\bar{\boldsymbol{x}}_\Delta, S_\Delta) = \frac{1}{(2\pi)^{\frac{d}{2}}\sqrt{\det(S_\Delta)}} e^{-\frac{1}{2}(\boldsymbol{x}-\bar{\boldsymbol{x}}_\Delta)^\top S_\Delta^{-1}(\boldsymbol{x}-\bar{\boldsymbol{x}}_\Delta)}$$

and similarly for class o.

Linear discriminant - a probabilistic view

If we use equal covariance in each class, $\bar{S} = \frac{1}{n_\Delta + n_o}(n_\Delta S_\Delta + n_o S_o)$, the classification boundary is linear and given by

$$\boldsymbol{w} = \bar{S}^{-1}(\bar{\boldsymbol{x}}_o - \bar{\boldsymbol{x}}_\Delta)$$

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From Fisher criterion, we got

$$\boldsymbol{w} \propto S_W^{-1}(\bar{\boldsymbol{x}}_o - \bar{\boldsymbol{x}}_\Delta) \quad \text{with} \quad S_W = S_\Delta + S_o \quad \text{and (e.g.)} \quad \beta = \frac{1}{2}(\mu_o + \mu_\Delta)$$

$\Rightarrow$ Same as above if $n_\Delta = n_o$

LDA summary

Problem	Classification
Model	$y = \text{sign}(\boldsymbol{w}^T x - \beta)$
Error function	$\text{argmax}_{\boldsymbol{w}} \frac{\boldsymbol{w}^T S_B \boldsymbol{w}}{\boldsymbol{w}^T S_W \boldsymbol{w}}$
Optimization	Closed form

LDA algorithm

Computes: Normal vector $\boldsymbol{w}$ of decision hyperplane, threshold β

Input: Data $\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)\}, x_i \in \mathbb{R}^d, \; y_i \in \{-1, +1\}$,

Compute class mean vectors

$\bar{\boldsymbol{x}}_- = 1/n_- \sum_{i \in \mathcal{Y}_-} \boldsymbol{x}_i$

$\bar{\boldsymbol{x}}_+ = 1/n_+ \sum_{j \in \mathcal{Y}_+} \boldsymbol{x}_j$

Compute averaged covariance matrix

$$\bar{S} = 1/(n_+ + n_-) \Big[\sum_{i \in \mathcal{Y}_-} (\boldsymbol{x}_i - \bar{\boldsymbol{x}}_-)(\boldsymbol{x}_i - \bar{\boldsymbol{x}}_-)^\top + \sum_{j \in \mathcal{Y}_+} (\boldsymbol{x}_j - \bar{\boldsymbol{x}}_+)(\boldsymbol{x}_j - \bar{\boldsymbol{x}}_+)^\top \Big]$$

Compute normal vector $\boldsymbol{w}$

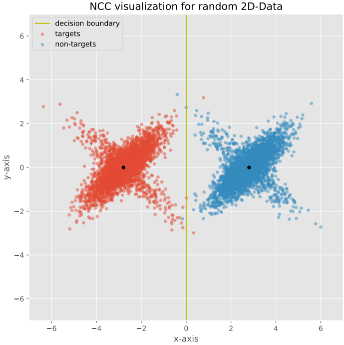
$\boldsymbol{w} = \bar{S}^{-1}(\bar{\boldsymbol{x}}_+ - \bar{\boldsymbol{x}}_-)$

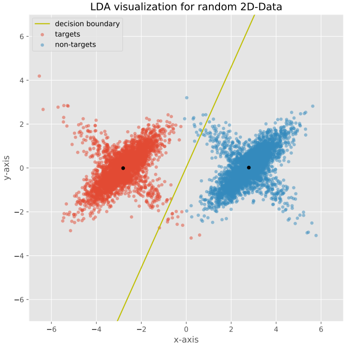
Compute threshold

$\beta = 1/2 \; \boldsymbol{w}^T (\bar{\boldsymbol{x}}_+ + \bar{\boldsymbol{x}}_-) + \log(n_- / n_+)$

Output: $\boldsymbol{w}$, β

Is LDA always better than NCC?





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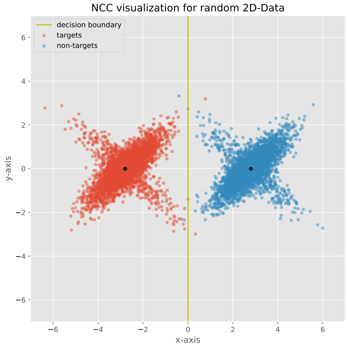
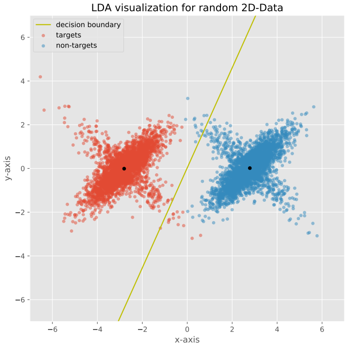
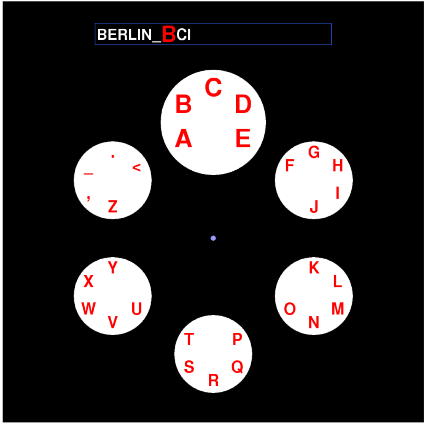


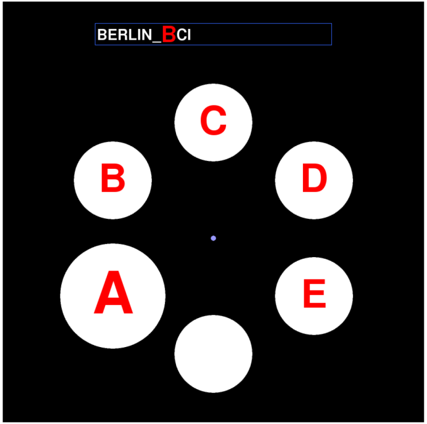


$\Rightarrow$ No, only if our assumption of equal covariance and Normal distribution for each class holds

Berlin Brain-Computer-Interface (BBCI)

Hex-o-spell: Writing with thoughts

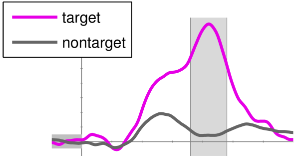


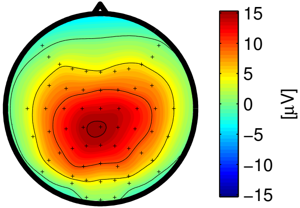


Demo: `http://iopscience.iop.org/1741-2552/8/6/066003/media`

BCI based on event-related potentials (ERPs)

- User concentrates on a symbol (the “target”)
- The six circles are intensified randomly
- Intensified targets elicit ERPs that differ from non-targets
- Training data is collected and an LDA classifier is trained
- The trained classifier can now be used for spelling





This Video explains the data gathering [00:43 - 3:05]

BCI with ML: calibration and feedback

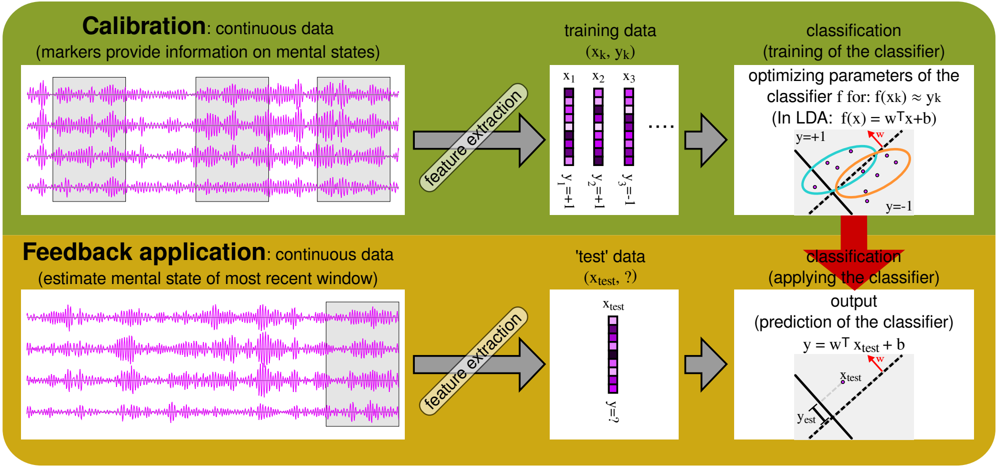


Illustration: single trials and ERPs

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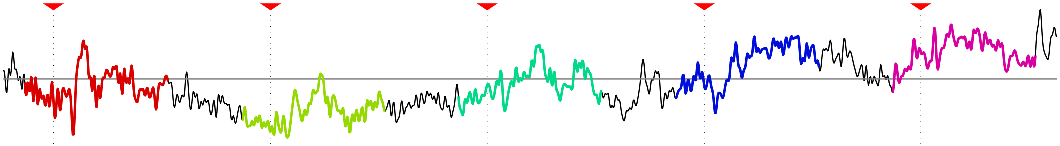
Continuous Signal (with markers)



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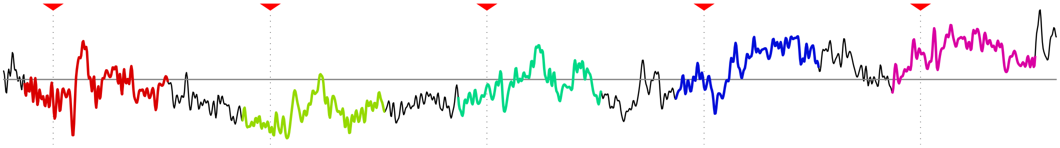
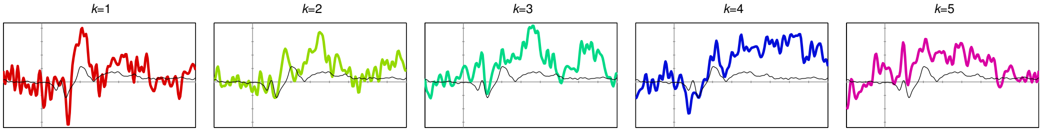
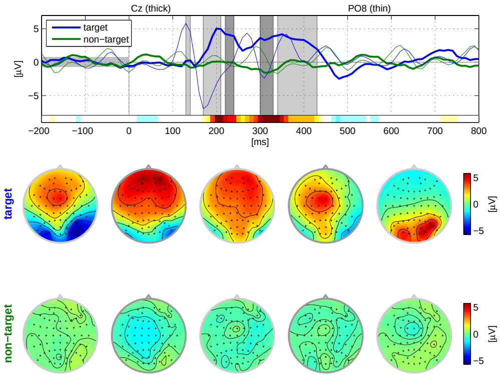


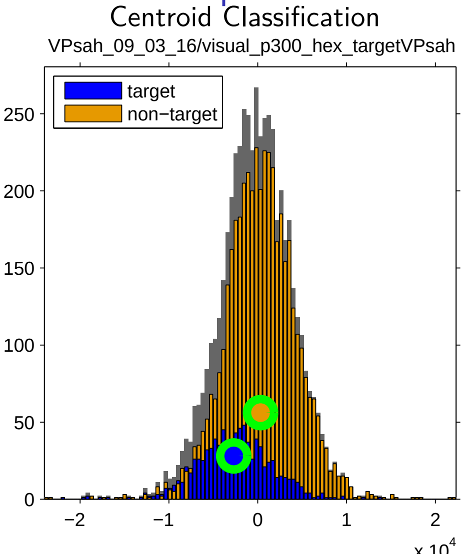
Segments (epochs) around stimulus markers



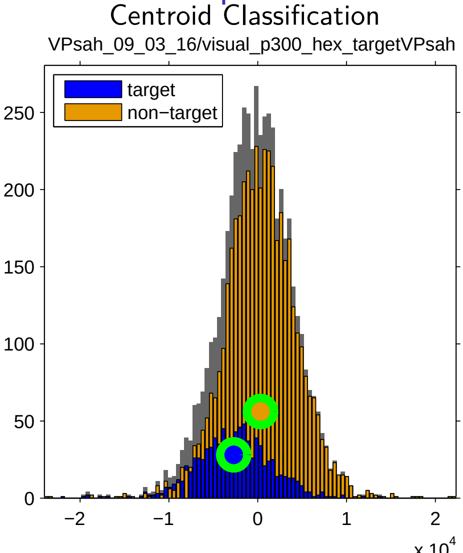
Scalp potentials in response to targets/non-targets

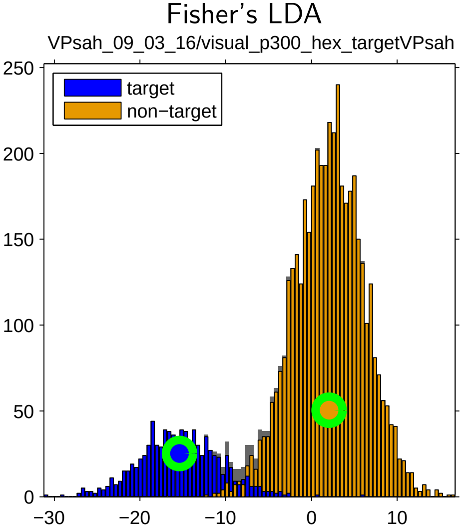


Berlin Brain-Computer-Interface



Berlin Brain-Computer-Interface





How can we properly evaluate a model?

If we use the following dataset $X \in \mathbb{R}^{d \times n}$:

$$
\begin{aligned}
p(\boldsymbol{x}) &= \mathcal{N}(\mathbf{0}, I) \\
p(y = +1 | \boldsymbol{x}) &= 0.5
\end{aligned}
$$

with $n_{train} = 100$, $d = 300$.

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Overfitting

The production of an analysis which corresponds too closely or exactly to a particular set of data, and may therefore fail to fit additional data or predict future observations reliably.

https://www.lexico.com/definition/overfitting

Generalization and model evaluation

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Generalization is the correct categorization/prediction of new (unseen) data

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How can we estimate generalization performance?

- Train model and choose parameters on main part of data
- Test model on other part of data, *that was not seen during training*, to estimate overall performance

Summary

Correlation. . .

- . . . is a measure of *linear relationship* between random variables
- . . . between features can affect classification accuracy

Linear Discriminant Analysis (LDA)

- LDA maximizes *between class variance* while minimizing *within class variance*
- For centered data, LDA is a NCC on whitened data
- If both classes follow a Gaussian with equal class covariances, then LDA is the optimal classifer

Model evaluation

- Only looking at performance on *training set* will give us an overly optimistic estimate of performance (*overfitting*)
- We want our model to *generalize* well