Cognitive Algorithms
Lecture 2

Linear Classification

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Summary Lecture 1

Psychologists postulated we learn **Prototypes**

- Prototypes can be the class means
- New data is associated with **closest** Prototype
- Prototype theory is closely related to linear classification

Artificial Neural Networks

- Inspired by biological neural networks
- Perceptron algorithm realizes linear classification

Linear Classification Revisited

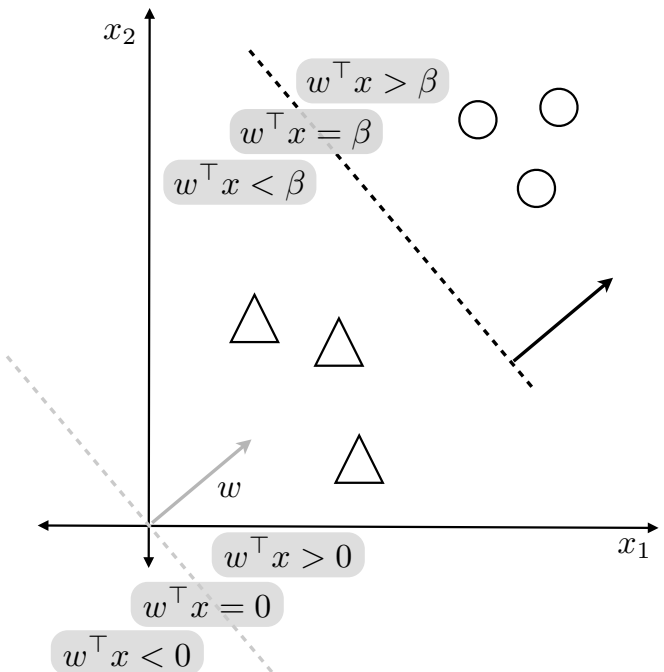
What do we mean by linear classification?

When the decision boundary is linear,

$$\text{i.e. } f(x) = \mathbf{w}^\top \mathbf{x} - \beta,$$

we talk about linear methods for classification.

Linear Classification Revisited



Comparison of distance to class means is equivalent to linear classification

$$\begin{aligned} \|\mathbf{x} - \mathbf{w}_\Delta\| &> \|\mathbf{x} - \mathbf{w}_o\| \\ \Leftrightarrow 0 &< \mathbf{w}^\top \mathbf{x} - \beta \end{aligned}$$

where

$$\mathbf{w} = \mathbf{w}_o - \mathbf{w}_\Delta$$

and

$$\begin{aligned} \beta &= 1/2 \cdot (\mathbf{w}_o^\top \mathbf{w}_o - \mathbf{w}_\Delta^\top \mathbf{w}_\Delta) \\ &= 1/2 \cdot \mathbf{w}^\top (\mathbf{w}_o + \mathbf{w}_\Delta) \end{aligned}$$

This simple linear classification rule is often called **Nearest Centroid Classifier**.

The Perceptron Learning Algorithm

Perceptron error $\mathcal{E}_{\mathcal{P}}(\mathbf{w}) = -\sum_{m \in \mathcal{M}} \mathbf{w}^\top \mathbf{x}_m y_m$
can be minimized *iteratively* using **stochastic gradient descent**
[Bottou, 2010; Robbins and Monro, 1951]

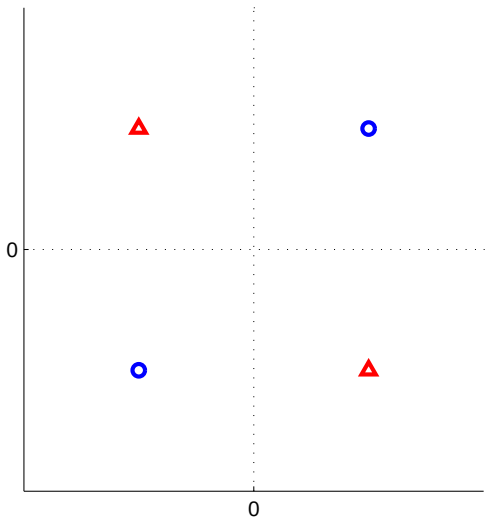
1. Initialize $\mathbf{w}^{\text{old}}$ (randomly, $1/n$, ...)
2. While there are misclassified data points
   Pick a random misclassified data point $\mathbf{x}_m$
   Descent in direction of the gradient at single data point $\mathbf{x}_m$

$$\begin{aligned} \mathcal{E}_m(\mathbf{w}) &= -\mathbf{w}^\top \mathbf{x}_m y_m \\ \nabla \mathcal{E}_m(\mathbf{w}) &= -\mathbf{x}_m y_m \end{aligned}$$

$$\mathbf{w}^{\text{new}} \leftarrow \mathbf{w}^{\text{old}} - \eta \nabla \mathcal{E}_m(\mathbf{w}^{\text{old}}) = \mathbf{w}^{\text{old}} + \eta \mathbf{x}_m y_m$$

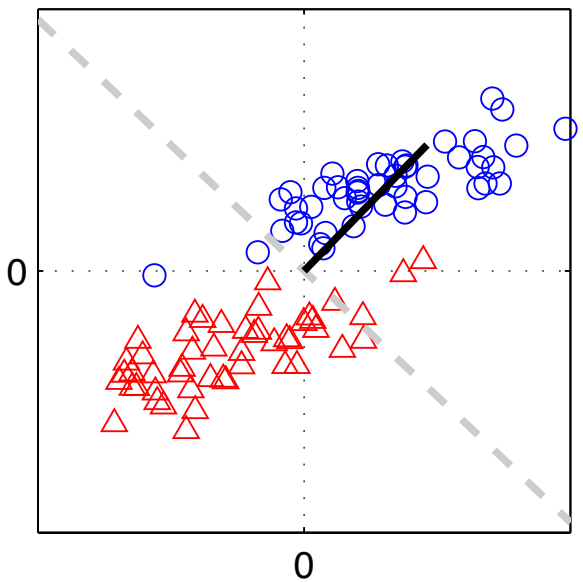
Problems with Nearest Centroid Classification

Non-linear Data



Solutions
Non-linear features,
Non-linear classification methods

Correlated Data



Solution
(Fisher's) Linear Discriminant Analysis

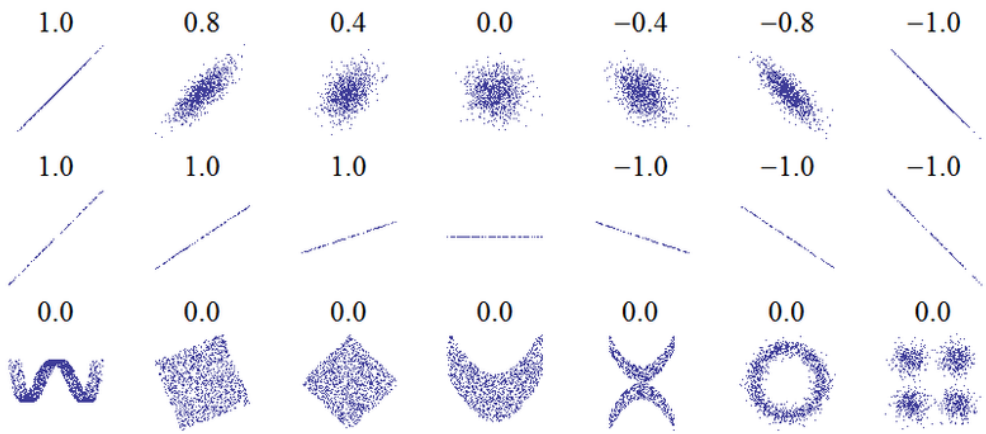
Covariance and Correlation

For two random variables X and Y, their **covariance** and **correlation** are defined as

$$\mathrm{Cov}(X, Y) := \mathrm{E}[(X - \mathrm{E}(X))(Y - \mathrm{E}(Y))] \geq 0$$

$$-1 \leq \mathrm{Corr}(X, Y) := \frac{\mathrm{Cov}(X, Y)}{\sqrt{\mathrm{Var}(X)}\sqrt{\mathrm{Var}(Y)}} \leq 1$$

Correlation measures the linear relationship between X and Y:



Correlation

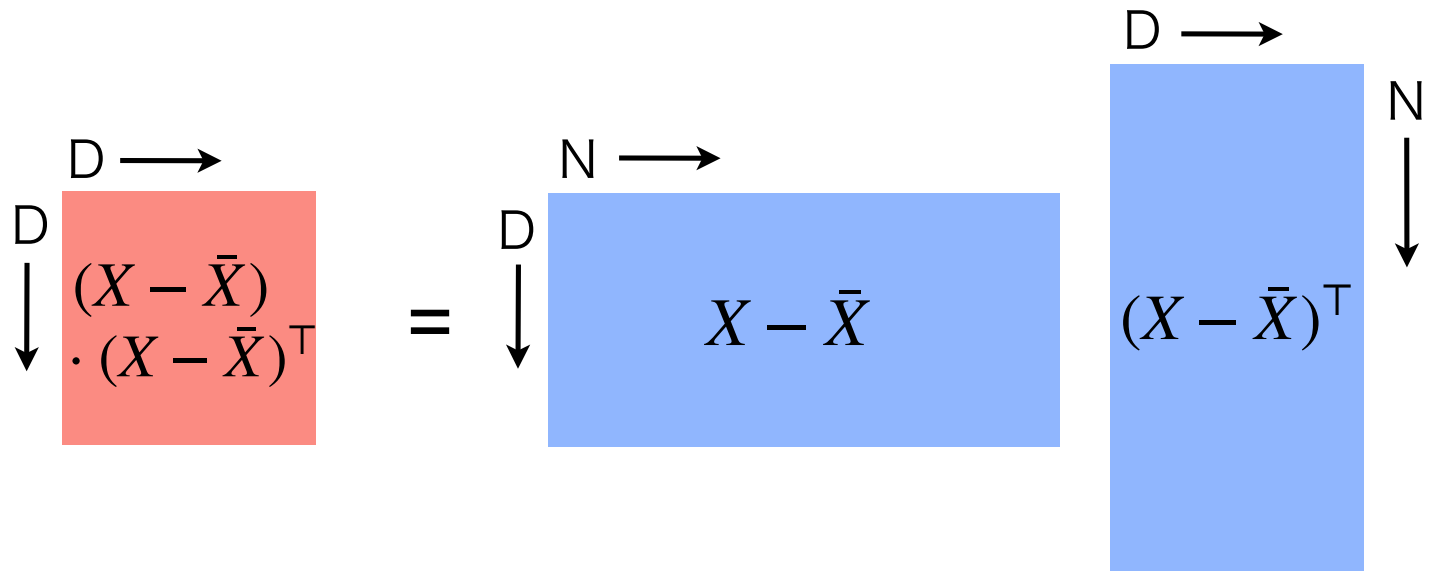
- indicates the strength of a linear relationship
- does not completely characterize their relationship

Covariance Matrices

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

$$S = \frac{1}{N} (X - \bar{X})(X - \bar{X})^\top \tag{1}$$

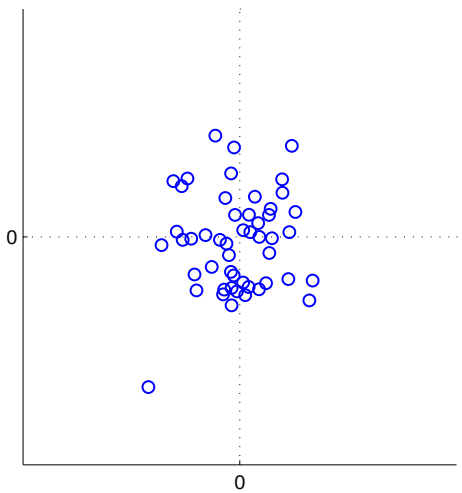
$$\text{where } \bar{X} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{x}_i. \tag{2}$$



Correlated Data and Linear Mappings

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 $S = XX^\top$

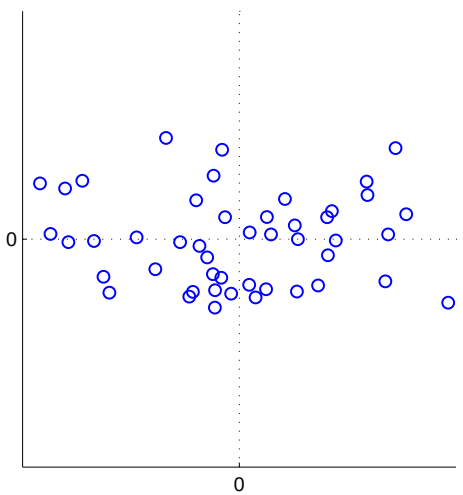
Uncorrelated



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

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

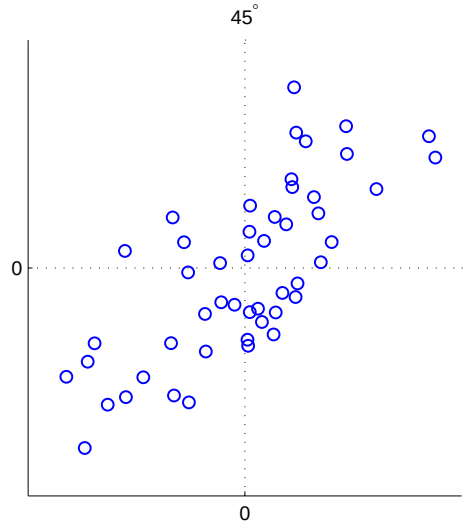
Uncorrelated, scaled



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

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

Scaled, rotated by 45°



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

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

Ronald A. Fisher

R.A. Fisher (1890 - 1962)

Founder of modern statistics

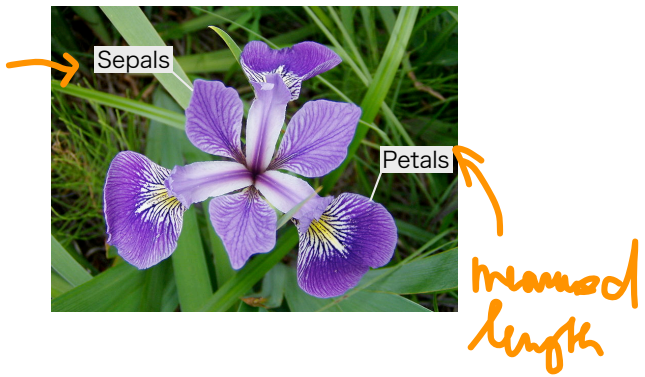
Interested in Biology

Suggested *Linear Discriminant Analysis* (LDA) [Fisher, 1936]

The *Iris* Flower Dataset

Iris Setosa

Iris Versicolor



Iris Virginica

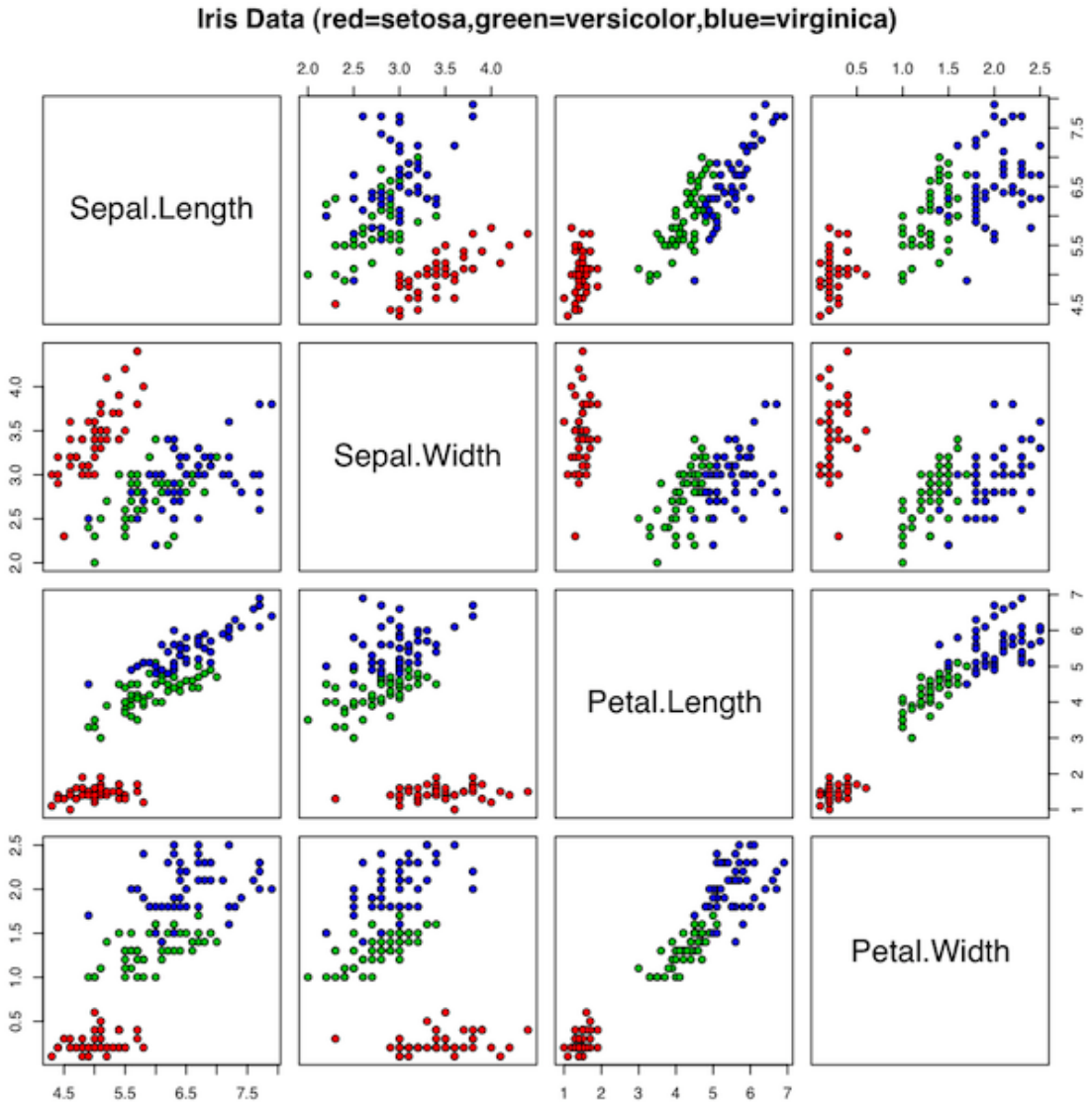
`http://en.wikipedia.org/wiki/Iris_flower_data_set`

50 flowers of each species were collected
"all from the same pasture, and picked on the same day and measured at the same time by the same person with the same apparatus"

Petal and Sepal length and width were measured

Very popular benchmark data set

The *Iris* Flower Dataset

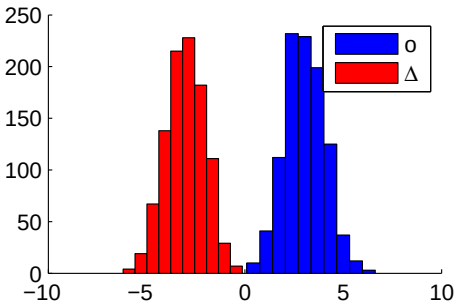


http://en.wikipedia.org/wiki/Iris_flower_data_set

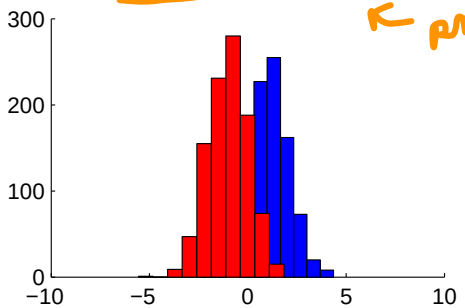
The Fisher Criterion - measure for class separability

Consider one dimensional data and two classes

Good Class Separation

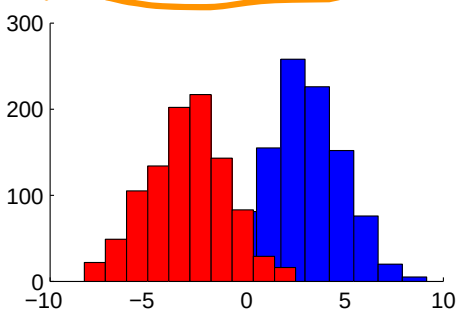


Bad Class Separation:
Close means



problem

Bad Class Separation:
Large Variance

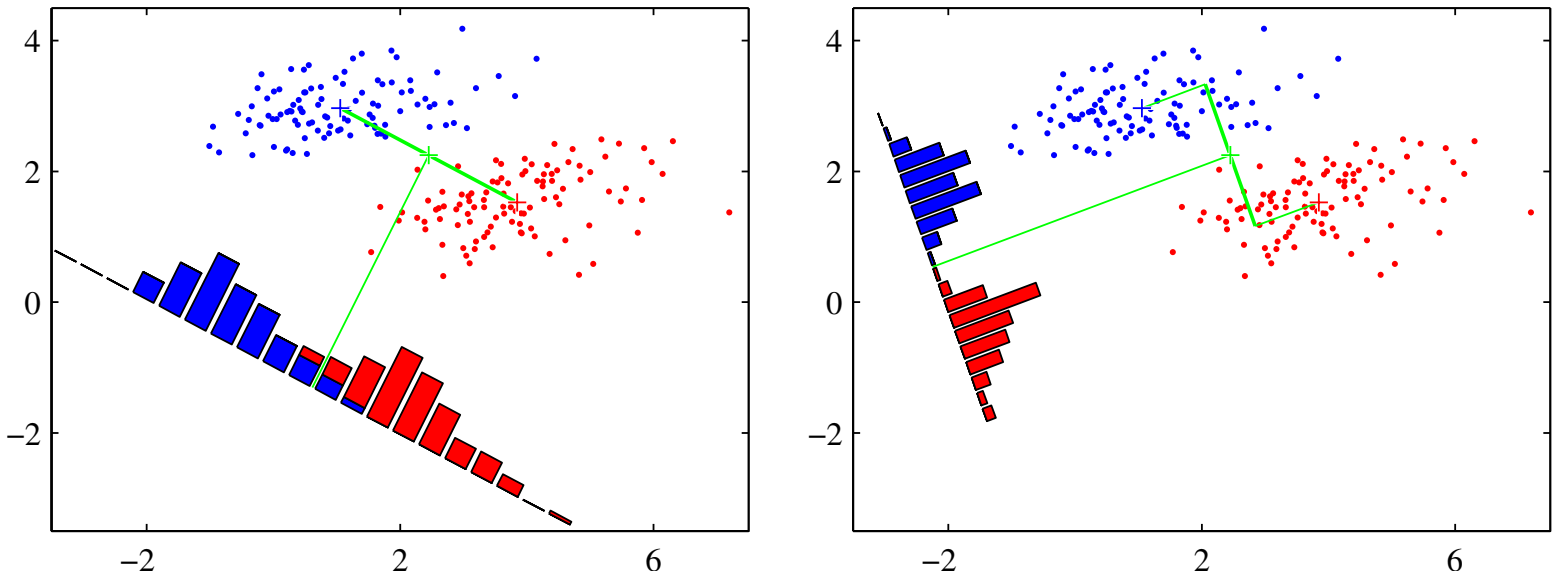


The fisher criterion:

$$\frac{\text{between class variance}}{\text{within class variance}} = \frac{(\mathbf{w}_o - \mathbf{w}_\Delta)^2}{\sigma_o^2 + \sigma_\Delta^2}$$

where $\mathbf{x}_{1o}, \ldots, \mathbf{x}_{N_o o} \in \mathbb{R}^D$ and
$\mathbf{w}_o = \frac{1}{N_o} \sum_{i=1}^{N_o} \mathbf{x}_{io}$ and $\sigma_o^2 = \frac{1}{N_o} \sum_{i=1}^{N_o} (\mathbf{x}_{io} - \mathbf{w}_o)^2$.

Linear Discriminant Analysis



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

Maximizes mean class difference, and

Minimizes variance in each class

Linear Discriminant Analysis

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

Maximizes mean class difference

$$(\mathbf{w}^\top \mathbf{w}_o - \mathbf{w}^\top \mathbf{w}_\Delta)^2 = \mathbf{w}^\top \underbrace{(\mathbf{w}_o - \mathbf{w}_\Delta)(\mathbf{w}_o - \mathbf{w}_\Delta)^\top}_{S_B - \text{"between class scatter"}} \mathbf{w} \tag{3}$$

Minimizes variance in each class

$$\frac{1}{N_o}\sum_{i=1}^{N_o}\left(\mathbf{w}^\top(\mathbf{x}_{oi} - \mathbf{w}_o)\right)^2 + \frac{1}{N_\Delta}\sum_{j=1}^{N_\Delta}\left(\mathbf{w}^\top(\mathbf{x}_{\Delta j} - \mathbf{w}_\Delta)\right)^2$$

$$= \mathbf{w}^\top \underbrace{\left(\frac{1}{N_o}\sum_{i=1}^{N_o}(\mathbf{x}_{oi} - \mathbf{w}_o)(\mathbf{x}_{oi} - \mathbf{w}_o)^\top + \frac{1}{N_\Delta}\sum_{j=1}^{N_\Delta}(\mathbf{x}_{\Delta j} - \mathbf{w}_\Delta)(\mathbf{x}_{\Delta j} - \mathbf{w}_\Delta)^\top\right)}_{S_W - \text{"within class scatter"}} \mathbf{w}$$

Linear Discriminant Analysis

Goal: Find a (normal vector of a linear decision boundary) $\mathbf{w}$ that

Maximizes mean class difference, $\mathbf{w}^\top S_B \mathbf{w}$ and

Minimizes variance in each class, $\mathbf{w}^\top S_W \mathbf{w}$

$\rightarrow$ maximize the *Fisher criterion*

$$\underset{\mathbf{w}}{\operatorname{argmax}} \frac{\mathbf{w}^\top S_B \mathbf{w}}{\mathbf{w}^\top S_W \mathbf{w}} \tag{4}$$

Linear Discriminant Analysis

$$\underset{\mathbf{w}}{\text{argmax}} \frac{\mathbf{w}^\top S_B \mathbf{w}}{\mathbf{w}^\top S_W \mathbf{w}}$$

To optimize the Fisher criterion, we set its derivative w.r.t $\mathbf{w}$ to 0

$$\begin{aligned}
\frac{(\mathbf{w}^\top S_W \mathbf{w}) S_B \mathbf{w} - (\mathbf{w}^\top S_B \mathbf{w}) S_W \mathbf{w}}{(\mathbf{w}^\top S_W \mathbf{w})^2} &= 0 \\
(\mathbf{w}^\top S_B \mathbf{w}) S_W \mathbf{w} &= (\mathbf{w}^\top S_W \mathbf{w}) S_B \mathbf{w} \\
S_W \mathbf{w} &= S_B \mathbf{w} \underbrace{\frac{\mathbf{w}^\top S_W \mathbf{w}}{\mathbf{w}^\top S_B \mathbf{w}}}_{\textit{scalar}}
\end{aligned}$$

Linear Discriminant Analysis

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

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

Note that

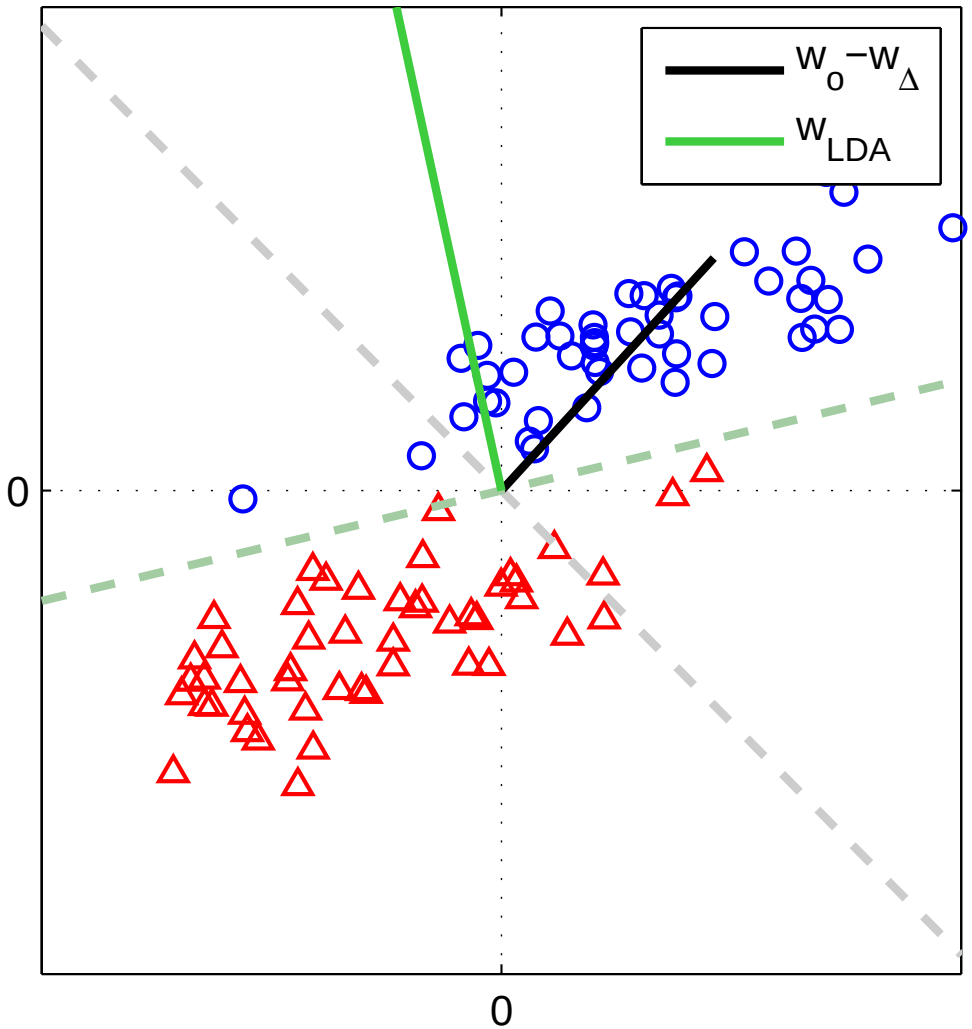
$$S_B \mathbf{w} = (\mathbf{w}_o - \mathbf{w}_\Delta) \underbrace{(\mathbf{w}_o - \mathbf{w}_\Delta)^\top \mathbf{w}}_{\text{scalar}}$$

thus left multiplying with S_W^{-1} yields

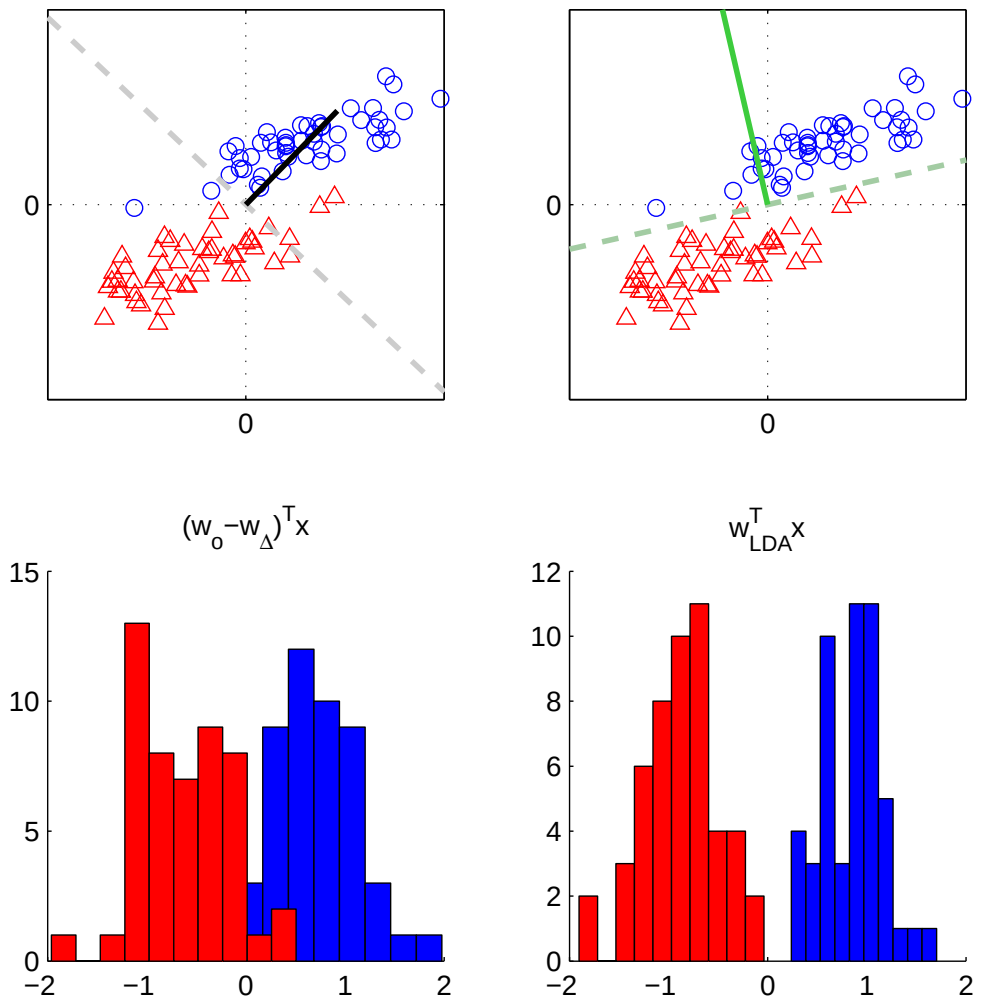
$$\mathbf{w} \propto S_W^{-1}(\mathbf{w}_o - \mathbf{w}_\Delta).$$

($\propto$ denotes proportional)

Linear Discriminant Analysis vs Nearest Centroid Classifier



Linear Discriminant Analysis vs Nearest Centroid Classifier



Linear Discriminant Analysis

If both classes have the same covariance matrix, LDA first *decorrelates* the data followed by nearest centroid classification:

$$\begin{aligned} \mathbf{x} &\mapsto \text{sign}(\mathbf{w}^T \cdot \mathbf{x} - \beta) \\ \mathbf{w} &\propto S_W^{-1}(\mathbf{w}_o - \mathbf{w}_\Delta) \end{aligned}$$

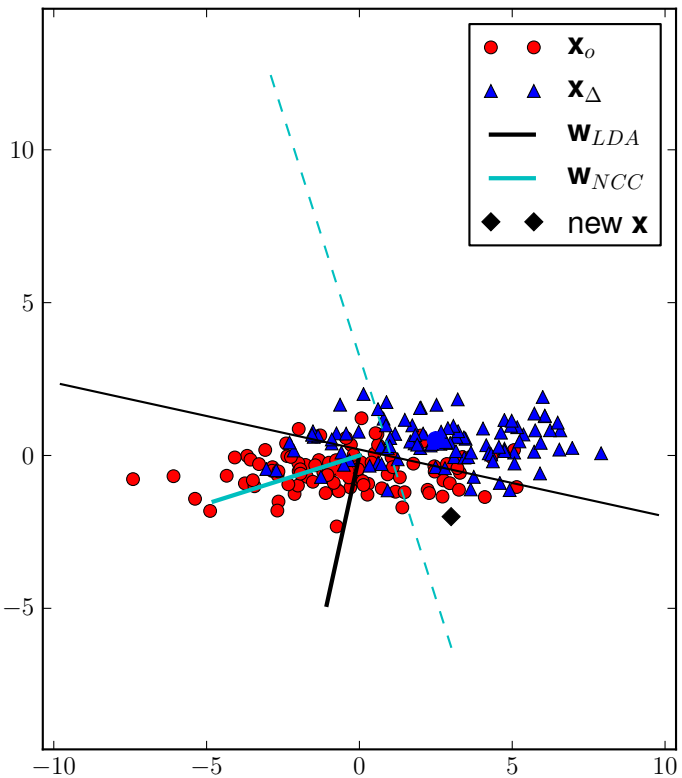
$$\mathbf{w}^T\mathbf{x} = (\mathbf{w}_o - \mathbf{w}_\Delta)^T S_W^{-1}\mathbf{x} = \underbrace{(\mathbf{w}_o - \mathbf{w}_\Delta)^T U\Lambda^{-1/2}}_{\substack{\text{mean class difference} \\ \text{of decorrelated data}}} \underbrace{\Lambda^{-1/2}U^T\mathbf{x}}_{\text{decorrelated } \mathbf{x}}$$

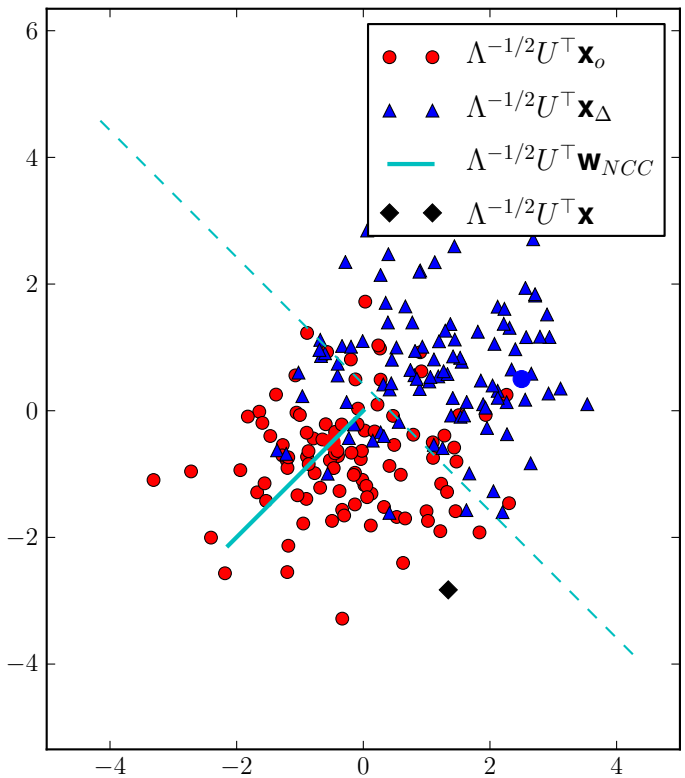
where $S_W = U\Lambda U^T$ is the eigenvalue decompostion of S_W

Linear Discriminant Analysis

LDA first *decorrelates* the data followed by nearest centroid classification:

$$\mathbf{w}^T\mathbf{x} = (\mathbf{w}_o - \mathbf{w}_\Delta)^T S_W^{-1}\mathbf{x} = \underbrace{(\mathbf{w}_o - \mathbf{w}_\Delta)^T U\Lambda^{-1/2}}_{\text{mean class difference of decorrelated data}} \underbrace{\Lambda^{-1/2}U^T\mathbf{x}}_{\text{decorrelated } \mathbf{x}}$$





Decision theory

Decision theory:
For a new data point $\mathbf{x} \in \mathbb{R}^D$

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

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

$$\begin{aligned} p(\Delta|\mathbf{x}) &= \frac{p(\Delta, \mathbf{x})}{p(\mathbf{x})} \\ &= \frac{p(\Delta)p(\mathbf{x}|\Delta)}{p(\mathbf{x})} \end{aligned}$$

Decision theory

Estimating $p(\mathbf{x}|\Delta)$ is difficult: already if each dimension of $\mathbf{x}$ can take 2 values $\rightarrow 2^D$ possible values.

One possibilty to deal with it:

Choose a distribution $p(\mathbf{x}|\Delta)$, $p(\mathbf{x}|o)$ that is easy to deal with

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

$$\mathbf{x} \in \mathbb{R}^D \sim \mathcal{N}(\mathbf{w}_\Delta, S_\Delta) = \frac{1}{(2\pi)^{\frac{D}{2}}\sqrt{|S_\Delta|}} e^{-\frac{1}{2}(\mathbf{x}-\mathbf{w}_\Delta)^\top S_\Delta^{-1}(\mathbf{x}-\mathbf{w}_\Delta)}$$

Linear Discriminant - a Probabilistic View

If we assume equal covariance in each class, $S_W = S_\Delta = S_o$ (i.e. rescale S_W), and equal class probabilities, $p(\Delta) = p(o) = 0.5$, the optimal classification boundary is linear and given by

$$\begin{aligned} \mathbf{w} &= S_W^{-1}(\mathbf{w}_o - \mathbf{w}_\Delta) \\ \beta &= \frac{1}{2}\mathbf{w}_o S_W^{-1}\mathbf{w}_o - \frac{1}{2}\mathbf{w}_\Delta S_W^{-1}\mathbf{w}_\Delta = \frac{1}{2}\mathbf{w}^T(\mathbf{w}_o + \mathbf{w}_\Delta) \end{aligned}$$

$\Rightarrow$ Linear decision boundaries arise from simple assumption about the distribution of the data.

Linear Discriminant - a Probabilistic View

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$\Rightarrow$ Linear decision boundaries arise from simple assumption about the distribution of the data.

Linear Discriminant Algorithm

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

Input: Data $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}, x_i \in \mathbb{R}^D,\ y_i \in \{-1, +1\}$,

Compute class mean vectors

$\mathbf{w}_{-1} = 1/N_- \sum_{i \in \mathcal{Y}_{-1}} \mathbf{x}_i$

$\mathbf{w}_{+1} = 1/N_+ \sum_{j \in \mathcal{Y}_{+1}} \mathbf{x}_j$

Compute *within-class* covariance matrices

$S_W = 1/(2N_-) \sum_{i \in \mathcal{Y}_{-1}} (\mathbf{x}_i - \mathbf{w}_{-1})(\mathbf{x}_i - \mathbf{w}_{-1})^\top$

$\quad +1/(2N_+) \sum_{j \in \mathcal{Y}_{+1}} (\mathbf{x}_j - \mathbf{w}_{+1})(\mathbf{x}_j - \mathbf{w}_{+1})^\top$

Compute normal vector $\mathbf{w}$

$\mathbf{w} = S_W^{-1}(\mathbf{w}_{+1} - \mathbf{w}_{-1})$

Compute threshold

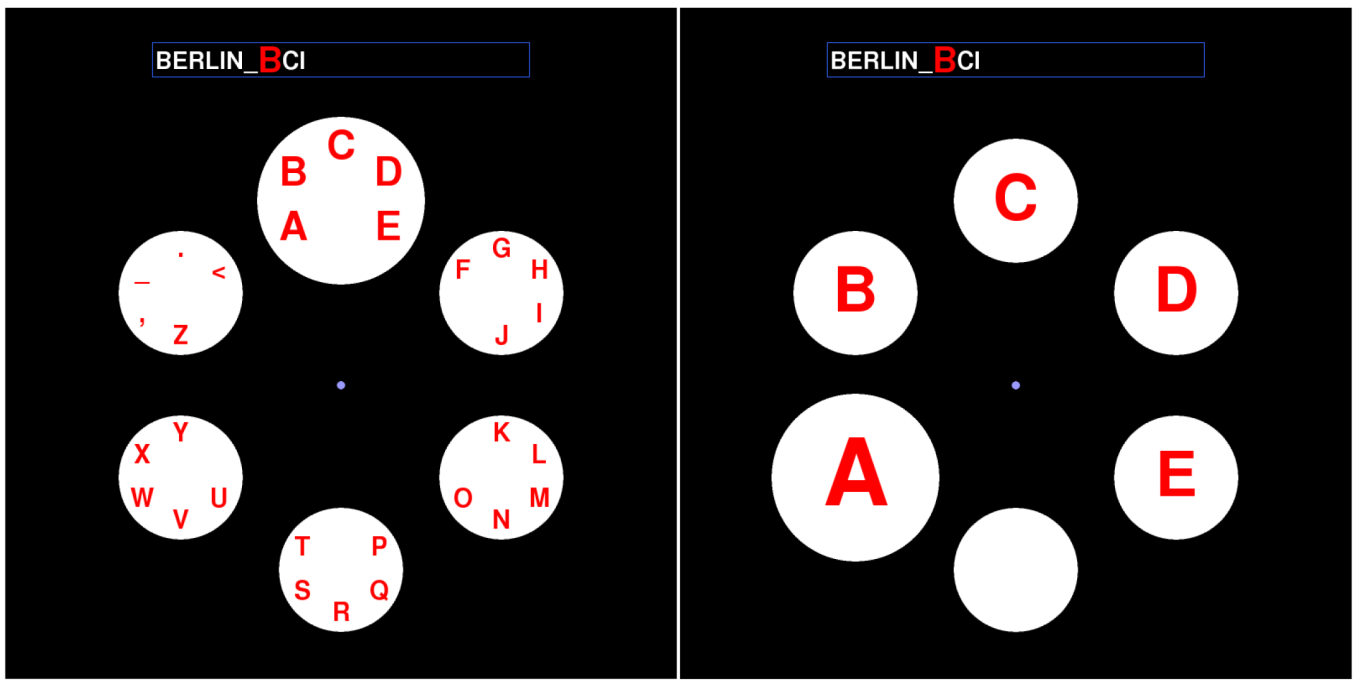
$\beta = 1/2\ \mathbf{w}^T(w_{+1} + \mathbf{w}_{-1}) + \log(N_-/N_+)$

Output: $\mathbf{w},\ \beta$

Berlin Brain-Computer-Interface (BBCI)

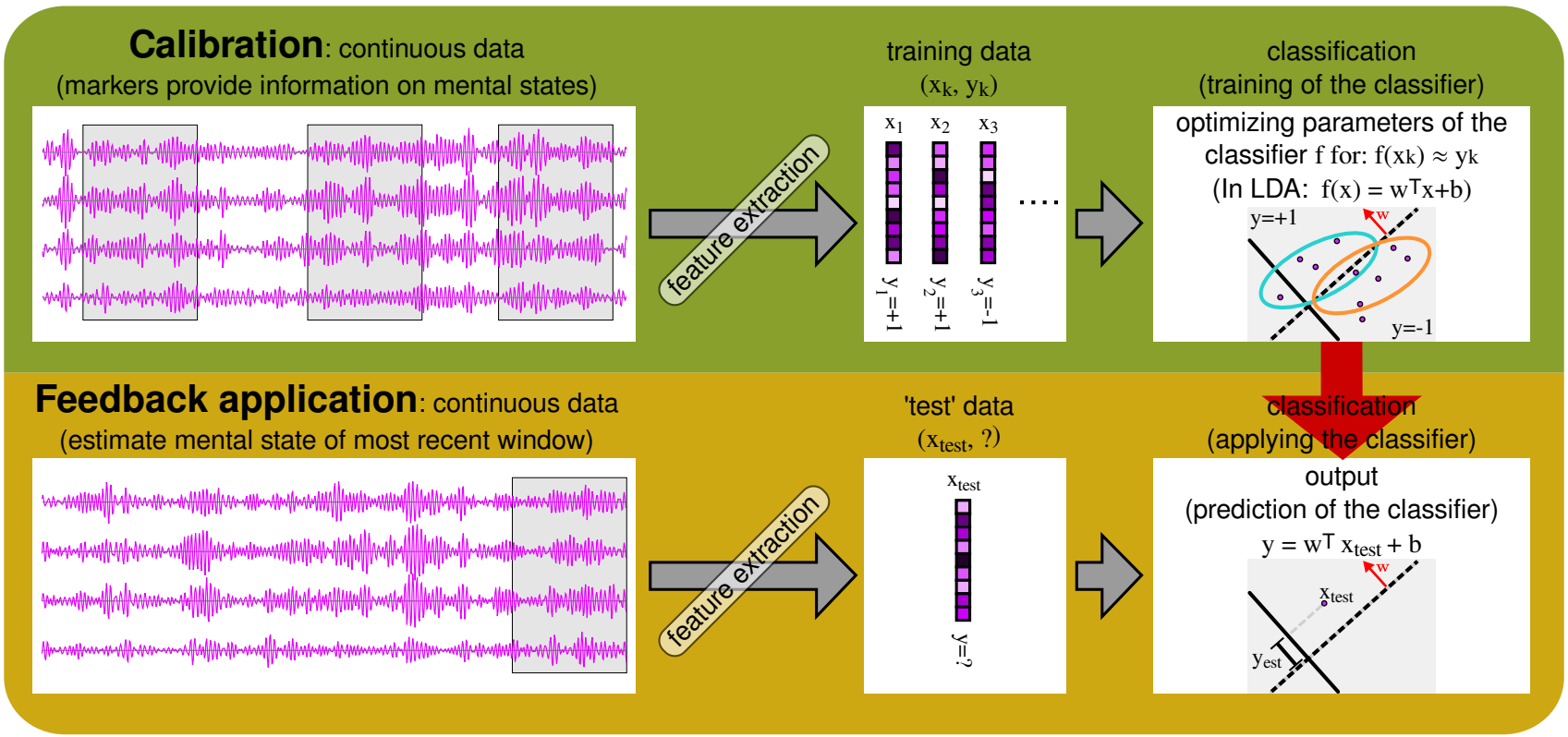
Hex-o-spell: Writing with thoughts

`http://www.bbci.de/`



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

BCI with ML: Calibration and Feedback



BCI Based on Event-Related Potentials (ERPs)

- User concentrates on a symbol
- Rows and columns are intensified randomly
- Target rows and columns elicit specific ERPs
- BCI detects target ERPs (averaged over few repetitions)

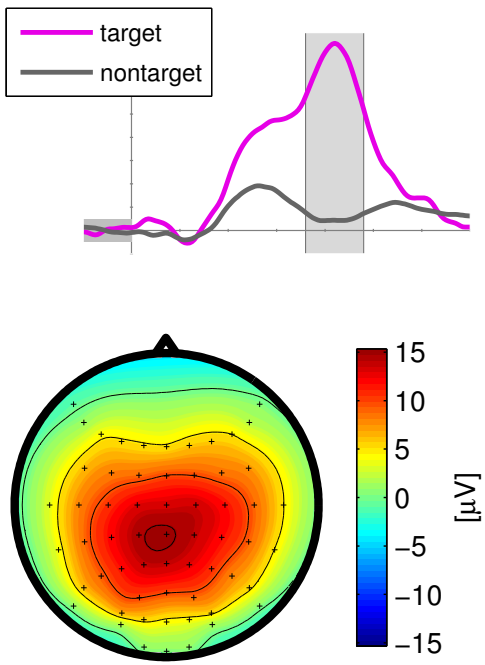
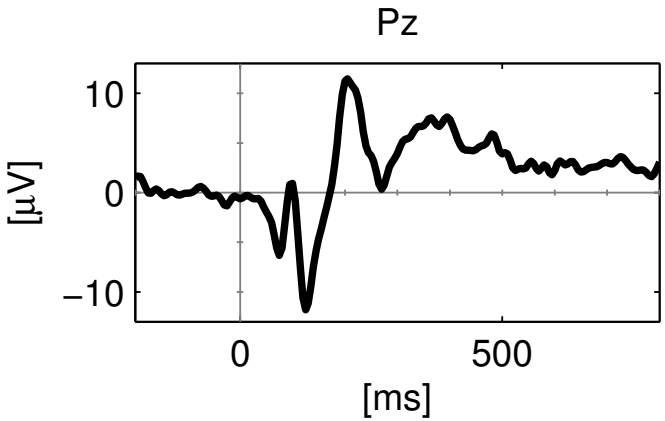
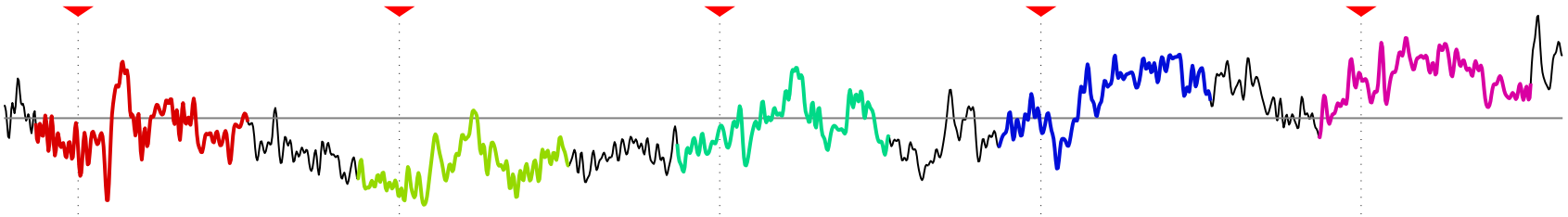


Illustration: Single-Trials and ERPs



Continous Signal (with markers):



Segments (epochs) around stimulus markers:

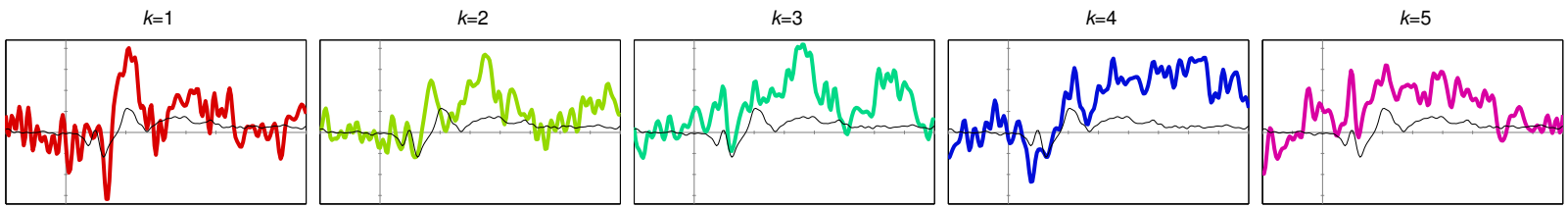
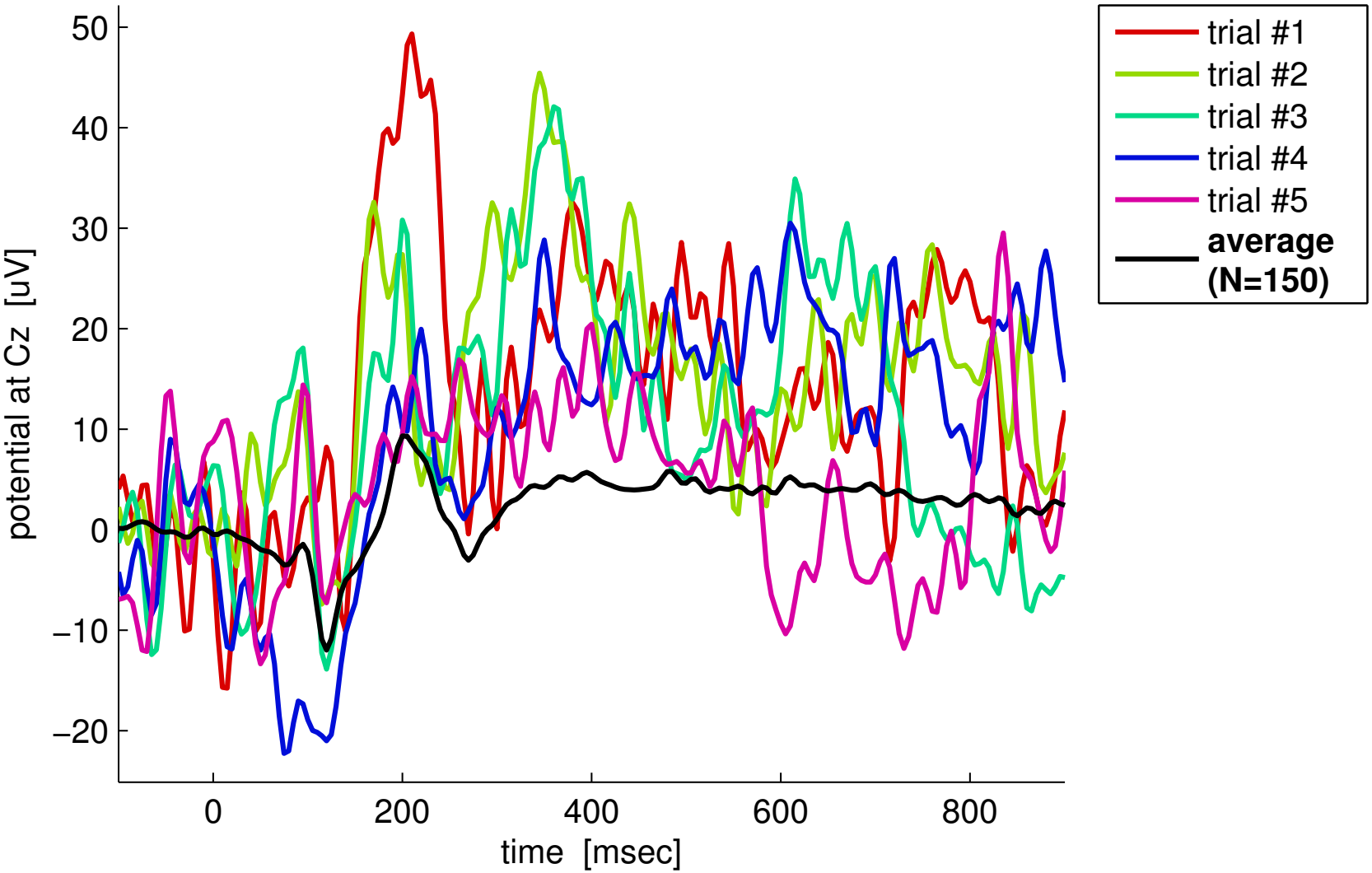
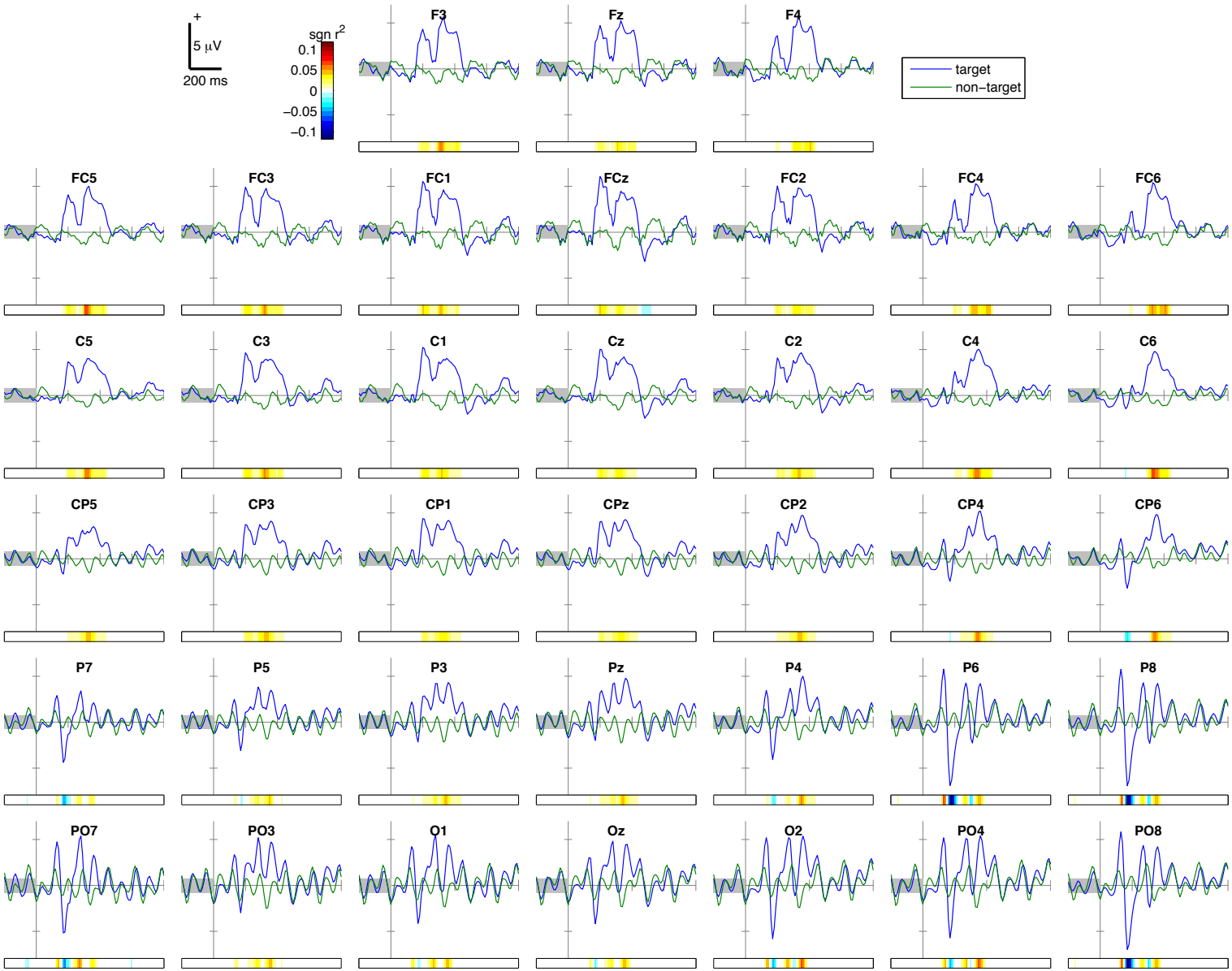


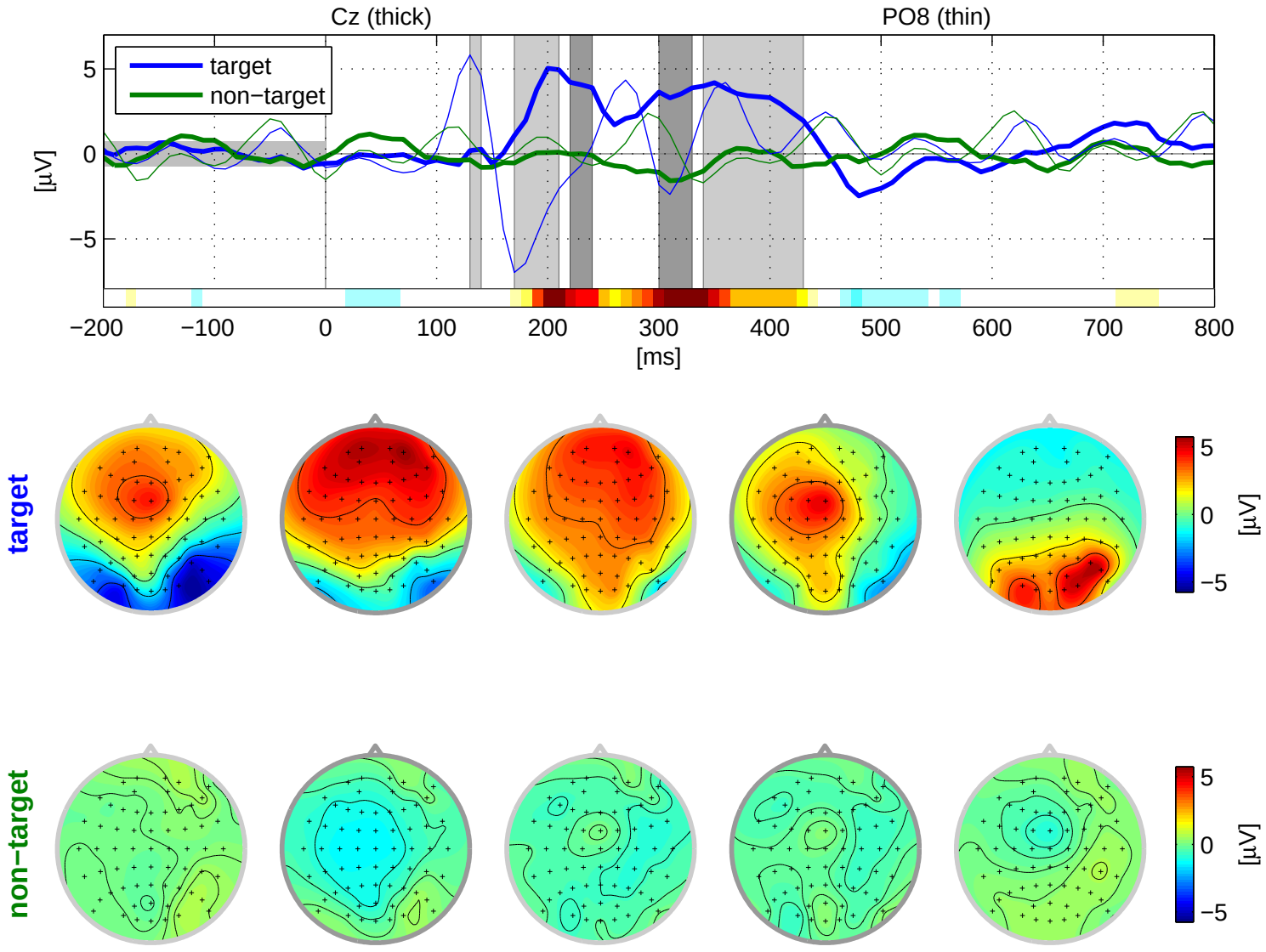
Illustration: Single-Trials and ERPs



Scalp Potentials In Response to Targets/Non-Targets

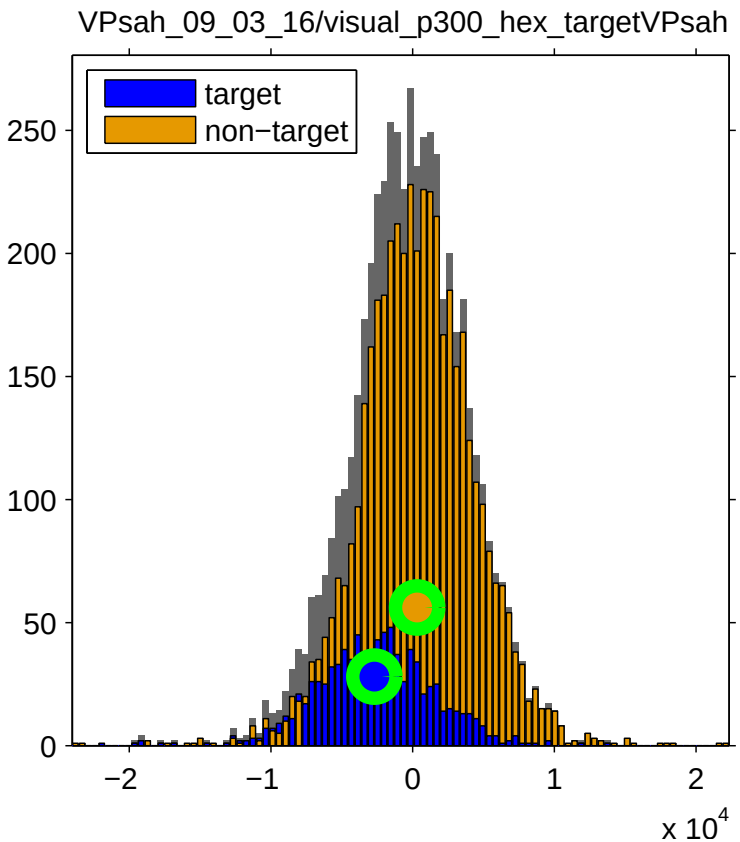


Berlin Brain-Computer-Interface

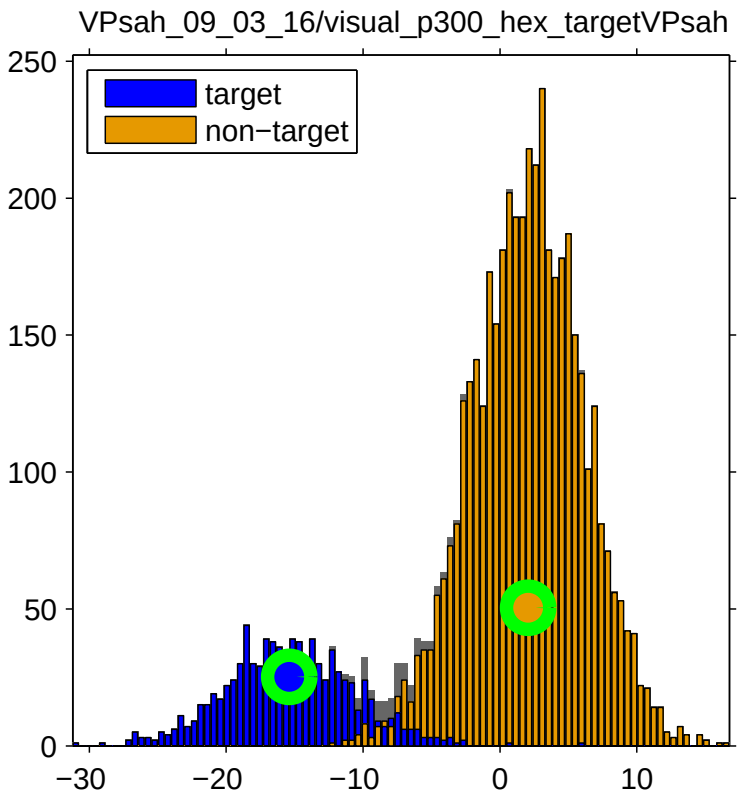


Berlin Brain-Computer-Interface

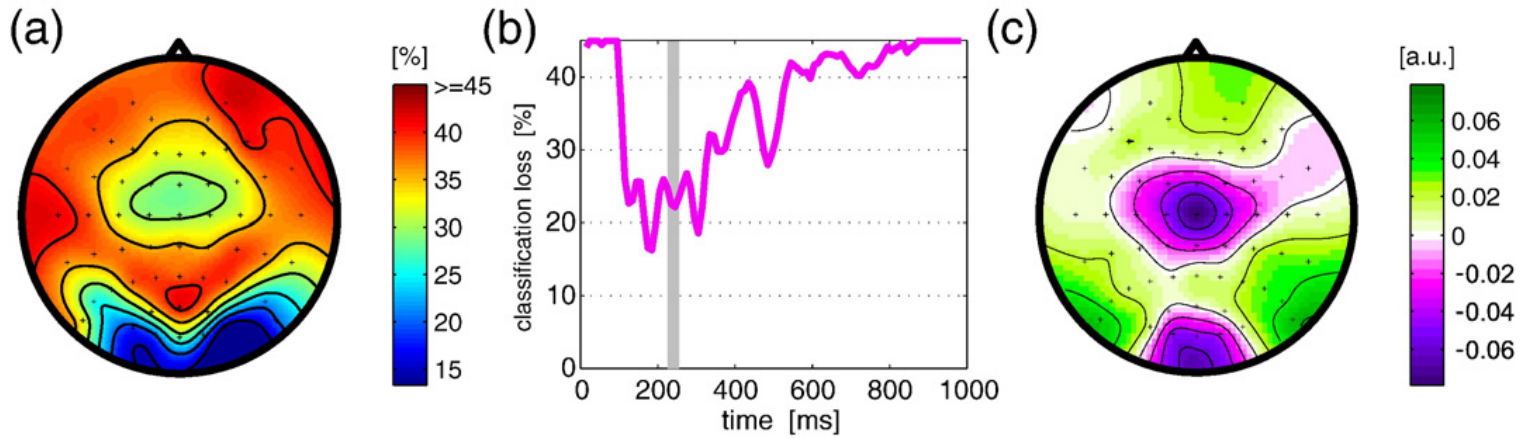
Centroid Classification



Fisher's LDA



Understanding the classifier



(a) Classification error on features from the time interval 115-535m
(b) Classification error for intervals of 30ms duration
(c) Weight vector of classification on features from the time interval 220-250ms
[Blankertz et al., 2011]

Generalization and Model Evaluation

The goal of classification is **generalization**: Correct categorization/prediction of new data

How can we estimate generalization performance?

→ **Cross-validation**:

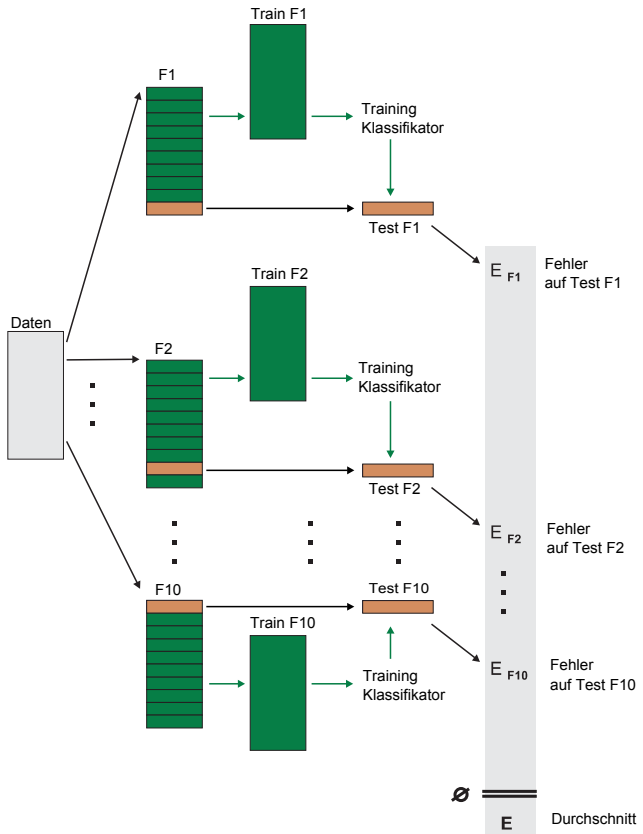
- Train model on part of data
- Test model on other part of data
- Repeat on different cross-validation *folds*
- Average performance on test set across all folds

Cross-Validation

Algorithm 1: Cross-Validation

Require: Data $(x_1, y_1) \ldots, (x_N, y_N)$, Number of CV folds F

1: # Split data in F **disjunct** folds
2: **for** folds $f = 1, \ldots, F$ **do**
3: # Train model on folds $\{1, \ldots, F\} \setminus f$
4: # Compute prediction error on fold f
5: **end for**
6: # Average prediction error



Summary

Correlations between features can affect classification accuracy

Fisher proposed Linear Discriminant Analysis (LDA)

LDA maximizes *between class variance* while minimizing *within class variance*

If data is Gaussian with equal class covariances, than LDA is the optimal classifer

LDA is used in state-of-the-art BCI systems

We can use Cross-validation for Model Evaluation

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