Machine learning with R

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What is machine learning?

- Learning the relations between properties of an object and its target value
- **example: vowel classification**
  F1=800Hz, F2=1200Hz, duration=0.1s $\longrightarrow$ *'/a:/'*
- **object:** vowel segment
- **target:** its category

What is machine learning?

Definitions

- **Features = independent variables:** properties of an object, e.g. *F1, F2, duration*
- **Feature vector:** object representation [*800, 1200, 0.1*]
- **Target = dependent variable:** value, feature vector is to be mapped on; e.g. *phoneme '/a:/'*

Machine Learning = Learning to map objects represented as feature vectors to their target values

Which method to choose?

Are targets known?

- yes: **supervised** learning method
- no: **unsupervised** learning method

Of what variable type is the target?

- categorical: **classification** task
- continuous: **regression** task

When to choose classical machine learning . . .

. . . instead of End-to-end Deep Neural Networks

- if data is sparse (e.g. clinical data)
- if one can/wants to rely on expert features

Contents

Supervised learning – the Caret package

Basics

- **C**lassification **a**nd **re**gression training
- wrapper around lots of machine learning methods provided by other packages
- allowing for a common workflow
- CRAN: `https://cran.r-project.org/web/packages/caret/index.html`
- Function reference: `https://cran.r-project.org/web/packages/caret/caret.pdf`
- Tutorial: `https://topepo.github.io/caret/index.html`

The Caret package

Workflow

1. split data into train and test partition
2. feature normalization
3. model hyperparameter optimization and training
4. evaluation

The Caret package

Data split

- to allow for testing whether or not the model can generalize from the examples it was trained on
- if not: **overadaption** to training data
- **stratified split:** same relative class proportions in training and test partition
- Function: *createDataPartition()*

Data preprocessing

- **normalization** for mean and standard deviation
  - features usually have different mean and range values (e.g. fundamental frequency vs. formants)
  - thus contribute to different extent to classification, e.g. distance between objects more determined by features with high range
  - solution: z-transform $x \leftarrow \frac{x - \mathrm{mean}(x)}{\mathrm{std}(x)}$, so that all features have mean 0 and std 1
  - *train(. . . preProc = c("center", "scale") . . .)*
- **decorrelation**
  - features might be highly correlated and thus are redundant in training
  - solution: orthogonalization by Principal component analysis
  - *train(. . . preProc = c("pca") . . .)*

The Caret package

Training

- **Tuning: hyperparameter optimization**
  - **grid-search:** loop over all hyperparameter value combinations
  - for each value combination, do an **n-fold cross-validation**, i.e.
  - divide training set *n* times into fitting and development partition
  - fit the model to the data in the fitting partition and evaluate it on the development partition.
  - Keep the hyperparameter combination with highest mean evaluation score
- **Fitting:** fit model with optimized hyperparameters on training partition
- specify training procedure: $tc \leftarrow trainControl()$
- training: $train(\ldots trControl = tc \ldots)$

The Caret package

Evaluation

- Apply the model to unseen test set: *predict()*
- measure model performance by comparing its output with the reference targets from test set
  - **Classification:** *confusionMatrix()*
  - **Regression:** *RMSE()*

Metrics

- **Classification**
  - classes balanced: **Accuracy**, i.e. percentage correct, **Mean F-Score**
  - classes not balanced: **Unweighted Average Recall or F-Score**
- **Regression**
  - distance matters: **Mean Absolute or Squared Error**
  - correlation matters, but not distance: **Pearson Correlation Coefficient**
  - both matters: **Concordance Correlation Coefficient**

Instance-based learning

Overview

- **supervised** learning method
- **task:** classification
- **features:** categorical, continuous
- **targets:** categorical
- **scenarios:** exemplar theory modeling
- **training:** store feature vectors with their corresponding class (*lazy learning*)
- **application:** for an object to be classified select the k nearest feature vectors. Assign to the object the **class with the highest support (weight sum)** among the retrieved feature vectors.
- **CARET method:** *kknn()*

Instance-based learning

Classification: $\hat{f}(y) = \arg\max_{c \in C} \sum_{i=1}^{k} w_i \delta(c, f(x_i))$

- y: object to be classified
- C: set of possible classes
- $\sum_{i=1}^{k} w_i \delta(c, f(x_i))$: support for class c
- k: number of nearest neighbors to be considered
- $f(x_i)$: class of neighbor x_i
- $\delta(a, b)$: 1 if a=b, else 0
- w_i: weight of neighbor x_i derived from its distance d to y by a Kernel function, e.g. the **inversion kernel** $\frac{1}{|d|}$
- **Parameters:**
  - *kmax* – maximum number k of neighbors
  - *distance* – parameter of **Minkowski distance** (1=Manhattan, 2=Euclidean)
  - *kernel* – to map distance to weight; 'rectangular' – unweighted, 'optimal' – design depends on *kmax* (i.e. for high k weight for high distance gets reduced more strongly), others – differ wrt extent the weight decreases with increasing distance

Classification and regression trees (CARTs)

Overview

- **supervised** learning method
- **tasks:** classification and regression
- **features:** categorical, continuous
- **targets:** categorical, continuous
- **training:** represent feature vectors as paths through tree, and targets as tree leaf labels
- **application:** follow path according to the object's feature vector. Assign to the object the terminal leaf label.
- **CARET method:** *rpart2()*
- **Parameter:** maximum tree depth *maxdepth*
  - deep trees can take more features and their interactions into account
  - flat trees are less prone to overadaption, and thus often generalize better

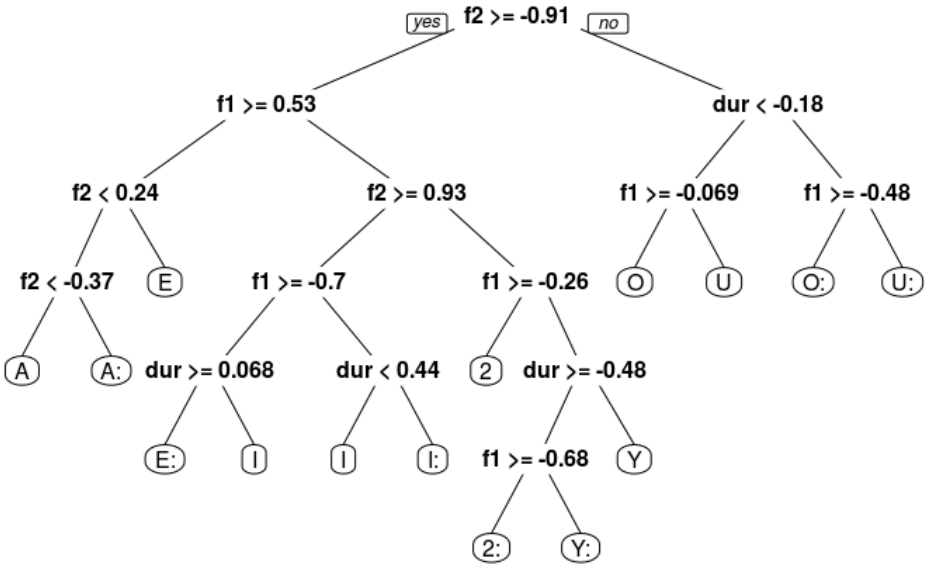
Classification and regression trees

Training procedure

- divide and conquer: recursive partitioning of an object set into subsets
- resulting tree with one leaf for each final subset
- **Regression tree:** for each subset a simple regression model is fitted (which simply corresponds to the subset mean value)
- **Classification Tree:** to each subset a class label is assigned (which is the most frequent class in this subset)

CART examples

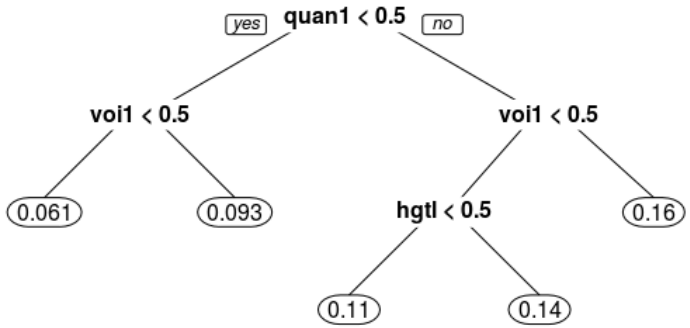
Classification



Target: Vowel class

Features: 1st and 2nd formant, duration

Regression



Target: Vowel duration

Features: Vowel height and position, voicing of neighbor-Cs

Split criteria

- according to which variable the objects are to be divided?
- **regression tree:** search over variables (and split points) to minimize the variation within a subset
  - **example:** target T = phone duration, features X_1 = prominence, X_2 = sentence mode
  - by X_1 the phones can be divided into 2 subsets one for long, the other for short vowels
  - by X_2 the division yields overlapping subsets wrt to phone duration
  - $\longrightarrow$ use X_1 to subdivide the objects

Classification and regression trees

- **classification tree:** use variable X containing the **highest information** about the target class T

$$\begin{aligned} \hat{X} &= \arg\max_{V}[MI(X;T)] \\ MI(X;T) &= H(T) - H(T|X) \end{aligned}$$

- $H(T)$: entropy (incertitude) of target value
- $H(T|X)$: remaining incertitude if value of X is known
  - **example** T = vowel class, X = F2
  - $MI(X;T)$: mutual information between the F2 and the vowel class
  - $H(T)$: the incertitude of predicting the vowel, if no cues are given
  - $H(T|X)$: the remaining incertitude to predict the vowel class if the F2-value is known

Termination criteria

- all objects in a subset have (about) the **same target value**
  - *classification:* all vowel objects in a subset are /i/s
  - *regression:* all phones in a subset have about the same duration
- the objects are **not further dividable** by their feature vectors
  - *all phones within a subset are in prominent position of a declarative sentence*
- the **number** of objects in a subset is **below** a specified **threshold**

Classification and regression trees

Leaf labels

- *classification:* class occuring most often in the subset at that leaf
- *regression:* mean value of all targets at that leaf

Application

- follow the tree from the node to a leaf according to the object's feature values
- assign the leaf label to the object

Ensemble models

Overview

- **supervised** learning method
- **tasks:** classification and regression
- **features:** categorical, continuous
- **targets:** categorical, continuous
- **CARET method:** e.g. *xgbTree()*
- **Parameters:** number of trees (*nrounds*) maximum tree depth (*max_depth*), minimum number of items at a leaf (*min_child_weight*), learning rate (weight of each subsequent tree in correcting the preceding tree's error; *eta*), proportion of features a single tree is trained on (*colsample_bytree*), proportion of training items a single tree is trained on (*subsample*), minimum required loss reduction to further split a tree (*gamma*)

Ensemble models

- e.g. Random Forests, Gradient Boosting, Extreme Gradient Boosting
- **Boosting:** combining several weak classifiers to built a strong one (cf *wisdom of crowds*).
- **Bagging:** combining classifiers trained on parts of the training data
- consists of many **classification (or regression) trees**
- **training:**
  - see CARTs, each tree trained on feature and/or data subset
  - **parallel training:** trees are trained independently in parallel (e.g. Random Forest)
  - **sequential training:** trees are trained sequentially (Gradient Boosting); the later trees are trained to predict the residual, which is the deviation of the previous tree's predictions from the target value; i.e. later trees correct the errors of the previous trees
  - for classification these residuals refer to class probabilities

Ensemble models

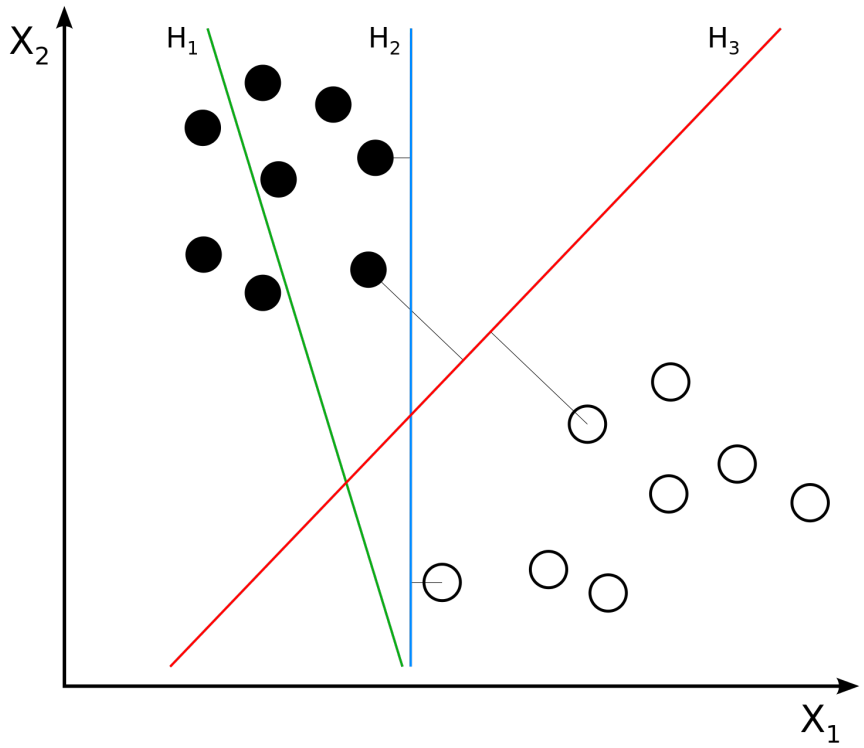
- **application:**
  - the feature vector is accordingly subdivided in the forest
  - each tree responds a class based on the feature values it sees
  - **classification result: most frequent class**, if trees are trained in parallel (e.g. Random Forests); **class with the highest summed probability**, if trees are trained sequentially (Gradient Boosting)
  - **regression result:** prediction **mean** (parallel training), or **sum** (sequential training)
- Fernández-Delgado et al. (2014): **Random forest as best performing classifier (next to SVMs)** for various data sets
- **XGBoost and SVMs are currently the overall best performing classical (i.e. non deep-learning) machine learning methods**

Support vector machines (SVM)

Overview

- for **supervised learning**
- **task:** binary classification, (regression)
- **features:** binary, continuous
- **targets:** categorical, (continuous)
- **Caret method:** *svmLinear()*
- **Parameters:** misclassification cost C
  - low values: **soft margin**, allowing for more errors
  - high values: **hard margin**, potentially overadapt to training data

Support vector machines (SVM)



Training:

- find the best plane (**H3**) in the feature space to separate two classes
- maximize the distance between the plane and the **support vectors**, i.e. the vectors closest to the plane

Support vector machines

Training cntd.

- **Kernel:**
  - similarity function $K(x, y) = f(x) \cdot f(y)$
  - inner product of feature vectors x and y that are mapped to a higher dimensional space by $f(\cdot)$
- **Kernel trick:** if classes are not separable, then map feature vectors to a higher dimensional feature space and try again (increase of separability – but also overadaption!)
- linear, polynomial, and RBF Kernel functions: different distance calculation in the feature space
- robust against outliers, since these are ignored
- **from two to n classes:**
  - one SVM for each class pair c_i vs c_j, or
  - one SVM for each class c_i vs $\neg c_i$

Bias and Variance

High bias, low variance

- **Simple model:** low number of neighbors (KNN), flat/few trees (CART, XGBoost), low misclassification cost (SVM), low learning rate (XGBoost)
- **Disadvantage:** does not make use of all information available in training data, e.g. feature interactions
- **Advantage:** robustness; does not over-adapt to training data and works equally well unseen data

Low bias, high variance

- **Complex model:** high number of neighbors (KNN), deep/many trees (CART, XGBoost), high misclassification cost (SVM), high learning rate (XGBoost)
- **Advantage:** powerful; can make use of more information in training data
- **Disadvantage:** might overfit to training data and thereafter not work well on unseen data

Hyperparameter tuning by cross validation to balance power (high variance) and robustness (high bias)

Contents

- What is machine learning?
- Which method to choose?
- Supervised learning
- Unsupervised learning
  - Clustering

Clustering

Overview

- **unsupervised** learning method
- **task:** partition of the data into similar objects
- **features:** categorical, continuous
- **targets:** yet unknown
- **scenarios:** intonation contour classification
- **R packages:** *stats*

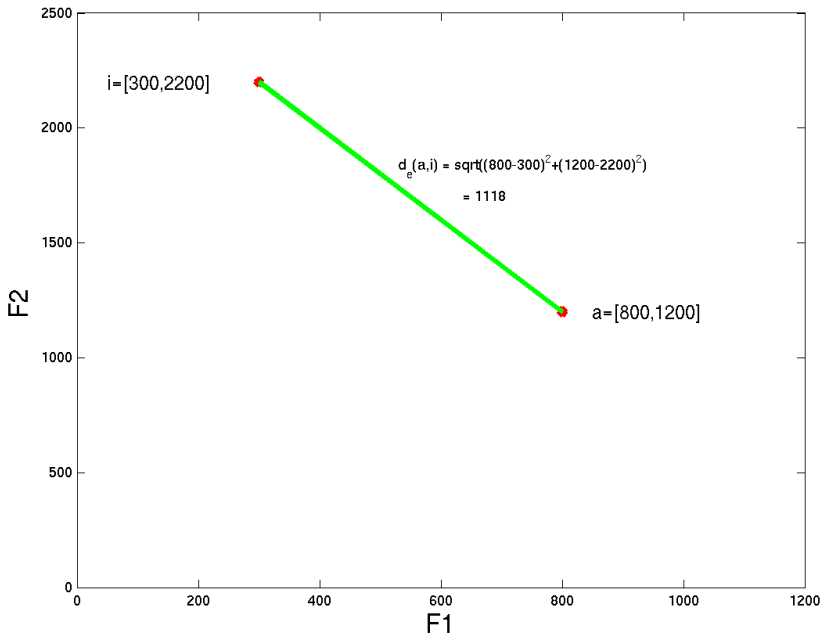
When to use?

- if no categories are available yet

Objects

- feature vectors
- points in a Cartesian coordinate system

Distance (between feature vectors a and b)



- **continuous variables:** e.g. *Euclidean distance*

$$d_e(a,b) = \sqrt{\sum_i (a_i - b_i)^2}$$

Clustering

- **categorical variables:** e.g. *Hamming distance*

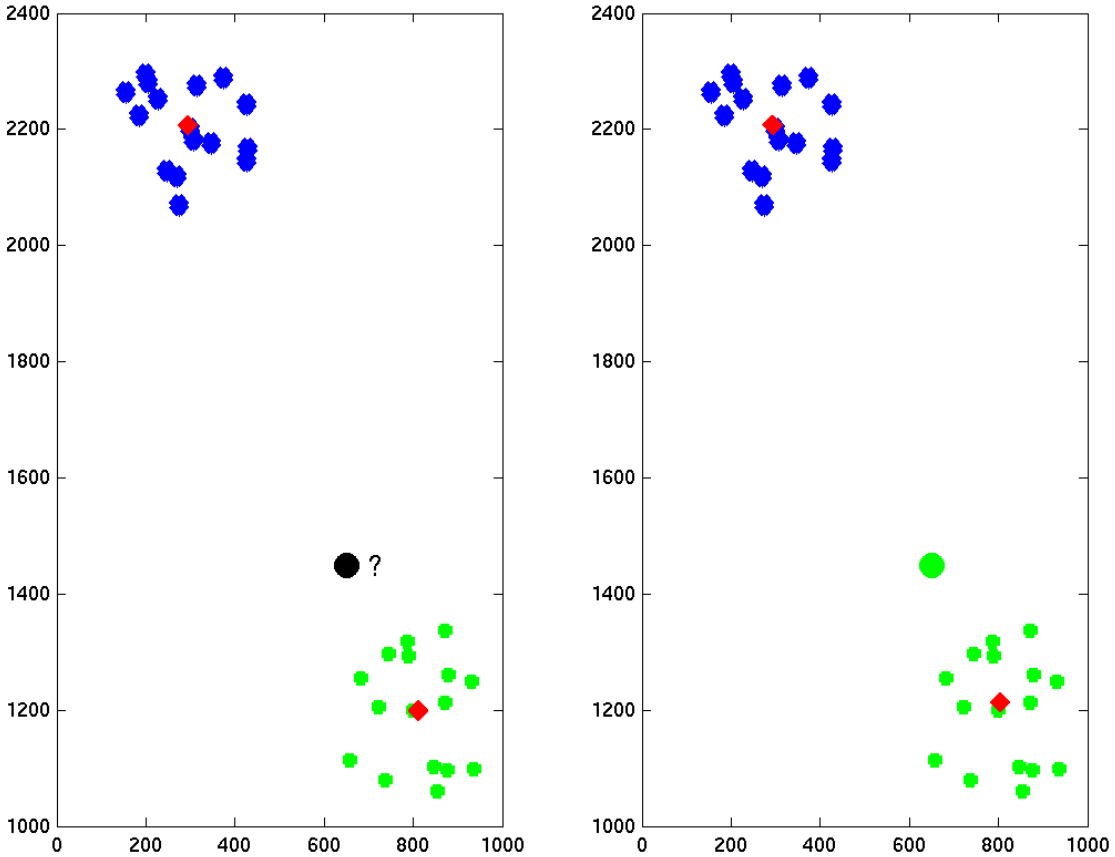
$$d_h = \frac{\sum_{i:a_i \neq b_i} 1}{\sum_i 1}$$

- **example: distinctive feature vectors for /a/ and /i/**
  /a/ [low, back, spread, lax]
  /i/ [high, front, spread, tense]
  $d_h(a, i) = \frac{3}{4} = 0.75$

kmeans Algorithm

$X \leftarrow$ objects to be clustered
$k \leftarrow$ intended number of clusters
init: determine k clusterCenters
until all clusters stable
  foreach $x \in X$
    $c \leftarrow$ closest cluster
    $c \leftarrow [c, x]$
    update clusterCenter(c)
  endforeach
enduntil

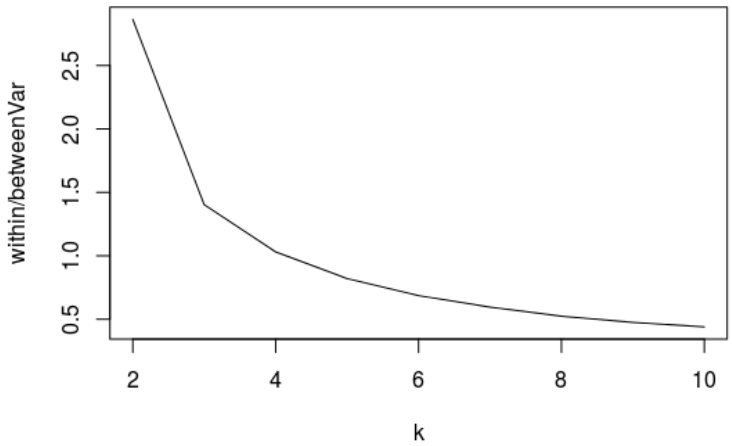
Clustering



- kmeans **cluster center: centroid** (mean vector)
- **closest** cluster: the cluster with the nearest centroid

Validation

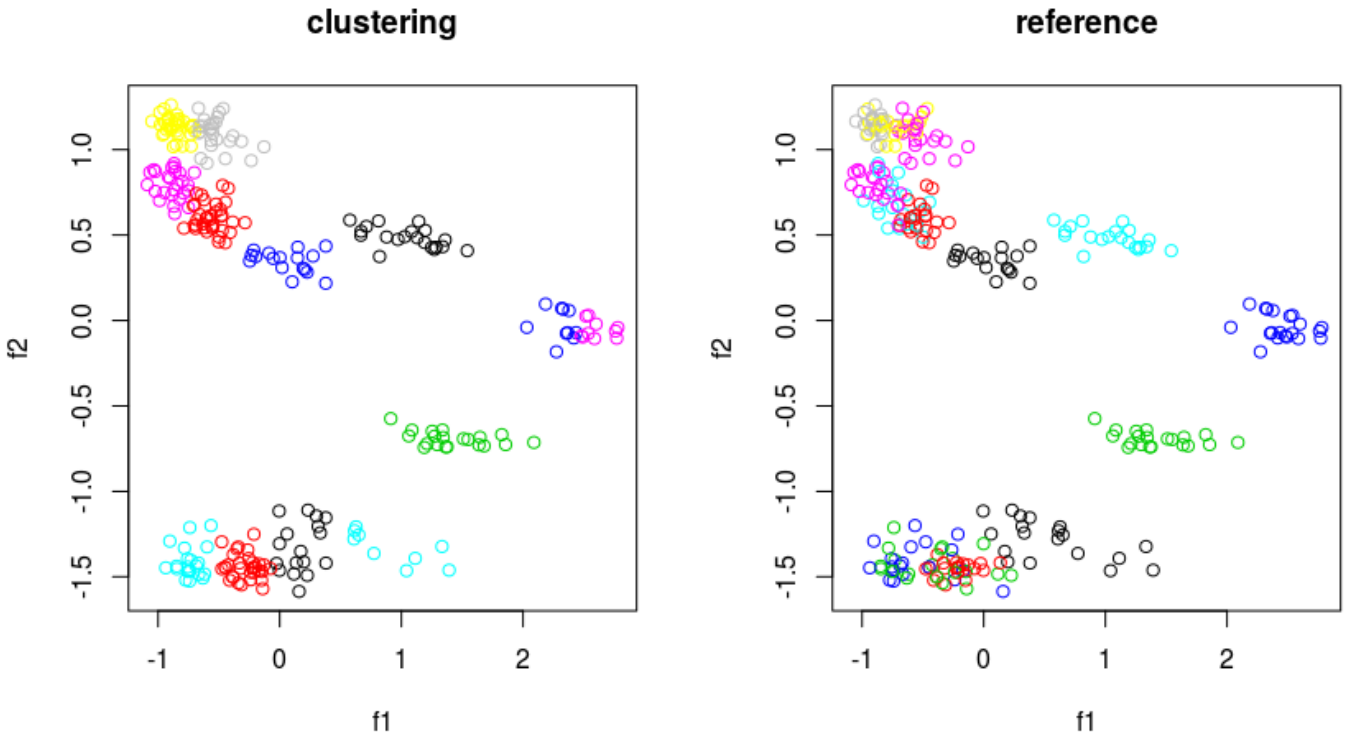
- how to determine a good number k of clusters?
- **Cohesion:** low within-cluster variability
- **Separation:** high between-cluster variability
- **Generalisation:** keep number of clusters as low as possible



- best k at some **breakpoint** in $\frac{\text{withinClusterVariability}(k)}{\text{betweenClusterVariabilty}(k)}$ curve
- here: e.g. 3 or 6

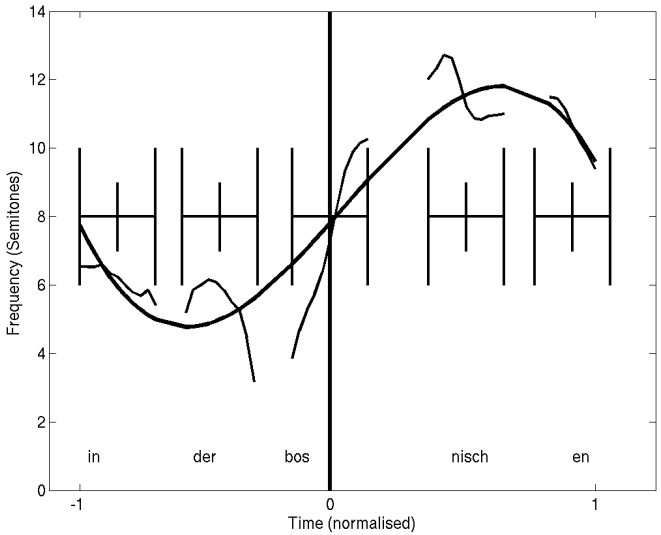
Clusters and reference

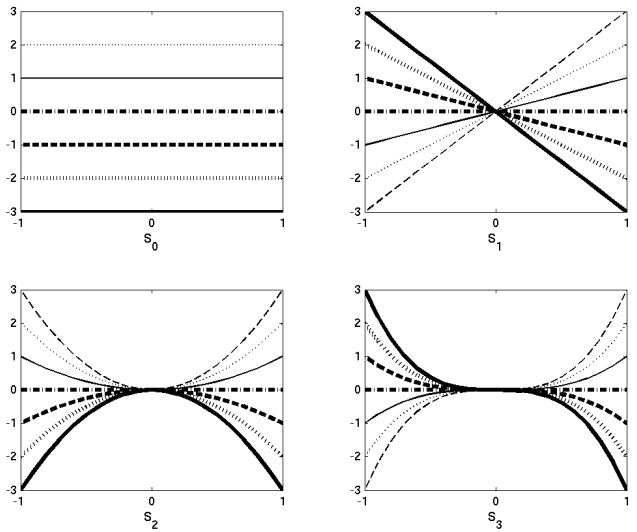
- Hungarian vowel classes by formants 1 and 2 (z-transformed)



Intonation contour classes

- derived from 3rd order polynomial stylization of f0 contours
- $f0 = \sum_{i=0}^{3} s_i t^i$ (t: time, s_i: coefficients to be fitted)





Resulting contour classes (k=6)