Naïve Bayes & kNN

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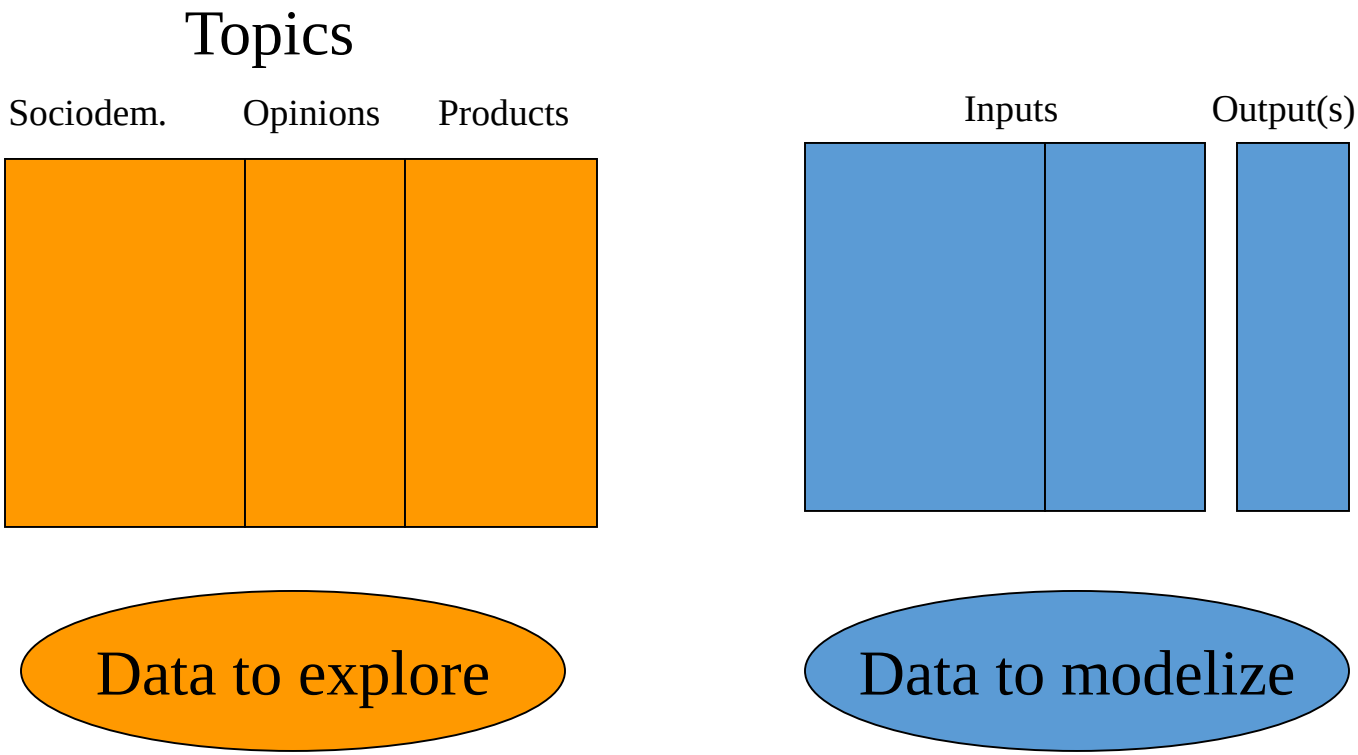
and on Mario Martin Slides

Contents

- Data
- Introduction
- Naive Bayes
- kNN
- Weighted kNN
- Distance Metrics

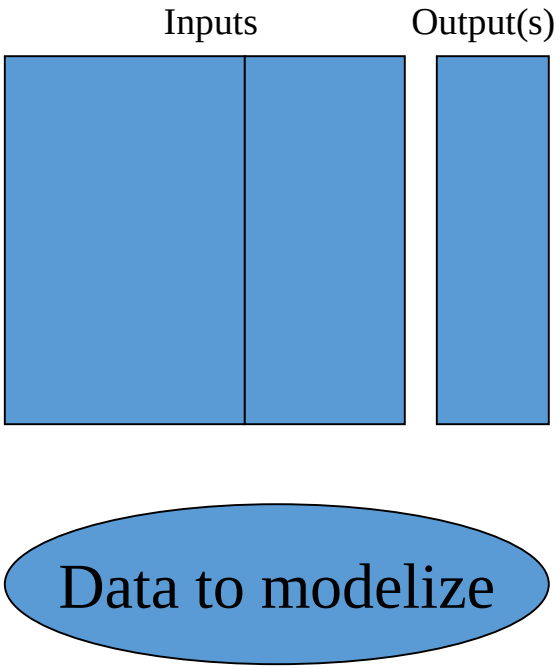
Data

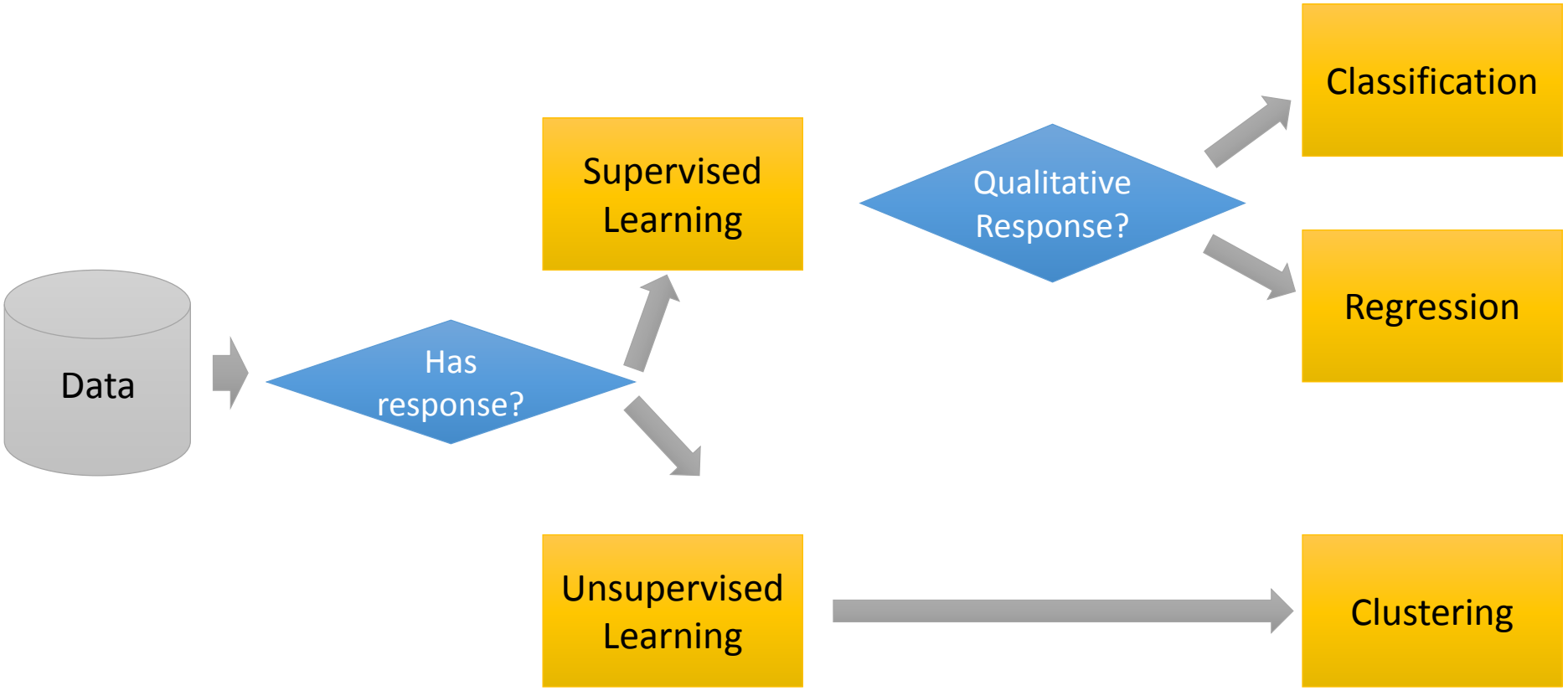
- Data in *Data Mining*:
  - massive, secondary, non-random, with errors, missings …



Data

- Supervised Learning
  - Input/Descriptors/Predictors
  - Output/Response/Class
    - Binary
      - Classification
    - Qualitative or Categorical
      - Classification
    - Quantitative or Numerical
      - Regression




Data
Has response?
Supervised Learning
Unsupervised Learning
Qualitative Response?
Classification
Regression
Clustering

Introduction

- Data mining in supervised mode has a target column.
- We have an objective way to measure the success of classifiers / regressors:
  - Test new cases with the classifier / regressor and check predicted labels/values with reality.
- There are a lot of different measures to qualify success of a classifier.

What is classification?

Supervised:

Assigning one individual to a group (previously defined). Decisional goal
= Discriminant Analysis
= Pattern recognition …

Unsupervised:

Unveiling the true existing populations
Partitioning of a population
= Clustering

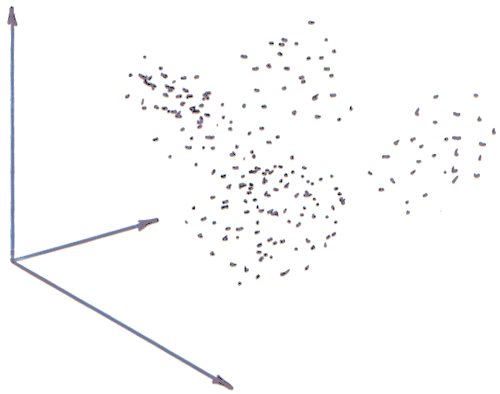
Definition of a classification rule (classifier):

We need a training file $X\ (n,p)$, where for each individual we know to each class it belongs to.

Individuals x_i are points in R^p space of variables (=features). Response variable is categorical.

We want to partition the R^p space into regions Ω_k, corresponding each regions to one class (problem of *separability* versus *random fluctuation*)

One individual belongs to Class C_k if $x_i \in \Omega_k$



Types of classifiers

Non parametric: *KNN, Kernel estimation of f(x/k)*
(without prob. hypothesis)

Parametric

Linear: *LDA, Logistic regression, …*
Non linear: *QDA*

Original feature space
or
Expanded feature space, introducing transformations of variables:
quadratic terms, interactions, basis expansions, the kernel trick (to achieve separability).

Assessment of the classification rules

Not trivial

The most obvious measure: estimate the ***error rate (= 1-accuracy)***
Every classification rule has its own missclassification probability (except for the case of perfect separability)

We can gain separabilty by means of increasing the complexity of the model

Confussion matrix

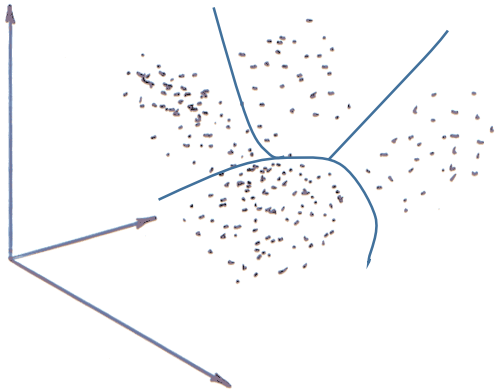
Error rate
Recall
Precision
F-measure
AUC
…

Classifiers

- Simple algorithms but effective
  - ***Naïve Bayes***
    - Parametric: Builds a probabilistic model of your data following some assumptions.
  - ***k-NN***
    - Non parametric method: In this case a lazy Instance Based Learning method that does not build any model.

Naive Bayes

The four probabilities



$f(k) = \pi_k$

$f(x/k)$

$$f(k/x) = \frac{\pi_k f(x/k)}{f(x)}$$

$$f(x) = \sum_{k=1}^{K} \pi_k f(x/k)$$

Bayes formula (Thomas Bayes, 1701-1761, presbyterian priest)
computing the probability of causes after having indirect evidences of facts

Bayesian classifier

A region Ω_k is defined by all points of R^p with max *f(k/x)*

Hence the objective is to estimate *f(k/x)* for *k=1..K* in every point *x* of R^p

The optimal rule

Bayes rule: Assign every point x of R^p to the $argmax_k\ f(k/x)$

It leads to the definition of ***decision surfaces***

Important property: It minimises the missclassification error

Discriminant function

$$f(k/x) \equiv \pi_k f(x/k) \equiv \delta(\pi_k f(x/k)) = \delta_k(x)$$

Every monotonic function of the posterior probability

Assign every point x of R^p to the $argmax_k\ \delta_k(x)$

Naïve Bayes

Data:

$$\begin{array}{c} \\ i_1 \\ \vdots \\ i_n \end{array} \begin{array}{c} \begin{array}{ccc} X_1 & \dots & X_M \end{array} \\ \begin{pmatrix} x_{11} & \cdots & x_{1M} \\ \vdots & \ddots & \vdots \\ x_{n1} & \dots & x_{nM} \end{pmatrix} \end{array}$$

1. For learning, with the examples, we estimate the likelihood of our data:

$$p(i_i|c_j) = p(x_{i1}, \dots, x_{iM}|c_j)$$

that means, probability that observation i_i with the M values of the M variables $(x_{i1}, x_{i2} \dots x_{iM})$ belongs to class *cj*

2. But for classifying, given an observation $i_{i'}$ $(x_{i'1}, x_{i'2} \dots x_{i'M})$, we look for the class that maximize the *a priori* probability of belonging to the class:

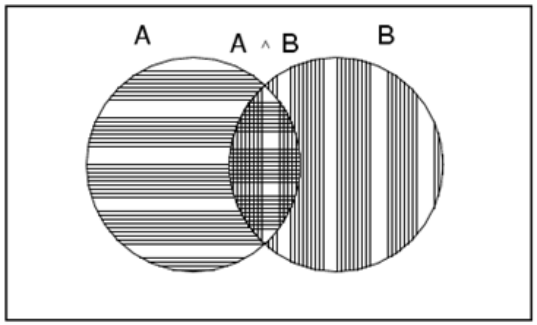
$$c_{MAP} = argmax_{c_j \in C} P(c_j|x_{i'1}, x_{i'2} \dots x_{i'M})$$

Naïve Bayes Classifier

- Bayes' theorem is used:

$$c_{MAP} = argmax_{c_j \in C} P(c_j | x_{i'1}, x_{i'2} \dots x_{i'M}) = argmax_{c_j \in C} \frac{P(x_{i'1}, x_{i'2} \dots x_{i'M} | c_j) P(c_j)}{P(x_{i'1}, x_{i'2} \dots x_{i'M})}$$

- Bayes' theorem



$$\begin{cases} P(A|B) = P(A \wedge B) / P(B) \\ P(B|A) = P(A \wedge B) / P(A) \end{cases}$$

$$\Rightarrow P(A \wedge B) = P(A|B)\, P(B) = P(B|A)\, P(A)$$

$$\Rightarrow \boxed{P(A|B) = \frac{P(B|A)\, P(A)}{P(B)}}$$

Computing Probabilities

- $P(c_j)$ - Proportion of elements in class j
- $P(x_{i'1}, x_{i'2} \dots x_{i'M} | c_j)$
  - Problem $|X|^M |C|$ parameters!
  - It can only be estimated from huge datasets.
    - Impractical
- Solution: **Independence assumption** (very Naïve)
  - Variables values are independent. So in this case, we can easily compute:

$$P(x_{i'1}, x_{i'2} \dots x_{i'M} | c_j) = \prod_{k=1..M} P(x_{i'k} | c_j)$$

Computing probabilities

- $P(x_{i'k}|c_j)$
  - Only needed M$|C|$ probability estimations
  - Very easy. Number of values with property X_k in class c_j over the complete number of cases in class c_j
- Solving $P(x_{i'1}, x_{i'2} \dots x_{i'M}|c_j) = \prod_{k=1..M} P(x_{i'k}|c_j)$ the class assigned to a new observation is :

$$c_{NB} = argmax_{c_j \in C} \frac{P(x_{i'1}, x_{i'2} \dots x_{i'M}|c_j)P(c_j)}{P(x_{i'1}, x_{i'2} \dots x_{i'M})} = \arg\max_{c_j \in C} P(c_j) \prod_{k=1..M} P(x_{i'k}|c_j)$$

Constant for all classes

Equation to solve

Example: Learning to classify texts

- Training set: X document corpus
- Each document is labeled with f(x)=*like/dislike*
- Goal: Learn function that permits given new document if you like it or not.
- Questions:
  - How do we represent documents?
  - How to compute probabilities?

Example: Learning to classify texts

- **How do we represent documents?**
  - Each document is represented as a *Bag of Words*
  - Variables: All words that appear in the document
  - So each document is represented as a Boolean vector with length N:
    - 0 – word does not appear ;
    - 1 – word appear
- Practical problem: A very huge table.
- Solution : Use sparse representation of matrixes

Example: Learning to classify texts

- Some numbers
  - 10.000 documents
  - 500 words per document
  - Maximum theoretical number of words: 50.000 (much less because of word repetitions)
- Reducing the number of variables
  - Removing the number (sing/plural) and verbal forms (*stemming*)
  - Remove conjunctions, propositions and articles (*stop words*)
  - Now we have about. 10.000 variables

Example: Learning to classify texts

- **How to compute probabilities?**
- For each word

$$V_{NB} = argmax_{v \in \{like, dislike\}} P(v) \prod_i p(x_i = word_i \,|v)$$

- "a priori" probability for like and dislike classes **$P(v_i)$**

$$\boldsymbol{P(v_{like}) = \frac{\#documents\ like}{total\ number\ of\ documents}}$$

$$\boldsymbol{P(v_{dislike}) = \frac{\#documents\ dislike}{total\ number\ of\ documents}}$$

Example: Learning to classify texts

$$V_{NB} = argmax_{v \in \{like, dislike\}} P(v) \prod_i p(x_i = word_i \,|v)$$

- Number of parameters $P(x_i = word_i|v)$
  - 10.000 words and 2 classes (so about 20000)

$$\boldsymbol{P(word_k|v) = \frac{\#docs\ v\ in\ training\ where\ word_k\ appears}{\#\ documents\ v} = \frac{n_{v_k}}{n_k}}$$

Example: Learning to classify texts

- Problem:

$$P(word_k|v) = \frac{\#docs\ v\ in\ training\ where\ word_k\ appears}{\#\ documents\ v} = \frac{n_{v_k}}{n_k}$$

  - When n_{v_k} is low, not an accurate probability
  - when n_{v_k} is 0 for $word_k$ for one class v, then any document with that word will never be assigned to v (independent of other appearing words)

Example: Learning to classify texts

- Solution: More robust computation of probabilities (Laplace *smoothing*)

$$P(word_k \mid v) = \frac{n_{v_k} + mp}{n_v + m}$$

Where:

- n_{v_k} is # of documents of class v in which word *k* appear
- n_v is # of documents with label *v*
- p it's a likelihood estimation of "a priori" $P(x_k|v)$ (f.i., uniform distribution)
- m is the number of labels

Example: Learning to classify texts

- *Smoothing*

$$P(x_k \mid v) = \frac{n_{v_k} + mp}{n_v + m}$$

More common “a priori” uniform distribution:

1. When two classes: p=1/2, m=2 (Laplace Rule)

$$P(x_k \mid v) = \frac{n_{v_k} + 1}{n_v + 2}$$

1. Generic case (c classes): p = 1/c, m=c

$$P(x_k \mid v) = \frac{n_{v_k} + 1}{n_v + c}$$

Example: Learning to classify texts

- Naïve Bayes return good accuracy results even when independence assumption is not fulfilled
  - In fact, Spam/not Spam implementation of Thunderbird work in this way
  - Applied to document filtering (ex. *Newsgroups* or *incoming mails*)
- Learning and testing time are linear with the number of variables!

Extension to Continuous Variables

- Assume each class follows a normal distribution for each variable:

$$f(x) = \frac{1}{\sqrt{2\pi\sigma}} e^{\frac{(x-\mu)^2}{2\sigma^2}}$$

- For instance, with an average of 73 for the variable temperature in class x, and std=26.2, the conditional probability in the following:

$$p(temperature = 66 \mid x) = \frac{1}{\sqrt{2\pi 6.2}} e^{\frac{(66-73)^2}{26.2^2}} = 0.034$$

Example: Sex classification

- Training set:

Person	height (feet)	weight (lbs)	foot size(inches)
male	6	180	12
male	5.92 (5'11")	190	11
male	5.58 (5'7")	170	12
male	5.92 (5'11")	165	10
female	5	100	6
female	5.5 (5'6")	150	8
female	5.42 (5'5")	130	7
female	5.75 (5'9")	150	9

- Mean and variance assuming Gaussian distribution:

Person	mean (height)	variance (height)	mean (weight)	variance (weight)	mean (foot size)	variance (foot size)
male	5.855	$3.5033*10^{-2}$	176.25	$1.2292*10^{2}$	11.25	$9.1667*10^{-1}$
female	5.4175	$9.7225*10^{-2}$	132.5	$5.5833*10^{2}$	7.5	1.6667

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- New instance to classify

Person	height (feet)	weight (lbs)	foot size(inches)
sample	6	130	8

- Determine which posterior probability is greater, male or female

$$\text{posterior (male)} = \frac{P(\text{male})\, p(\text{height} \mid \text{male})\, p(\text{weight} \mid \text{male})\, p(\text{foot size} \mid \text{male})}{evidence}$$

$$\text{posterior (female)} = \frac{P(\text{female})\, p(\text{height} \mid \text{female})\, p(\text{weight} \mid \text{female})\, p(\text{foot size} \mid \text{female})}{evidence}$$

$$\begin{aligned}\text{evidence} = {} & P(\text{male})\, p(\text{height} \mid \text{male})\, p(\text{weight} \mid \text{male})\, p(\text{foot size} \mid \text{male}) \\ & + P(\text{female})\, p(\text{height} \mid \text{female})\, p(\text{weight} \mid \text{female})\, p(\text{foot size} \mid \text{female})\end{aligned}$$

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- Determine which posterior probability is greater, male or female

$$\text{posterior (male)} = \frac{P(\text{male})\,p(\text{height} \mid \text{male})\,p(\text{weight} \mid \text{male})\,p(\text{foot size} \mid \text{male})}{evidence}$$

$$P(\text{male}) = 0.5$$

$$p(\text{height} \mid \text{male}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{-(6-\mu)^2}{2\sigma^2}\right) \approx 1.5789,$$

$$p(\text{weight} \mid \text{male}) = 5.9881 \cdot 10^{-6}$$

$$p(\text{foot size} \mid \text{male}) = 1.3112 \cdot 10^{-3}$$

$$\text{posterior numerator (male)} = \text{their product} = 6.1984 \cdot 10^{-9}$$

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- New instance to classify

Person	height (feet)	weight (lbs)	foot size(inches)
sample	6	130	8

- Determine which posterior probability is greater, male or female

$$\text{posterior (female)} = \frac{P(\text{female})\, p(\text{height} \mid \text{female})\, p(\text{weight} \mid \text{female})\, p(\text{foot size} \mid \text{female})}{evidence}$$

$$P(\text{female}) = 0.5$$

$$p(\text{height} \mid \text{female}) = 2.2346 \cdot 10^{-1}$$

$$p(\text{weight} \mid \text{female}) = 1.6789 \cdot 10^{-2}$$

$$p(\text{foot size} \mid \text{female}) = 2.8669 \cdot 10^{-1}$$

$$\text{posterior numerator (female)} = \text{their product} = 5.3778 \cdot 10^{-4} > \text{posterior numerator (male)} = 6.1984 \cdot 10^{-9}$$

The posterior probability of female is greater => it predicts the sample is female!

k-NN

- Probably the simpliest classifier
- Simple idea: a new instance is labeled with label of its closest neighbour/s.
- No model is learnt or trained
  - Lazy learning: generalization of the training data is delayed until a query is made
    - defers the majority of computation to consultation time

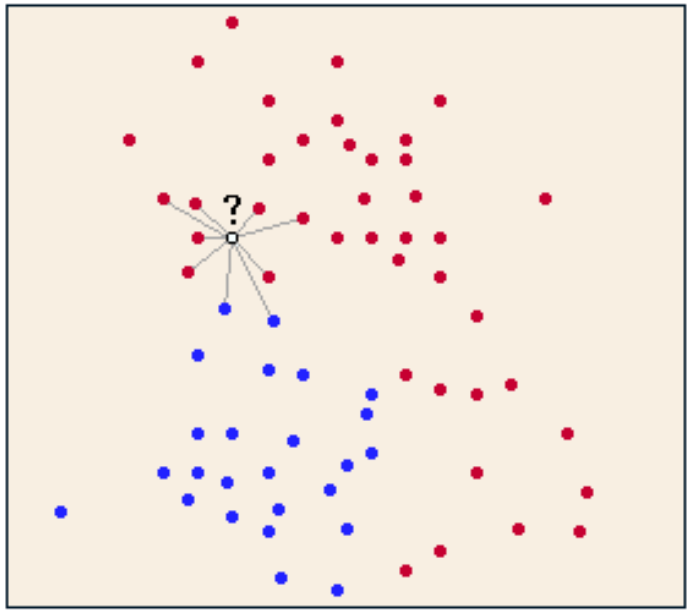
k-NN origins

- k-nn (k nearest neighbours)
- First paper with the name:
  - *Cover TM, Hart PE (1967). "Nearest neighbor pattern classification" (PDF). IEEE Transactions on Information Theory.* ***13*** *(1): 21–27.*
  - That paper shows what happens if a very large aselectively chosen training set is used.
- Before Cover and Hart the rule was mentioned by Nilsson (1965) who called it “minimum distance classifier” and by Sebestyen (1962), who called it “proximity algorithm”. Fix and Hodges in their very early discussion on non-parametric discrimination (1951) already pointed to the NN rule as well.

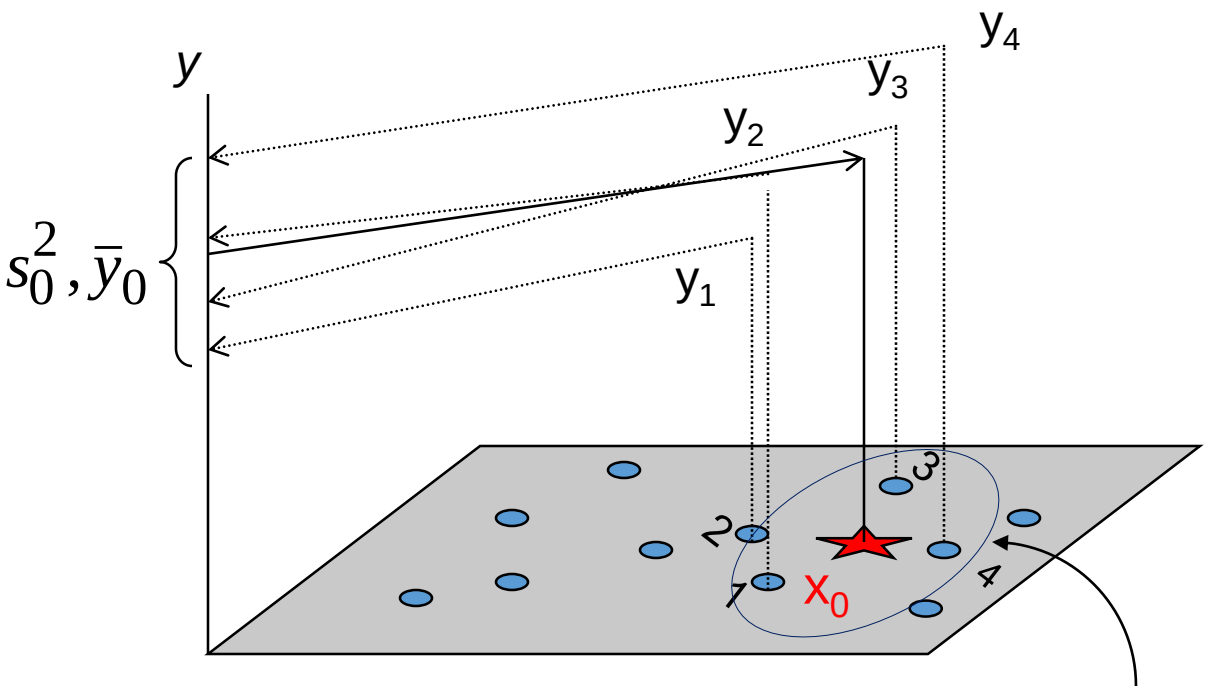
Local Discrimination

- k-NN
  - Universal Aproximator
  - Requires a big dataset for training

  - *“curse of dimensionality”*



k-NN. Theorical basis



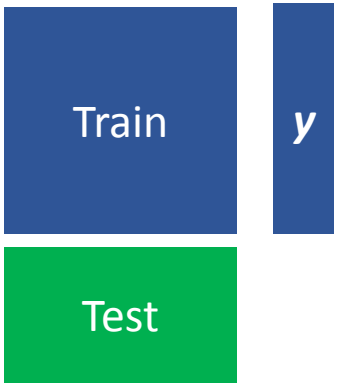
If $K \to \infty, \quad K/n \to 0$

V_0 Neighbourhood of x_0

$$\bar{y}_0 \to E(y|x_0) \quad s_0^2 \to V(y|x_0)$$ *(numerical response)*

$$\hat{f}(j|x) = \frac{k_j}{k \times V_0} \to f(j|x)$$ *(categorical response)*

Correspondence Graph of k-NN




```
knn(train, test, y, k)
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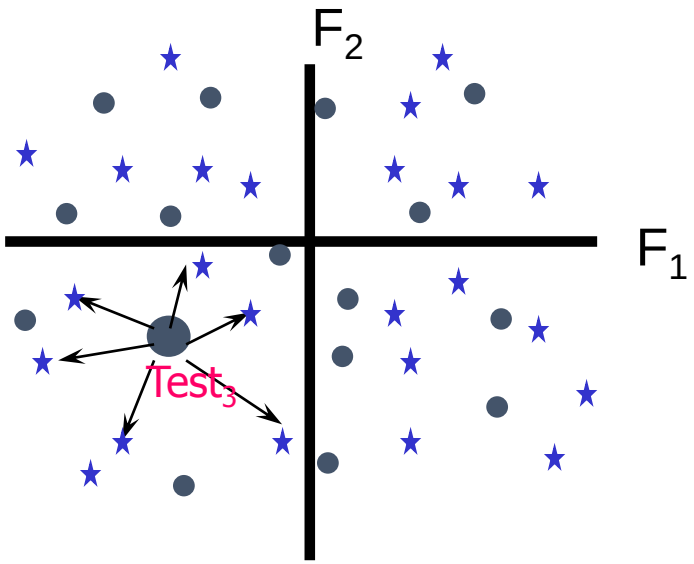
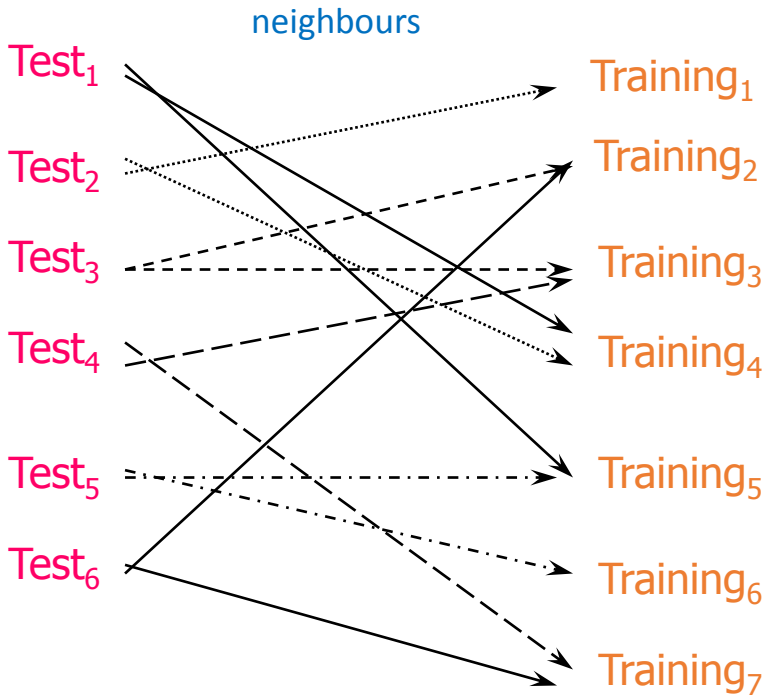




k-NN

- Non-parametric
- Lazy algorithm
- Instance-based Learning method
- Not builds any model

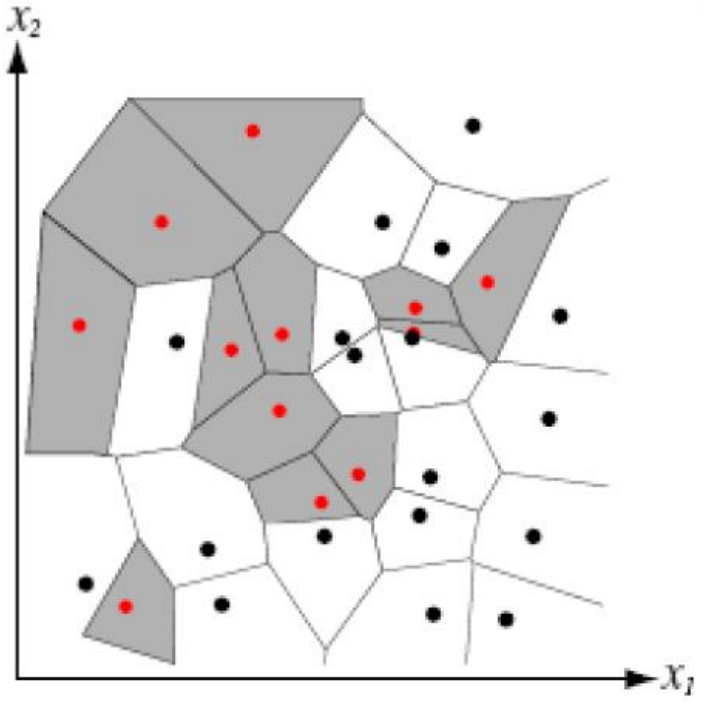
- Requeriments:
  - A training set
  - A similarity measure

k-NN

- K-Nearest neighbor algorithm
  - It interprets each example as a point in a space defined by the features describing the data
  - In that space a similarity measure allows as to classify new examples.
  - Class is assigned depending on the *K* closest examples

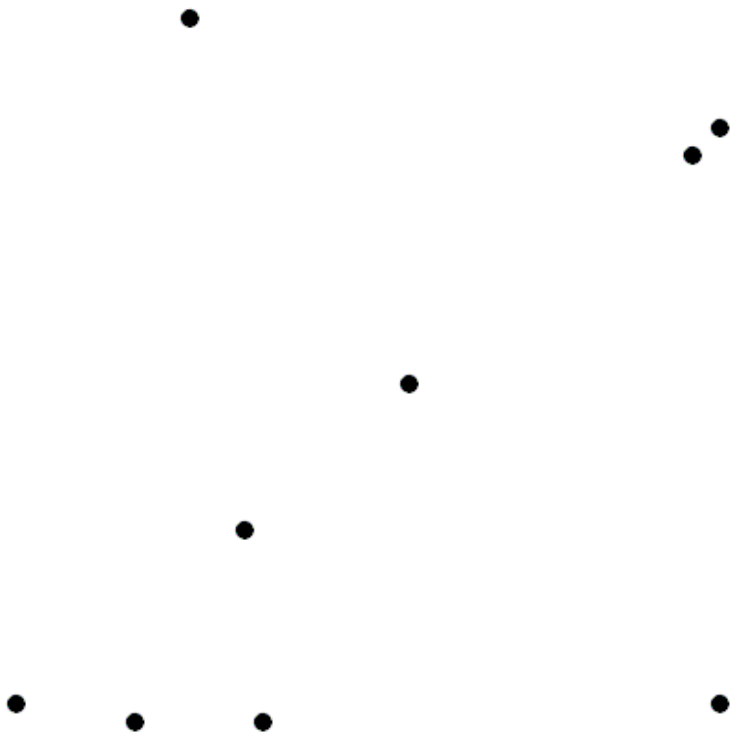
1-NN Example

- Two real variables (x1, x2) define the space
- Each red point is a positive example. Black points are negative examples



Equivalent to draw the Voronoi space of your data.

Voronoi Space



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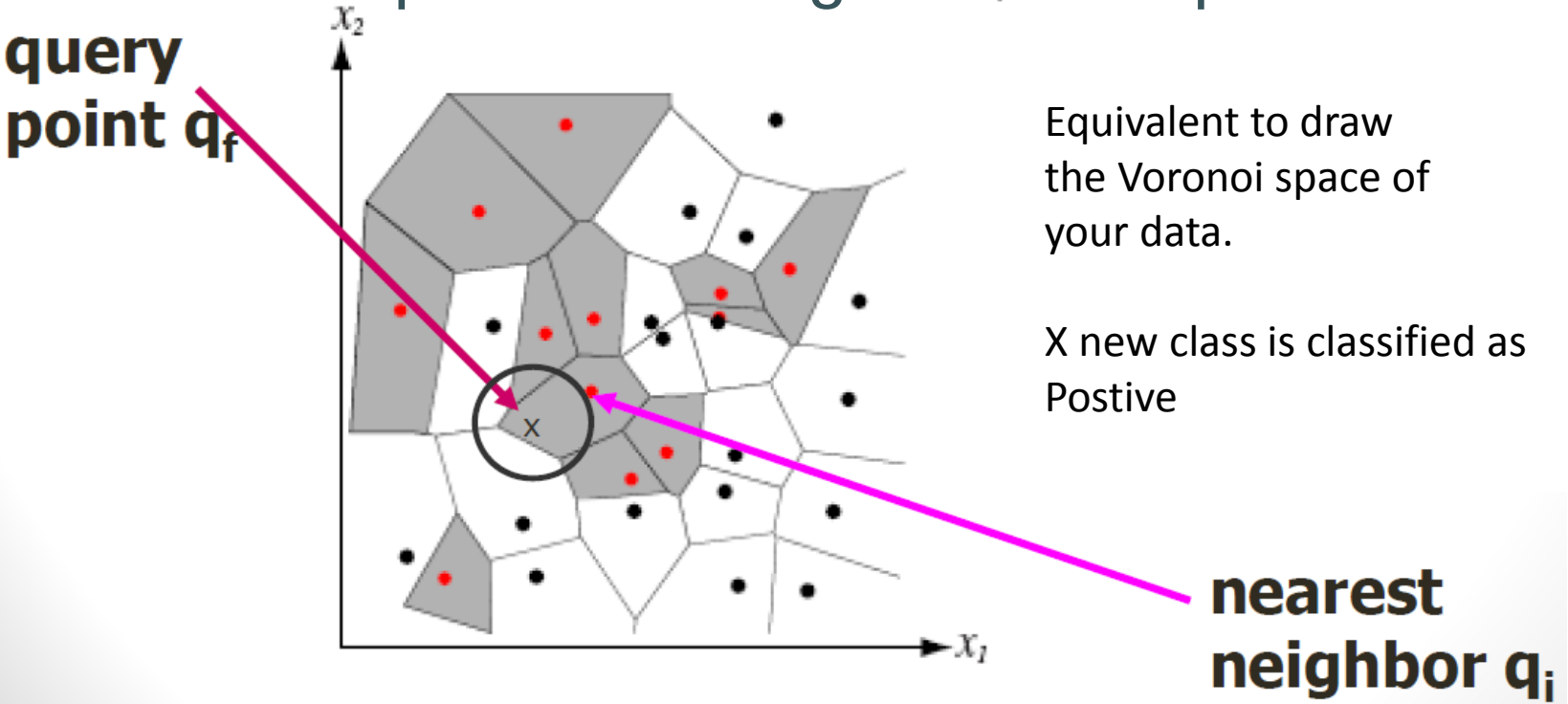
  Black points are negative examples



Equivalent to draw the Voronoi space of your data.

X new class is classified as Postive

Distance Measure

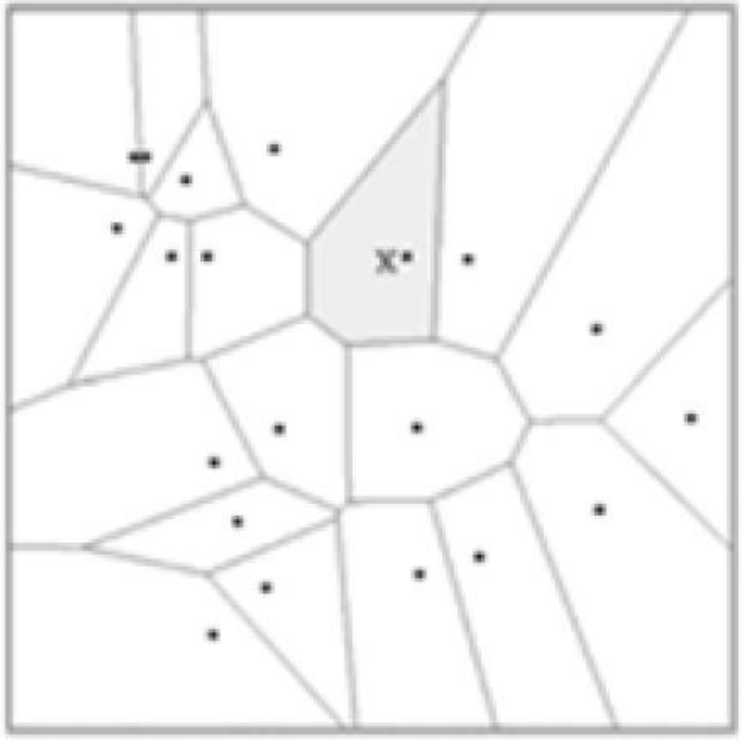
- Euclidean

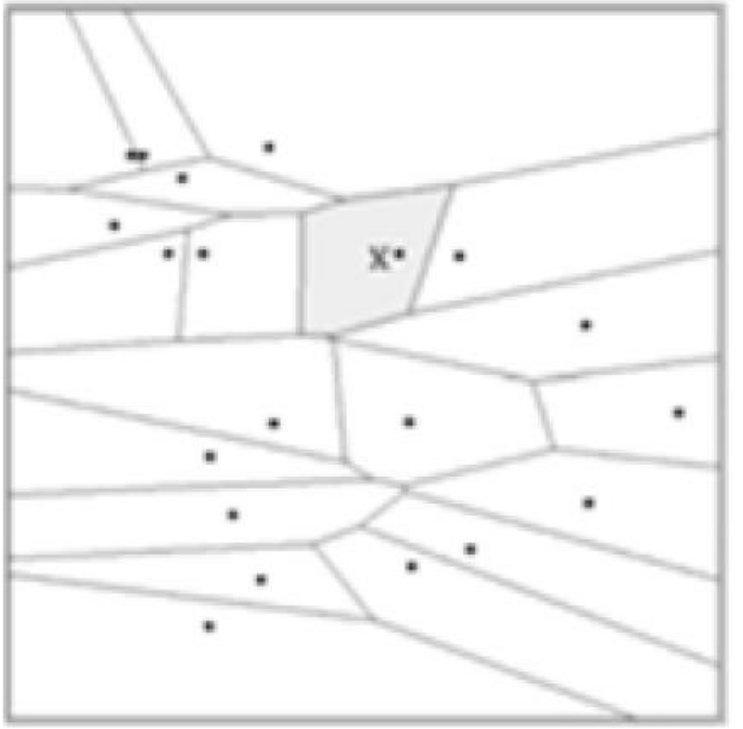
$$d(x_i, x_j) = \sqrt{\sum_{k=1}^{M} (x_{ik} - x_{jk})^2}$$

- Weighted Euclidean

$$d(x_i, x_j) = \sqrt{\sum_{k=1}^{M} w_k (x_{ik} - x_{jk})^2}$$

Weighting Effect





$$d^2(x_i,x_j) = (x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2$$

$$d^2(x_i,x_j) = 9(x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2$$

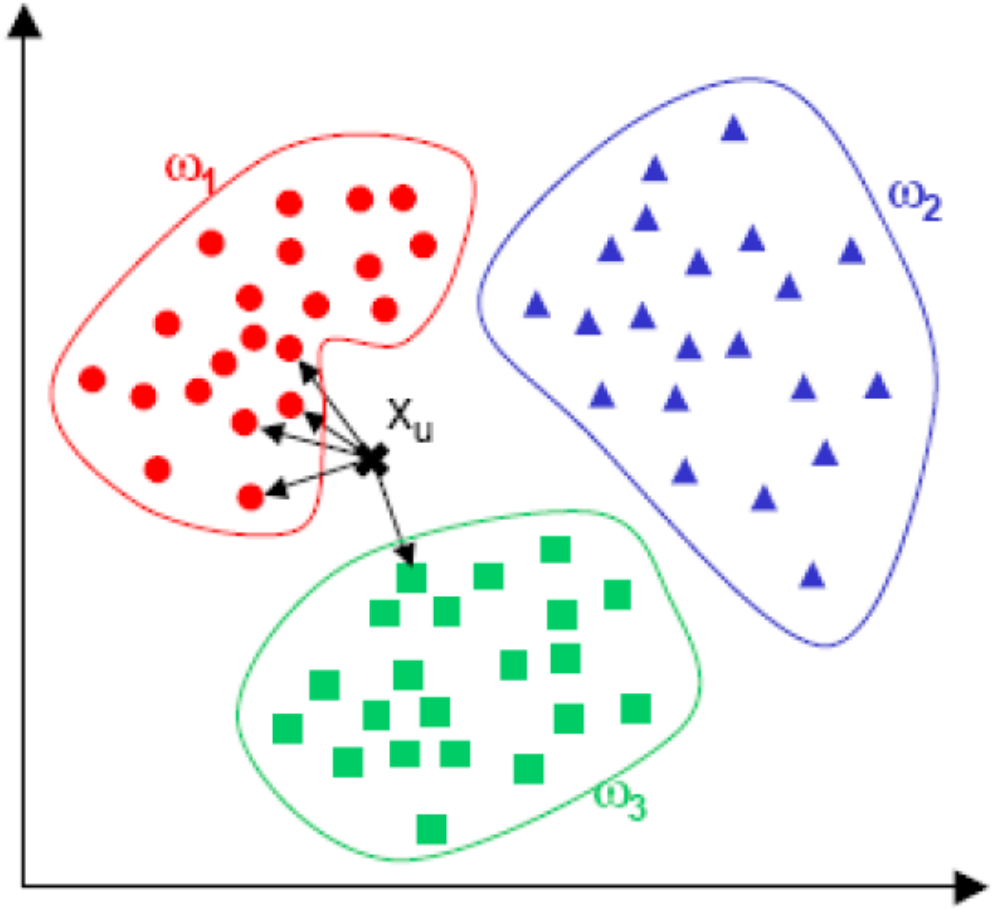
k-NN

- Advantages:
  - Fast training
  - Ability to learn very complex functions
- Problems:
  - Very slow in testing. Needed some smart structure representation of data in trees
  - Fooled by noise
  - Fooled when irrelevant features

- Building more robust classifiers
  - Results do not depend on the closest example
  - but on the k closest examples (so *k-nearest neighbours* (kNN) name)

Example

- kNN; k = 5

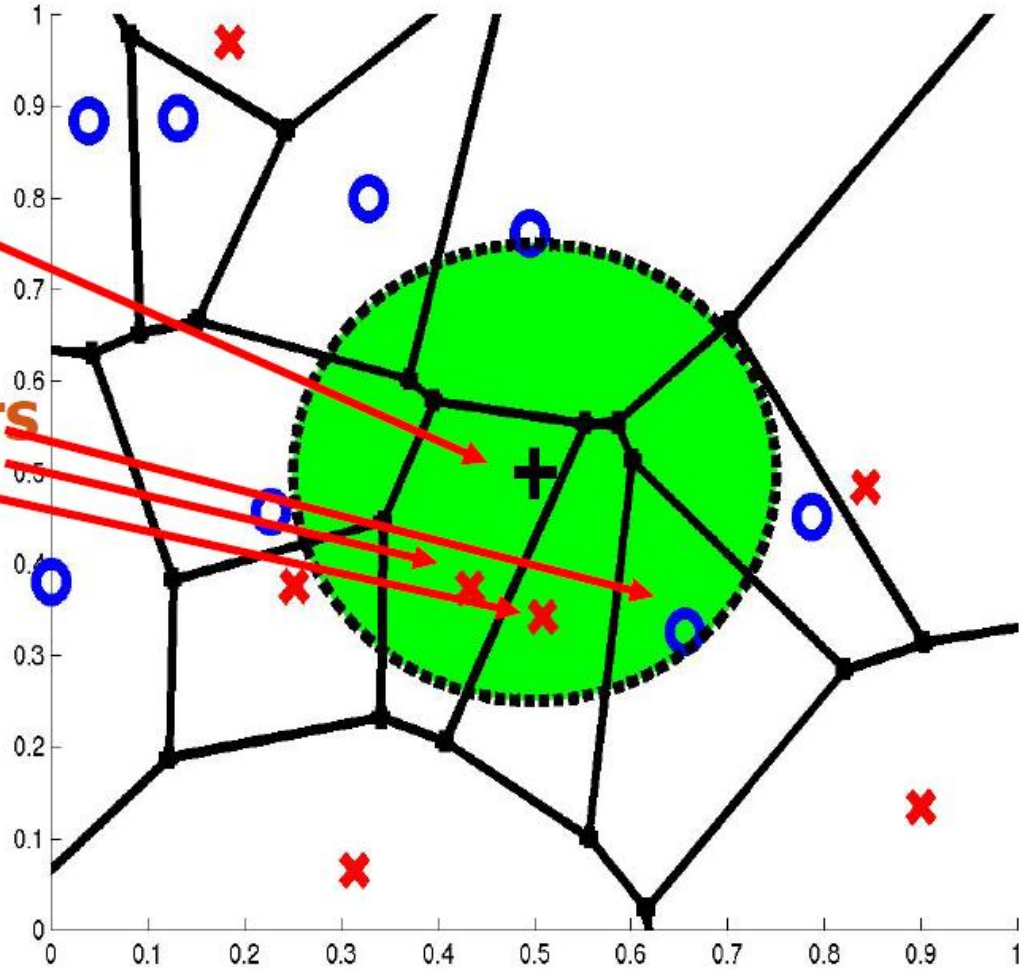


3-nearest neighbours

query point q_f

3 nearest neighbors

2x,1o

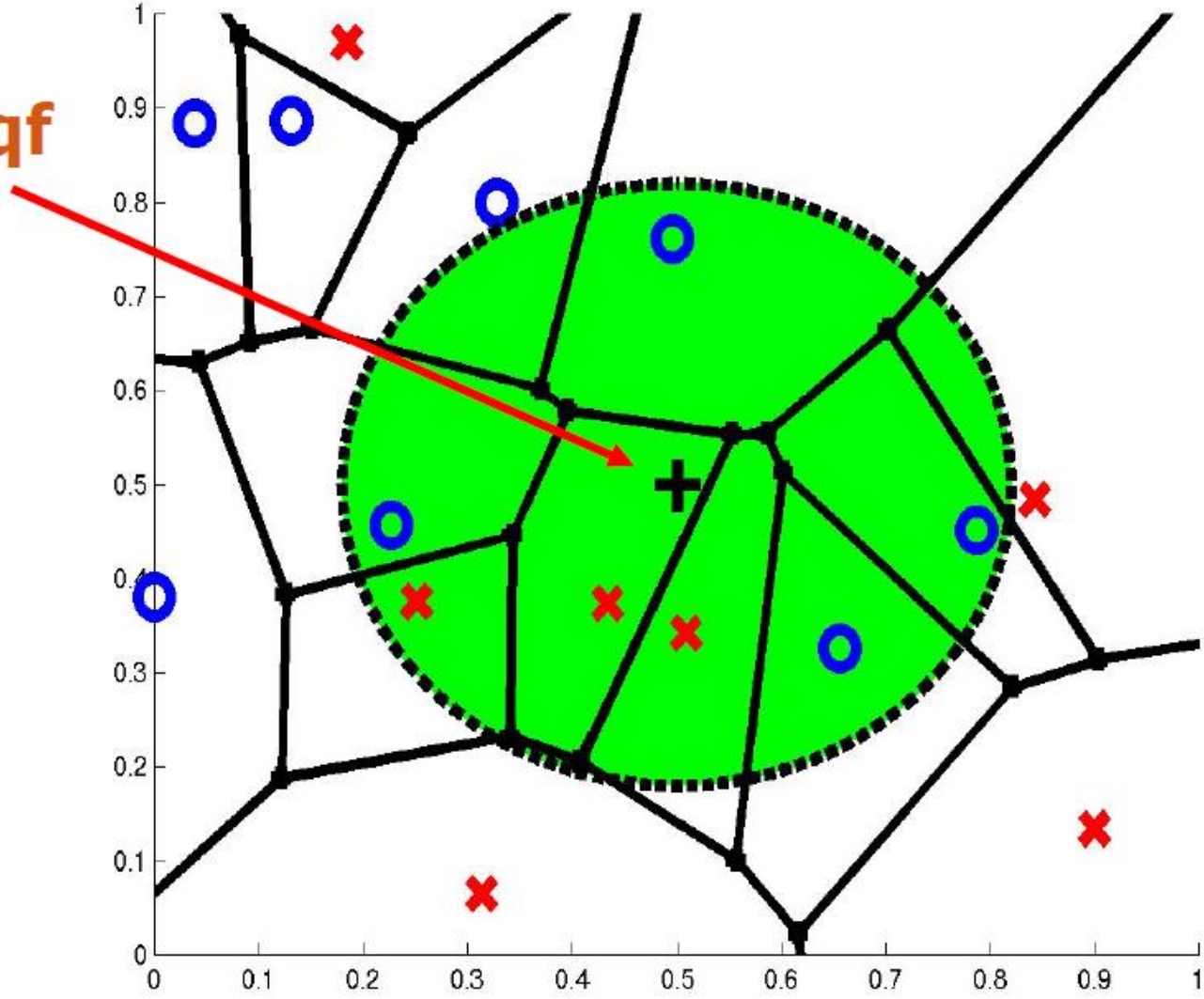


7-nearest neighbours

query point qf

7 nearest neighbors

3x,4o



k-NN Algorithm

- **Parameters**:
  - Natural number *k (even number)*
  - Training set
  - Distance measure
- Algorithm:
  1. Store all training set $<i_i, label(i_i)>$
  2. Given new observation, i' compute the nearest k neighbors
  3. Let vote the nearest k neighbors to assign the label to the new data.

Drawbacks of k-NN

- The parameter that defines the complexity is the number of neighbours ***k***
- A higher ***k*** more bias
- A lower ***k*** more variance
- Problem with high dimensional data (*curse of dimensionality*)
- Problem when unbalanced classes (need of having balanced samples)
- Black hole effect. Tends to produce results a little worse than with other methods.

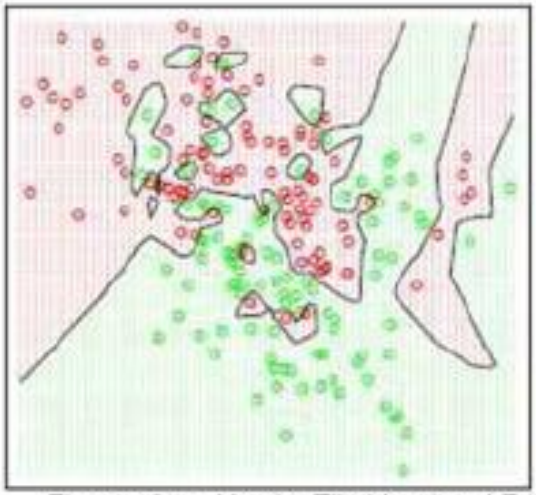
How to select k?

- High number of k show two advantages:
  - Smother frontiers
  - Reduces sensibility to noise
- But too large values are bad because
  - We lose locality in the decision because very distant points can interfere in assigning labels
  - Computation time is increased
- K-value usually is chosen by cross-validation

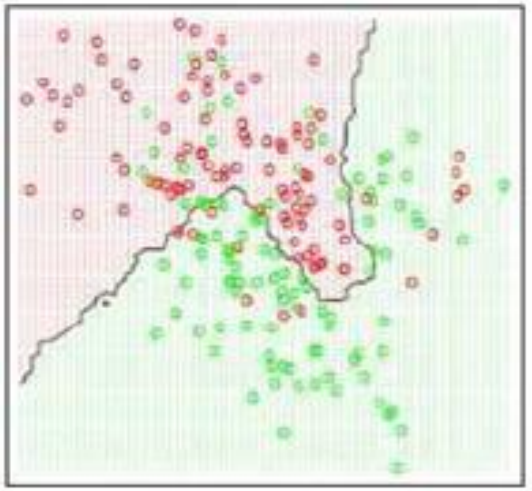
Decision boundary defined from data

Effect of K

K=1



K=15



Figures from Hastie, Tibshirani and Friedman (Elements of Statistical Learning)

Larger k produces smoother boundary effect and can reduce the impact of class label noise.

But when k is too large, say k=N, we always predict the majority class

Distance Weighted k-NN

- A smart variation of k-NN.
- When voting, all k neighbors have the same influence, but some of them are more distant than the others (so they should influence less in decisions)
- Solution: Given more weight to closest examples

Distance Weighted kNN

- Label is assigned by the weighted addition:

$$f_l = \sum_{i}^{k} w_i l(x_i)$$

where $l(x_i) \in \{-1,1\}$ the label of example x_i

$w_i = K(d(x_q, x_i))$ is the weight of example i

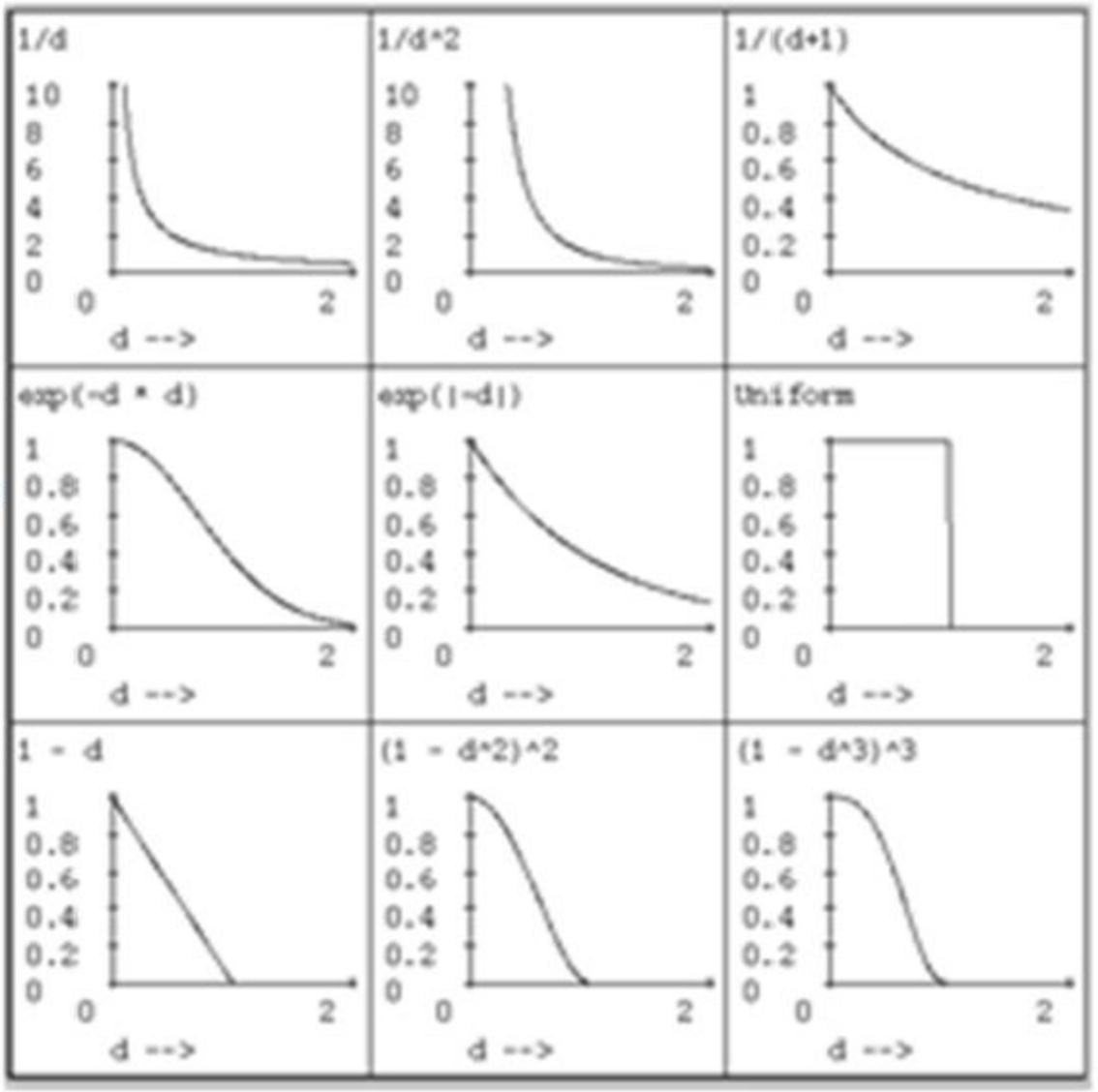
$K(d)$ is a weight functions depending on distance, and

$d(x_q, x_i)$ is distance from x_q to x_i

Distance Weighted kNN

$$d = d(x_i, x_{query})$$

Common Weighting Functions

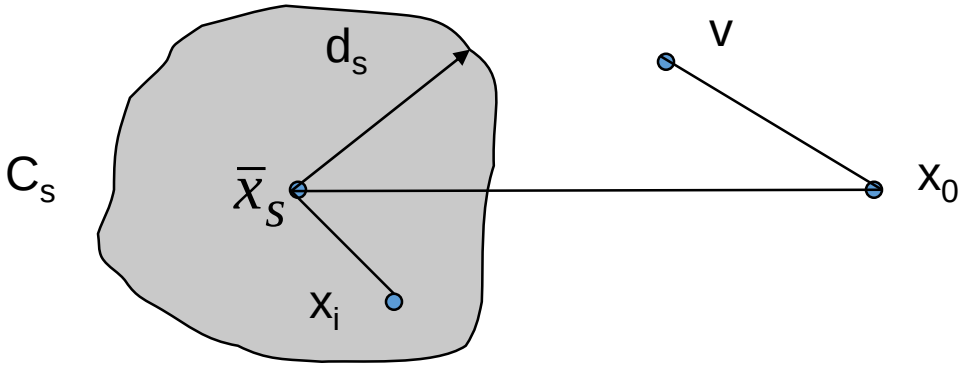


Problems with irrelevant features

- kNN is fooled when irrelevant features.
  - Lets assume examples described with 20 attributes, but only 2 are relevant to the classification
  - kNN will be lost easily in this case
- Solution: consist in feature removal:
  - Find weights $z_1, \ldots, z_n$, one for each feature, that minimize error in a validation data set (so use cross-validation to choose weights)
  - Notice that setting $z_j = 0$ means removing the feature

Finding the k-NN
(Fukunaga&Narendra)

1. Classify the n individuals into a big number of classes (ex. using k-means)



c_s: *class s*
$\bar{x_s}$: *centroid of class* c_s
d_s: *diameter of class* c_s
x_i: *point in class* c_s
v: *point not in class* c_s
x_o: *point to classify*

2. Algorithm branch&bound:

Discard of a class: $d(\bar{x}_s, x_0) - d_s > d(x_0, v)$

Discarting individuals: $d(\bar{x}_s, x_0) - d(\bar{x}_s, x_i) > d(x_0, v)$

k-NN

- Advantages:
  - Fast training
  - Ability to learn very complex functions
  - Incremental
    - Hability of adaptation to new cases
- Problems:
  - Very slow in testing. Needed some smart structure representation of data in trees
  - Fooled by noise
  - Fooled when irrelevant features

Management of heterogeneous data matrices

- **Heterogeneous matrices faced. Several approaches [Anderberg 73]:**
  - **Variables partitioning**
  - **Variables converting**
  - **Compatibility measures**
    - **Mixed metrics required**

Distance between individuals

- Quantitative Variables
  - Euclidean
  - Manhattan
  - Minkowski
- Qualitative Variables
  - χ^2 [Benzécri 80]
- Heterogeneous variables (compatibility measures):
  - Gower [71]
  - Gowda i Diday [91]
  - Gibert's Mixed [91]
  - Ichino i Yaguchi [94]
  - Ralambondrainy [95]

Distance for Numerical Variables

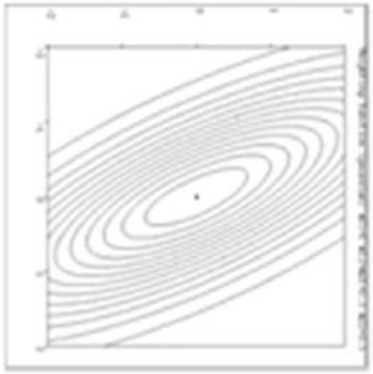
- *Minkowski*

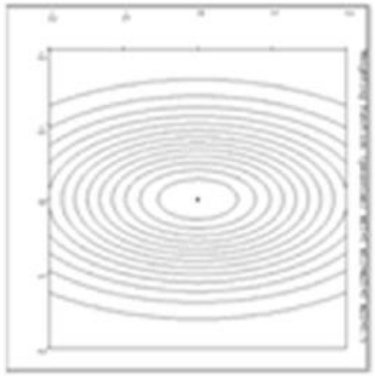
$$d(x_i, x_j) = \sqrt[r]{\sum_{k=1}^{M} (x_{ik} - x_{jk})^r}$$

  - r = 1 Manhattan
  - r = 2 Euclidean

Other Measures for Numerical

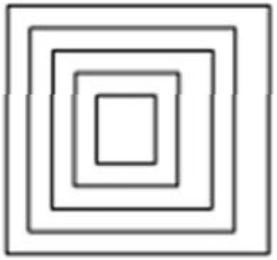
Mahalanobis





Scaled Euclidian (L_2)

$L_{infinity}$ *(max) norm*



L_1 norm (absolute)

Distances for Qualitative Variables

- Chi-Square Distance

$$\chi^2 = \sum_{k=1}^{p} \sum_{j=1}^{q} \frac{\left(n_{kj} - \frac{n_k n_j}{n}\right)^2}{\frac{n_k n_j}{n}}$$

- Jaccard index (binary variables)

$$d(i, i') = \frac{n_{11} + n_{oo}}{n}$$

Mixed Metric - Gower

$$d_G(i,j) = \frac{\sum_k \delta_{ii\prime k} \ * \ d_k(i,i')}{\sum_k \delta_{ii\prime k}}$$

$$d_k(i,i') = \begin{cases} 0 & if\ X_k\ binary\ \wedge x_{ik} = x_{i\prime k} = TRUE \\ 0 & if\ X_k\ categorical\ \wedge x_{ik} = x_{i\prime k} \\ \dfrac{|x_{ik} - x_{i\prime k}|}{\max_k - min_k} & if\ X_k\ es\ numerical \\ \dfrac{|r_{ik} - r_{i\prime k}|}{\max_{r_k} - 1} & if\ X_k\ is\ ordered (r_{ik} = índex\ of\ the\ category) \\ 1 & otherwise \end{cases}$$

$$\delta_{ii\prime k} = \begin{cases} 0 & if\ x_{ik} = MISSING\ or\ x_{i\prime k} = MISSING \\ 0 & if\ X_k\ assymetric\ binary \wedge x_{ik} = x_{i\prime k} = 0\ or\ x_{ik} = x_{i\prime k} = FALSE \\ 1 & otherwise \end{cases}$$

Mixed Metric - Gowda-Diday [Gow 91]

$$D(i,i') = \sum_{k=1}^{K} D_k(i_k, i'_k)$$

$$D_k(i,i') = D_p(i,i') + D_s(i,i') + D_c(i,i')$$

- Component Position

$$D_{kp}(i,i') = \begin{cases} \dfrac{|x_{ik} - x_{i'k}|}{R_k} & if\,(X_k numerical) and\ R_k is\ range\ of\ X_k \\ 0 & if\,(X_k qualitative) \end{cases}$$

- Component Span

$$D_{ks}(i,i') = \begin{cases} 0 & if X_k numerical \\ 1 & if\ X_k qualitative\ and\ not\ multi-valued \end{cases}$$

- Component Content

$$D_{kc}(i,i') = \begin{cases} 0 & if X_k numerical \\ 0 & if\,(X_k qualitative) and\ (x_{ik} = x_{i'k}) \\ 1 & if\,(X_k qualitative) and\ (x_{ik} \neq x_{i'k}) \end{cases}$$

Mixed Metric [Gibert 91]

$$d^2_{(\alpha,\beta)}(i,i') = \alpha d^2_{\varsigma}(i,i') + \beta d_Q(i,i')$$

$$d^2_{\varsigma}(i,i') = \sum_{\forall k \in \varsigma} \frac{(x_{ik} - x_{i'k})^2}{s_k^2}$$

$$d^2_Q(i,i') = \begin{cases} 0 \quad if\ x_{ik} = x_{i'k} \\ \frac{1}{I_{k^i}} + \frac{1}{I_{k^{i'}}} \quad otherwise, for\ compact\ i\ and\ i'w.r.t\ X_k \\ \frac{\left(f_i^{k_s} - 1\right)^2}{I^{k_s}} + \sum_{j \neq s}^{n_k} \frac{\left(f_i^{k_j}\right)^2}{I^{k_j}} \quad if\ x_{ik} = c_s^k, an\ extendend\ i'w.r.t\ X_k \\ \sum_{j=1}^{n_k} \frac{\left(f_i^{k_j} - f_{i'}^{k_j}\right)^2}{I^{k_j}} \quad fori, i'extended\ w.r.t\ X_k \end{cases}$$

Proposal

$$\alpha = \frac{n_{\varsigma}}{d^2_{\varsigma}\max *} \qquad \beta = \frac{n_Q}{d^2_Q max\ *}$$

Example: Sex classification

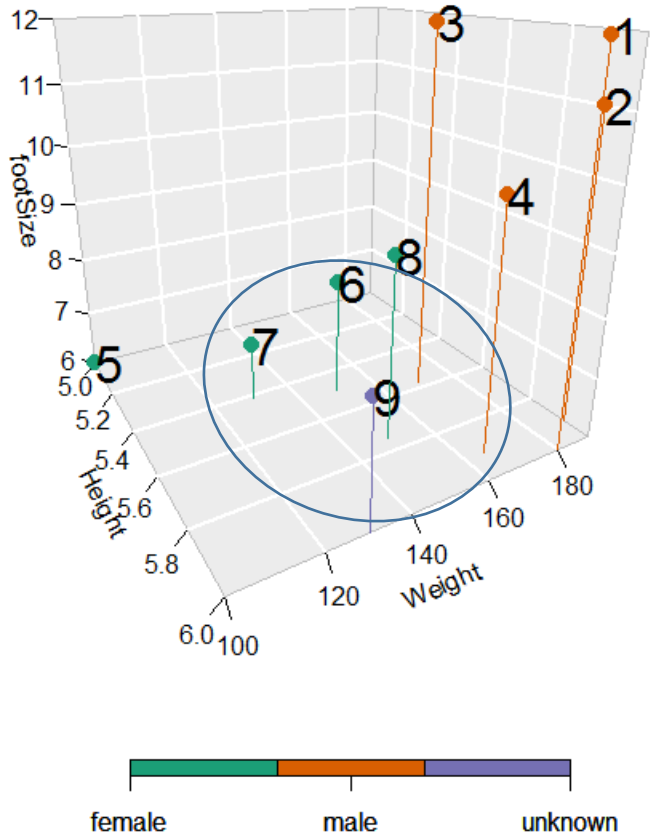
- Training set:

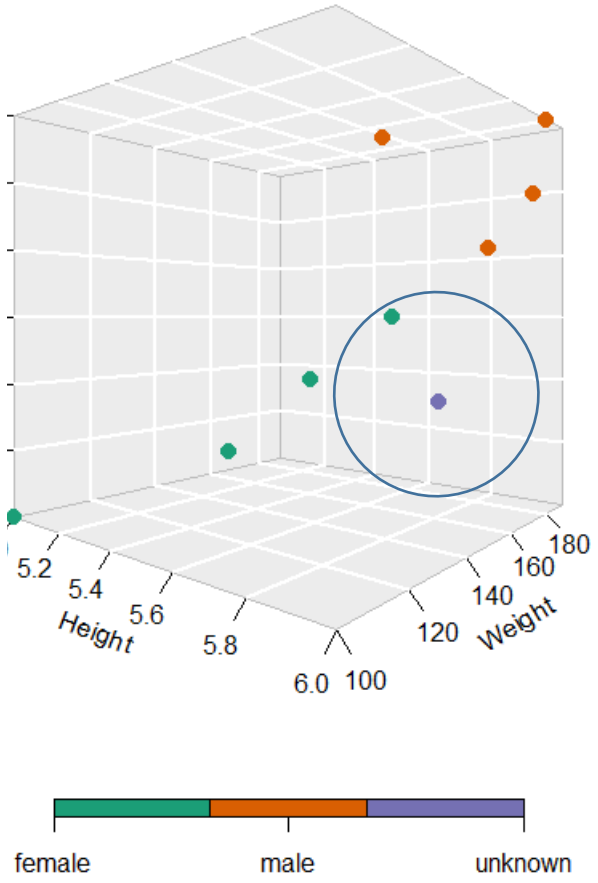
Person	height (feet)	weight (lbs)	foot size(inches)
male	6	180	12
male	5.92 (5'11")	190	11
male	5.58 (5'7")	170	12
male	5.92 (5'11")	165	10
female	5	100	6
female	5.5 (5'6")	150	8
female	5.42 (5'5")	130	7
female	5.75 (5'9")	150	9

- New instance to classify

Person	height (feet)	weight (lbs)	foot size(inches)
sample	6	130	8

Example: Sex classification





Example: Sex classification

- $1 - NN$
- Class=female

Person	height (feet)	weight (lbs)	foot size(inches)
sample	6	130	8

	Class	Euclidean	Manhattan	Minkowski r=100	Gower
i_1	Male	50.16	54	50	0.41
i_2	Male	60.07	63.03	60	0.42
i_3	Male	40.20	44.42	40	0.51
i_4	Male	35.06	37.08	35	0.27
i_5	Female	30.08	33	30	0.56
i_6	Female	20.00	20.50	20	0.24
i_7	Female	**1.16**	**1.58**	**1**	0.25
i_8	Female	20.03	21.25	20	**0.22**

Example: Sex classification

- $1 - NN$
  - Class=female
- 2-NN
  - Class=female

Person	height (feet)	weight (lbs)	foot size(inches)
sample	6	130	8

	Class	Euclidean	Manhattan	Minkowski r=100	Gower
i_1	Male	50.16	54	50	0.41
i_2	Male	60.07	63.03	60	0.42
i_3	Male	40.20	44.42	40	0.51
i_4	Male	35.06	37.08	35	0.27
i_5	Female	30.08	33	30	0.56
i_6	Female	**20.00**	**20.50**	**20**	**0.24**
i_7	Female	**1.16**	**1.58**	**1**	0.25
i_8	Female	20.03	21.25	20	**0.22**

Example: Sex classification

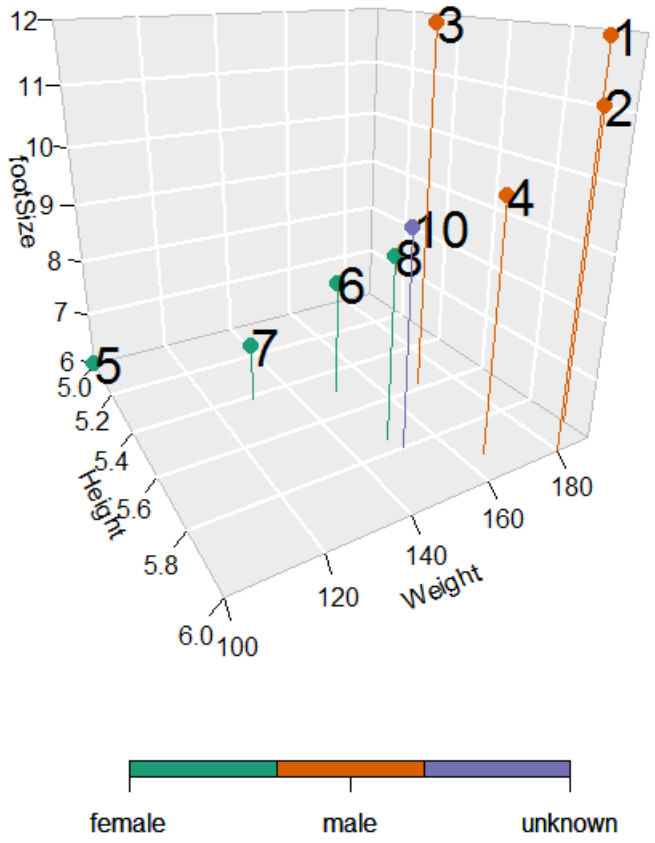
- $1 - NN$
  - Class=female
- 2-NN
  - Class=female
- 4-NN
  - Class=female
- 7-NN
  - Minkowsky
    - Class=female
  - Gower
    - **Class=Male**

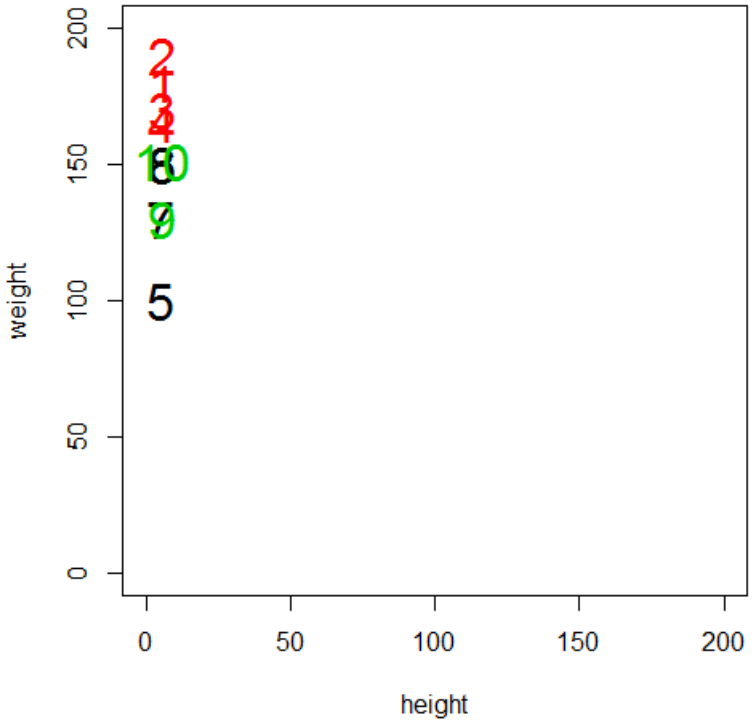
Person	height (feet)	weight (lbs)	foot size(inches)
sample	6	130	8

	Class	Euclidean	Manhattan	Minkowski r=100	Gower
i_1	Male	**50.16**	**54**	**50**	**0.41**
i_2	Male	60.07	63.03	60	**0.42**
i_3	Male	**40.20**	**44.42**	**40**	**0.51**
i_4	Male	**35.06**	**37.08**	**35**	**0.27**
i_5	Female	**30.08**	**33**	**30**	0.56
i_6	Female	**20.00**	**20.50**	**20**	**0.24**
i_7	Female	**1.16**	**1.58**	**1**	**0.25**
i_8	Female	**20.03**	**21.25**	**20**	**0.22**

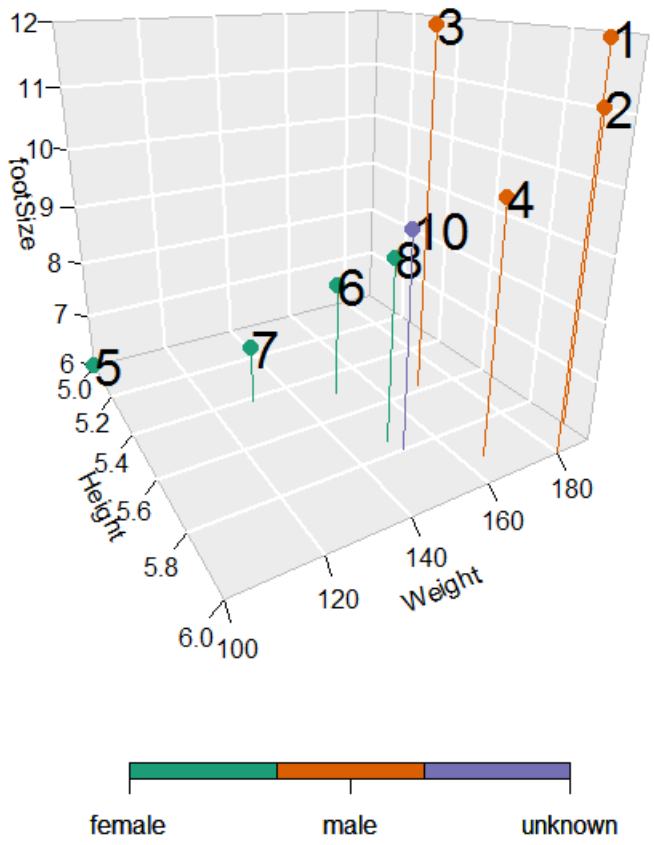
Example: Sex classification -

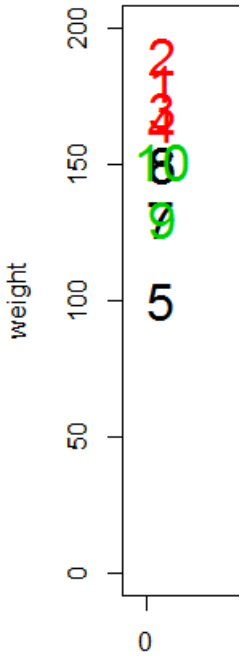
Range(Weight)=[100..190]
Range(Height)=[5..6]
Range(FoodSize)=[6..12]

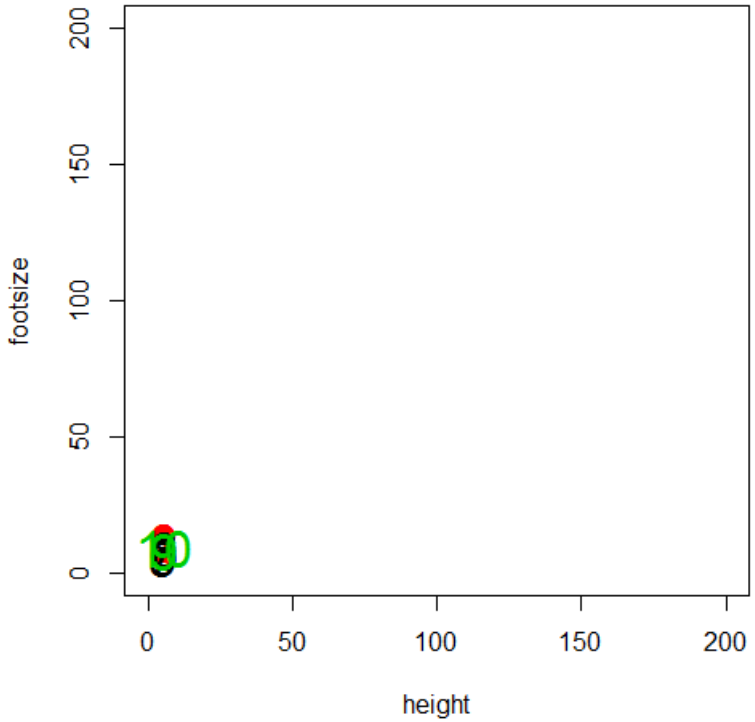




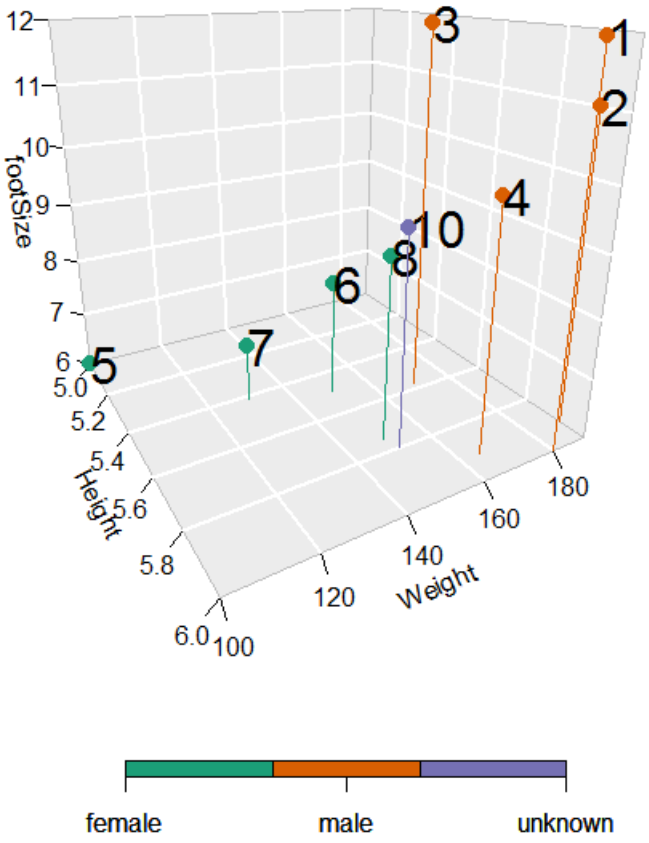
Example: Sex classification -

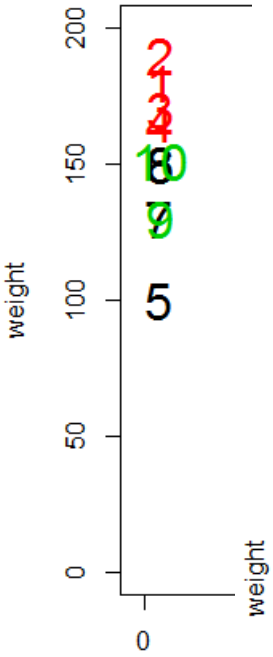


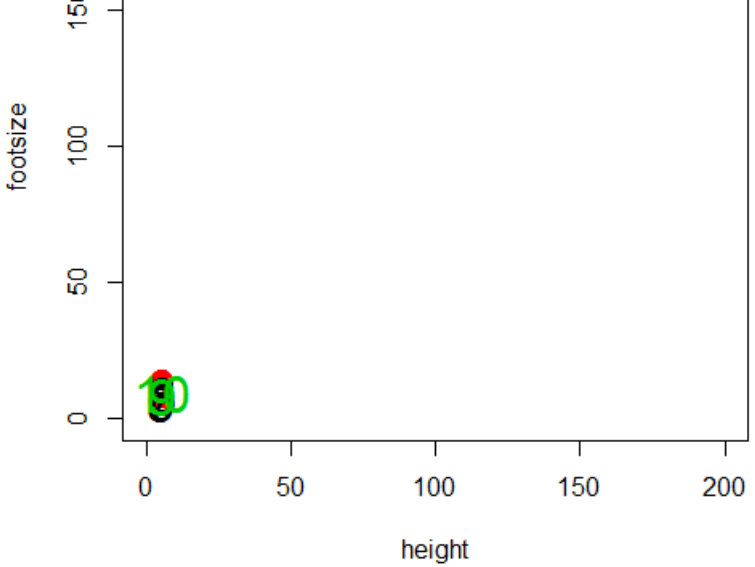


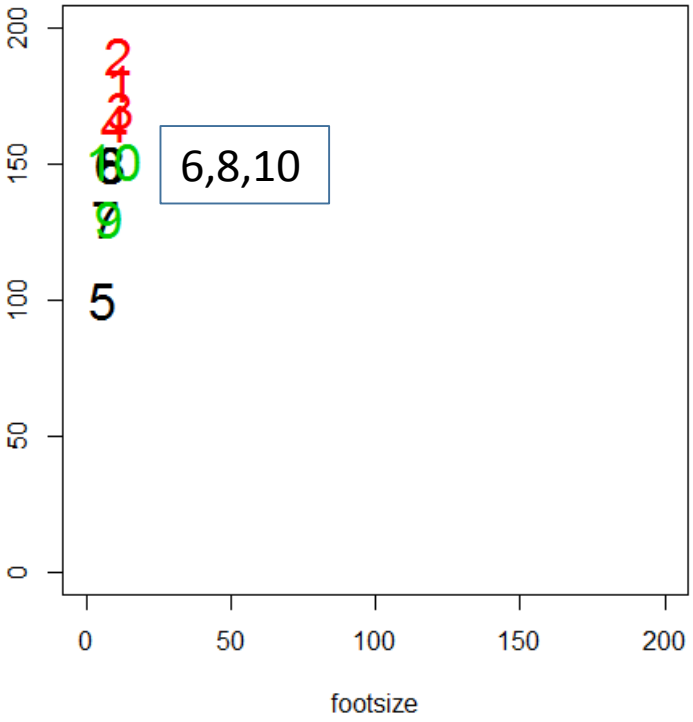


Example: Sex classificatio









Example: Sex classification

Person	height (feet)	weight (lbs)	foot size(inches)
sample	6	130	8

- $1 - NN$
  - Class=female
  - Scaled centered
    - Class=Male
- 2-NN
  - Euclidean=Female
  - Rest: Tie

	Class	Euclidean	Standardized Euclidean	Normalize Euclidean	Gower	Standardized Gower
i_1	Male	29.11	1.75	0.31	0.32	0.32
i_2	Male	39.03	1.68	0.284	0.27	0.27
i_3	Male	19.17	1.58	0.28	0.28	0.28
i_4	Male	14.00	**0.69**	**0.10**	**0.12**	**0.12**
i_5	Female	51.13	3.59	0.49	0.65	0.65
i_6	Female	**1.83**	**1.19**	0.16	0.19	0.19
i_7	Female	21.15	1.88	0.29	0.34	0.34
i_8	Female	**1.12**	1.25	**0.05**	**0.05**	**0.05**

Example: Sex classification

Person	height (feet)	weight (lbs)	foot size(inches)
sample	6	130	8

- $1 - NN$
  - Class=female
  - Scaled centered
    - Class=Male
- 2-NN
  - Euclidean=Female
  - Rest: Tie
- 5-NN
  - Euclidean
    - Class= Female
  - Rest
    - Class=Male

	Class	Euclidean	Standardized Euclidean	Normalized Euclidean	Gower	Standardized Gower
i_1	Male	29.11	1.75	0.31	0.32	0.32
i_2	Male	39.03	1.68	0.284	0.27	0.27
i_3	Male	19.17	1.58	0.28	0.28	0.28
i_4	Male	14.00	**0.69**	**0.10**	**0.12**	**0.12**
i_5	Female	51.13	3.59	0.49	0.65	0.65
i_6	Female	**1.83**	**1.19**	0.16	0.19	0.19
i_7	Female	21.15	1.88	0.29	0.34	0.34
i_8	Female	**1.12**	1.25	**0.05**	**0.05**	**0.05**

Example: Sex classification

Person	height (feet)	weight (lbs)	foot size(inches)
sample	6	130	8

- Weighted k-NN
- weight: 1/(d+1)
- Labels: male=-1 and female=1
- Euclidean
  - 2-NN:
    - $\frac{1}{0.05+1} * 1 + \frac{1}{0.1+1} * (-1) = 0{,}04$
  - 3-NN: 0.91
  - 4-NN: 0.12
- Gower:
  - 2-NN: 0.06
  - 3-NN: 0.89
  - 4-NN: 0.11
- All females

	Class	Normalized Euclidean	Gower
i_1	Male	0.31	0.32
i_2	Male	**0.284**	**0.27**
i_3	Male	**0.28**	**0.28**
i_4	Male	**0.10**	**0.12**
i_5	Female	0.49	0.65
i_6	Female	**0.16**	**0.19**
i_7	Female	0.29	0.34
i_8	Female	**0.05**	**0.05**

Example: Sex classification

Person	height (feet)	weight (lbs)	foot size(inches)
sample	6	130	8

- Weighted k-NN
- weight: 1/(d+1) or (1-d)
- Labels: male=-1 and female=1

	1/(d+1)		1-d	
	Euclidean	Gower	Euclidean	Gower
2-NN	0.04	0.06	0.05	0.07
3-NN	0.91	0.89	0.89	0.88
4-NN	0.12	0.11	0.27	0.15

	Class	Normalized Euclidean	Gower
i_1	Male	0.31	0.32
i_2	Male	0.284	**0.27**
i_3	Male	**0.28**	0.28
i_4	Male	**0.10**	**0.12**
i_5	Female	0.49	0.65
i_6	Female	**0.16**	**0.19**
i_7	Female	0.29	0.34
i_8	Female	**0.05**	**0.05**

- All females

R

- Naïve Bayes
  - Naivebayes from library e1071
- kNN
  - knn, knn.cv from class library
  - Knn.dist , knn.predict from KODAMA library
  - Train(“knn”) caret library
  - kNN from VIM library

  - Dummy variables for categorical and then treat as numierical?

Generalization error

To have an honest estimate of the error rate it must be computed on an independent data different from the training set. Called *test data* or *hold-out data* Then, it is called the ***Generalization error***

Let be a model: $\hat{y} = f(X, w)$

- f represents a class of functions to predict y
- X is the matrix of explanatory variables
- w represents the coefficients of the model

Generalization error (=Loss function): $L\left(y, f(X, w)\right)$

= Expected loss with independent data

$= \left[y - \hat{y}\right]^2$ (if regression)

$= \left[y \neq \hat{y}\right]$ (if classification)

$$Risk_{theoretical} = E\left[L\right] = \int L(y, f(X, w))dP(X, y)$$

Empirical Generalization error

Generalization error in the training:

$$Risk_{learn} = \frac{1}{n}\sum L(y, f(X, w))$$

If computed in the learning data we call it $Risk_{learn}$

What we expect from $Risk_{learn}$?
if $n \to \infty$

- If regression: $\frac{\sum (y - f(X, w))^2}{n}$
- If classification: *percentage of misclassified* (error rate)

$$\frac{\sum (y \neq f(X, w))}{n}$$

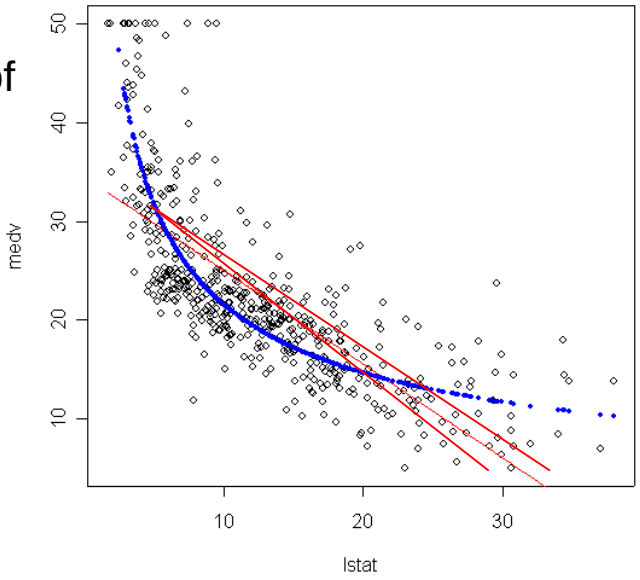
Components of the generalization error

Components of the Risk (Generalization Error) in regression:

$$GE(\hat{y}) = E\left[y_0 - \hat{y}_0\right]^2 = E\left[\hat{y}_0 - r(x_0)\right]^2 + \sigma_0^2 = \sigma_0^2 + \mathrm{var}(\hat{y}_0) + \left(E\left[\hat{y}_0\right] - r(x_0)\right)^2$$

Risk = Generalization (Prediction) Error

1. **Random fluctuation** of the phenomenon (deviation of the actual data respect to the true model due to multiple small and unknown causes)
2. **Variance** of fit (deviation of the prediction trained model respect to its average, i.e. with another sample we would obtained a different fit)
3. **Bias** (deviation of the true model respect to the average prediction of the trained model)

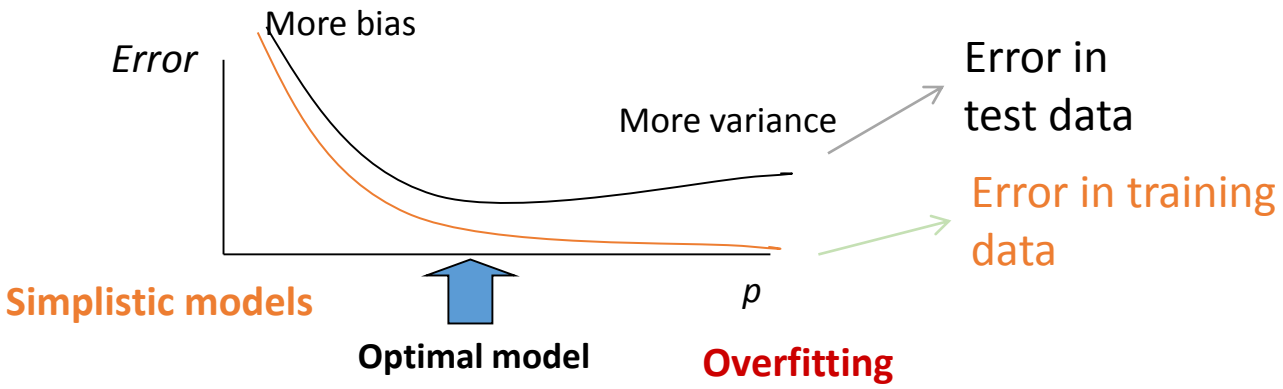


Trade off of the generalization error

$$GE(\hat{y}) = E\left[y_0 - \hat{y}_0\right]^2 = \sigma_0^2 + \mathrm{var}(\hat{y}_0) + \left(E\left[\hat{y}_0\right] - r(x_0)\right)^2$$

The GE depends on the complexity of the model
With *p* predictors we have 2^p-1 posible models

Trade-off between bias and variance



Components of bias:

Bad specification of the classifier function *r*
Not including all the relevant predictors in the model

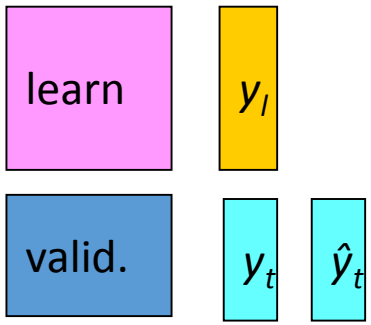
Components of prediction variance:

Complexity of the model

Finding the optimal model for prediction: Validation sample

To obtain reliable estimations we need to estimate it applying the model in an ***independent*** sample, from the one used to estimate the model, i.e. we divide the learning sample in two parts (learn and validation).
Instead of the *GE*, we can compute the R^2 (if regression).

Validation sample



$$GE_{valid}(\hat{y}) = \frac{1}{n_{valid}} \sum_{i=1}^{n_{test}} (y_i^{valid} - \hat{y}_i^{valid})^2$$

$$R^2_{valid} = 1 - \frac{GE_{valid}(\hat{y})}{\frac{1}{n_{valid}} \sum_{i=1}^{n_{valid}} (y_i^{valid} - \bar{y}^{valid})^2}$$

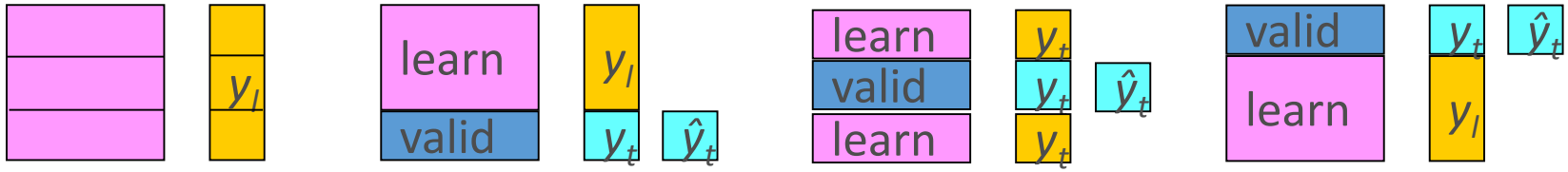
We split the available data in two parts at random, one used for learning (2/3) the other used to validate the model (1/3).

Evaluation of the generalization error in **R** with a validation sample

```
> ypred = predict(l1, data=dd.valid)
> 1-(sum((ypred-yvalid)^2)/sum((yvalid-mean(yvalid))^2))
```

Finding the optimal model for prediction: Cross-validation

We split the learning data in *k* parts at random



$$GE_{cv}(\hat{y}) = PRESS = \frac{1}{n}\sum_{k=1}^{R}\sum_{i\in k}(y_i^{valid} - \hat{y}_{-i}^{valid})^2$$

$$R^2_{cv} = 1 - \frac{GE_{cv}(\hat{y})}{\frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

$$MGE_{CV}(\hat{y}) = \frac{1}{n}PRESS = \frac{1}{n}\sum_{i=1}^{n}\left(e_i \big/ (1-h_{ii})\right)^2$$

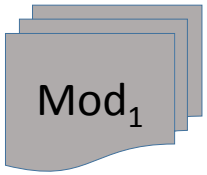
LOO (leave one out crossvalidation) each individual is a part, *k=n*

```
> n      = length(medv)
> ECMPcv = sum((l1$residuals/(1-ls.diag(l1)$hat))^2)/n
> R2cv   = 1 - ECMPcv*n/(var(medv)*(n-1))
> R2cv
```

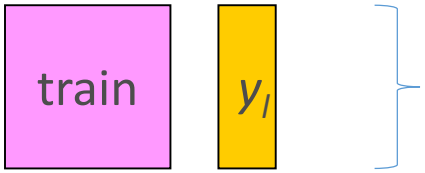
The process of modeling

1. Selecting the optimal model

Competing models:



Define for each model the best parameters with the training data



Selection of the optimal model:

- Crossvalidation
- Validation sample
- Likelihood penalization for complexity: AIC, BIC.

2. Estimation of the optimal model

Estimation of the selected optimal model in the whole training data

3. Computing honest estimates of the goodness of the model

Estimation of quality measures (error rate, …) in the test data