Machine Learning
Decision Trees, Neural Networks and nonparametric Methods

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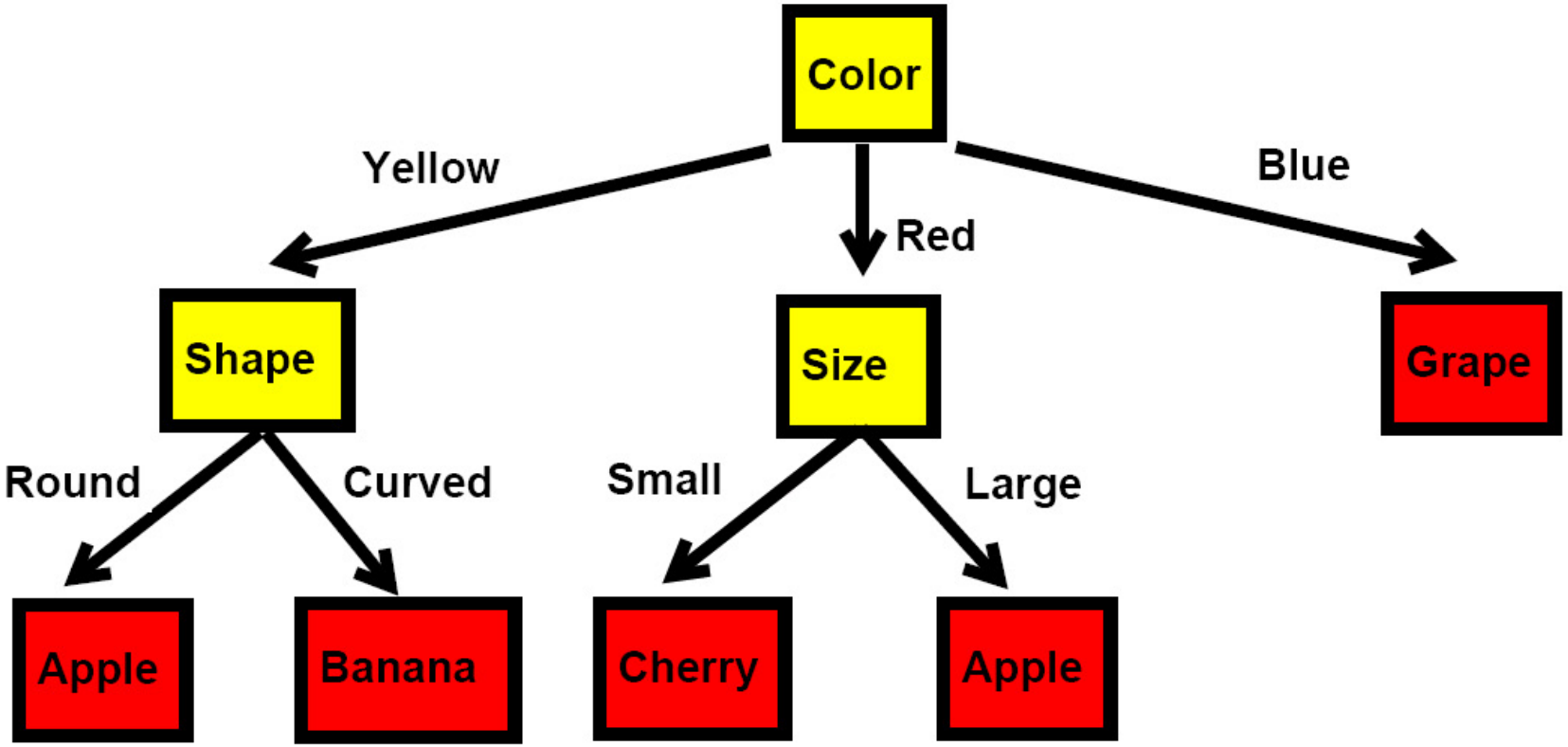
Roadmap of today and wednesday

Classification methods:

- Boosting (how to get a good classifier from a set of simple ones)
- **Decision Trees**,
- **Neural Networks**,
- **Nearest Neighbor Methods, Parzen-Window**,

(Binary) Decision trees



Properties and questions:

- Designed for categorical features (but real-valued ones are possible),
- How to grow the tree, when to stop and how to prune the tree?

Decision trees II

Why binary trees ?

Any tree can be rewritten in terms of a binary tree.

What is the binary decision if we have a group of attributes ?

We partition the group of attributes into two sets.

What is the binary decision for real-valued features ?

A simple split of the coordinate.

How to classify a node ?

Let $p_N(k)$ be the fraction of training points at node N of class k.

$\Longrightarrow$ Classification by majority vote: $f(N) = \underset{k=1,\ldots,K}{\arg\max}\, p_N(k)$.

How to grow a decision tree ?

- Measures of **node impurity** $I(N)$ of node N,

$$\text{Entropy:} \qquad I(N) = -\sum_{k=1}^{K} p_N(k) \log p_N(k),$$

$$\text{Gini Index:} \qquad I(N) = \sum_{k \neq l} p_N(k) p_N(l),$$

$$\text{Zero one loss:} \qquad I(N) = 1 - \max_{k=1,\ldots,K} p_N(k).$$

- Determine for each feature the best split by minimizing

$$\frac{N_L}{N} I(N_L) + \frac{N_R}{N} I(N_R)$$

- Take the feature and the corresponding split with minimal impurity.

Decision trees IV

When to stop ?

- cross validation,
- minimal decrease in impurity or minimal number of training points in each node.

Alternative: grow the tree until each leaf is maximal pure, then prune it.

How to prune ?

- collapse successively the pair of leafs which leads to a minimal increase of the complexity criterion

$$\sum_{i=1}^{|T|} N_i \, I(N_i) + \alpha |T|.$$

- choose α by cross validation.

Many variants: ID3, C4.5, CART - works also for regression.

Decision trees V

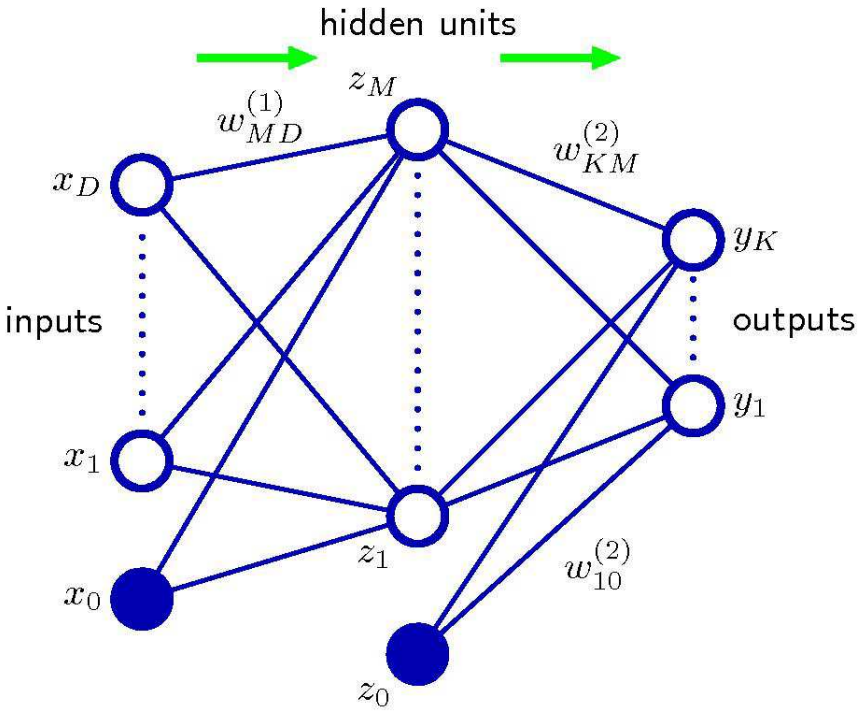
Pro

- if tree is small allows an easy interpretation (simple rules),
- very fast classifiers (real-time performance).

Contra

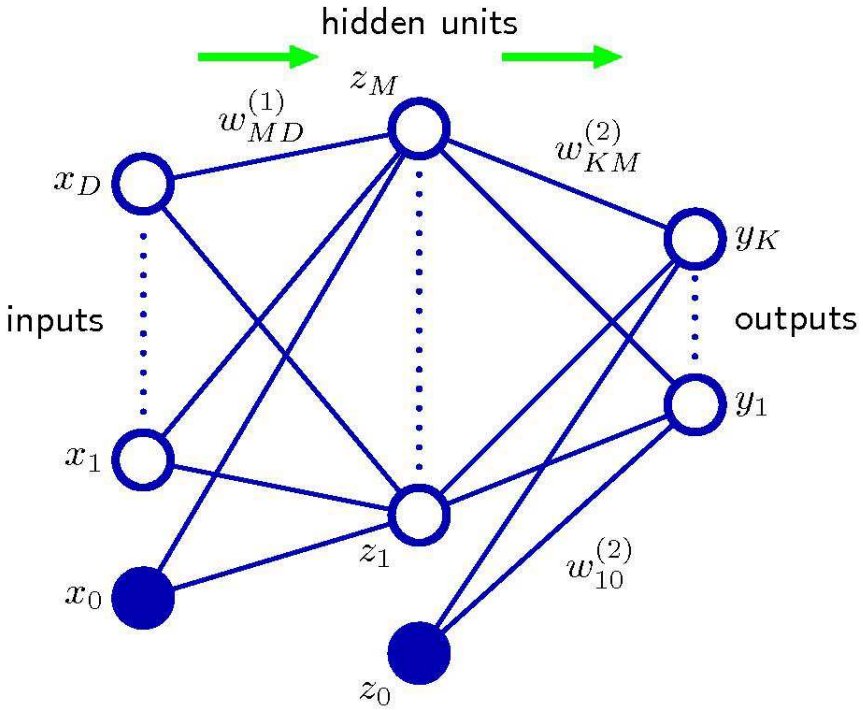
- often bad accuracy (the larger the tree (possibly better accuracy), the less interpretable),
- tree construction is quite unstable (greedy procedure),
- complex decision boundaries are difficult to model,
- forward/backward selection of features - no joint model.

What is a neural network ?



- **Input:** D features (real-valued),
- **Output:** K classes,

What is a neural network ? parameterized function model



- **Input:** D features (real-valued),
- **Output:** K classes,
- **Hidden layer:** M units.

$$f_k(x, w) = \sigma\Big(\sum_{j=1}^{M} w^{(2)}_{kj}\,\sigma\Big(\sum_{i=1}^{D} w^{(1)}_{ji} x_i + w^{(1)}_{j0}\Big) + w^{(2)}_{k0}\Big).$$

Parameters of a neural network

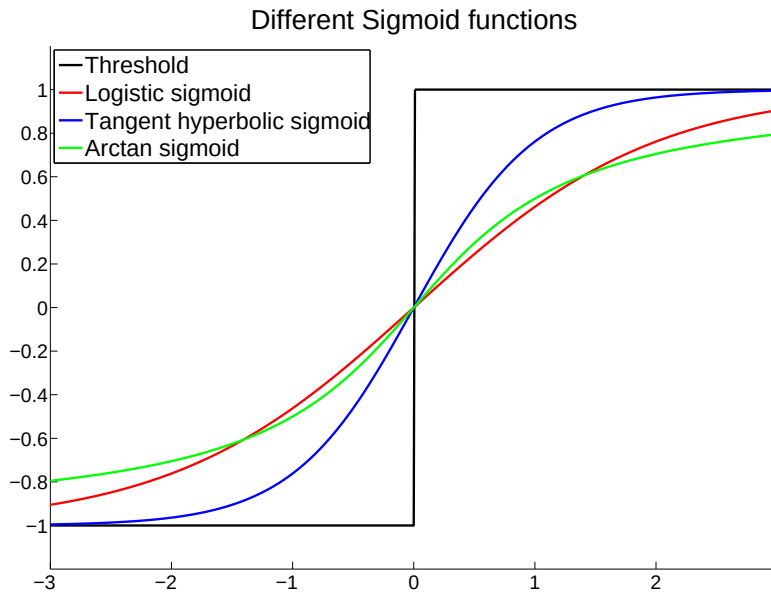
- Number of hidden layers L,
- Number of hidden units for each hidden layer M_l,
- choice of the sigmoid or activation function σ,

$$\text{threshold: } \sigma(x) = \begin{cases} 1 & \text{if } x > 0, \\ -1 & \text{if } x \leq 0. \end{cases}$$

$$\text{logistic sigmoid: } \quad \sigma(x) = \frac{1 - e^{-x}}{1 + e^{x}},$$

$$\text{tangent hyp.: } \quad \sigma(x) = \tanh(x),$$

$$\text{arctan sigmoid: } \quad \sigma(x) = \frac{2}{\pi} \arctan(x).$$



Objective function of a neural network

- **Common loss functions:** squared loss or so called cross-entropy,
- **Regularization:** penalty on the weights (often squared L_2-norm).

Objective $F(w)$ could look like this,

$$F(w) = \frac{1}{n}\sum_{i=1}^{n} \|f(X_i, w) - Y_i\|^2 + \lambda \sum_{l=1}^{L}\sum_{j=1}^{M_l}\sum_{i=1}^{M_{l-1}} {w^{(l)}}_{ji}^2,$$

where the label of each training input Y_i is a k-dimensional vector,

$$Y_{ij} = 1, \text{ if } j \text{ is the true label of } X_i, \text{ and } Y_{ij} = -1 \text{ else.}$$

$\Longrightarrow$ **Complicated non-convex optimization problem !**

$$w_{ij}^l = w_{ij}^l + \gamma\, \Delta w_{ij}^l.$$

- gradient descent $\Longrightarrow$ backpropagation (chain rule to compute gradient),
- stepsize of descent step $\Longrightarrow$ learning rate γ.

Some theory for neural networks

Results for two classes: $K = 2$.

Theorem

Let $\mathcal{F}_k$ be the set of all functions which can be represented by a neural network with one hidden layer with k units and an arbitrary, monotonically increasing sigmoid function $\sigma(x)$. Then

$$\lim_{k \to \infty} \inf_{f \in \mathcal{F}_k} R(f) = R^*.$$

Conclusion:

- Neural networks can represent any function in the limit of infinite hidden units (same result holds for SVM with Gaussian kernel for $n \to \infty$),
- Is the function class used by neural networks better suited for problems in nature than kernel expansions ("deep versus shallow methods") ?
- Since the optimization is non-convex only convergence to local minima is guaranteed and theoretical analysis considers the global

Biological motivation of neural networks

Biology:

- Neurons cause other neurons to fire (**activation** of other neurons). All-or-none principle (either fires or not).
- Neural network tries to model sensory input, **but:** only V1 (visual cortex) is well understood, understanding of higher order activity is poor.
- Only in recent years multiple neurons are recorded in order to understand the interaction of neurons in the (monkey) brain.

Comments:

- It is very interesting to understand how the brain works !
- Neural networks are a very coarse approximation of the brain,
- Biological plausibility is o.k. if method has well-founded statistical and mathematical foundation.

$\Longrightarrow$ **Neural networks are nested parameterized function classes !**

Summary of neural networks

Pro

- heavily used in industry - currently again a hype topic
- has a well-founded theoretical underpinning independent of the biological motivation,
- dependent of the number of hidden layers and units can still be reasonably fast at test time.

Contra

- difficult to train (slow convergence and local minima) but recent improvements,
- design of network (number of hidden units, layers) requires expert knowledge,
- too many free parameters.
- generalization to non-linear input spaces seems difficult.

Nearest neighbor methods

What is a nearest neighbor method ?

Classify or estimate the function value of a test point based on the nearest neighbors in the training set.

Properties:

- one of the most simple and oldest classification method,
- despite its simplicity it often yields reasonable performance,
- no training required - testing is more expensive,
- well studied theory - many variants of such classifiers,
- very flexible - can be applied to any kind of data !

Nearest neighbor methods II

What is a nearest neighbor method ?

Let $X_{(1)}, \ldots, X_{(k)}$ be the k training points which have the smallest distance to the given test point x, $w(x)_{(i)}$ the associated positive weights and $Y_{(1)}, \ldots, Y_{(k)}$ their corresponding label.

- **Classification**

$$f(x) = \begin{cases} 1, & \text{if } \operatorname{sign}(\sum_{i=1}^{k} w(x)_i Y_i) > 0, \\ -1, & \text{else.} \end{cases}$$

Simple: $w(x)_i = 1 \Longrightarrow$ majority vote - use odd values of k to avoid ties.

- **Regression:**

$$f(x) = \frac{\sum_{i=1}^{k} w(x)_i Y_i}{\sum_{i=1}^{k} w(x)_i}.$$

$\Longrightarrow$ simple weighted average - but choice of the weights $w(x)_i$ and the number of neighbors can significantly influence the result.

Nearest neighbor method - Classification

Classification in Euclidean space

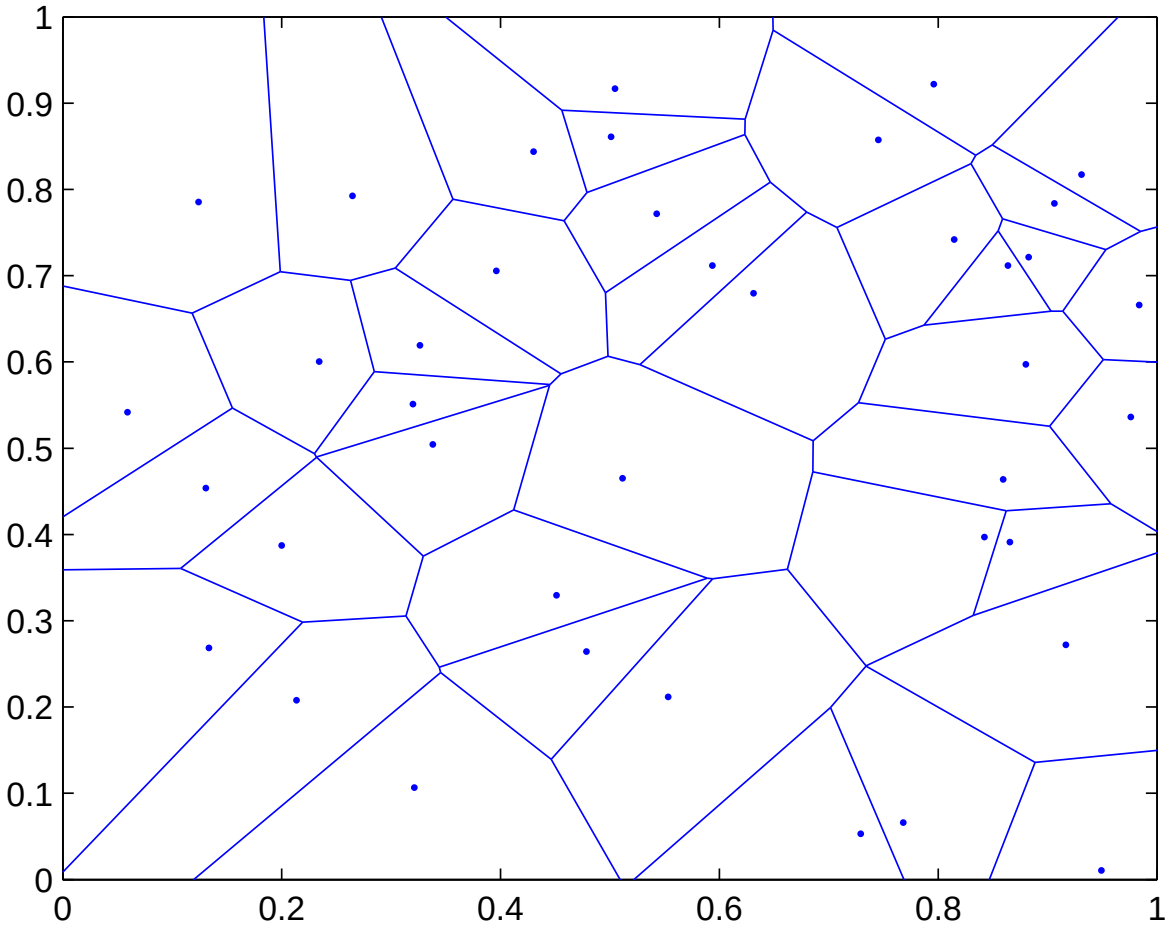
$$f(x) = \begin{cases} 1, & \text{if } \operatorname{sign}(\sum_{i=1}^{k} w(x)_i Y_i) > 0, \\ -1, & \text{else.} \end{cases}$$

Choices for the weights:

- Gaussian weights $w(x)_i = e^{-\lambda \left\| x - X_{(i)} \right\|^2} \Longrightarrow \lambda$ is determined by cross-validation (problems if high- and low density regions vary),
- Adaptive Gaussian weights $w(x)_i = e^{-\frac{\left\| x - X_{(i)} \right\|^2}{r_k^2}}$, where $r_k = \left\| x - X_{(k)} \right\|$ is the distance of the k-nearest neighbor.

Multi-class Extension: Classify test point by majority vote using the labels of the k nearest neighbors - break ties either randomly (no weights) or use weights for each point.

Nearest neighbor - Voronoi diagram



The Voronoi-diagram shows the influence region for each point corresponding to the nearest neighbor.

Theoretical results for nearest neighbor classification

Theorem

Let R_n be the classification error made by the k-nearest neighbor classifier in $\mathbb{R}^d$. Assume that X has a density with respect to the Lebesgue measure. If $k \to \infty$, $k/\log n \to \infty$ and $k/n \to 0$, then for every $\varepsilon > 0$ there exists an n_0 such that for $n \geq n_0$,

$$\mathrm{P}(R_n - R^* > \varepsilon) \leq 2\, e^{-\frac{n\varepsilon^2}{72\gamma_d^2}},$$

where γ_d is a constant depending only on the dimension.

Basic idea:

- as $k \to \infty$ and $k/n \to 0$, we have $r_k \to 0$.
- One averages over decreasing neighborhoods and since $k \to \infty$ the majority vote converges to $\arg\max_{m=1,\ldots,K} \mathrm{P}(Y = m | X = x)$.
- note that any rate for k faster than $\log n$ is sufficient to get convergence.

Theoretical results for nearest neighbor classification II

What happens when we keep k fixed and $n \to \infty$? One can compute the asymptotic error

$$R_{kNN} = \lim_{n \to \infty} R_n,$$

for a k nearest neighbor classifier with fixed k as

- $R_{1NN} = 2\,\mathbb{E}[\mathrm{P}(Y = 1|X)(1 - \mathrm{P}(Y = 1|X)],$
- $R_{3NN} = \mathbb{E}\Big[\mathrm{P}(Y = 1|X)\big[(1 - \mathrm{P}(Y = 1|X)) + 4(1 - \mathrm{P}(Y = 1|X))^2\big]\Big]$

Reminder: the Bayes error

$$R^* = \mathbb{E}_X[\min\{\mathrm{P}(Y = 1|X), \mathrm{P}(Y = -1|X)\}],$$

We have

$$\begin{aligned} R_{1NN} &= 2\,\mathbb{E}[\mathrm{P}(Y = 1|X)\mathrm{P}(Y = -1|X)] \\ &= 2\,\mathbb{E}[\min\{\mathrm{P}(Y = 1|X), \mathrm{P}(Y = -1|X)\}\max\{\mathrm{P}(Y = 1|X), \mathrm{P}(Y = -1| \\ &\leq 2\,\mathbb{E}[\min\{\mathrm{P}(Y = 1|X), 1 - \mathrm{P}(Y = 1|X)\}] = 2\,R^* \end{aligned}$$

Metric space

Metric spaces:

Definition

A **metric space** is a set $\mathcal{X}$ with a distance function $d : \mathcal{X} \times X \to \mathbb{R}$ such that:

- $d(x, y) \geq 0$,
- $d(x, y) = 0$ if and only if $x = y$,
- $d(x, y) = d(y, x)$, (symmetry)
- $d(x, y) \leq d(x, z) + d(z, y)$. (triangle inequality)

It is denoted as $(\mathcal{X}, d)$.

- We can define nearest neighbor classifier on any metric space !
- **More general:** we can define nearest neighbor classifier for any set with a similarity function (instead of nearest neighbors take **most similar points**).

Examples of distances

Examples of distances on $\mathbb{R}^d$:

- For $x, y \in \mathbb{R}^d$, use $d(x,y) = \|x-y\|_p = \left(\sum_{i=1}^d (x_i - y_i)^p\right)^{\frac{1}{p}}$, with the extreme case $p = \infty$,

$$d(x,y) = \|x-y\|_\infty = \max_{1 \leq i \leq d} |x_i - y_i|.$$

- Mahalanobis distance - a weighted Euclidean distance,

$$d(x,y) = \left(\sum_{i,j=1}^d A_{ij}(x_i - y_i)(x_j - y_j)\right)^{\frac{1}{2}} = \sqrt{\langle x-y, A(x-y)\rangle},$$

where A is a positive-definite matrix,

Distance on the sphere in $\mathbb{R}^d$:

$$d(x,y) = \arccos(\langle x, y\rangle).$$

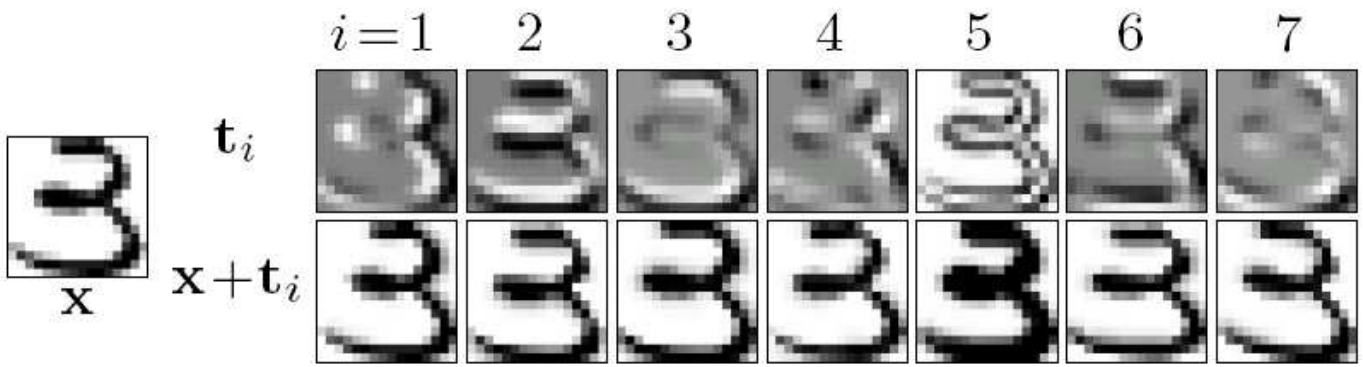
The famous cosine measure in text classification is a similarity measure !

Tangent distance

A dissimilarity measure designed for a particular application

small changes of digit images $\Longrightarrow$ label does not change !

but: Euclidean distance changes dramatically !



Degrees of freedom:

- **Geometric transformations:** 1+2) translation, 3) scaling, 4) rotation,
- **Application specific:** 5) line thickness, 6+7) shear.

Idea: build distance measure which is invariant under the transformations !

Tangent distance II

Definition of general tangent distance

Definition

Let x, y be two instances in $\mathcal{X}$ and $T(\alpha), T(\beta)$ be a group action G on $\mathcal{X}$,

$$T : \mathcal{X} \times \mathcal{G} \mapsto \mathcal{X}, \quad (x, \alpha) \to T(\alpha)x,$$

with which we want to be invariant. Then define the general tangent distance on $\mathcal{X}$ as,

$$d'(x, y) = \min_{\alpha,\beta \in G} d(T(\alpha)\, x, T(\beta)\, y),$$

where $d(x, y)$ is the original metric on $\mathcal{X}$.

- generally does not yield a metric (even if d is a metric !),
- the tangent distance minimizes usually only over group elements close to the identity (tangent elements),
- quite expensive to compute.

Nearest neighbor method - Regression

Regression:

$$f(x) = \frac{\sum_{i=1}^{k} w(x)_i Y_i}{\sum_{i=1}^{k} w(x)_i}.$$

For the specific choice of weights,

$$w(x)_i = k(\|x - X_i\| / h),$$

where $k : \mathbb{R}_+ \to \mathbb{R}$ satisfies

- $k(x)$ is monotonically decreasing,
- $k(x)$ is always positive,
- the number of neighbors k is equal to n.

then f is called the **Nadaraya-Watson estimator**,

$$f(x) = \frac{\sum_{i=1}^{n} k(\|x - X_i\| / h) Y_i}{\sum_{i=1}^{n} k(\|x - X_i\| / h)}.$$

Motivation of the Nadaraya-Watson estimator:

Proposition

The Nadaraya-Watson estimator $f(x)$ at x is the result of the following optimization problem,

$$f(x) = \arg\min_{c \in \mathbb{R}} \sum_{i=1}^{n} k(\|x - X_i\| / h)(Y_i - c)^2.$$

Proof: The Functional $F(c) = \sum_{i=1}^{n} k(\|x - X_i\| / h)(Y_i - c)^2$ is convex in c, and thus we find the minimizer by solving,

$$\frac{\partial F}{\partial c} = 2 \sum_{i=1}^{n} k(\|x - X_i\| / h)(Y_i - c) = 0.$$

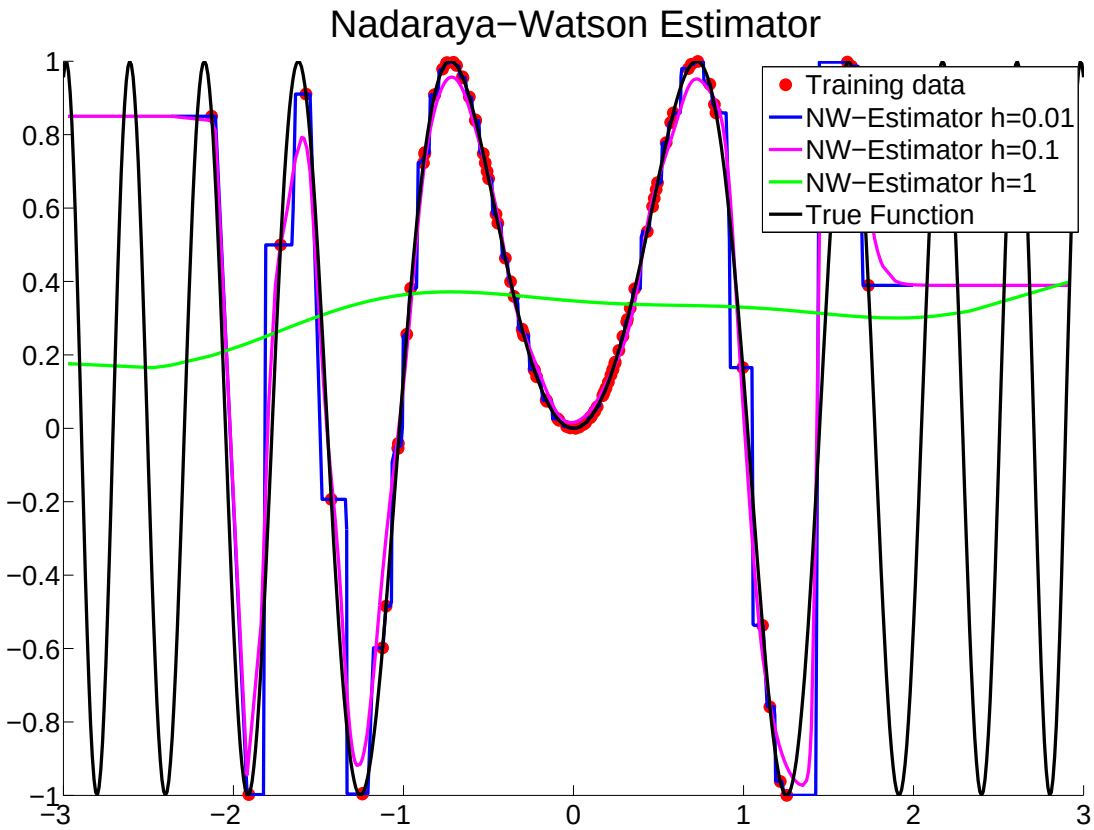
which yields,

$$c = \frac{\sum_{i=1}^{n} k(\|x - X_i\| / h) Y_i}{\sum_{i=1}^{n} k(\|x - X_i\| / h)}.$$

Parameters of the Nadaraya-Watson estimator:

h is the so called bandwidth and influences the smoothness of f,

$$f(x) = \frac{\sum_{i=1}^{n} k(\|x - X_i\| / h) Y_i}{\sum_{i=1}^{n} k(\|x - X_i\| / h)}.$$



Distances in high dimensions

Lemma

Let $x, y \in \mathbb{R}^d$ and $\epsilon_1, \epsilon_2 \sim N(0, \sigma^2)$ and define $X = x + \epsilon_1$ and $Y = y + \epsilon_2$, then

$$\mathbb{E}\,\|X - Y\|^2 = \|x - y\|^2 + 2\,d\,\sigma^2,$$
$$\mathrm{Var}\,\|X - Y\|^2 = 8\sigma^2\,\|x - y\|^2 + 8\,d\,\sigma^4.$$

Distances in high dimensions

Lemma

Let $x, y \in \mathbb{R}^d$ *and* $\epsilon_1, \epsilon_2 \sim N(0, \sigma^2)$ *and define* $X = x + \epsilon_1$ *and* $Y = y + \epsilon_2$, *then*

$$\mathbb{E}\,\|X - Y\|^2 = \|x - y\|^2 + 2\,d\,\sigma^2,$$
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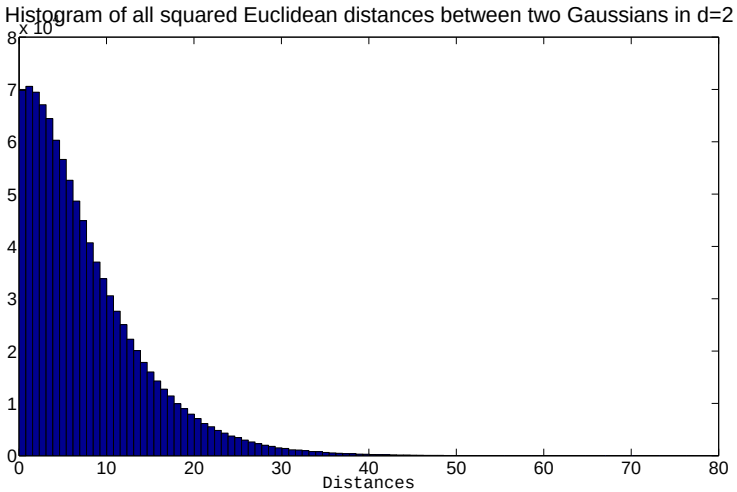
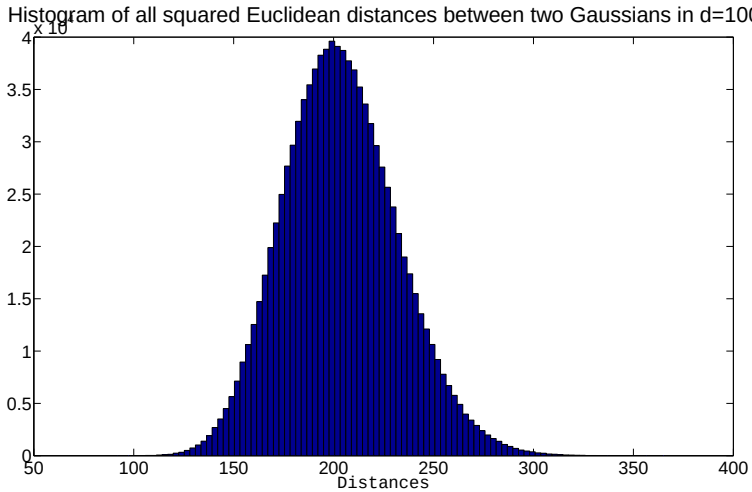
- Distances start to concentrate in high dimensions !
- All points have almost all the same distance.





Summary of nearest neighbor methods

Pro

- easy to understand,
- flexible, can be used with any user-specified similarity or distance,
- often competitive in performance,
- requires no training.

Contra

- Problems in high dimensions - distances are almost all equal,
- No interpretation,
- Slow at test time (but depends heavily on the dimension and the use of efficient data structures to compute the distances).