

Machine Learning

3. Nearest Neighbor and Kernel Methods

Lars Schmidt-Thieme

Information Systems and Machine Learning Lab (ISMLL)
Institute for Business Economics and Information Systems
& Institute for Computer Science
University of Hildesheim
<http://www.ismll.uni-hildesheim.de>

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim
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Machine Learning



1. Distance Measures

2. k -Nearest Neighbor Method

3. Parzen Windows

Motivation

So far, regression and classification methods covered in the lecture can be used for

- numerical variables,
- binary variables (re-interpreted as numerical), and
- nominal variables (coded as set of binary indicator variables).

Often one is also interested in more complex variables such as

- set-valued variables,
- sequence-valued variables (e.g., strings),
- . . .

Motivation

There are two kinds of approaches to deal with such variables:

feature extraction:

try to derive binary or numerical variables,
then use standard methods on the feature vectors.

kernel methods:

try to establish a distance measure between two variables,
then use methods that use only distances between objects
(but no feature vectors).

Distance measures

Let d be a **distance measure** (also called **metric**) on a set \mathcal{X} , i.e.,

$$d : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}_0^+$$

with

1. d is **positiv definite**: $d(x, y) \geq 0$ and $d(x, y) = 0 \Leftrightarrow x = y$

2. d is **symmetric**: $d(x, y) = d(y, x)$

3. d is **subadditive**: $d(x, z) \leq d(x, y) + d(y, z)$
(triangle inequality)

(for all $x, y, z \in \mathcal{X}$.)

Example: **Euclidean metric** on $\mathcal{X} := \mathbb{R}^n$:

$$d(x, y) := \left(\sum_{i=1}^n (x_i - y_i)^2 \right)^{\frac{1}{2}}$$

Minkowski Metric / L_p metric

Minkowski Metric / L_p metric on $\mathcal{X} := \mathbb{R}^n$:

$$d(x, y) := \left(\sum_{i=1}^n |x_i - y_i|^p \right)^{\frac{1}{p}}$$

with $p \in \mathbb{R}, p \geq 1$.

$p = 1$ (**taxicab distance; Manhattan distance**):

$$d(x, y) := \sum_{i=1}^n |x_i - y_i|$$

$p = 2$ (**euclidean distance**):

$$d(x, y) := \left(\sum_{i=1}^n (x_i - y_i)^2 \right)^{\frac{1}{2}}$$

$p = \infty$ (**maximum distance; Chebyshev distance**):

$$d(x, y) := \max_{i=1}^n |x_i - y_i|$$

Minkowski Metric / L_p metric / Example

Example:

$$x := \begin{pmatrix} 1 \\ 3 \\ 4 \end{pmatrix}, \quad y := \begin{pmatrix} 2 \\ 4 \\ 1 \end{pmatrix}$$

$$d_{L_1}(x, y) = |1 - 2| + |3 - 4| + |4 - 1| = 1 + 1 + 3 = 5$$

$$d_{L_2}(x, y) = \sqrt{(1 - 2)^2 + (3 - 4)^2 + (4 - 1)^2} = \sqrt{1 + 1 + 9} = \sqrt{11} \approx 3.32$$

$$d_{L_\infty}(x, y) = \max\{|1 - 2|, |3 - 4|, |4 - 1|\} = \max\{1, 1, 3\} = 3$$

Similarity measures

Instead of a distance measure sometimes **similarity measures** are used, i.e.,

$$\text{sim} : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}_0^+$$

with

- sim is symmetric: $\text{sim}(x, y) = \text{sim}(y, x)$.

Some similarity measures have stronger properties:

- sim is **discerning**: $\text{sim}(x, y) \leq 1$ and $\text{sim}(x, y) = 1 \Leftrightarrow x = y$
- $\text{sim}(x, z) \geq \text{sim}(x, y) + \text{sim}(y, z) - 1$.

Some similarity measures have values in $[-1, 1]$ or even \mathbb{R} where negative values denote “dissimilarity”.

Distance vs. Similarity measures

A discerning similarity measure can be turned into a semi-metric (pos. def. & symmetric, but not necessarily subadditive) via

$$d(x, y) := 1 - \text{sim}(x, y)$$

In the same way, a metric can be turned into a discerning similarity measure (with values eventually in $] - \infty, 1]$).

Cosine Similarity

The angle between two vectors in \mathbb{R}^n is used as similarity measure: **cosine similarity**:

$$\text{sim}(x, y) := \arccos\left(\frac{\langle x, y \rangle}{\|x\|_2 \|y\|_2}\right)$$

Example:

$$x := \begin{pmatrix} 1 \\ 3 \\ 4 \end{pmatrix}, \quad y := \begin{pmatrix} 2 \\ 4 \\ 1 \end{pmatrix}$$

$$\begin{aligned} \text{sim}(x, y) &= \arccos \frac{1 \cdot 2 + 3 \cdot 4 + 4 \cdot 1}{\sqrt{1 + 9 + 16} \sqrt{4 + 16 + 1}} = \arccos \frac{18}{\sqrt{26} \sqrt{21}} \\ &\approx \arccos 0.77 \approx 0.69 \end{aligned}$$

cosine similarity is not discerning as vectors with the same direction but of arbitrary length have angle 0 and thus similarity 1.

Distances for Nominal Variables

For binary variables there is only one reasonable distance measure:

$$d(x, y) := 1 - I(x = y) \quad \text{with } I(x = y) := \begin{cases} 1 & \text{if } x = y \\ 0 & \text{otherwise} \end{cases}$$

This coincides with the L_∞ distance for the indicator/dummy variables.

The same distance measure is useful for nominal variables with more than two possible values.

For hierarchical variables, i.e., a nominal variable with levels arranged in a hierarchy, there are more advanced distance measures (not covered here).

Distances for Set-valued Variables

For set-valued variables (which values are subsets of a set A) the **Hamming distance** often is used:

$$d(x, y) := |(x \setminus y) \cup (y \setminus x)| = |\{a \in A \mid I(a \in x) \neq I(a \in y)\}|$$

(the number of elements contained in only one of the two sets).

Example:

$$d(\{a, e, p, l\}, \{a, b, n\}) = 5, \quad d(\{a, e, p, l\}, \{a, e, g, n, o, r\}) = 6$$

Also often used is the similarity measure **Jaccard coefficient**:

$$\text{sim}(x, y) := \frac{|x \cap y|}{|x \cup y|}$$

Example:

$$\text{sim}(\{a, e, p, l\}, \{a, b, n\}) = \frac{1}{6}, \quad \text{sim}(\{a, e, p, l\}, \{a, e, g, n, o, r\}) = \frac{2}{8}$$

Distances for Strings / Sequences

edit distance / Levenshtein distance:

$d(x, y) :=$ minimal number of deletions, insertions or substitutions to transform x in y

Examples:

$$d(\text{man}, \text{men}) = 1$$

$$d(\text{house}, \text{spouse}) = 2$$

$$d(\text{order}, \text{express order}) = 8$$

Distances for Strings / Sequences

The edit distance is computed recursively. With

$$x_{1:i} := (x_{i'})_{i'=1,\dots,i} = (x_1, x_2, \dots, x_i), \quad i \in \mathbb{N}$$

we compute the number of operations to transform $x_{1:i}$ into $y_{1:j}$ as

$$c(x_{1:i}, y_{1:j}) := \min \left\{ \begin{array}{ll} c(x_{1:i-1}, y_{1:j}) + 1, & // \text{ delete } x_i, x_{1:i-1} \rightsquigarrow y_{1:j} \\ c(x_{1:i}, y_{1:j-1}) + 1, & // x_{1:i} \rightsquigarrow y_{1:j-1}, \text{ insert } y_j \\ c(x_{1:i-1}, y_{1:j-1}) + I(x_i \neq y_j) \end{array} \right\} // x_{1:i-1} \rightsquigarrow y_{1:j-1}, \text{ substitute } y_j \text{ for } x_i$$

starting from

$$\begin{array}{l} c(x_{1:0}, y_{1:j}) = c(\emptyset, y_{1:j}) := j // \text{ insert } y_1, \dots, y_j \\ c(x_{1:i}, y_{1:0}) = c(x_{1:i}, \emptyset) := i // \text{ delete } x_1, \dots, x_i \end{array}$$

Such a recursive computing scheme is called **dynamic programming**.

Distances for Strings / Sequences

Example: compute $d(\text{excused}, \text{exhausted})$.

<i>d</i>	9								
<i>e</i>	8								
<i>t</i>	7								
<i>s</i>	6								
<i>u</i>	5								
<i>a</i>	4								
<i>h</i>	3								
<i>x</i>	2								
<i>e</i>	1								
	0	1	2	3	4	5	6	7	
$y[j]/x[i]$		<i>e</i>	<i>x</i>	<i>c</i>	<i>u</i>	<i>s</i>	<i>e</i>	<i>d</i>	

Distances for Strings / Sequences

Example: compute $d(\text{excused}, \text{exhausted})$.

<i>d</i>	9	8	7	7	6	5	4	3	
<i>e</i>	8	7	6	6	5	4	3	4	
<i>t</i>	7	6	5	5	4	3	3	4	
<i>s</i>	6	5	4	4	3	2	3	4	
<i>u</i>	5	4	3	3	2	3	4	5	
<i>a</i>	4	3	2	2	2	3	4	5	
<i>h</i>	3	2	1	1	2	3	4	5	
<i>x</i>	2	1	0	1	2	3	4	5	
<i>e</i>	1	0	1	2	3	4	5	6	
	0	1	2	3	4	5	6	7	
$y[j]/x[i]$		<i>e</i>	<i>x</i>	<i>c</i>	<i>u</i>	<i>s</i>	<i>e</i>	<i>d</i>	

Distances for Strings / Sequences

Example: compute $d(\text{excused}, \text{exhausted})$.

<i>d</i>	9	8	7	7	6	5	4	3
<i>e</i>	8	7	6	6	5	4	3	4
<i>t</i>	7	6	5	5	4	3	3	4
<i>s</i>	6	5	4	4	3	2	3	4
<i>u</i>	5	4	3	3	2	3	4	5
<i>a</i>	4	3	2	2	2	3	4	5
<i>h</i>	3	2	1	1	2	3	4	5
<i>x</i>	2	1	0	1	2	3	4	5
<i>e</i>	1	0	1	2	3	4	5	6
	0	1	2	3	4	5	6	7
$y[j]/x[i]$		<i>e</i>	<i>x</i>	<i>c</i>	<i>u</i>	<i>s</i>	<i>e</i>	<i>d</i>

1. Distance Measures

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Neighborhoods

Let d be a distance measure.

For a dataset

$$D \subseteq X \times Y$$

and $x \in X$ let

$$D = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$$

be an enumeration with increasing distance to x , i.e., $d(x, x_i) \leq d(x, x_{i+1})$ (ties broken arbitrarily).

The first $k \in \mathbb{N}$ points of such an enumeration, i.e.,

$$N_k(x) := \{(x_1, y_1), (x_2, y_2), \dots, (x_k, y_k)\}$$

are called a **k -neighborhood** of x (in D).

Nearest Neighbor Regression

The **k -nearest neighbor regressor**

$$\hat{Y}(x) := \frac{1}{k} \sum_{(x', y') \in N_k(x)} y'$$

The **k -nearest neighbor classifier**

$$\hat{p}(Y = y | x) := \frac{1}{k} \sum_{(x', y') \in N_k(x)} I(y = y')$$

and then predict the class with maximal predicted probability

$$\hat{Y}(x) := \operatorname{argmax}_{y \in \mathcal{Y}} \hat{p}(Y = y | x)$$

i.e., the majority class w.r.t. the classes of the neighbors.

Decision Boundaries

For 1-nearest neighbor, the predictor space is partitioned in regions of points that are closest to a given data point:

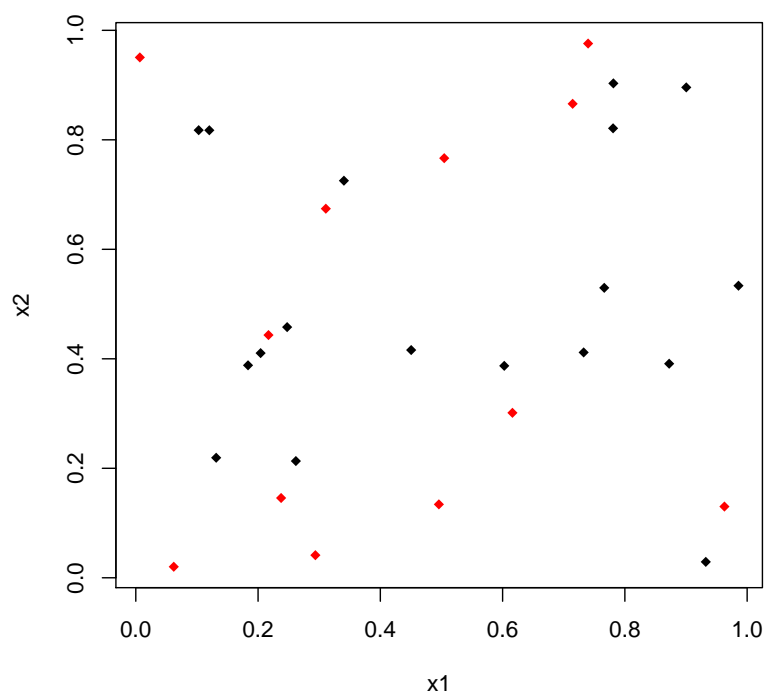
$$\text{region}_D(x_1), \text{region}_D(x_2), \dots, \text{region}_D(x_n)$$

with

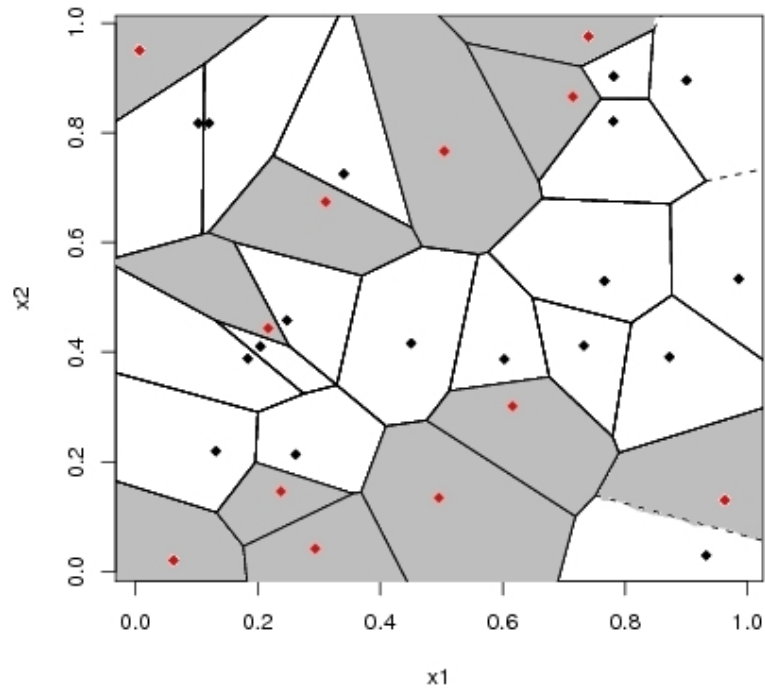
$$\text{region}_D(x) := \{x' \in \mathcal{X} \mid d(x', x) \leq d(x', x'') \quad \forall (x'', y'') \in D\}$$

These regions often are called **cells**, the whole partition a **Voronoi tessellation**.

Decision Boundaries



Decision Boundaries



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Expected error

To assess the quality of a classifier $\hat{y}(x)$, one can use the **expected error**, i.e., the probability to predict the wrong class if cases are picked at random:

$$p(\text{error}) = E(I(y \neq \hat{y})) = \int_{\mathcal{X}} I(y \neq \hat{y}) dx = \int_{\mathcal{X}} (1 - p(Y = \hat{y}(x) | x)) p(x) dx$$

Bayes Classifier

The minimal expected error can be achieved, if for each point x the class y with the largest conditional probability $p(y | x)$ is predicted, i.e.,

$$y^*(x) := \operatorname{argmax}_{y \in \mathcal{Y}} p(y | x)$$

This classifier is called **Bayes classifier** y^* , its error **Bayes error** $p^*(\text{error})$.

The Bayes classifier assumes the ideal case that the conditional class probabilities $p(Y | X)$ are known.

Bayes error

In the case of a deterministic dependency of y on x , i.e., for each x there is an y with $p(y | x) = 1$, the Bayes error is

$$p^*(\text{error}) = 0$$

In the case that for each x there is a uniform distribution of the classes y , i.e., for k classes $p(y | x) = 1/k$ for all y , the Bayes error is maximal

$$p^*(\text{error}) = \frac{k-1}{k}$$

Error rate for nearest-neighbor rule (Cover and Hart 1967)

If we have unlimited data, the error rate of the nearest neighbor classifier is bound as follows:

$$p^*(\text{error}) \leq \lim_{n \rightarrow \infty} p_n(\text{error}) \leq p^*(\text{error}) \left(2 - \frac{k}{k-1} p^*(\text{error})\right)$$

where $p_n(\text{error})$ denotes the error rate for the nearest neighbor classifier in a sample of n points.

Roughly spoken “at least half of the classification information in an infinite data set resides in the nearest neighbor” (Duda et al. 2001).

Error rate for nearest-neighbor rule / proof

A strict proof of the error bounds is not so easy. A more informal argument is as follows (cf. Duda et al. 2001, p. 179–182):

For x_0 denote by x'_n the nearest neighbor of x_0 in a sample of n points.

$$p_n(\text{error}|x_0, x'_n) = 1 - \sum_y p(y_0 = y, y'_n = y|x_0, x'_n) = 1 - \sum_y p(y_0 = y|x_0)p(y'_n = y|x'_n)$$

$$\begin{aligned} \lim_{n \rightarrow \infty} p_n(\text{error}|x_0) &= \lim_{n \rightarrow \infty} \int p_n(\text{error}|x_0, x'_n) p(x'_n|x_0) dx'_n \\ &= \lim_{n \rightarrow \infty} \int \left(1 - \sum_y p(y_0 = y|x_0)p(y'_n = y|x'_n)\right) p(x'_n|x_0) dx'_n \\ &= \int \left(1 - \sum_y p(y_0 = y|x_0)p(y'_n = y|x'_n)\right) \delta(x'_n - x_0) dx'_n \\ &= 1 - \sum_y p(y_0 = y|x_0)^2 \end{aligned}$$

Error rate for nearest-neighbor rule / proof

Now let $y^*(x) := \operatorname{argmax}_y p(y|x)$ the Bayes classifier:

$$\begin{aligned} \sum_y p(y_0 = y|x_0)^2 &= p(y_0 = y^*(x_0)|x_0)^2 + \sum_{y \neq y^*(x_0)} p(y_0 = y|x_0)^2 \\ &\geq (1 - p^*(\mathbf{error}|x_0))^2 + \frac{1}{k-1} p^*(\mathbf{error}|x_0)^2 \\ &= 1 - 2p^*(\mathbf{error}|x_0) + \frac{k}{k-1} p^*(\mathbf{error}|x_0)^2 \end{aligned}$$

because the sum is minimal if all $p(y_0 = y|x_0)$ are equal, and thus

$$p(y_0 = y|x_0) = \frac{1}{k-1} (1 - p(y_0 = y^*(x_0)|x_0)) = \frac{1}{k-1} p^*(\mathbf{error}|x_0)$$

Error rate for nearest-neighbor rule / proof

Then we continue

$$\lim_{n \rightarrow \infty} p_n(\mathbf{error}|x_0) = 1 - \sum_y p(y_0 = y|x_0)^2 \leq 2p^*(\mathbf{error}|x_0) - \frac{k}{k-1} p^*(\mathbf{error}|x_0)^2$$

Now

$$\begin{aligned} \lim_{n \rightarrow \infty} p_n(\mathbf{error}) &= \lim_{n \rightarrow \infty} \int p_n(\mathbf{error}|x_0) p(x_0) dx_0 \\ &\leq \int (2p^*(\mathbf{error}|x_0) - \frac{k}{k-1} p^*(\mathbf{error}|x_0)^2) p(x_0) dx_0 \\ &= 2p^*(\mathbf{error}) - \frac{k}{k-1} \int p^*(\mathbf{error}|x_0)^2 p(x_0) dx_0 \end{aligned}$$

Error rate for nearest-neighbor rule / proof

And finally as

$$\begin{aligned} V(p^*(\mathbf{error})) &= \int (p^*(\mathbf{error}|x_0) - p^*(\mathbf{error}))^2 p(x_0) dx_0 \\ &= \int p^*(\mathbf{error}|x_0)^2 p(x_0) dx_0 - p^*(\mathbf{error})^2 \geq 0 \end{aligned}$$

$$\Rightarrow \int p^*(\mathbf{error}|x_0)^2 p(x_0) dx_0 \geq p^*(\mathbf{error})^2$$

we get

$$\begin{aligned} \lim_{n \rightarrow \infty} p_n(\mathbf{error}) &\leq 2p^*(\mathbf{error}) - \frac{k}{k-1} \int p^*(\mathbf{error}|x_0)^2 p(x_0) dx_0 \\ &\leq 2p^*(\mathbf{error}) - \frac{k}{k-1} p^*(\mathbf{error})^2 \end{aligned}$$

Complexity of k -Nearest Neighbor Classifier

The k -Nearest Neighbor classifier does not need any learning algorithm as it just stores all the training examples.

On the other hand, predicting using a k -nearest neighbor classifier is slow:

- To predict the class of a new point x , the distance $d(x, x_i)$ from x to each of the n training examples $(x_1, y_1), \dots, (x_n, y_n)$ has to be computed.
- If the predictor space is $\mathcal{X} := \mathbb{R}^p$, for one such computation we need $O(p)$ operations.
- We then keep track of the k points with the smallest distance.

So in total one needs $O(npk)$ operations.

Accelerations: partial distances

In practice, nearest neighbor classifiers often can be accelerated by several methods.

Partial distances:

Compute the distance to each training point x' only partially, e.g.,

$$d_r(x, x') := \left(\sum_{i=1}^r (x_i - x'_i)^2 \right)^{\frac{1}{2}}, \quad r \leq p$$

As d_r is non-decreasing in r , once $d_r(x, x')$ exceeds the k -th smallest distance computed so far, the training point x' can be dropped.

This is a heuristic:

it may accelerate computations, but it also may slow it down (as there are additional comparisons of the partial distances with the k smallest distance).

Accelerations: search trees

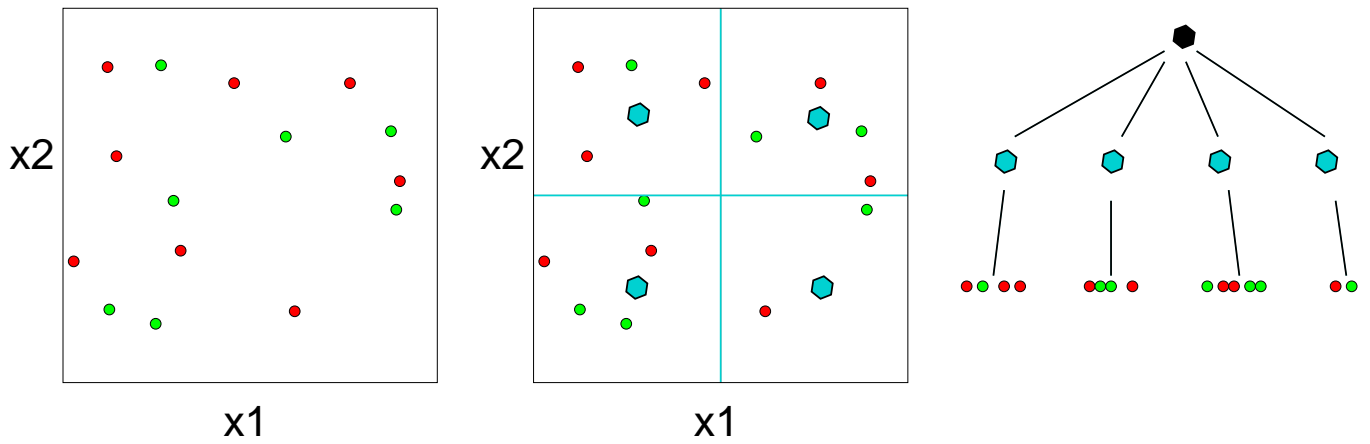
Search trees:

Do not compute the distance of a new point x to **all** training examples, but

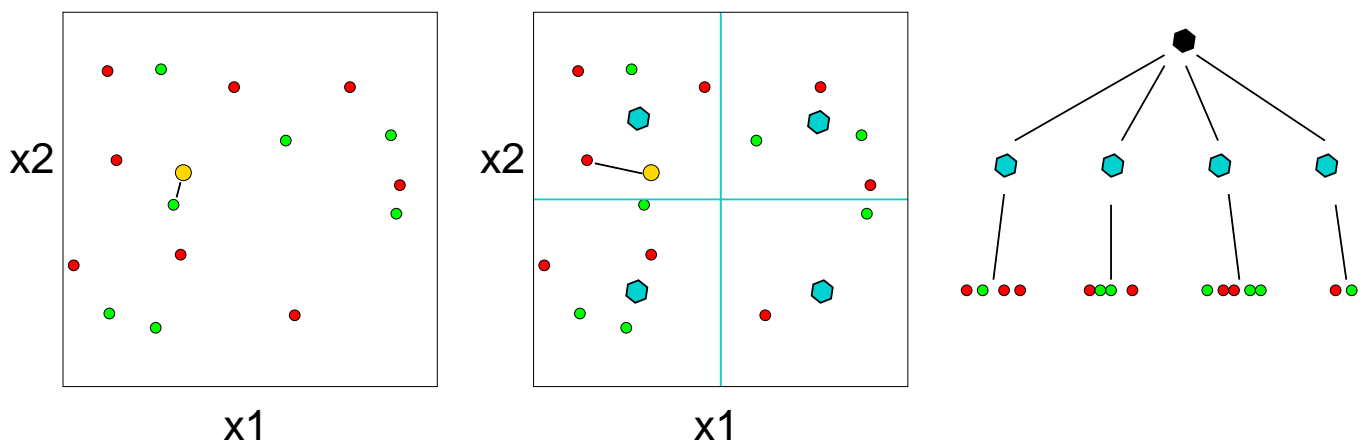
1. organize the training examples as a tree (or a DAG) with
 - sets of training examples at the leaves and
 - a prototype (e.g., the mean of the training examples at all descendent leaves) at each intermediate node.
2. starting at the root, recursively
 - compute the distance to all children of the actual node and
 - branch to the child with the smallest distance,
3. compute distances only to training examples in the leaf finally found.

This is an approximation.

Accelerations: search trees



Accelerations: search trees



Accelerations: editing

Editing / Pruning / Condensing:

shrink the set of training data points,

e.g., select a subset of the original training data points.

Example: remove all points with cells that are surrounded by cells of points of the same class.

$$X_{\text{edited}} := \{(x, y) \in X \mid \exists(x', y') \in X, R(x') \cap R(x) \neq \emptyset \text{ and } y' \neq y\}$$

This basic editing algorithms

- retains the decision function,
- has complexity $O(d^3 n^{\lfloor \frac{d}{2} \rfloor} \log n)$
(with $\lfloor x \rfloor := \max\{n \in \mathbb{N} \mid n < x\}$; Duda et al. 2001, p. 186).

See e.g., Ottmann/Widmayer 2002, p. 501–515 for computing Voronoi diagrams in two dimensions.

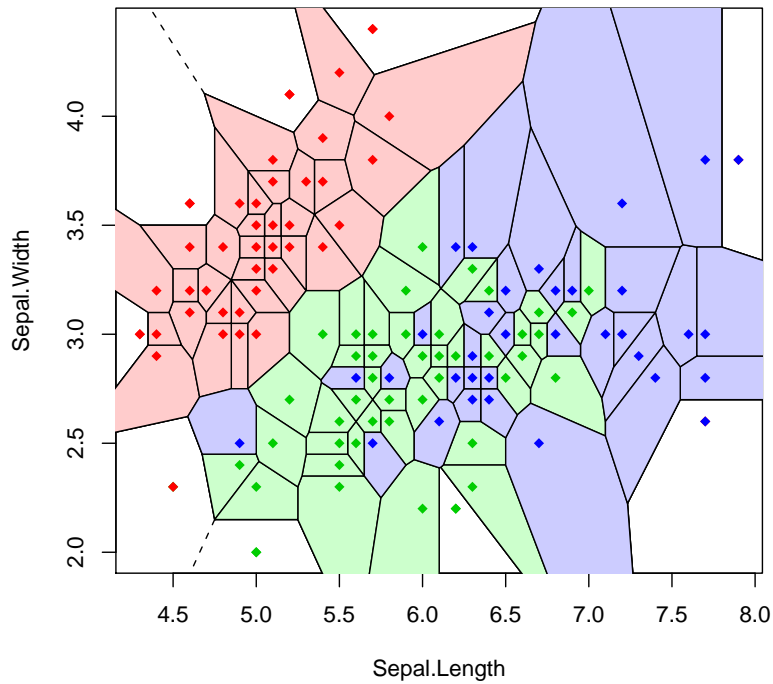
Accelerations: editing

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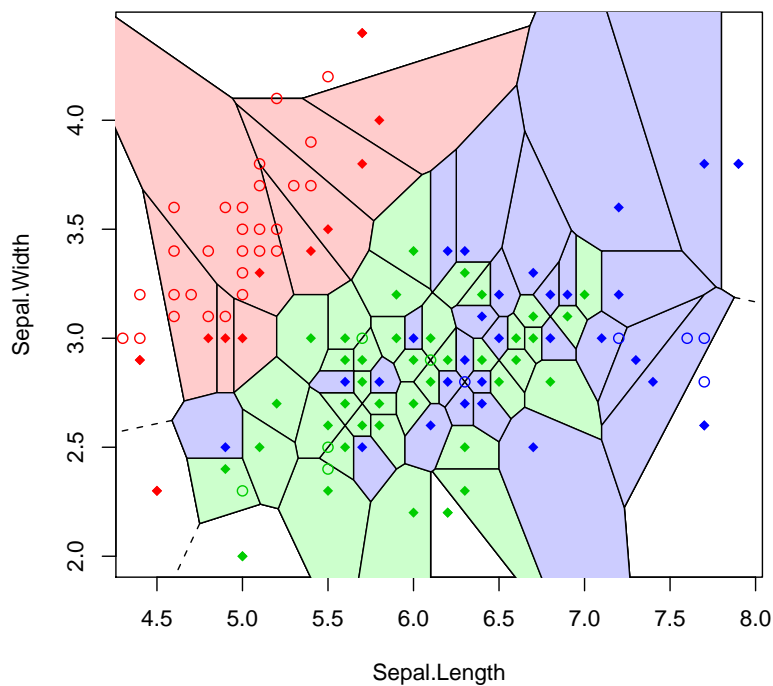
1 knn-edit-training-data(training data  $X$ ) :
2   compute Voronoi cells  $R(x) \quad \forall(x, y) \in X$ ,
3   esp. Voronoi neighbors  $N(x) := \{(x', y') \in X \mid R(x') \cap R(x) \neq \emptyset\}$ 
4    $E := \emptyset$ 
5   for  $(x, y) \in X$  do
6      $hasNeighborOfOtherClass := false$ 
7     for  $(x', y') \in N(x)$  do
8       if  $y \neq y'$ 
9          $hasNeighborOfOtherClass := true$ 
10      fi
11     od
12     if not  $hasNeighborOfOtherClass$ 
13        $E := E \cup \{(x, y)\}$ 
14     fi
15   od
16   for  $(x, y) \in E$  do
17      $X := X \setminus \{(x, y)\}$ 
18   od

```

Accelerations: editing



Accelerations: editing



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Machine Learning / 3. Parzen Windows

Example

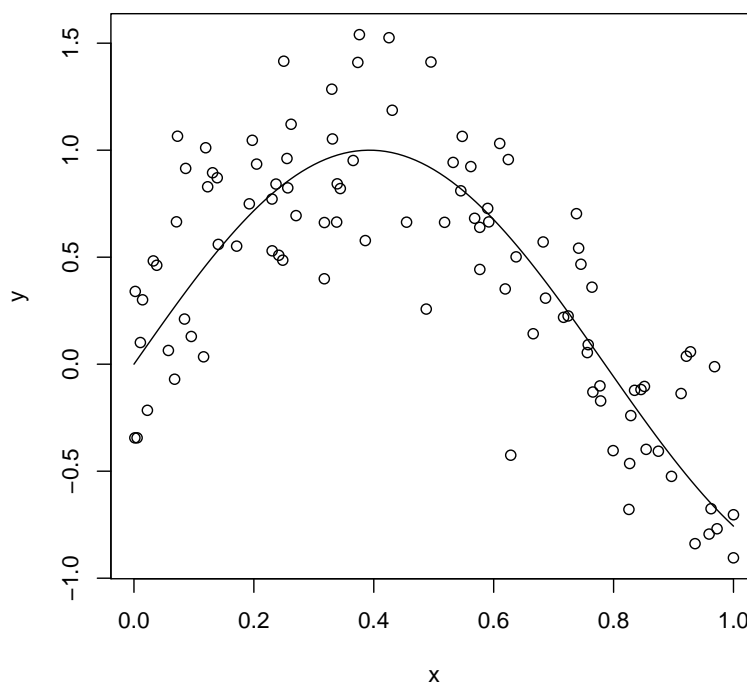


Figure 8: Points generated by the model $y = \sin(4x) + \mathcal{N}(0, 1/3)$ with $x \sim \text{unif}(0, 1)$.

Example / k-Nearest-Neighbor

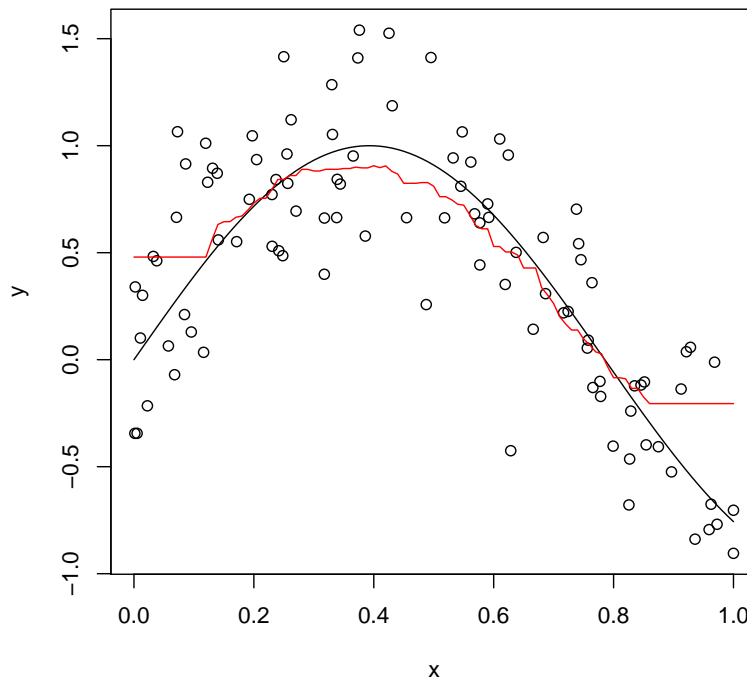


Figure 9: Points generated by the model $y = \sin(4x) + \mathcal{N}(0, 1/3)$ with $x \sim \text{unif}(0, 1)$. 30-nearest-neighbor regressor.

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 k -Nearest Neighbor is locally constant

k -nearest neighbor models are

- based on discrete decisions if a point is a k -nearest neighbor or not,
- in effect, locally constant,
- and thus not continuous.

Discrete decisions can be captured by binary window functions,

i.e.,

instead of

$$K_{x_0}(x, x_0) := \begin{cases} 1, & \text{if } (x, y) \in N_k(x_0) \\ 0, & \text{otherwise} \end{cases}$$

$$\hat{y}(x_0) = \frac{\sum_{(x,y) \in X} K(x, x_0) y}{\sum_{(x,y) \in X} K(x, x_0)}$$

$$\hat{y}(x_0) = \frac{\sum_{(x,y) \in N_k(x_0)} y}{k}$$

k -Nearest Neighbor is locally constant

In k -nearest neighbor the size of the window varies from point to point: it depends on the density of the data:

in dense parts

the effective window size is small,

in sparse parts

the effective window size is large.

Alternatively, it is also possible to set the size of the windows to a constant λ , e.g.,

$$K_\lambda(x, x_0) := \begin{cases} 1, & \text{if } |x - x_0| \leq \lambda \\ 0, & \text{otherwise} \end{cases}$$

Kernel Regression

Instead of discrete windows, one typically uses continuous windows, i.e., continuous weights

$$K(x, x_0)$$

that reflect the distance of a training point x to a prediction point x_0 , called **kernel** or **Parzen window**, e.g.,

$$K(x, x_0) := \begin{cases} 1 - \frac{|x - x_0|}{\lambda}, & \text{if } |x - x_0| \leq \lambda \\ 0, & \text{otherwise} \end{cases}$$

Instead of a binary neighbor/not-neighbor decision, a continuous kernel captures a “degree of neighborhood”.

Kernels can be used for prediction via **kernel regression**, esp. **Nadaraya-Watson kernel-weighted average**:

$$\hat{y}(x_0) := \frac{\sum_{(x,y) \in X} K(x, x_0) y}{\sum_{(x,y) \in X} K(x, x_0)}$$

Epanechnikov Kernel

Kernels are similarity measures:
the closer two points, the larger the kernel value.

Epanechnikov kernel

$$K_\lambda(x, y) := D\left(\frac{|x - y|}{\lambda}\right)$$

with

$$D(t) := \begin{cases} \frac{3}{4}(1 - t^2), & t < 1 \\ 0, & \text{otherwise} \end{cases}$$

The constant $\lambda \in \mathbb{R}^+$ is called **kernelwidth**.

More kernels

Tri-cube kernel

$$D(t) := \begin{cases} (1 - t^3)^3, & t < 1 \\ 0, & \text{otherwise} \end{cases}$$

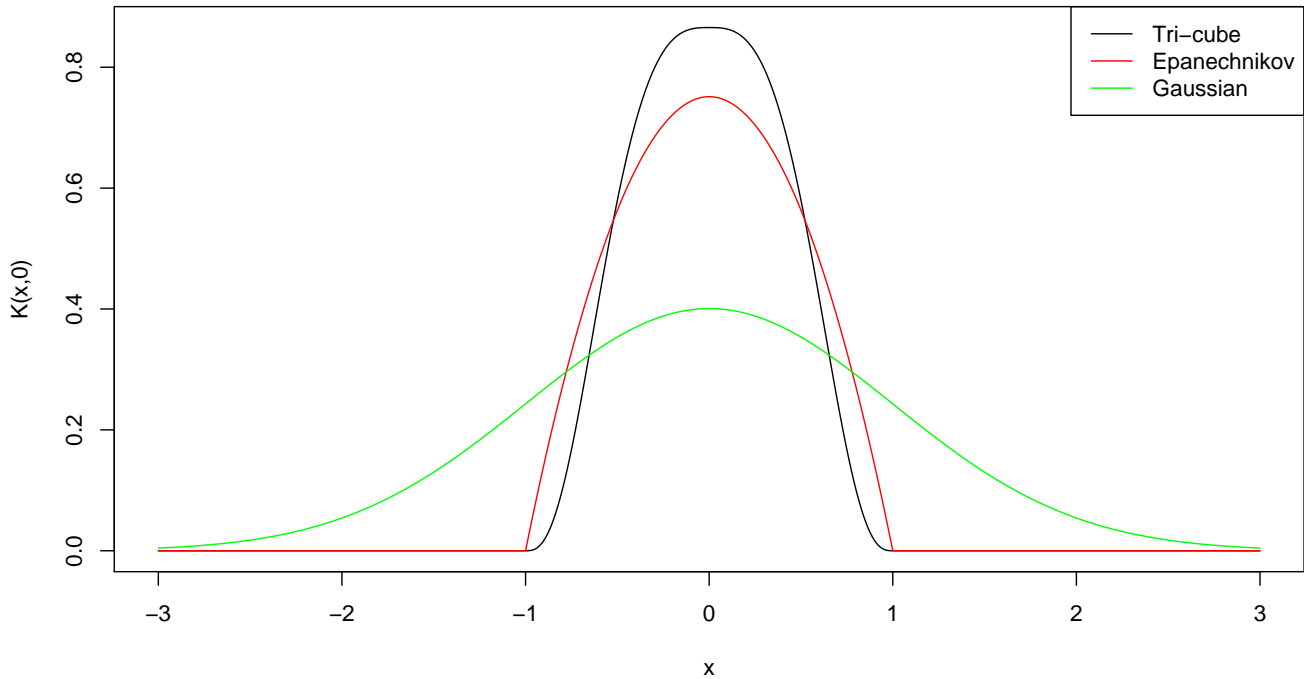
Gaussian kernel

$$D(t) := \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}t^2}$$

The Epanechnikov and Tri-cube kernel have compact support $[x_0 - \lambda, x_0 + \lambda]$.

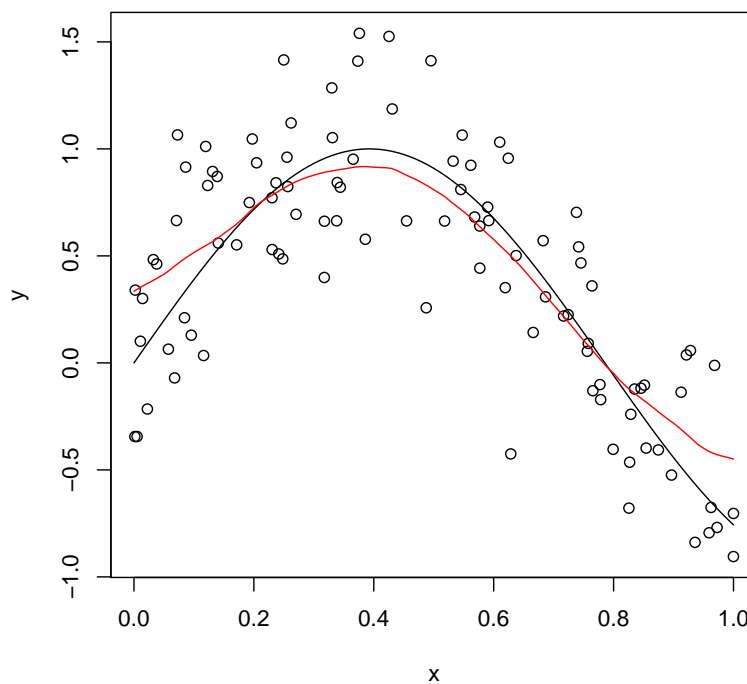
The Gaussian kernel has noncompact support, λ acts as standard deviance.

Kernels



Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim
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Example / Epanechnikov Kernel, $\lambda = 0.2$ 

Choosing the Kernelwidth

If the kernelwidth λ is small

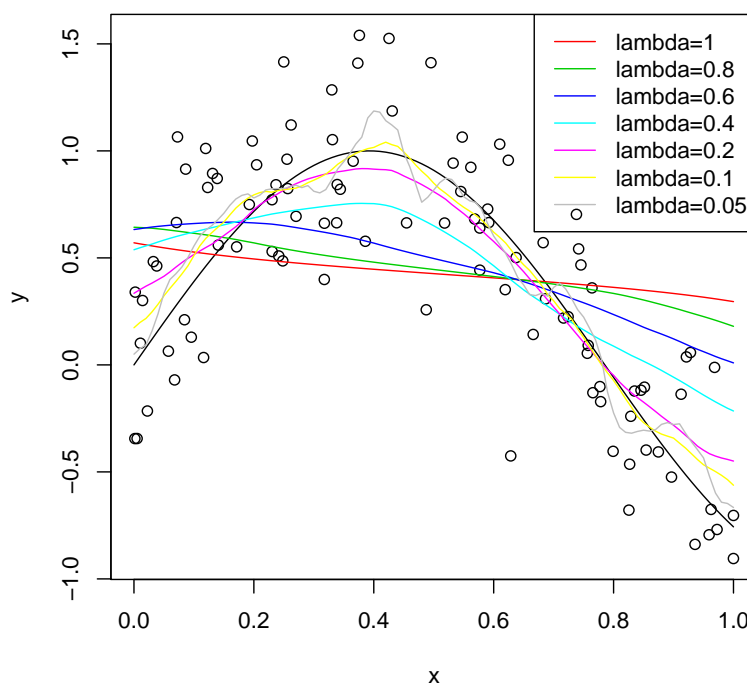
larger variance – as averaged over fewer points
 smaller bias – as closer instances are used
 \Rightarrow risks to be too bumpy

If the kernelwidth λ is large

smaller variance – as averaged over more points
 larger bias – as instances further apart are used
 \Rightarrow risks to be too rigid / over-smoothed

The kernelwidth λ is a parameter (sometimes called a **hyperparameter**) of the model that needs to be optimized / estimated by data.

Example / Epanechnikov Kernel, various kernelwidths



Space-averaged Estimates

The probability that an instance x is within a given region $R \subseteq \mathcal{X}$:

$$p(x \in R) = \int_R p(x) dx$$

For a sample

$$x_1, x_2, \dots, x_n \sim p$$

it is

$$(x_i \in R) \sim \text{binom}(p(x \in R))$$

Let k be the number of x_i that are in region R :

$$k := |\{x_i \mid x_i \in R, i = 1, \dots, n\}|$$

then we can estimate

$$\hat{p}(x \in R) := \frac{k}{n}$$

Space-averaged Estimates

If p is continuous and R is very small, $p(x)$ is almost constant in R :

$$p(x \in R) = \int_R p(x) dx \approx p(x) \text{vol}(R), \quad \text{for any } x \in R$$

where $\text{vol}(R)$ denotes the volume of region R .

$$p(x) \approx \frac{k/n}{\text{vol}(R)}$$

Space-averaged Estimates

For unlimited data, i.e., $n \rightarrow \infty$, we can estimate p more and more accurately:

$$\hat{p}_n(x) = \frac{k_n/n}{V_n}, \quad \text{with } V_n := \text{vol}(R_n).$$

It must be assured that

$$\begin{aligned} V_n &\rightarrow 0 \\ k_n &\rightarrow \infty \\ k_n/n &\rightarrow 0 \end{aligned}$$

There are two methods to accomplish this:

1. nearest-neighbor method:

$$k_n := \sqrt{n}, \quad V_n \text{ is set adaptive to the data}$$

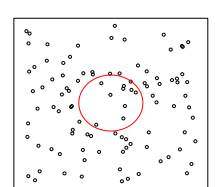
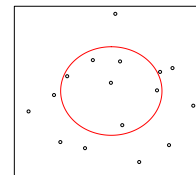
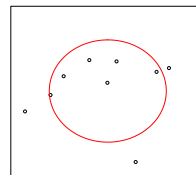
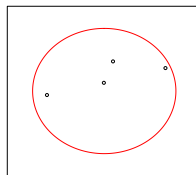
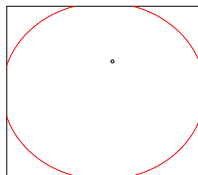
2. Parzen windows:

$$V_n := \frac{1}{\sqrt{n}}, \quad k_n \text{ is set adaptive to the data}$$

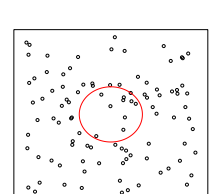
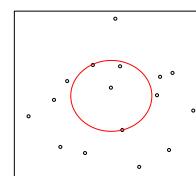
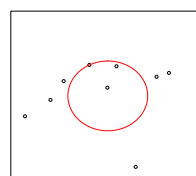
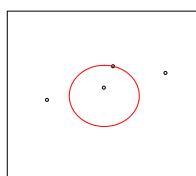
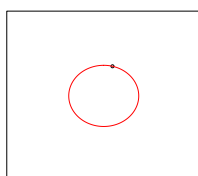
Space-averaged Estimates

 $n = 1$
 $n = 4$
 $n = 9$
 $n = 16$
 $n = 100$

$V_n = 1/\sqrt{n}$



$k_n = \sqrt{n}$



Summary

- Simple classification and regression models can be built by
 - averaging over target values (regression)
 - counting the occurrences of the target class (classification) of training instances close by (measured in some **distance measure**).
- If always a fixed number of nearest points is taken into account,
⇒ the model is called **nearest neighbor**,
if points are weighted with some similarity measure
(called **kernel** or **Parzen window**),
⇒ the model is called **kernel regression** and **kernel classification**.
- There is no learning tasks for these models, as simply all training instances are stored (“memory-based methods”).
- Therefore, to compute predictions is more costly than for say linear models. — There are several acceleration techniques (partial distances, search trees, editing).
- The error rate of the 1-nearest-neighbor classifier is bound by twice
the Bayes error rate.