Syllabus

Fri. 27.10.	(1)	0. Introduction
		A. Supervised Learning: Linear Models & Fundamentals
Fri. 3.11.	(2)	A.1 Linear Regression
Fri. 10.11.	(3)	A.2 Linear Classification
Fri. 17.11.	(4)	A.3 Regularization
Fri. 24.11.	(5)	A.4 High-dimensional Data
		B. Supervised Learning: Nonlinear Models
Fri. 1.12.	(6)	B.1 Nearest-Neighbor Models
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Fri. 19.1.	(10)	B.5 A First Look at Bayesian and Markov Networks
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Outline

1. Distance Measures
2. K-Nearest Neighbor Models
3. Scalable Nearest Neighbor

Outline

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 called **scalar variables**.

Often one is also interested in more complex variables such as

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

often called **structured variables** or **complex variables**.

Note: A complex variable in this sense has nothing to do with complex numbers.

Motivation

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

I. **feature extraction**
   1. derive binary or numerical variables,
   2. then use standard methods on the feature vectors.

II. **kernel methods**
   1. establish a distance measure between two values,
   2. 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.,

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

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 $\mathcal{X} := \mathbb{R}^n$:

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

Minkowski Metric / L_p metric

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

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

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):

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

$p = \infty$ (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.,

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

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 possibly in $]-\infty, 1]$).

Cosine Similarity

The angle between two vectors in $\mathbb{R}^N$ can be used as distance measure

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

To avoid the arccos, often the cosine of the angle is used as similarity measure (**cosine similarity**):

$$\text{sim}(x,y) := \cos\text{angle}(x,y) := \frac{\langle x,y\rangle}{||x||_2\,||y||_2}$$

Example:

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

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

Distances for Nominal Variables

1. **Binary variables**:
   - there is only one reasonable distance measure:

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

   - This coincides with
     - L_∞, $\frac{1}{2}L_1$ and $\frac{1}{\sqrt{2}}L_2$ distance

     for the indicator/dummy variables.

2. **Nominal variables** (with more than two possible values):
   - The same distance measure is useful.

3. **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:

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

(= 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**:

$$d(x, y) := \text{minimal number of single character deletions, insertions or substitutions to transform } x \text{ in } y$$

Examples:

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

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

Distances for Strings / Sequences

edit distance / **Levenshtein distance**:

$$d(x, y) := \text{minimal number of single character deletions, insertions or substitutions to transform } x \text{ in } y$$

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

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

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

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

starting from

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

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

Distances for Strings / Sequences

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

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

Machine Learning

Distances for Strings / Sequences

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

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

Distances for Strings / Sequences

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

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

Outline

Neighborhoods

Let d be a distance measure.
For a dataset

$$D \subseteq X \times Y$$

and $x \in \mathcal{X}$ let

$$D = \{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$$

be an enumeration with increasing distance to x, i.e.,

$$d(x, x_n) \leq d(x, x_{n+1}), \quad n = 1, \ldots, N$$

(ties broken arbitrarily).
The first $K \in \mathbb{N}$ points of such an enumeration, i.e.,

$$C_K(x) := \{(x_1, y_1), (x_2, y_2), \ldots (x_K, y_K)\}$$

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

Nearest Neighbor Regression and Classification Models

The **K-nearest neighbor regressor**

$$\hat{y}(x) := \frac{1}{K} \sum_{(x', y') \in C_K(x)} y'$$

The **K-nearest neighbor classifier**

$$\hat{p}(Y = y \mid x) := \frac{1}{K} \sum_{(x', y') \in C_K(x)} \mathbb{I}(y = y')$$

and then predict the class with maximal predicted probability

$$\hat{y}(x) := \arg\max_{y \in \mathcal{Y}} \hat{p}(Y = y \mid x)$$

i.e., the majority class in the neighborhood.

Nearest Neighbor Regression Algorithm

predict-knn-reg$(q \in \mathbb{R}^M, \mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\} \in \mathbb{R}^M \times \mathbb{R}, K \in \mathbb{N}, d)$:
  allocate array D of size N
  for $n := 1 : N$:
    $D_n := d(q, x_n)$
  $C := \textbf{argmin-k}(D, K)$
  $\hat{y} := \frac{1}{K} \sum_{k=1}^{K} y_{C_k}$
  return $\hat{y}$

Nearest Neighbor Classification Algorithm

predict-knn-class$(q \in \mathbb{R}^M, \mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\} \in \mathbb{R}^M \times \mathcal{Y}, K \in \mathbb{N}, d)$:
  allocate array D of size N
  for $n := 1 : N$:
    $D_n := d(q, x_n)$
  $C := \textbf{argmin-k}(D, K)$
  allocate array $\hat{p}$ of size $|\mathcal{Y}|$
  for $k := 1 : K$:
    $\hat{p}_{C_k} := \hat{p}_{C_k} + 1/K$
  return $\hat{p}$

Compute the argmin

```
1  argmin-k(x ∈ ℝ^N, K ∈ ℕ) :
2     allocate  array  T of size K
3     for  n = 1 : min(K, N):
4        insert-bottomk(T_{1:n}, n, π_x, 1)
5     for  n = K + 1 : N:
6        if  x_n < x_{T_K}:
7           insert-bottomk(T, n, π_x, 0)
8     return  T
9
10 insert-bottomk(T ∈ 𝒳^K, n ∈ 𝒳, π : 𝒳 → ℝ, s ∈ ℕ) :
11    k := find-sorted(T_{1:K−s}, n, π)
12    for  l := K : k + 1 decreasing:
13       T_l := T_{l−1}
14    T_{k+1} := n
```

Note: $\pi_x(n) := x_n$ comparison by x-values. Here, $\mathcal{X} := \mathbb{N}$.

Compute the argmin / find (naive)

```
1  find-sorted-linear(x ∈ 𝒳^K, z ∈ 𝒳, π : X → ℝ) :
2     k := K
3     while  k > 0 and π(z) < π(x_k):
4        k := k − 1
5     return  k
```

- requires
  - x is sorted (increasingly w.r.t. π)
- returns smallest index k with $\pi(x_k) \leq \pi(z)$
  - 0, if $\pi(z) < \pi(x_1)$

Note: Esp. for larger K it is better to use binary search.

Decision Boundaries

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

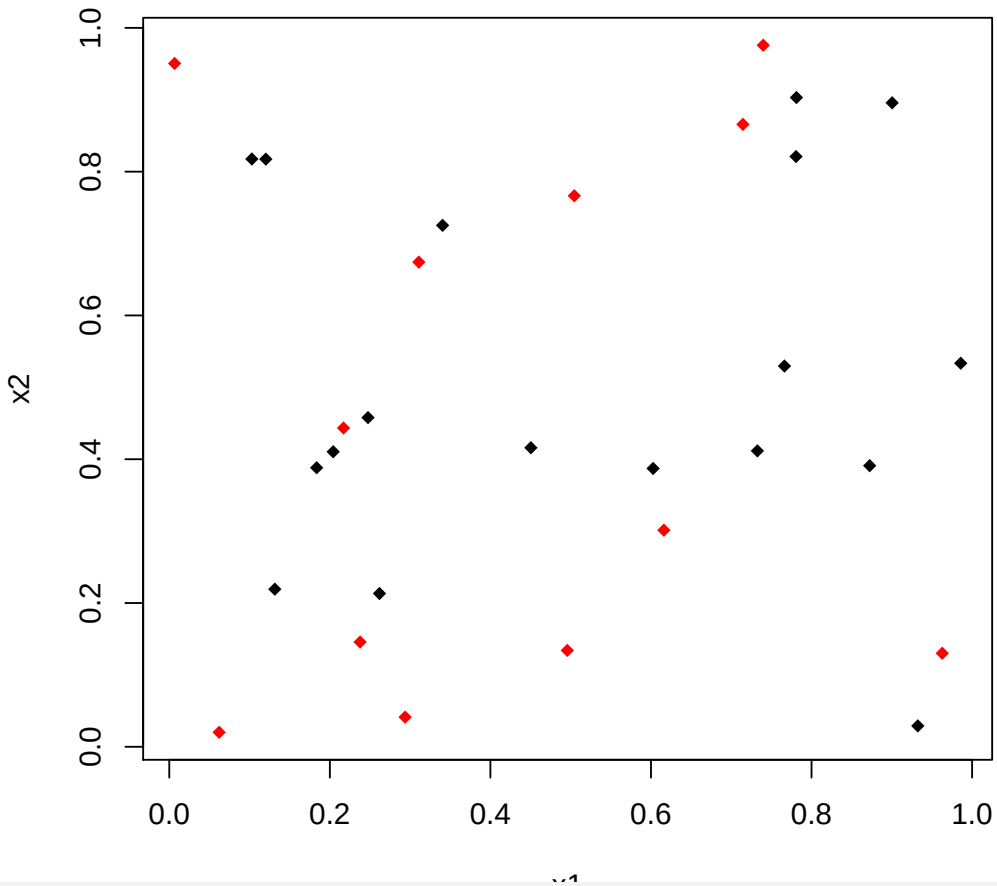
$$\text{region}_D(x_1), \text{region}_D(x_2), \ldots, \text{region}_D(x_N)$$

with

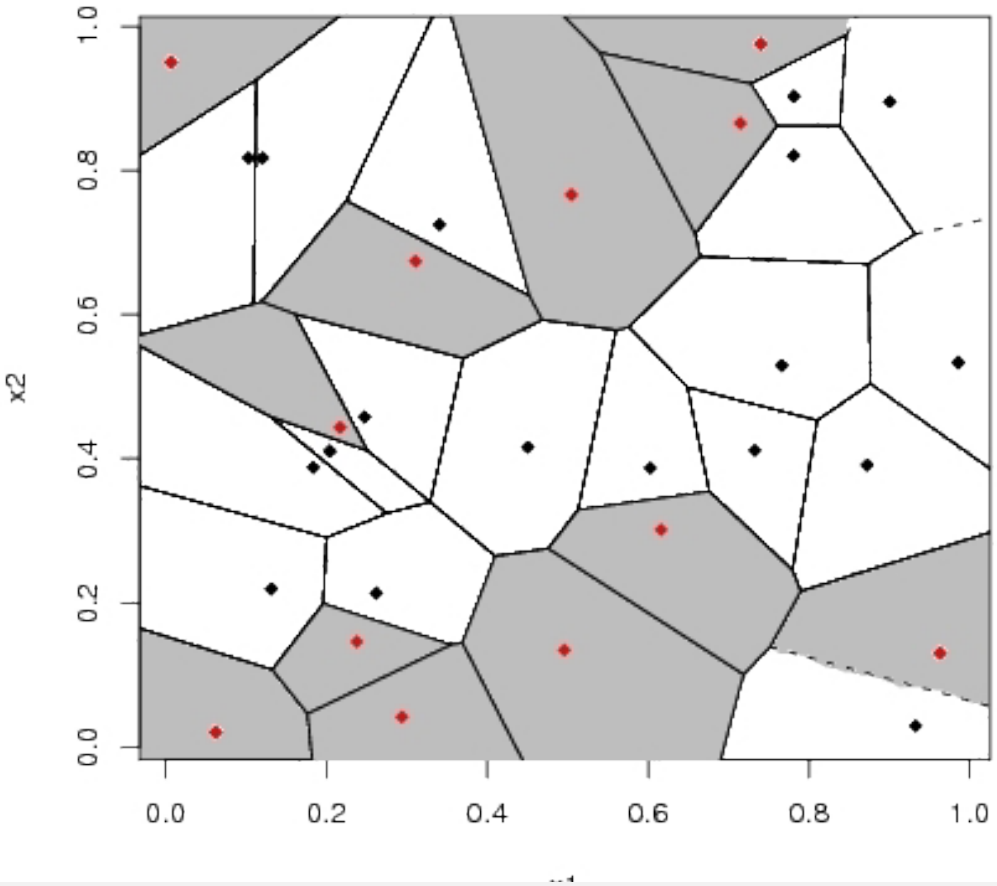
$$\text{region}_D(x) := \{x' \in \mathcal{X} \mid d(x', x) \leq d(x', x'') \quad \forall (x'', y'') \in D\}$$

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

Decision Boundaries



Decision Boundaries



Outline

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 $(x_1, y_1), \ldots, (x_N, y_N)$ has to be computed.
- For a predictor space $\mathcal{X} := \mathbb{R}^M$, each such computation needs $O(M)$ operations.
- We then keep track of the K points with the smallest distance.

In total one needs $O(NM + NK)$ operations.

Partial Distances / Lower Bounding

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.,

$$d_r(x, x') := \left(\sum_{m=1}^{r} (x_m - x'_m)^2\right)^{\frac{1}{2}}, \quad r \leq M$$

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).

Nearest Neighbor Classification Algorithm

predict-knn-reg$(q \in \mathbb{R}^M, \mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\} \in \mathbb{R}^M \times \mathbb{R}, K \in \mathbb{N}, d)$:
  allocate array D of size N
  for $n := 1 : N$:
    $D_n := d(q, x_n)$
  $C := \textbf{argmin-k}(D, K)$
  $\hat{y} := \frac{1}{K} \sum_{k=1}^{K} y_{C_k}$
  return $\hat{y}$

Machine Learning

predict-knn-reg$(q \in \mathbb{R}^M, \mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\} \in \mathbb{R}^M \times \mathbb{R}, K \in \mathbb{N}, d)$:
  allocate array D of size N
  for $n := 1 : N$:
    $D_n := d(q, x_n)$
  $C := \textbf{argmin-k}(D, K)$
  $\hat{y} := \frac{1}{K} \sum_{k=1}^{K} y_{C_k}$
  return $\hat{y}$

predict-knn-class$(q \in \mathbb{R}^M, \mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\} \in \mathbb{R}^M \times \mathbb{R}, K \in \mathbb{N}, d)$:
  $C := \pi_1(\text{ARGCLOS-K}(q, x_1, x_2, \ldots, x_N, K))$
  $\hat{y} := \frac{1}{K} \sum_{k=1}^{K} y_{C_k}$
  return $\hat{y}$

argclos-k$(q \in \mathbb{R}^M, x_1, \ldots, x_N \in \mathbb{R}^M, K \in \mathbb{N})$:
  allocate array D of size N
  for $n := 1 : N$:
    $D_n := d(q, x_n)$
  $C := \textbf{argmin-k}(D, K)$
  return $\{(C_k, D_{C_k}) \mid k = 1 : |C|\}$

Find Neighbors / Without Lower Bounding

argclos-k$(q \in \mathbb{R}^M, x_1, \ldots, x_N \in \mathbb{R}^M, K \in \mathbb{N})$:
  allocate array T of size K for pairs $\mathbb{N} \times \mathbb{R}$
  for $n = 1 : \min(K, N)$:
    $d := \sum_{m=1}^{M} (q_m - x_{n,m})^2$
    insert-bottomk$(T, (n, d), \pi_2, 1)$
  for $n = K + 1 : N$:
    $d := \sum_{m=1}^{M} (q_m - x_{n,m})^2$
    if $d < \pi_2(T_K)$:
      insert-bottomk$(T, (n, d), \pi_2, 0)$
  return T

Note: ARGCLOS-K returns the K points closest to q and their distances.
$\pi_2(n, d) := d$ comparison by second component (distance).

Find Neighbors / With Lower Bounding

argclos-k$(q \in \mathbb{R}^M, x_1, \ldots, x_N \in \mathbb{R}^M, K \in \mathbb{N})$:
  allocate array T of size K for pairs $\mathbb{N} \times \mathbb{R}$
  for $n = 1 : \min(K, N)$:
    $d := \sum_{m=1}^{M} (q_m - x_{n,m})^2$
    insert-bottomk$(T, (n, d), \pi_2, 1)$
  for $n = K + 1 : N$:
    $d := 0$
    $m := 1$
    while $m \leq M$ and $d < \pi_2(T_K)$:
      $d := d + (q_m - x_{n,m})^2$
      $m := m + 1$
    if $d < \pi_2(T_K)$:
      insert-bottomk$(T, (n, d), \pi_2, 0)$
  return T

Note: ARGCLOS-K returns the K points closest to q and their distances.
$\pi_2(n, d) := d$ comparison by second component (distance).

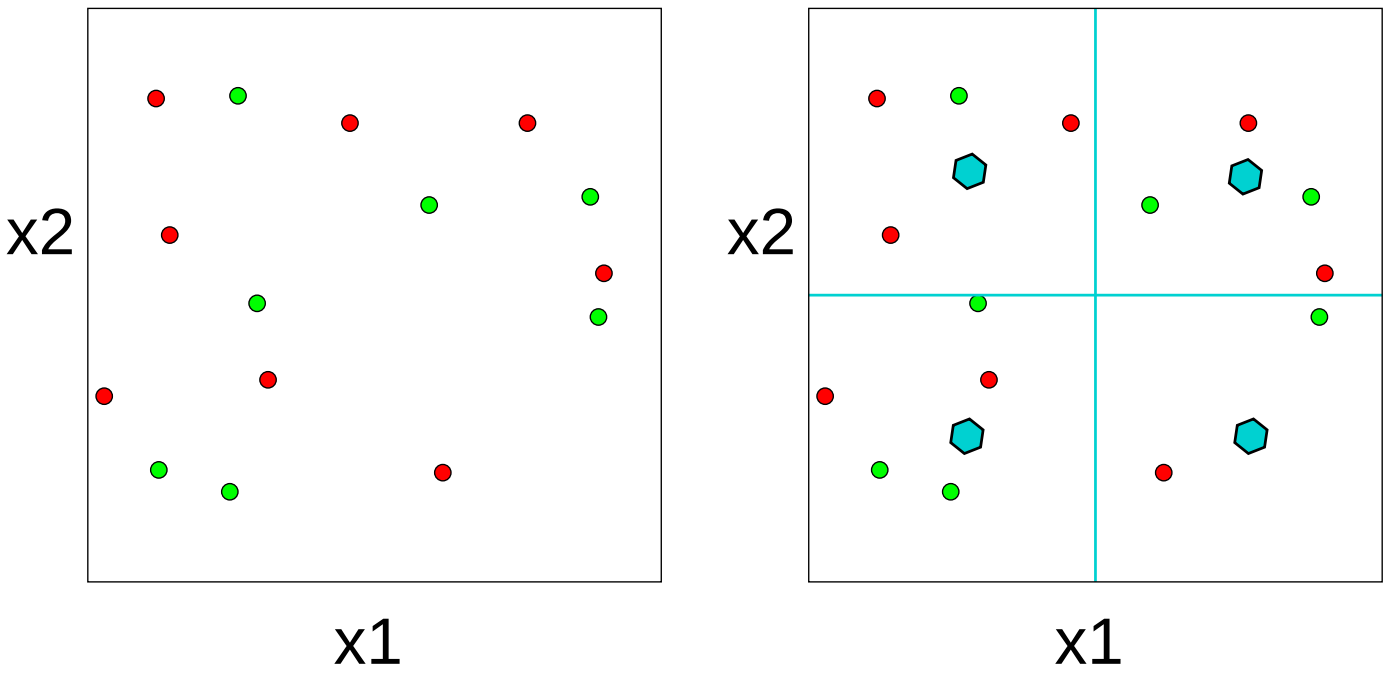
Search trees

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

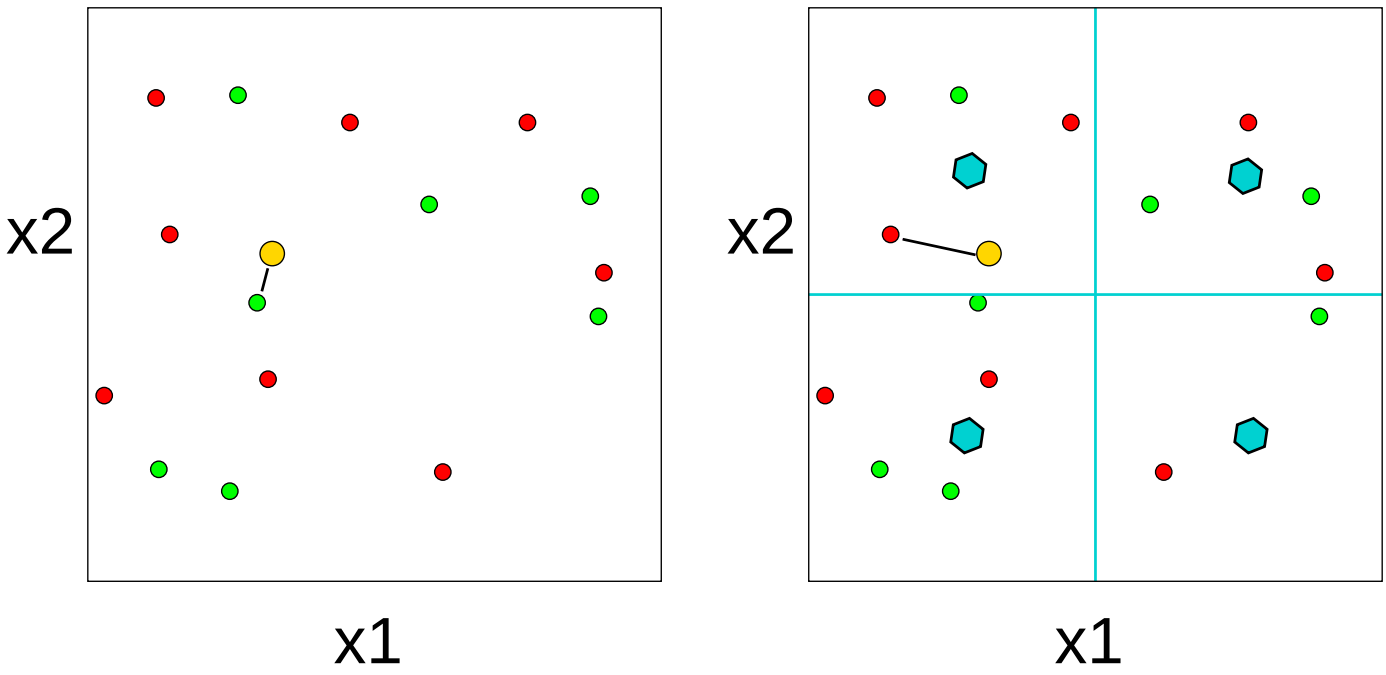
1. organize the training examples as a tree (or a DAG) with
   - sets of training examples at the leaves and
   - a prototype (e.g., the mean of the training examples at all descendent leaves) at each intermediate node.
2. starting at the root, recursively
   - compute the distance to all children of 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.

Search trees



Search trees



Approximate Nearest Neighbor

- for low dimensions, **k-d trees** (k-dimensional trees) can be used
  - only useful for very low dimensions (2d, 3d)
  - in computational geometry, computer graphics, computer vision
- for higher dimensions **locality-sensitive hashing** performs better
  - only works with specific distances (Euclidean/L2, L1, Hamming)

Locality-Sensitive Hashing [Datar et al., 2004]

- idea: create a hash key function h that puts
  - close instances into the same bin, but
  - far instances into different bins.

  allowing some errors.
- for $x \in \mathbb{R}^M$, the **discretized projection on a random line** is

$$h_{a,b,r}(x) := \left\lfloor \frac{a^T x + b}{s} \right\rfloor, \quad a \in \mathbb{R}^M, b \in [0, s], s \in \mathbb{R}^+$$

$$\text{where } a_m \sim \mathcal{N}(0,1), b \sim \text{unif}(0, s)$$

- use the concatenation of L such projection keys as hash key

$$h_{A,b,r}(x) := (h_{A_{l,.},b_l,s}(x))_{l=1,\ldots,L}$$
$$= (\left\lfloor \frac{1}{s}(Ax + b)_l \right\rfloor)_{l=1,\ldots,L}, \quad A \in \mathbb{R}^{L \times M}, b \in [0, s]^L, s \in \mathbb{R}^+$$

- build H such hash maps and test all points found in any of them.

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 algorithm

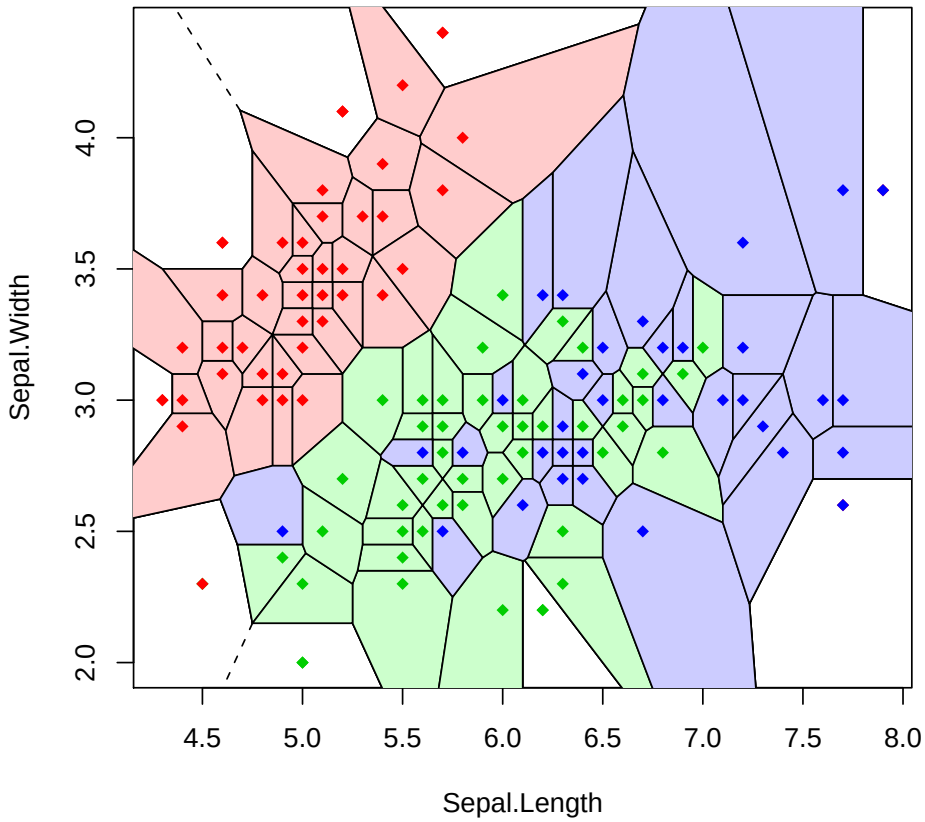
- retains the decision function,
- has complexity $O(M^3 N^{\lfloor \frac{M}{2} \rfloor} \log N)$
  (with $\lfloor x \rfloor := \max\{n \in \mathbb{N} \mid n \leq x\}$; Duda et al. 2001, p. 186).

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

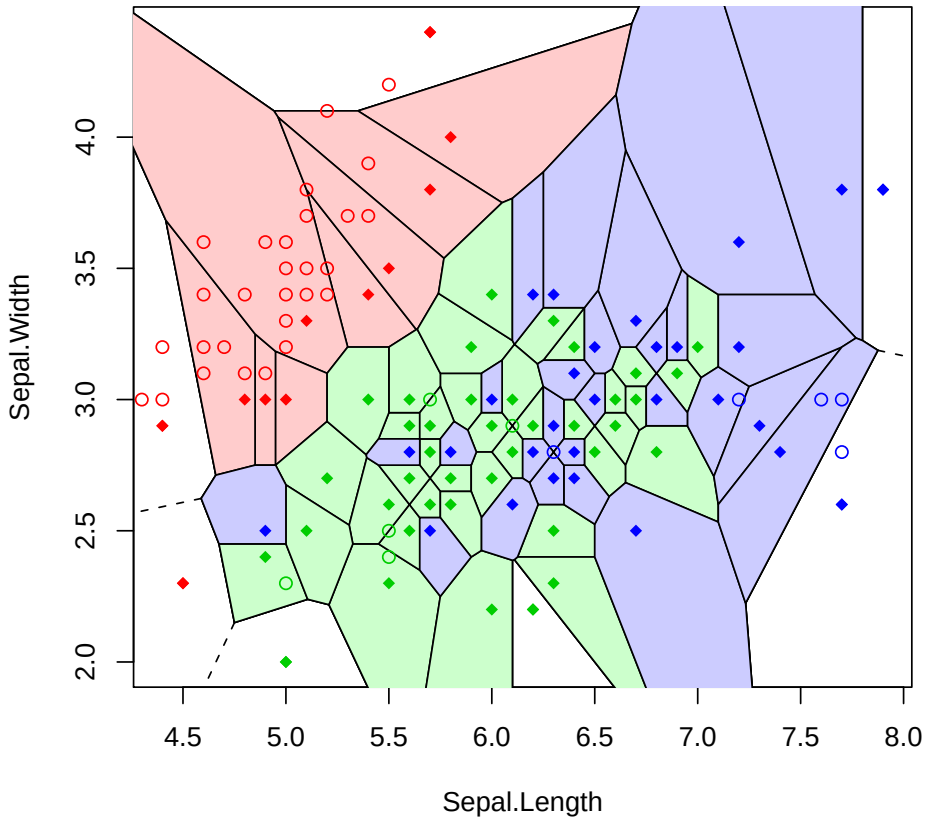
Editing

1: **procedure** KNN-EDIT-TRAINING-DATA($\mathcal{D}^{\text{train}} \subseteq \mathbb{R}^M \times \mathcal{Y}$)
2: compute Voronoi cells $R(x)$ for all $(x, y) \in \mathcal{D}^{\text{train}}$,
3: esp. Voronoi neighbors $N(x) := \{(x', y') \in \mathcal{D}^{\text{train}} \mid R(x) \cap R(x') \neq \emptyset\}$
4: $E := \emptyset$
5: **for** $(x, y) \in \mathcal{D}^{\text{train}}$ **do**
6: hasNeighborOfOtherClass := false
7: **for** $(x', y') \in N(x)$ **do**
8: **if** $y \neq y'$ **then**
9: hasNeighborOfOtherClass := true
10: **if** not hasNeighborOfOtherClass **then**
11: $E := E \cup \{(x, y)\}$
12: **return** $\mathcal{D}^{\text{train}} \setminus E$

Editing



Editing



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**).
- The **nearest neighbor** takes always a fixed number K of nearest points into account.
  - Alternatively, one also could weight points with some similarity measure (called **kernel** or **Parzen window**),
    $\Rightarrow$ the model is called **kernel regression** and **kernel classification**.
- There are 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 / lower bounding**
  - **search trees** / **locality-sensitive hashing**
  - **editing**

Further Readings

- [Hastie et al., 2005, chapter 13.3, 2.3.2], [Murphy, 2012, chapter 1.4.2, 14.1+2+4], [James et al., 2013, chapter 2.2.3,].

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