Data Mining and Machine Learning

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Instance-Based Learning

- Rote Learning
- k Nearest-Neighbor Classification
  - Prediction, Weighted Prediction
  - choosing k
  - feature weighting (RELIEF)
  - instance weighting (PEBLS)
  - efficiency
  - kD-trees

- IBL and Rule Learning
  - NEAR: Nearest Nested Hyper-Rectangles
  - RISE

Acknowledgements:
Some slides adapted from
- Tom Mitchell
- Eibe Frank & Ian Witten
- Kan, Steinbach, Kumar
- Ricardo Gutierrez-Osuna
- Gunter Grieser

Instance Based Classifiers

- No model is learned
  - The stored training instances themselves represent the knowledge
  - Training instances are searched for instance that most closely resembles new instance

  → *lazy learning*

- Examples:
  - Rote-learner
    - Memorizes entire training data and performs classification only if attributes of record match one of the training examples exactly

A Sample Task

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Day	Temperature	Outlook	Humidity	Windy	Play Golf?
07-05	hot	sunny	high	false	no
07-06	hot	sunny	high	true	no
07-07	hot	overcast	high	false	yes
07-09	cool	rain	normal	false	yes
07-10	cool	overcast	normal	true	yes
07-12	mild	sunny	high	false	no
07-14	cool	sunny	normal	false	yes
07-15	mild	rain	normal	false	yes
07-20	mild	sunny	normal	true	yes
07-21	mild	overcast	high	true	yes
07-22	hot	overcast	normal	false	yes
07-23	mild	rain	high	true	no
07-26	cool	rain	normal	true	no
07-30	mild	rain	high	false	yes
today	cool	sunny	normal	false	yes
tomorrow	mild	sunny	normal	false	?

Instance Based Classifiers

- No model is learned
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  → *lazy learning*

- Examples:
  - Rote-learner
    - Memorizes entire training data and performs classification only if attributes of record match one of the training examples exactly
  - Nearest-neighbor classifier
    - Uses k “closest” points (nearest neigbors) for performing classification

Nearest Neighbor

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07-05	hot	sunny	high	false	no
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07-07	hot	overcast	high	false	yes
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07-10	cool	overcast	normal	true	yes
07-12	mild	sunny	high	false	no
07-14	cool	sunny	normal	false	yes
07-15	mild	rain	normal	false	yes
07-20	mild	sunny	normal	true	yes
07-21	mild	overcast	high	true	yes
07-22	hot	overcast	normal	false	yes
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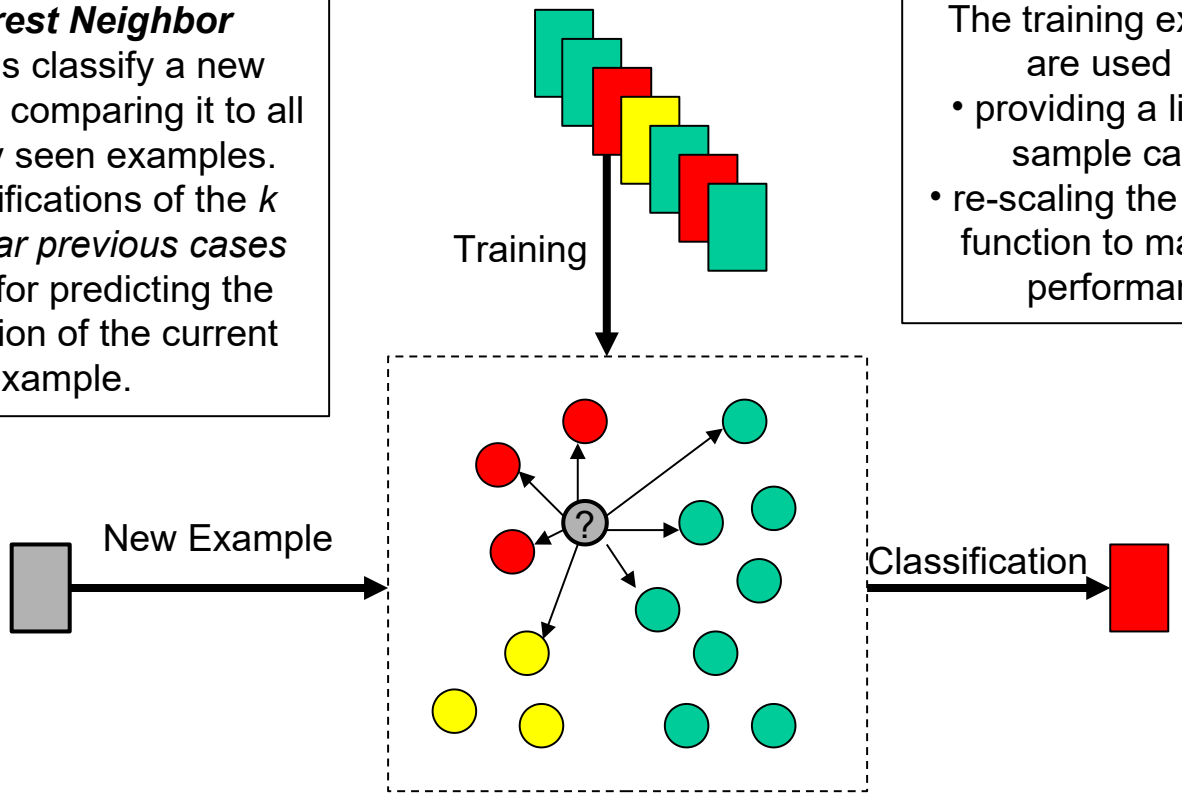
07-26	cool	rain	normal	true	no
07-30	mild	rain	high	false	yes
today	cool	sunny	normal	false	yes
tomorrow	mild	sunny	normal	false	yes

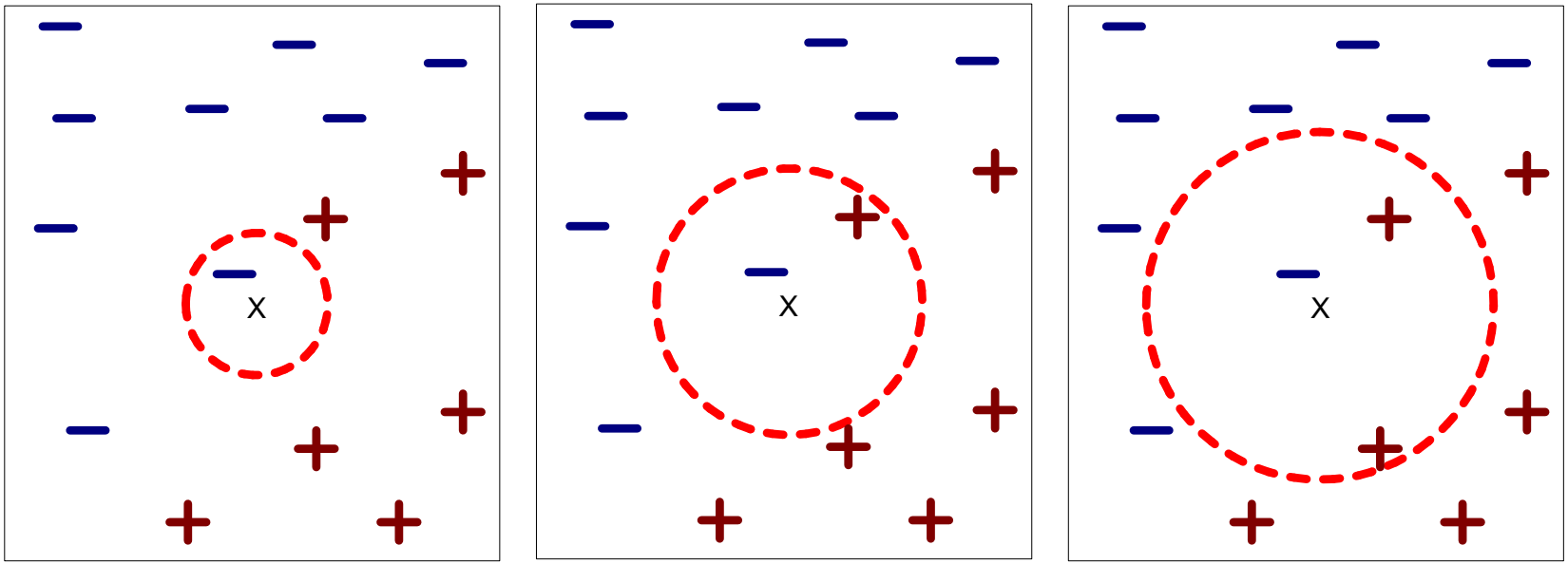
Nearest Neighbor Classifier

K-Nearest Neighbor algorithms classify a new example by comparing it to all previously seen examples. The classifications of the *k most similar previous cases* are used for predicting the classification of the current example.



The training examples are used for
- providing a library of sample cases
- re-scaling the similarity function to maximize performance

Nearest Neighbors



(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

k nearest neighbors of an example x are the data points that have the k smallest distances to x

Prediction

The predicted class is determined from the nearest neighbor list

- classification
  - take the majority vote of class labels among the k-nearest neighbors

$$\hat{y} = \max_c \sum_{i=1}^{k} \begin{cases} 1 & \text{if } y_i = c \\ 0 & \text{if } y_i \neq c \end{cases} = \max_c \sum_{i=1}^{k} \mathbf{1}(y_i = c)$$

indicator function

- can be easily be extended to regression
  - predict the average value of the class value of the k-nearest neighbors

$$\hat{y} = \frac{1}{k} \sum_{i=1}^{k} y_i$$

Weighted Prediction

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- Often prediction can be improved if the influence of each neighbor is weighted

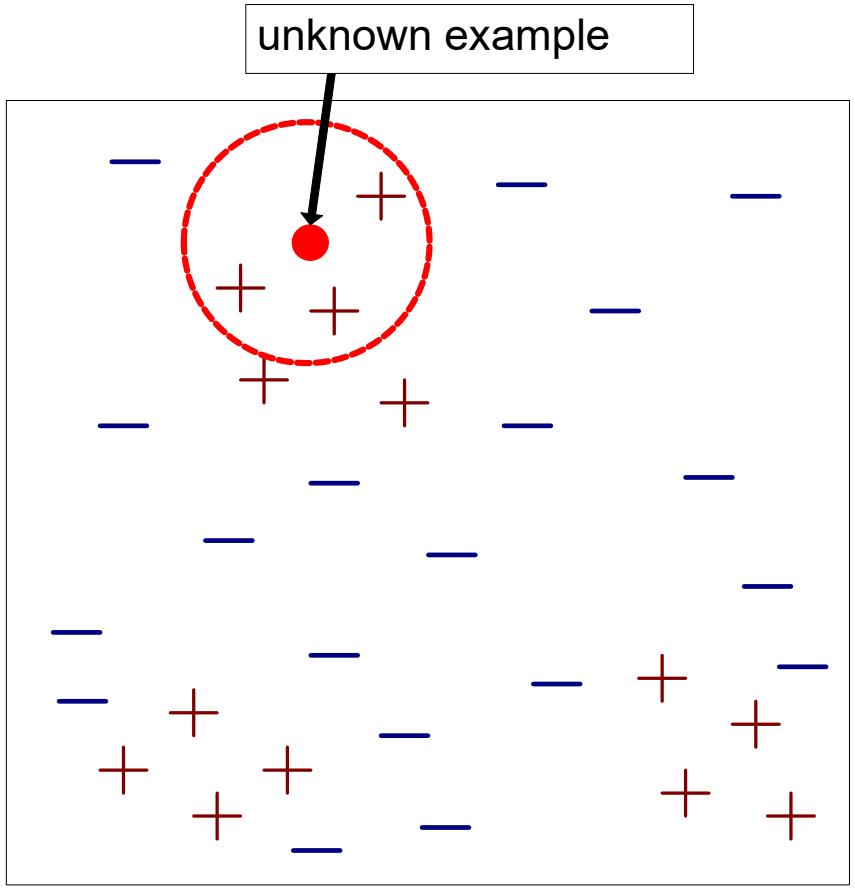
$$\hat{y} = \frac{\sum_{i=1}^{k} w_i \cdot y_i}{\sum_{i=1}^{k} w_i}$$

- Weights typically depend on distance, e.g.

$$w_i = \frac{1}{d(x_i, x)^2}$$

- Note:
  - with weighted distances, we could use all examples for classifications (→ Inverse Distance Weighting)

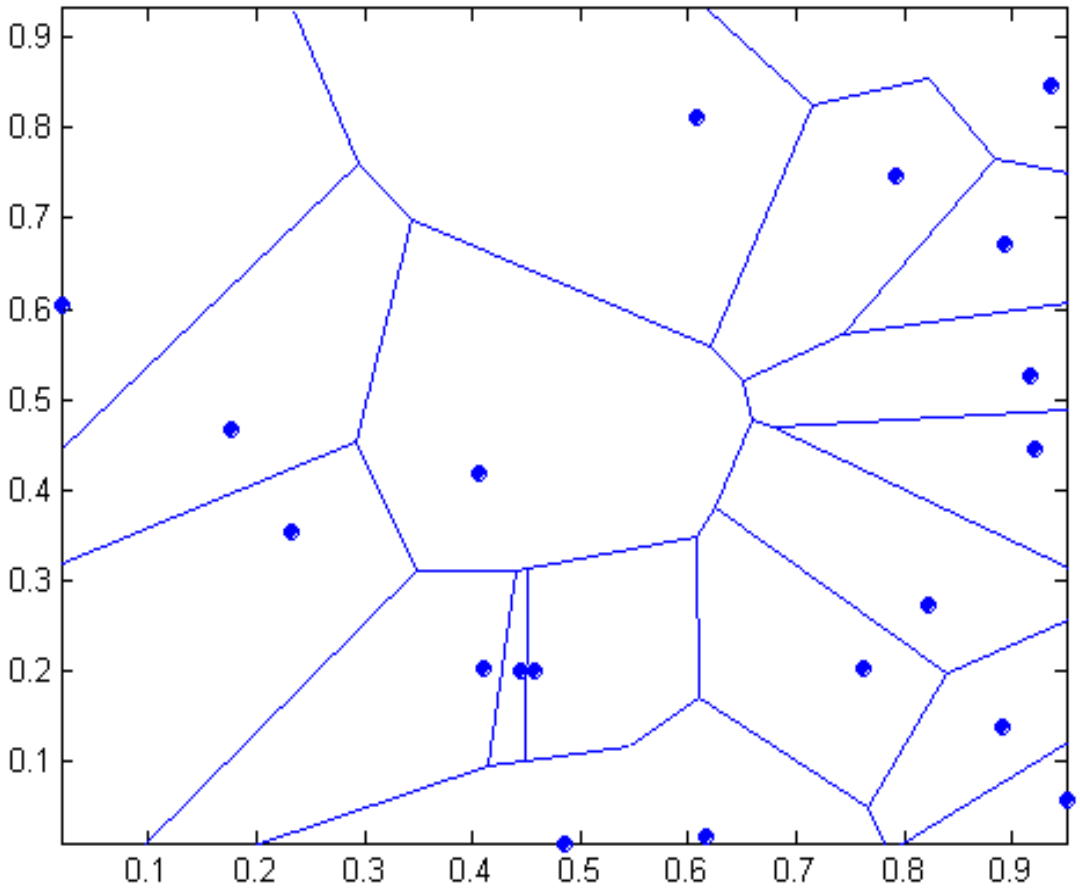
Nearest-Neighbor Classifiers



- Require three things
  - The set of stored examples
  - Distance Metric to compute distance between examples
  - The value of *k*, the number of nearest neighbors to retrieve
- To classify an unknown example:
  - Compute distance to other training examples
  - Identify *k* nearest neighbors
  - Use class labels of nearest neighbors to determine the class label of unknown example (e.g., by taking majority vote)

Voronoi Diagram

- shows the regions of points that are closest to a given set of points
- boundaries of these regions correspond to potential decision boundaries of 1NN classifier



Lazy Learning Algorithms

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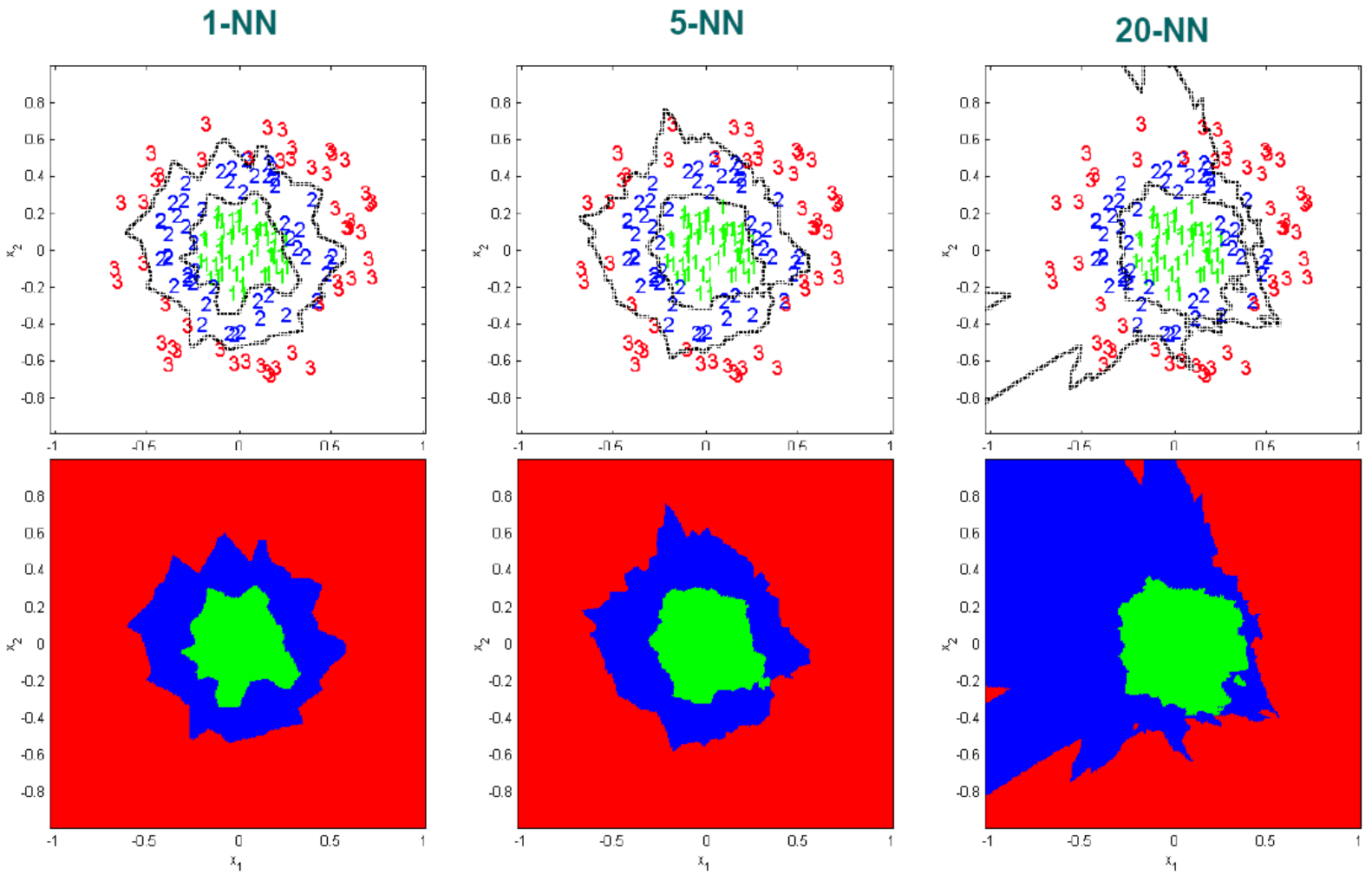
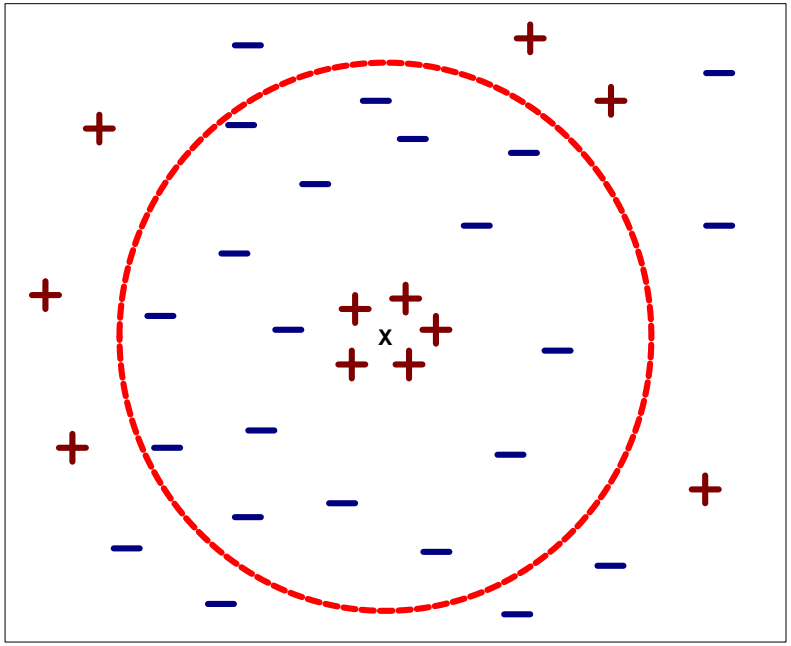
- kNN is considered a lazy learning algorithm
  - Defers data processing until it receives a request to classify an unlabelled example
  - Replies to a request for information by combining its stored training data
  - Discards the constructed answer and any intermediate results
- Other names for lazy algorithms
  - Memory-based, Instance-based , Exemplar-based , Case-based, Experiencebased
- This strategy is opposed to eager learning algorithms which
  - Compiles its data into a compressed description or model
  - Discards the training data after compilation of the model
  - Classifies incoming patterns using the induced model

Choosing the value of k



Choosing the value of k

- If k is too small
  - sensitive to noise in the data (misclassified examples)
- If k is too large
  - neighborhood may include points from other classes
  - limiting case: $k \geq |D|$
    - all examples are considered
    - largest class is predicted



- good values can be found
  - e.g, by evaluating various values with cross-validation on the training data

Distance Functions

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- Computes the distance between two examples
  - so that we can find the “nearest neighbor” to a given example
- General Idea:
  - reduce the distance $d(x_1, x_2)$ of two examples to the distances $d_A(v_1, v_2)$ between two values for attribute A
- Popular choices
  - Euclidean Distance: $d(x_1, x_2) = \sqrt{\sum_A d_A(v_{1,A}, v_{2,A})^2}$
    - straight-line between two points
  - Manhattan or City-block Distance: $d(x_1, x_2) = \sum_A d_A(v_{1,A}, v_{2,A})$
    - sum of axis-parallel line segments

Distance Functions for Numerical Attributes

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- Numerical Attributes:
  - distance between two attribute values

$$d_A(v_{1,}v_2)=|v_1-v_2|$$

- Normalization:
  - Different attributes are measured on different scales

    → values need to be normalized in [0,1]:

$$\hat{v}_i=\frac{v_i-\min v_j}{\max v_j-\min v_j}$$

  - Note:
    - This normalization assumes a (roughly) uniform distribution of attribute values
    - For other distributions, other normalizations might be preferable
      - e.g.: logarithmic for salaries?

Distance Functions for Symbolic Attributes

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- 0/1 distance

$$d_A(v_1, v_2) = \begin{cases} 0 & \text{if} \quad v_1 = v_2 \\ 1 & \text{if} \quad v_1 \neq v_2 \end{cases}$$

- Value Difference Metric (VDM) (Stanfill & Waltz 1986)
  - two values are similar if they have approximately the same distribution over all classes (similar relative frequencies in all classes)
  - sum over all classes the difference of the percentage of examples with value v_1 in this class and examples with value v_2 in this class

$$d_A(v_1, v_2) = \sum_c \left| \frac{n_{1,c}}{n_1} - \frac{n_{2,c}}{n_2} \right|^k$$

k is a user-settable parameter (e.g., k=2)

  - used in PEBLS with $k = 1$
    (Parallel Exemplar-Based Learning System; Cost & Salzberg, 1993)

VDM Example

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Class	Marital Status		
	Single	Married	Divorced
Yes	2	0	1
No	2	4	1

Distance between values:

$$d(\text{Single},\text{Married}) = |2/4 - 0/4| + |2/4 - 4/4| = 1$$

$$d(\text{Single},\text{Divorced}) = |2/4 - 1/2| + |2/4 - 1/2| = 0$$

$$d(\text{Married},\text{Divorced}) = |0/4 - 1/2| + |4/4 - 1/2| = 1$$

VDM Example

Tid	Refund	Marital Status	Taxable Income	Cheat
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8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Class	Refund	
	Yes	No
Yes	0	3
No	3	4

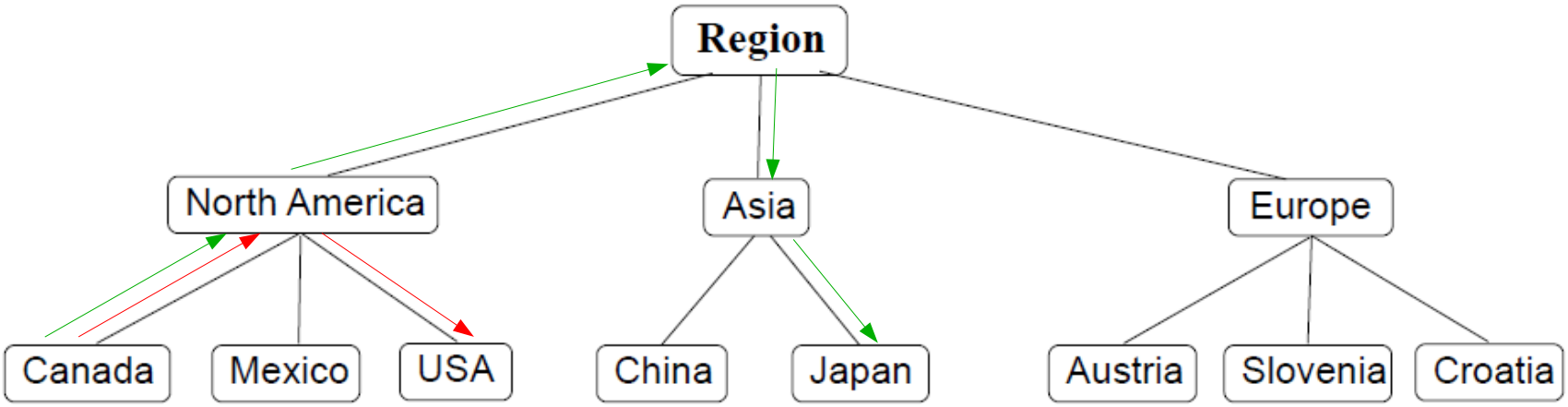
Distance between values:

d(Refund=Yes,Refund=No)

$$= | 0/3 - 3/7 | + | 3/3 - 4/7 | = 6/7$$

Other Distance Functions

- Other distances are possible
  - hierarchical attributes
    - distance of the values in the hierarchy
    - e.g., length of shortest path form v_1 to v_2



$$d(\text{Canada}, \text{USA}) = 2, \; d(\text{Canada}, \text{Japan}) = 4$$

Other Distance Functions

- Other distances are possible
  - hierarchical attributes
    - distance of the values in the hierarchy
    - e.g., length of shortest path form v_1 to v_2
  - string values
    - edit distance

Virginia
Verginia
Verminia
Vermonia
Vermonta
Vermont

$$d(\text{Virginia}, \text{Vermont}) = 5$$

Other Distance Functions

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- Other distances are possible
  - hierarchical attributes
    - distance of the values in the hierarchy
    - e.g., length of shortest path form v_1 to v_2
  - string values
    - edit distance
- in general
  - distances are domain-dependent
  - can be chosen appropriately

Distances for Missing Values

- not all attribute values may be specified for an example
- Common policy:
  - assume missing values to be maximally distant

Feature Weighting

- Not all dimensions are equally important
  - comparisons on some dimensions might even be completely irrelevant for the prediction task
  - straight-forward distance functions give equal weight to all dimensions
- Idea:
  - use a weight for each attribute to denote its importance
  - e.g., Weighted Euclidean Distance:

$$d(x_1, x_2) = \sqrt{\sum_A w_A \cdot d_A(v_{1,A}, v_{2,A})^2}$$

  - weights w_A can be set by user or determined automatically
- Survey of feature weighting algorithms:

Dietrich Wettschereck, David W. Aha, Takao Mohri:
A Review and Empirical Evaluation of Feature Weighting Methods for a Class of Lazy Learning Algorithms.
Artificial Intelligence Review 11(1-5): 273-314 (1997)

RELIEF
(Kira & Rendell, ICML-92)

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Basic idea:

in a local neighborhood around an example x a good attribute A should

- allow to discriminate x from all examples of different classes (the set of *misses*)
  - therefore the probability that the attribute has a different value for x and a miss m should be high
- have the same value for all examples of the same class as x (the set of *hits*)
  - therefore the probability that the attribute has a different value for x and a hit h should be low

→ try to estimate and maximize $w_A = Pr(v_x \neq v_m) - Pr(v_x \neq v_h)$

where v_x is the value of attribute A in example x

- this probability can be estimated via the average distance

RELIEF
(Kira & Rendell, ICML-92)

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1. set all attribute weights $w_A = 0.0$
2. for $i = 1$ to r (← user-settable parameter)
   - select a random example x
   - find
     - h: nearest neighbor of same class (*near hit*)
     - m: nearest neighbor of different class (*near miss*)
   - for each attribute A

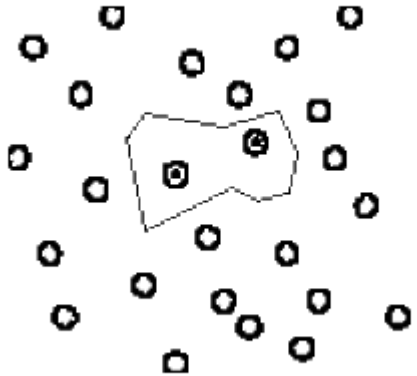
$$w_A \leftarrow w_A + \frac{1}{r} \cdot (d_A(m, x) - d_A(h, x))$$

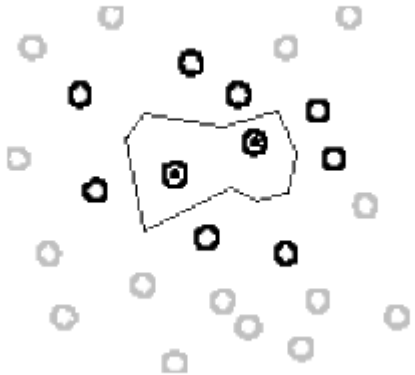
where $d_A(x,y)$ is the distance in attribute A between examples x and y (normalized to [0,1]-range).

Note: when used for feature weighting, all $w_A < 0.0$ are set to 0 in the end.

Learning Prototypes

- Only those instances involved in a decision need to be stored
  - Noisy instances should be filtered out
- Idea:
  - only use prototypical examples





Learning Prototypes: IB-algorithms

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- Case Study for prototype selection
  - Aha, Kibler and Albert: Instance-based learning. *Machine Learning,*1991.
- **IB1:** Store all examples
  - high noise tolerance
  - high memory demands
- **IB2:** Store new example only if misclassified by stored examples
  - low noise tolerance
  - low memory demands
- **IB3:** like IB2, but
  - maintain a counter for the number of times the example participated in correct and incorrect classifications
  - use a significant test for filtering noisy examples
    - improved noise tolerance
    - low memory demands

Instance Weighting

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- Idea:
  - we assign a weight to each instance
  - instances with lower weights are always distant
    - hence have a low impact on classification
    - instance weight $w_x = 0$ completely ignores this instance x

  → Selecting instances is a special case of instance weighting

- Similarity function used in PEBLS (Cost & Salzberg, 1993)

$$d(x_1, x_2) = \frac{1}{w_{x_1} \cdot w_{x_2}} \cdot \sum_A d_A(v_1, v_2)^k$$

where $$w_x = \frac{\text{Number of times } x \text{ has correctly predicted the class}}{\text{Number of times } x \text{ has been used for prediction}}$$

  - $w_x \approx 1$ if instance x predicts well
  - $w_x < 1$ if instance x does not predict well

Efficiency of NN algorithms

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- very efficient in training
  - only store the training data
- not so efficient in testing
  - computation of distance measure to every training example
  - much more expensive than, e.g., rule learning

- What is more efficient: k-NN or 1-NN?
  - retrieving the k nearest neighbors is (almost) no more expensive than retrieving a single nearest neighbor
  - k nearest neighbors can be maintained in a queue

    → k-NN and 1-NN are equal in terms of efficiency

Finding nearest neighbors efficiently

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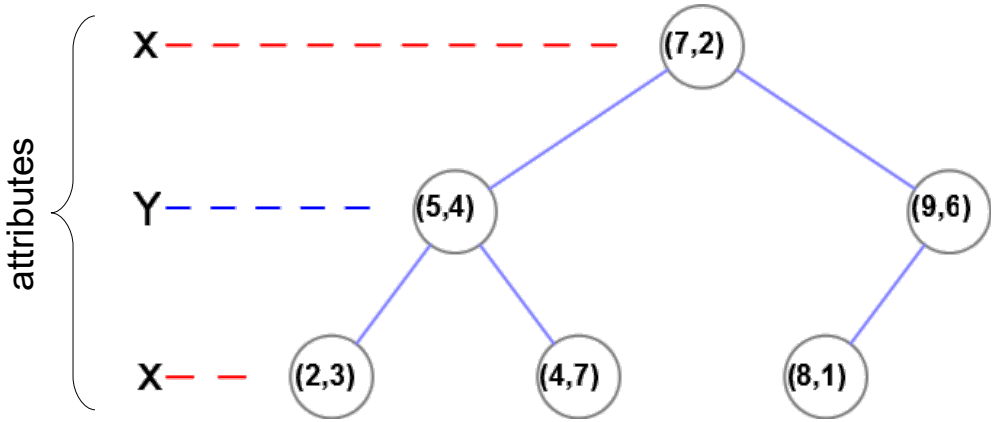
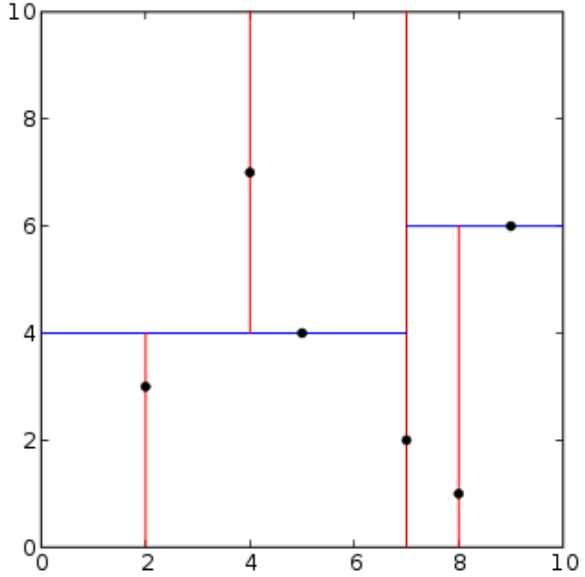
- Simplest way of finding nearest neighbour:
  - linear scan of the data
  - classification takes time proportional to the product of the number of instances in training and test sets
- Nearest-neighbor search can be done more efficiently using appropriate data structures
  - kD-trees
  - ball trees

kD-Trees

- common setting (others possible)
  - each level corresponds to one of the attributes
    - order of attributes can be arbitrary, fixed, and cyclic
  - each level splits according to its attribute
    - ideally use the median value (results in balanced trees)
    - often simply use the value of the next example





Building kD-trees incrementally

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- Big advantage of instance-based learning: classifier can be updated incrementally
  - Just add new training instance after it arrives!
- Can we do the same with kD-trees?
- Heuristic strategy:
  - Find leaf node containing new instance
  - If leaf is empty
    - place instance into leaf
  - Else
    - split leaf according to the next dimension
    - Alternatively: split according to the longest dimension
      - idea: preserve squareness
- Tree should be re-built occasionally
  - e.g., if depth grows to twice the optimum depth

Using kD-trees: example

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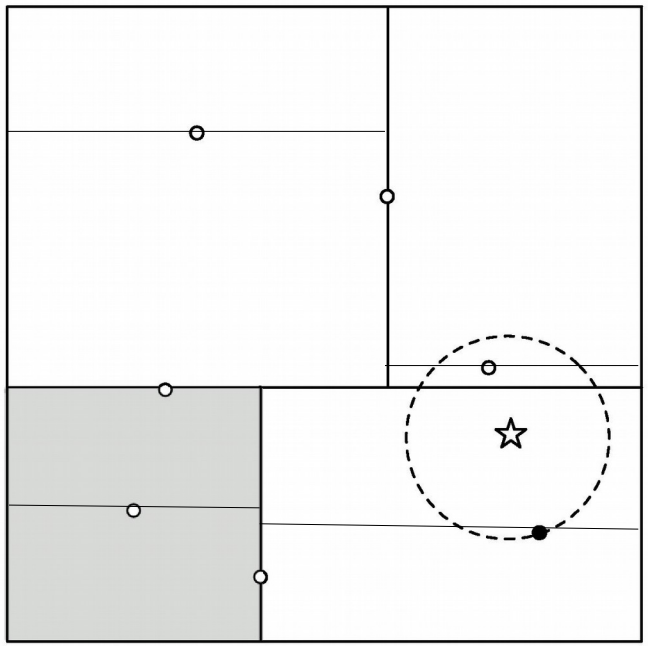
- The effect of a kD-tree is to partition the (multi-dimensional) sample space according to the underlying data distribution
  - finer partitioning in regions with high density
  - coarser partitioning in regions with low density
- For a given query point
  - descending the tree to find the data points lying in the cell that contains the query point
  - examine surrounding cells if they overlap the ball centered at the query point and the closest data point so far
    - recursively back up one level and check distance to the split point
    - if overlap also search other branch

→ only a few cells have to be searched



Using kD-trees: example

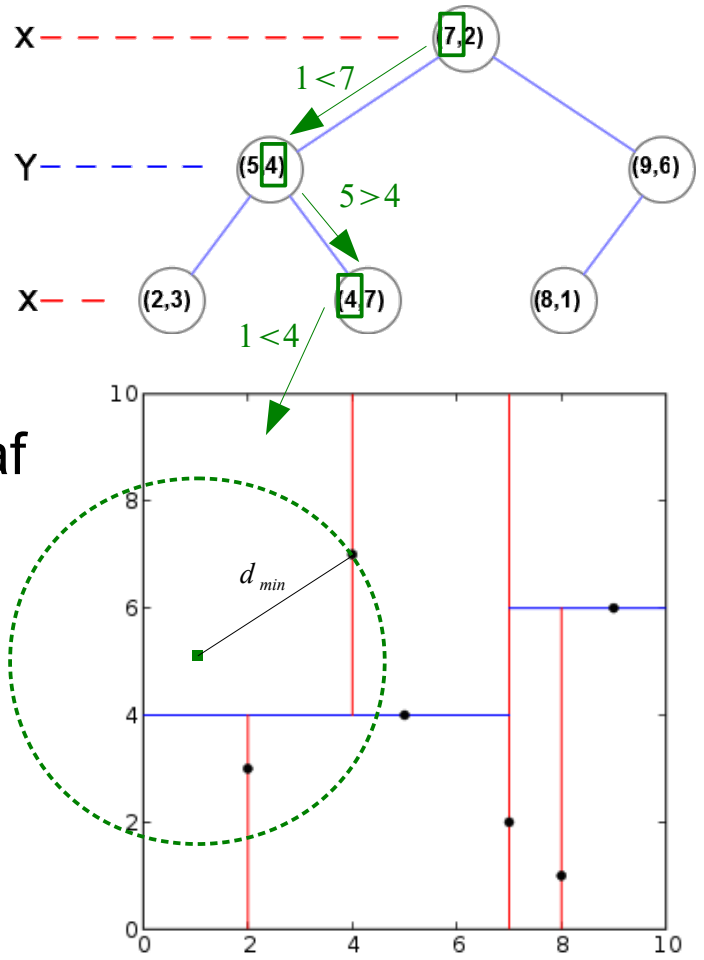
- Assume we have example [1,5]
  - Unweighted Euclidian distance

$$d(e_1,e_2)=\sqrt{\sum_A d_A(e_1,e_2)^2}$$

- sort the example down the tree:
  - ends in the left successor of [4,7]
- compute distance to example in the leaf

$$d([1,5],[4,7])=\sqrt{(1-4)^2+(5-7)^2}=\sqrt{13}$$

- now we have to look into rectangles that may contain a nearer example
  - remember the difference to the closest example $d_{min}=\sqrt{13}$



Using kD-trees: example

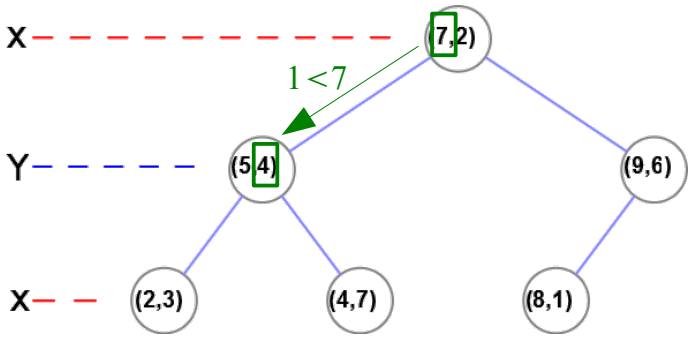
- go up one level (to example [4,7])
- compute distance to the closest point on this split (difference only on X)

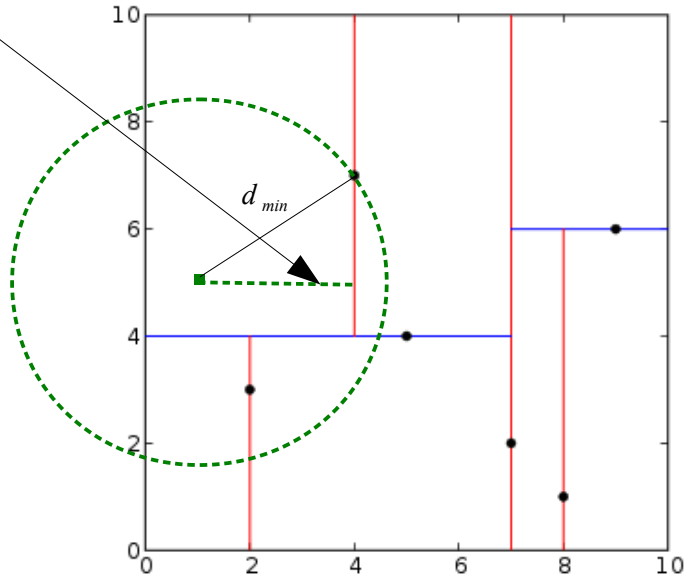
$$d([1,5],[4,*])=\sqrt{(4-1)^2+0^2}=3$$

- If the difference is smaller than the current best difference

$$d([1,5],[4,*])=3<\sqrt{13}=d_{min}$$

- then we could have a closer example in the right subtree of [4,7]
  - which in our case does not contain any example → done





Using kD-trees: example

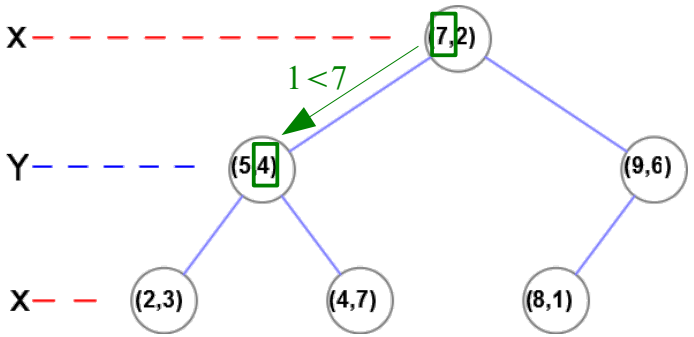
- go up one level (to example [5,4])
- compute distance to the closest point on this split (difference only on Y)

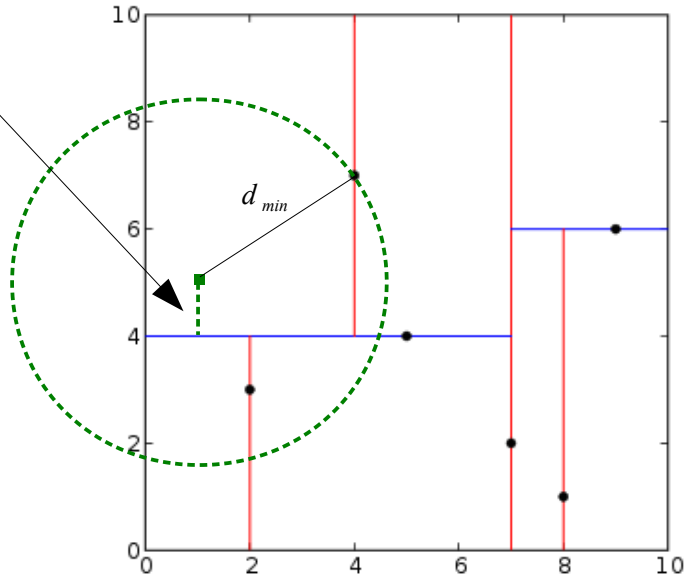
$$d([1,5],[*,4])=\sqrt{0^2+(5-4)^2}=1$$

- if the difference is smaller than the current best difference

$$d([1,5],[*,4])=1<\sqrt{13}=d_{min}$$

- then we could have a closer example in area $Y < 4$.
  - go down the other branch
  - and repeat recursively





Using kD-trees: example

- go down to leaf [2,3]
- compute distance to example in this leaf

$$d([1,5],[2,3])=\sqrt{(1-2)^2+(5-3)^2}=\sqrt{5}$$

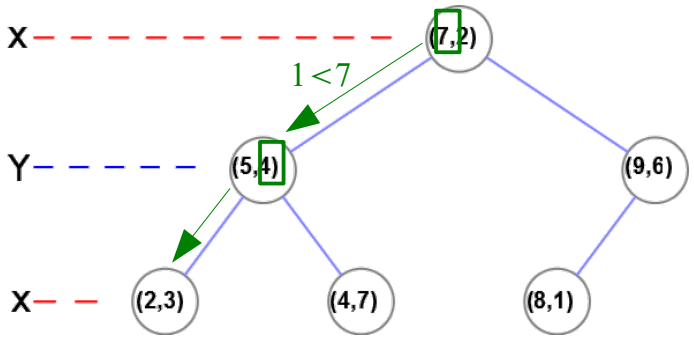
- if the difference is smaller than the current best difference

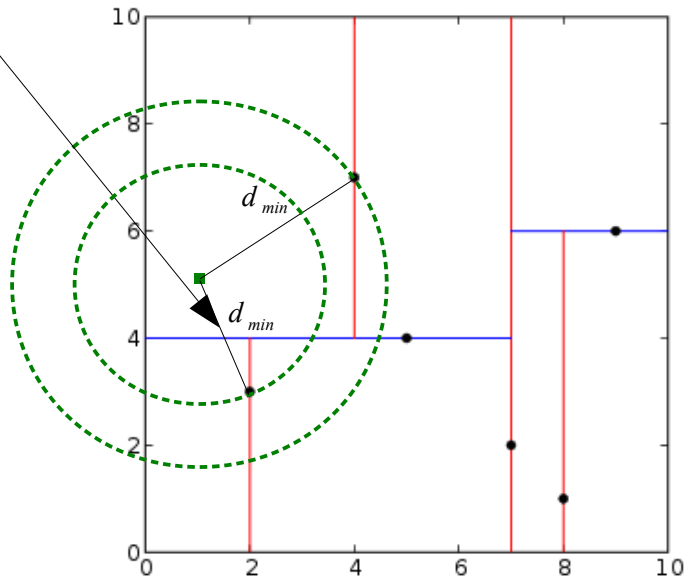
$$d([1,5],[2,3])=\sqrt{5}<\sqrt{13}=d_{min}$$

- then the example in the leaf is the new nearest neighbor and

$$d_{min}=\sqrt{5}<\sqrt{13}$$

- this is recursively repeated until we have processed the root node
  - no more distances have to be computed



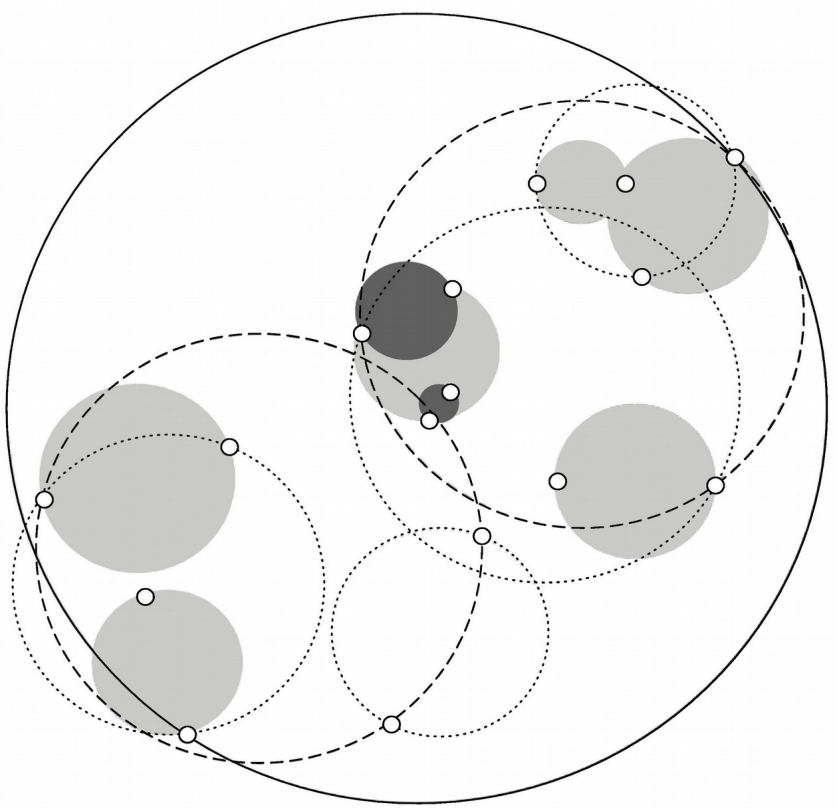


Ball trees

- Problem in kD-trees: corners
- Observation:
  - There is no need to make sure that regions don't overlap

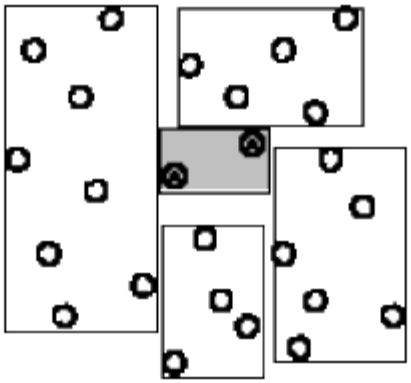
→ We can use balls (hyperspheres) instead of hyperrectangles

  - A ball tree organizes the data into a tree of k-dimensional hyperspheres
  - Normally allows for a better fit to the data and thus more efficient search

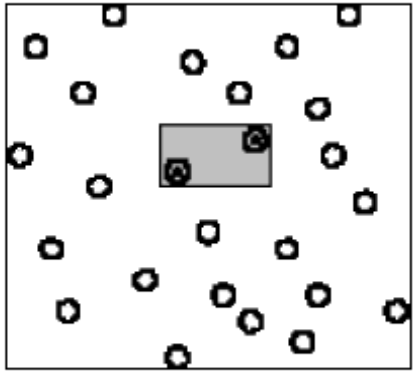


Nearest Hyper-Rectangle

- Nearest-Neighbor approaches can be extended to compute the distance to the nearest hyper-rectangle
  - a hyper-rectangle corresponds to a rule
  - conditions are intervals along each dimension



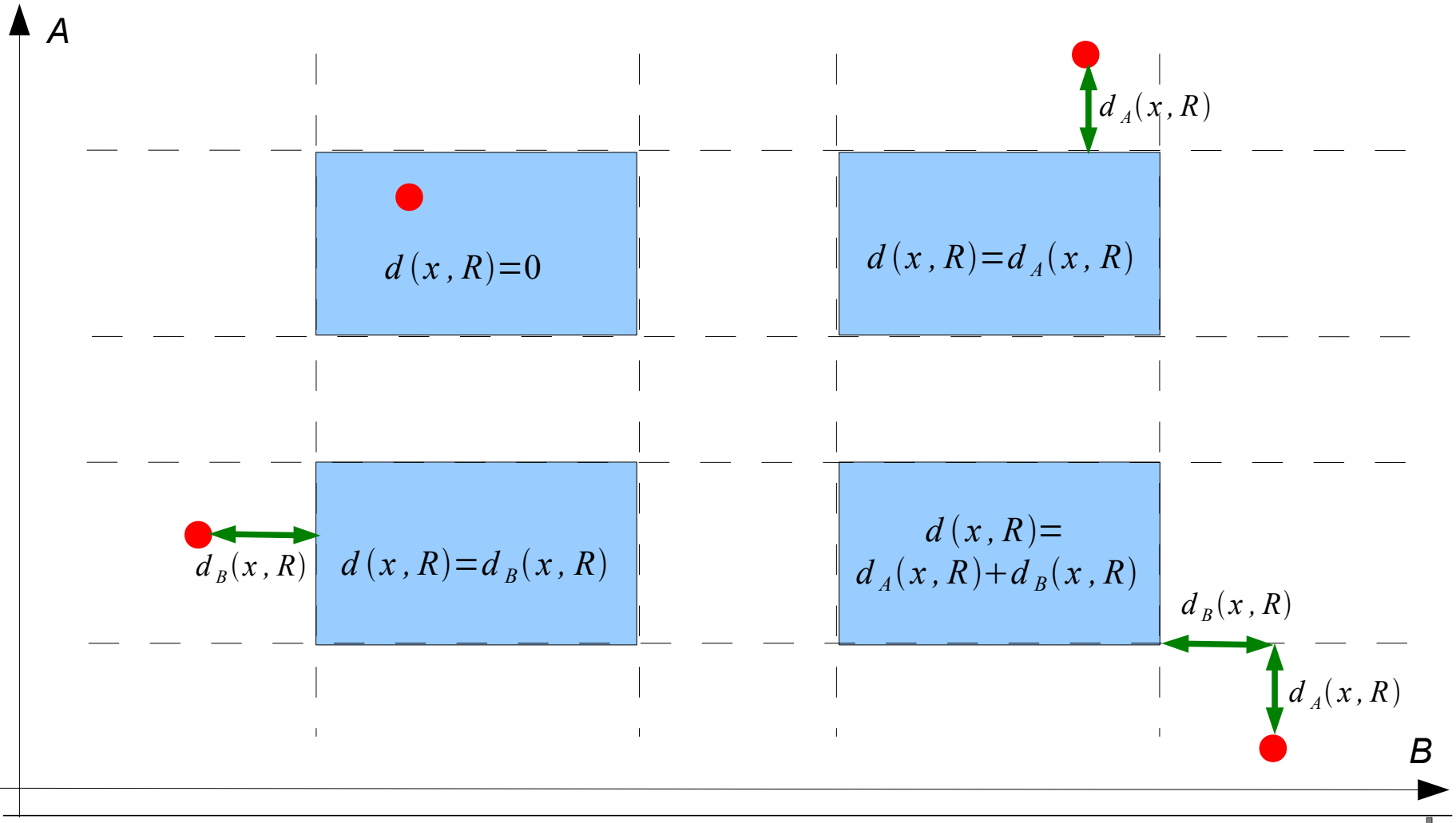
non-overlapping rectangles



nested rectangles

- To do so, we need to adapt the distance measure
  - distance of a point to a rectangle instead of point-to-point distance

Rectangle-to-Point Distance



Rectangle-to-Point Attribute Distance

- numeric Attributes
  - distance of the point to the closest edge of the rectangle along this attribute (i.e., distance to the upper/lower bound of the interval)

$$d_A(v, R) = \begin{cases} 0 & \text{if } v_{min,A_R} \le v \le v_{max,A_R} \\ v - v_{max,A_R} & \text{if } v > v_{max,A_R} \\ v_{min,A_R} - v & \text{if } v < v_{min,A_R} \end{cases}$$

if rule R uses $v_{min,A_R} \le A \le v_{max,A_R}$ as condition for attribute A

- symbolic attributes
  - 0/1 distance $d_A(v, R) = \begin{cases} 0 & \text{if } v = v_{A_R} \\ 1 & \text{if } v \neq v_{A_R} \end{cases}$

if rule R uses $A = v_{A_R}$ as condition for attribute A

One can also adapt other distances. RISE uses a version of the VDM.

NEAR (Salzberg, 1991)

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1. randomly choose r seed examples
   - convert them into rules
2. for each example x
   - choose rule $R_{min} = \arg\min_R d(x, R)$
   - if x is classified correctly by R_{min}
     - enlarge the condition of R_{min} so that x is covered
       - for each numeric attribute enlarge the interval if necessary
       - for each symbolic attribute delete the condition if necessary
   - else if x is classified incorrectly by R_{min}
     - add example x as a new rule

NEAR uses both instance and feature weighting

$$d(x, R) = w_x \sqrt{\sum_A w_A^2 d_A(x, R)^2}$$

Instance and Feature Weighting in NEAR

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Instance Weighting as in PEBLS

Feature Weights are computed incrementally

- if an example is incorrectly classified
  - the weights of all matching attributes are increased by a fixed percentage (20%)
    - this has the effect of moving the example farther away along these dimensions
  - the weights of all attributes that do not match are decreased by a fixed percentage (20%)
- if an example is correctly classified
  - do the opposite (decrease matching and increase non-matching weights analogously)

Second Chance Heuristic

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An improved version used a Second Chance Heuristic

- if the nearest rule did not classify correctly, try the second one
  - if this one matches → expand it to cover the example
  - if not → add the example as a new rule
- this can lead to the generation of nested rules
  - i.e., rectangles inside of other rectangles
  - at classification time, use the smallest matching rectangle
    - but this did not work well (overfitting?)
  - such nested rules may be interpreted as rules with exceptions

RISE (Domingos, 1996)

(Rule Induction from a Set of Exemplars)

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1. turn each example into a rule resulting in a theory T
2. repeat
   - for each rule R in T
     i. choose uncovered example $x_{min} = \arg\min_x d(x, R)$
     ii. R' = minimalGeneralisation(R,x_{min})
     iii. replace R with R' if this does not decrease the accuracy of T
     iv. delete R' if it is already part of T (duplicate rule)
3. until no further increase in accuracy

- RISE uses the simple distance function

$$d(x, R) = \sum_A d_A(x, R)^k$$

RISE (Domingos, 1996)

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- Classification of an example:
  - use the rule that is closest to the example
  - if multiple rules have the same distance, use the one with the highest Laplace-corrected precision

- Leave-one-out estimation of accuracy of a theory:
  - For classifying an example, the rule that encodes it is ignored
    - but only if it has not been generalized yet
  - can be computed efficiently if each examples remembers the distance to the rule by which it is classified
    - if a rule is changed, go once through all examples and see if the new rule classifies any examples that were classified by some other rule before
    - count the improvements (+1) or mistakes (-1) only for those examples, and see whether their sum is > 0 or < 0.

Differences NEAR and RISE

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- NEAR
  - focuses on examples
  - incremental training
  - instance weighted and feature-weighted Euclidean distance
  - tie breaking using the smallest rule
- RISE
  - focuses on rules
  - batch training
  - straight-forward Manhattan distance
  - tie breaking with Laplace heuristic

Discussion

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- Nearest Neighbor methods are often very accurate
  - Assumes all attributes are equally important
    - Remedy: attribute selection or weights
  - Possible remedies against noisy instances
    - Take a majority vote over the *k* nearest neighbors
    - Removing noisy instances from dataset (difficult!)
  - Statisticians have used k-NN since early 1950s
    - If $n \rightarrow \infty$ and $k/n \rightarrow 0$, error approaches minimum
    - can model arbitrary decision boundaries
- ...but somewhat inefficient (at classification time)
  - straight-forward application maybe too slow
  - kD-trees become inefficient when number of attributes is too large (approximately > 10)
  - Ball trees work well in higher-dimensional spaces
- several similarities with rule learning