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
  - EACH: 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
## Rote Learning

<table>
<thead>
<tr>
<th>Day</th>
<th>Temperature</th>
<th>Outlook</th>
<th>Humidity</th>
<th>Windy</th>
<th>Play Golf?</th>
</tr>
</thead>
<tbody>
<tr>
<td>07-05</td>
<td>hot</td>
<td>sunny</td>
<td>high</td>
<td>false</td>
<td>no</td>
</tr>
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today: cool sunny normal false yes
## Nearest Neighbor Classification

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| tomorrow | mild | sunny | normal | false | yes |
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
  - Nearest-neighbor classifier
    - Uses k “closest” points (nearest neighbors) for performing classification
**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
    \[
    \hat{y} = \max_c \sum_{i=1}^k \begin{cases} 
      1 & \text{if } y_i = c \\
      0 & \text{if } y_i \neq c 
    \end{cases}
    = \max_c \sum_{i=1}^k 1(y_i = c)
    \]

- 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

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

\[ \hat{y} = \frac{\sum_{i=1}^{k} w_i y_i}{\sum_{i=1}^{k} w_i} \]

- 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
Choosing the value of $k$

1-NN

5-NN

20-NN
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

- 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

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

- **0/1 distance**

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

- **Value Difference Metric (VDM)** (Stanfill & Waltz 1986)
  - two values are similar if they have approximately the same distribution over all classes (similar 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

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

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

$$d(\text{Refund}=\text{Yes}, \text{Refund}=\text{No})$$

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

<table>
<thead>
<tr>
<th>Tid</th>
<th>Refund</th>
<th>Marital Status</th>
<th>Taxable Income</th>
<th>Cheat</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Yes</td>
<td>Single</td>
<td>125K</td>
<td>No</td>
</tr>
<tr>
<td>2</td>
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<td>Married</td>
<td>100K</td>
<td>No</td>
</tr>
<tr>
<td>3</td>
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<td>70K</td>
<td>No</td>
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<tr>
<td>4</td>
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<td>No</td>
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<td>No</td>
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Distance between values:

\[
d(\text{Single}, \text{Married}) = | \frac{2}{4} - \frac{0}{4} | + | \frac{2}{4} - \frac{4}{4} | = 1
\]

\[
d(\text{Single}, \text{Divorced}) = | \frac{2}{4} - \frac{1}{2} | + | \frac{2}{4} - \frac{1}{2} | = 0
\]

\[
d(\text{Married}, \text{Divorced}) = | \frac{0}{4} - \frac{1}{2} | + | \frac{4}{4} - \frac{1}{2} | = 1
\]
Other Distance Functions

- Other distances are possible
  - hierarchical attributes
    - distance of the values in the hierarchy
    - e.g., length of shortest path from $v_1$ 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 from $v_1$ 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:
**RELIEF**
(Kira & Rendell, ICML-92)

**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

\[ w_A = Pr(v_x \neq v_m) - Pr(v_x \neq v_h) \]

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)

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 $A$
     - \[ w_A \leftarrow w_A + \frac{1}{r} \left( d_A(m, x) - d_A(h, x) \right) \]
     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

- Case Study for prototype selection

- **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

- Selecting instances is a special case of instance weighting
- Idea:
  - all instances are assigned weights
  - instances with higher weights are always distant
    - hence have a low impact on classification
    - instance weight $w_x = 0$ ignores this instance $x$

- 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

- 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

- Note that kNN and 1NN are equal in terms of efficiency
  - 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
Finding nearest neighbors efficiently

- 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 this attribute
    - ideally use the median value (results in balanced trees)
    - often simply use the value of the next example
Building kD-trees incrementally

- 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

- 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 Euclidean distance
    \[ d(e_1, e_2) = \sqrt{\sum \Delta d_A(e_1, e_2)^2} \]
- sort the example down the tree:
  - ends in leaf \([4,7]\)
- 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 \(d_{\text{min}} = \sqrt{13}\)
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
  \[ d([1,5],[*,4]) = 1 < \sqrt{13} = d_{\text{min}} \]
- 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

- 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**

\[ d(x, R) = d_A(x, R) + d_B(x, R) \]
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)
  
  \[
  d_A(v, R) = \begin{cases} 
  0 & \text{if } v_{min, A_R} \leq v \leq v_{max, A_R} \\
  v - v_{max, A_R} & \text{if } v > v_{max, A_R} \\
  v_{min, A_R} - v & \text{if } v < v_{min, A_R}
  \end{cases}
  \]

  if rule \( R \) uses \( v_{min, A_R} \leq A \leq v_{max, A_R} \) 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.
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

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

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)

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. \( R' = \text{minimalGeneralisation}(R, x_{\min}) \)
     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)

- 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

- **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

- 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 $n \to \infty$ and $k/n \to 0$, 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