Instance-Based Learning

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Some of the slides in these lectures have been adapted/borrowed from materials developed by Tom Dietterich, Pedro Domingos, Tom Mitchell, David Page, and Jude Shavlik

Goals for the lecture

you should understand the following concepts

- k-NN classification
- k-NN regression
- edited nearest neighbor
- k-d trees for nearest neighbor identification

Nearest-neighbor classification

learning task

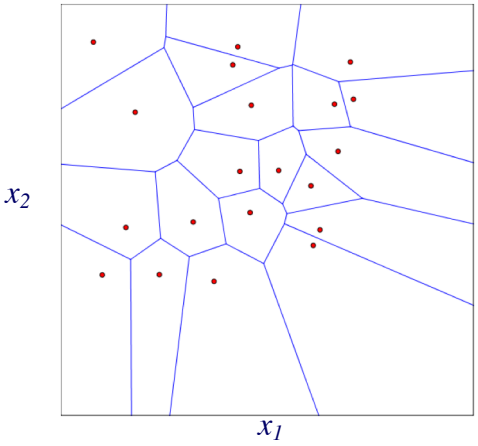
- given a training set $\left(\mathbf{x}^{(1)}, y^{(1)}\right) \ldots \left(\mathbf{x}^{(m)}, y^{(m)}\right)$, do nothing (it's sometimes called a *lazy learner*)

classification task

- **given**: an instance $\boldsymbol{x}^{(q)}$ to classify
- find the training-set instance $\boldsymbol{x}^{(i)}$ that is most similar to $\boldsymbol{x}^{(q)}$
- return the class value $y^{(i)}$

The decision regions for nearest-neighbor classification

Voronoi diagram: each polyhedron indicates the region of feature space that is in the nearest neighborhood of each training instance



k-nearest-neighbor classification

classification task

- **given**: an instance $\boldsymbol{x}^{(q)}$ to classify
- find the k training-set instances $\left(\mathbf{x}^{(1)}, y^{(1)}\right) \ldots \left(\mathbf{x}^{(k)}, y^{(k)}\right)$ that are most similar to $\boldsymbol{x}^{(q)}$
- return the class value

$$\hat{y} \leftarrow \arg\max_{v \in \text{values}(Y)} \sum_{i=1}^{k} \delta(v, y^{(i)}) \qquad \delta(a,b) = \begin{cases} 1 \text{ if } a = b \\ 0 \text{ otherwise} \end{cases}$$

(i.e. return the class that the plurality of the neighbors have)

How can we determine similarity/distance

suppose all features are discrete

- Hamming distance: count the number of features for which two instances differ

suppose all features are continuous

- Euclidean distance:

$d(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \sqrt{\sum_f \left(x_f^{(i)} - x_f^{(j)}\right)^2}$ where $x_f^{(i)}$ represents the f^{th} feature of $\boldsymbol{x}^{(i)}$

- Manhattan distance:

$d(\boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)}) = \sum_f \left| x_f^{(i)} - x_f^{(j)} \right|$

How can we determine similarity/distance

- if we have a mix of discrete/continuous features:

$$d(\mathbf{x}^{(i)},\mathbf{x}^{(j)}) = \sum_f \begin{cases} \left|x_f^{(i)} - x_f^{(j)}\right| & \text{if } f \text{ is continuous} \\ 1 - \delta\left(x_f^{(i)}, x_f^{(i)}\right) & \text{if } f \text{ is discrete} \end{cases}$$

- typically want to apply to continuous features some type of normalization (values range 0 to 1) or standardization (values distributed according to standard normal)
- many other possible distance functions we could use…

Standardizing numeric features

- given the training set D, determine the mean and stddev for feature x_i

$$\mu_i = \frac{1}{|D|}\sum_{d=1}^{|D|} x_i^{(d)} \qquad \sigma_i = \sqrt{\frac{1}{|D|}\sum_{d=1}^{|D|}\left(x_i^{(d)} - \mu_i\right)^2}$$

- standardize each value of feature x_i as follows

$$\hat{x}_i^{(d)} = \frac{x_i^{(d)} - \mu_i}{\sigma_i}$$

- do the same for test instances, using the same μ_i and σ_i derived from the training data

k-nearest-neighbor *regression*

learning task

- given a training set $\left(\mathbf{x}^{(1)}, y^{(1)}\right) \ldots \left(\mathbf{x}^{(m)}, y^{(m)}\right)$, do nothing

prediction task

- **given**: an instance $\boldsymbol{x}^{(q)}$ to make a prediction for
- find the k training-set instances $\left(\mathbf{x}^{(1)}, y^{(1)}\right) \ldots \left(\mathbf{x}^{(k)}, y^{(k)}\right)$ that are most similar to $\boldsymbol{x}^{(q)}$
- return the value

$$\hat{y} \leftarrow \frac{1}{k} \sum_{i=1}^{k} y^{(i)}$$

Distance-weighted nearest neighbor

We can have instances contribute to a prediction according to their distance from $\boldsymbol{x}^{(q)}$

classification:

$$\hat{y} \leftarrow \arg\max_{v \in \text{values}(Y)} \sum_{i=1}^{k} w_i \ \delta(v, y^{(i)}) \qquad w_i = \frac{1}{d(x^{(q)}, x^{(i)})^2}$$

regression:

$$\hat{y} \leftarrow \frac{\sum_{i=1}^{k} w_i \ y^{(i)}}{\sum_{i=1}^{k} w_i}$$

Speeding up k-NN

- k-NN is a "lazy" learning algorithm – does virtually nothing at training time
- but classification/prediction time can be costly when the training set is large

- two general strategies for alleviating this weakness
  - don't retain every training instance (edited nearest neighbor)
  - use a smart data structure to look up nearest neighbors (e.g. a k-d tree)

Edited instance-based learning

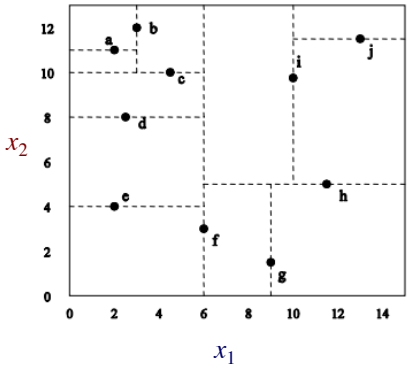
- select a subset of the instances that still provide accurate classifications

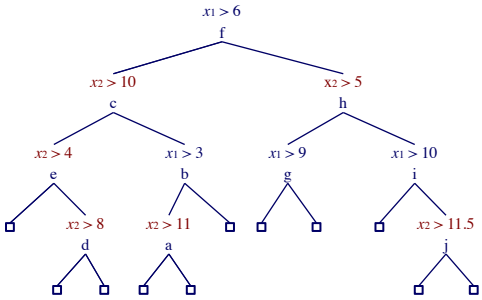
- *incremental deletion*
  start with all training instances in memory
  for each training instance $(\boldsymbol{x}^{(i)}, y^{(i)})$
    if other training instances provide correct classification for $(\boldsymbol{x}^{(i)}, y^{(i)})$
      delete it from the memory

- *incremental growth*
  start with an empty memory
  for each training instance $(\boldsymbol{x}^{(i)}, y^{(i)})$
    if other training instances in memory **don't** correctly classify $(\boldsymbol{x}^{(i)}, y^{(i)})$
      add it to the memory

k-d trees

- a *k-d tree* is a data structure for indexing a set of instances
- each internal node
  - stores one instance
  - has a Boolean test on the median value of the feature having the highest variance (left branch corresponds to *false* in the figure)





Finding nearest neighbors with a k-d tree

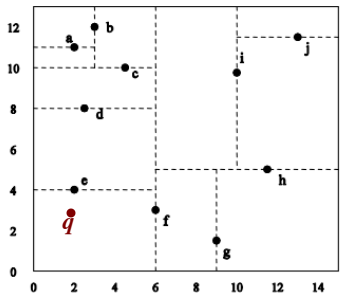
- use branch-and-bound search
- priority queue stores
  - nodes considered
  - lower bound on their distance to query instance
- lower bound given by distance using a single feature
- average case: $O(\log_2 m)$
- worst case: $O(m)$ where m is the size of the training-set

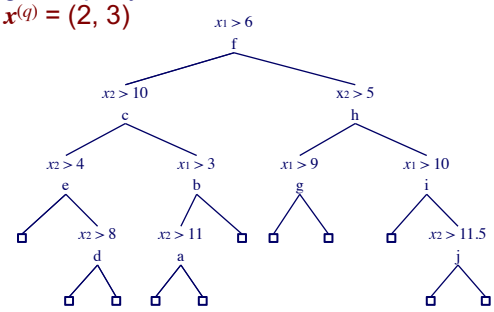
Finding nearest neighbors in a k-d tree

```
NearestNeighbor(instance x^(q))
    PQ = { }                                          // minimizing priority queue
    best_dist = ∞                                     // smallest distance seen so far
    PQ.push(root, 0)
    while PQ is not empty
        (node, bound) = PQ.pop();
        if (bound ≥ best_dist)
            return best_node.instance                 // nearest neighbor found
        dist = distance(x^(q), node. instance)
        if (dist < best_dist)
            best_dist = dist
            best_node = node
        if (q[node.feature] – node.threshold > 0)
            PQ.push(node.left, x^(q)[node.feature] – node.threshold)
            PQ.push(node.right, 0)
        else
            PQ.push(node.left, 0)
            PQ.push(node.right, node. threshold - x^(q) [node.feature])
    return best_node. instance
```

k-d tree example (Manhattan distance)

given query
$x^{(q)} = (2, 3)$





	distance	best distance	best node	priority queue
		∞		(f, 0)
pop f	4.0	4.0	f	(c, 0) (h, 4)
pop c	10.0	4.0	f	(e, 0) (h, 4) (b, 7)
pop e	1.0	1.0	e	(d, 1) (h, 4) (b, 7)
pop d	return e			

Strengths of instance-based learning

- simple to implement
- "training" is very efficient
- adapts well to on-line learning
- robust to noisy training data (when k > 1)
- often works well in practice

Limitations of instance-based learning

- sensitive to range of feature values
- sensitive to irrelevant and correlated features, although…
  - there are variants (such as locally weighted regression) that learn weights for different features
  - later we'll talk about *feature selection* methods
- classification/prediction can be inefficient, although edited methods and k-d trees can help alleviate this weakness
- doesn't provide much insight into problem domain because there is no explicit model