Machine learning

Instance Based Learning

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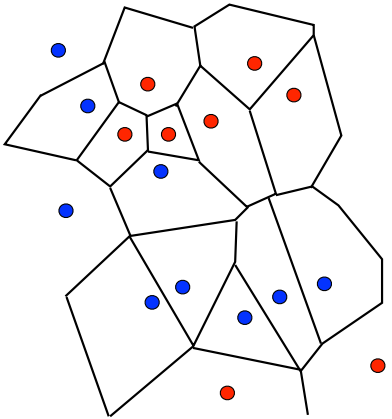
Introduction

1. The methods described before such as decision tree
   1.1 finding a hypothesis
   1.2 using this hypothesis for classification/regression of new test examples.
2. These methods are called eager learning.
3. The instance based learning algorithms such as k-NN
   3.1 store all of the training examples
   3.2 classify a new example x by finding some neighboring training example (x_i, y_i) of x according to some distance functions.
4. Instance based classifiers do not explicitly compute decision boundaries.
5. However, the boundaries form a subset of the Voronoi diagram of the training data.



Nearest neighbor algorithms

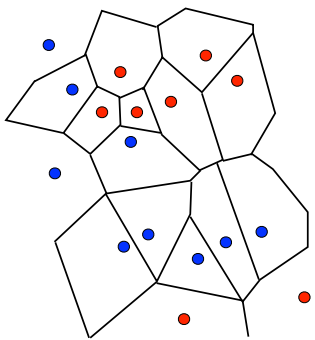
1. Fix $k \geq 1$ and let $t_i \in \{0, 1\}$, given the training set

$$S = \{(x_1, t_1), \ldots, (x_N, t_N)\}$$

2. The k-NN for all test examples x returns the hypothesis h defined by

$$h(x) = \mathbb{I}\left[\sum_{i, t_i = 1} w_i > \sum_{i, t_i = 0} w_i\right].$$

3. Weights $w_1, \ldots, w_N$ are chosen such that $w_i = \frac{1}{k}$ if x_i is among the k nearest neighbors of x.
4. The boundaries form a subset of the Voronoi diagram of the training data.



1. The k-NN only requires
   - An integer k.
   - A set of labeled examples S.
   - A metric to measure closeness.
2. For all points x, y, z, a metric d must satisfy the following properties.
   - Non-negativity : $d(x, y) \geq 0$.
   - Reflexivity : $d(x, y) = 0 \Leftrightarrow x = y$.
   - Symmetry : $d(x, y) = d(y, x)$.
   - Triangle inequality : $d(x, y) + d(y, z) \geq d(x, z)$.

1. The Minkowski distance for D-dimensional examples is the L_p norm.

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

2. The Euclidean distance is the L_2 norm

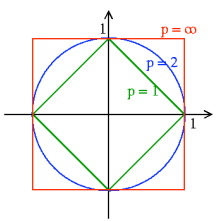
$$L_2(x, y) = \left(\sum_{i=1}^{D} |x_i - y_i|^2 \right)^{\frac{1}{2}}$$

3. The Manhattan or city block distance is the L_2 norm

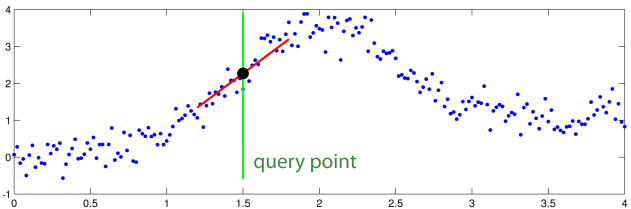
$$L_1(x, y) = \sum_{i=1}^{D} |x_i - y_i|$$

4. The L_∞ norm is the maximum of distances along axes

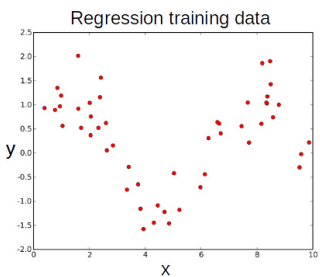
$$L_\infty(x, y) = \max_i |x_i - y_i|$$

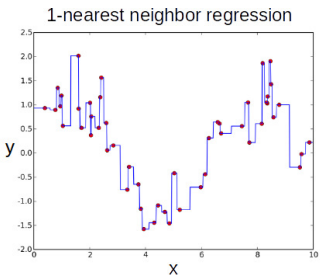


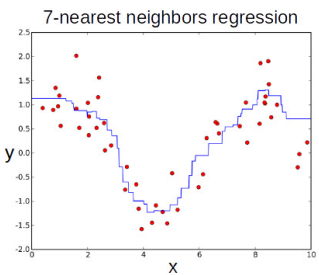
1. The k-NN algorithm adapted for approximating continuous-valued target function.
2. Calculate the mean of k nearest neighboring examples instead of majority vote : $\hat{f}(x) = \frac{\sum_{i=1}^{k} f(x_i)}{k}$.



3. The effect of k on the performance of algorithm [1]







[1] Pictures are taken from P. Rai slide.

1. The k-NN algorithm is a lazy learning algorithm.
   - It defers the hypothesis finding until a test example x arrives.
   - For test example x, the k-NN uses the stored training data.
   - Discards the the found hypothesis and any intermediate results.
2. This strategy is opposed to an eager learning algorithm which
   - It finds a hypothesis h using the training set
   - It uses the found hypothesis h for classification of test example x.
3. Trade offs
   - During training phase, lazy algorithms have fewer computational costs than eager algorithms.
   - During testing phase, lazy algorithms have greater storage requirements and higher computational costs.
4. What is inductive bias of k-NN?

Properties of nearest neighbor algorithms

1. Advantages
   - Analytically tractable
   - Simple implementation
   - Use local information, which results in highly adaptive behavior.
   - It parallel implementation is very easy.
   - Nearly optimal in the large sample ($N \to \infty$).

$$E(Bayes) < E(NN) < 2 \times E(Bayes).$$

2. Disadvantages
   - Large storage requirements.
   - It needs a high computational cost during testing.
   - Highly susceptible to the irrelevant features.
3. Large values of k
   - Results in smoother decision boundaries.
   - Provides more accurate probabilistic information
4. But large values of k
   - Increases computational cost.
   - Destroys the locality of estimation.

Distance-weighted nearest neighbor algorithms

1. One refinement of k-NN is to weight the contribution of each k neighbors to their distance to the query point x.
2. For two class classification

$$h(x) = \mathbb{I}\left[\sum_{i,t_i=1} w_i > \sum_{i,t_i=0} w_i\right].$$

   where

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

3. For C class classification

$$h(x) = \underset{c \in C}{argmax} \sum_{i=1}^{k} w_i \delta(c, t_i).$$

4. For regression

$$\hat{f}(x) = \frac{\sum_{i=1}^{k} w_i f(x_i)}{w_i}.$$

Locally weighted regression

1. In locally weighted regression (LWR), we use a linear model to do the local approximation $\hat{f}$:

$$\hat{f}(x) = w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_D x_D.$$

2. Suppose we aim to minimize the total squared error:

$$E = \frac{1}{2} \sum_{x \in S} (f(x) - \hat{f}(x))^2$$

3. Using gradient descent

$$\Delta w_j = \eta \sum_{x \in S} (f(x) - \hat{f}(x)) x_j$$

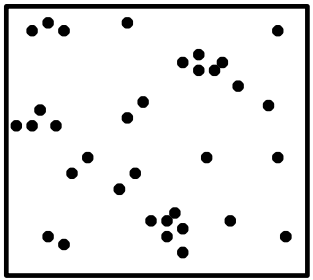
where η is a small number (the learning rate).

1. How shall we modify this procedure to derive a local approximation rather than a global one?
2. The simple way is to redefine the error criterion E to emphasize fitting the local training examples.
3. Three possible criteria are given below. Note we write the error $E(x_q)$ to emphasize the fact that now the error is being defined as a function of the query point x_q.
   - Minimize the squared error over just the k nearest neighbors:
   $$E_1(x_q) = \frac{1}{2} \sum_{x \in KNN(x_q)} (f(x) - \hat{f}(x))^2$$
   - Minimize 1 squared error over the set S of training examples, while weighting the error of each training example by some decreasing function k of its distance from x_q
   $$E_2(x_q) = \frac{1}{2} \sum_{x \in S} (f(x) - \hat{f}(x))^2 K(d(x_q, x))$$
   - Combine 1 and 2:
   $$E_3(x_q) = \frac{1}{2} \sum_{x \in KNN(x_q)} (f(x) - \hat{f}(x))^2 K(d(x_q, x))$$
4. If we choose criterion (3) and re-derive the gradient descent rule, we obtain
   $$\Delta w_j = \eta \sum_{x \in KNN(x_q)} K(d(x_q, x))(f(x) - \hat{f}(x)) x_j$$
   where η is a small number (the learning rate).

5. Criterion (2) is perhaps the most esthetically pleasing because it allows every training example to have an impact on the classification of x_q.
6. However, this approach requires computation that grows linearly with the number of training examples.
7. Criterion (3) is a good approximation to criterion (2) and has the advantage that computational cost is independent of the total number of training examples; its cost depends only on the number k of neighbors considered.

Finding $KNN(x)$ efficiently

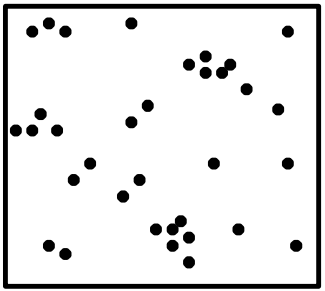
1. How efficiently find $KNN(x)$?
2. Tree-based data structures: pre-processing.
3. Often *kd*-trees (*k*-dimensional trees) used in applications.
4. A *kd*-tree is a generalization of binary tree in high dimensions
   - 4.1 Each internal node is associated with a hyper-rectangle and the hyper-plans is orthogonal to one of its coordinates.
   - 4.2 The hyper-plan splits the hyper-rectangle to two parts, which are associated with the child nodes.
   - 4.3 The partitioning goes on until the number of data points in the hyper-plane falls below some given threshold.



X	Y
.15	.1
.03	.55
.95	.1
...	...

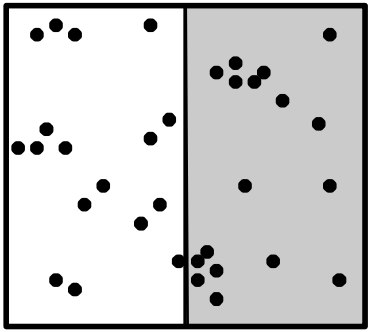
5. Splitting order : Widest first
6. Splitting value : Median
7. Stop condition : fewer than a threshold or box hit some minimum width.

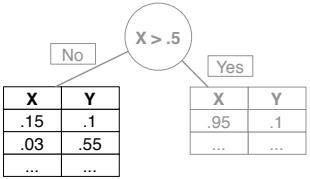
1. initial data set



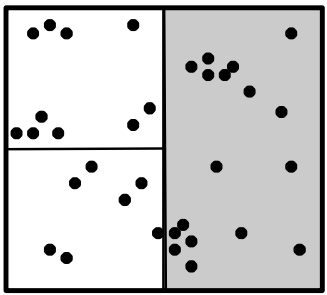
X	Y
.15	.1
.03	.55
.95	.1
...	...

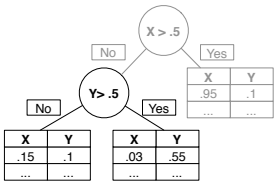
2. After first split



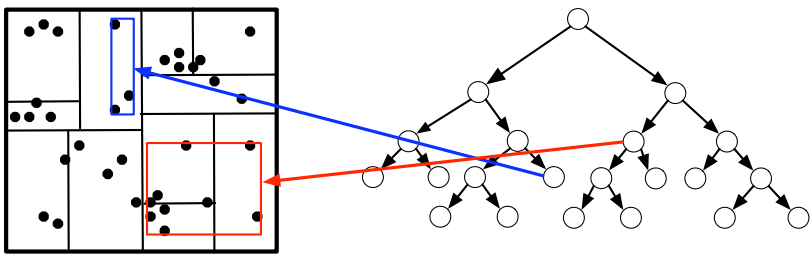


1. After second split

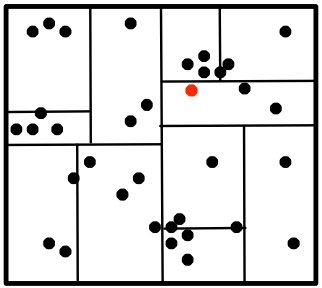


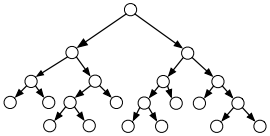


2. Final split.

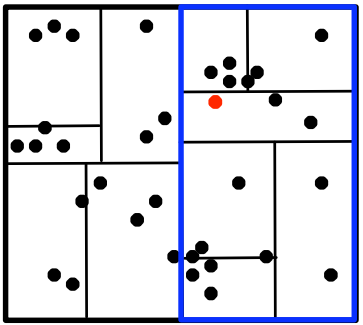


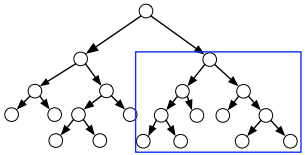
1. Traverse tree looking for the nearest neighbor of the query point.





2. Explore a branch of tree that is closest to the query point first





Reading

1. Chapter 8 of Machine Learning Book (Mitchell 1997).

 Mitchell, Tom M. (1997). *Machine Learning*. McGraw-Hill.

Questions?