

CSCE 478/878 Lecture 8: Instance-Based Learning

Stephen D. Scott
(Adapted from Tom Mitchell's slides)

November 10, 2008

Outline

- k -Nearest Neighbor
- Locally weighted regression
- Radial basis functions
- Case-based reasoning
- Lazy and eager learning

Nearest Neighbor

Key idea: just store all training examples $\langle x_i, f(x_i) \rangle$

Need some **distance measure** between instances (e.g. Euclidean distance, Hamming distance)

Nearest neighbor:

- Given query instance x_q , first locate nearest training example x_n , then estimate $\hat{f}(x_q) = f(x_n)$

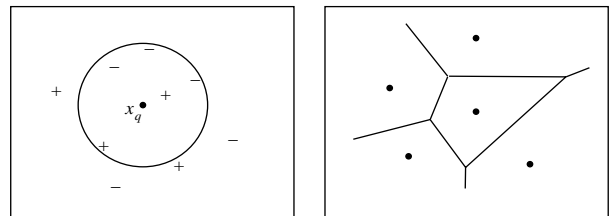
k -Nearest neighbor:

- Given x_q , take vote among its k nearest neighbors (if discrete-valued target function)
 - Let k not be divisible by number of possible labels
- Take mean of f values of k nearest neighbors if f real-valued

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

Voronoi Diagram

Decision surface for 1-NN



When To Consider Nearest Neighbor

- Instances map to points in \mathcal{R}^n (or, at least, one can define some distance measure between instances)
- Less than 20 attributes per instance
 - To avoid **curse of dimensionality**, where many irrelevant attributes causes distance to be large, but distance is small if only relevant attributes used
 - Also, large number of attributes increases classification complexity
- Lots of training data

Advantages:

- Robust to noise
- Stable
- Training is very fast
- Learn complex target functions
- Don't lose information

Disadvantages:

- Slow at query time (active research area: fast indexing and accessing algorithms)
- Easily fooled by irrelevant attributes

5

Nearest Neighbor's Behavior in the Limit

Consider $p(x)$ defines probability that instance x will be labeled 1 (positive) versus 0 (negative).

Nearest neighbor ($k = 1$):

- As number of training examples $\rightarrow \infty$, approaches Gibbs Algorithm

Recall Gibbs has at most twice the expected error of Bayes optimal

k -Nearest neighbor:

- As number of training examples $\rightarrow \infty$ and k gets large, approaches Bayes optimal (best possible with given hyp. space and prior information)

Bayes optimal: if $p(x) > .5$ then predict 1, else 0

6

Distance-Weighted k -NN

Might want weight nearer neighbors more heavily:

$$\hat{f}(x_q) \leftarrow \operatorname{argmax}_{v \in V} \sum_{i=1}^k w_i \delta(v, f(x_i))$$

for discrete-valued ($\delta(v, f(x_i)) = 1$ if $v = f(x_i)$ and 0 otherwise), and

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

for continuous

where

$$w_i \equiv \frac{1}{d(x_q, x_i)^2}$$

and $d(x_q, x_i)$ is distance between x_q and x_i

Note now it makes sense to use *all* training examples instead of just k (**Shepard's method**), but then get increased time to classify instances

7

Curse of Dimensionality

Imagine instances described by 20 attributes, but only 2 are relevant to target function

Curse of dimensionality: nearest neighbor is easily misled by high-dimensional X

One approach:

- Stretch j th axis by weight z_j , where z_1, \dots, z_n chosen to minimize prediction error
- Use cross-validation to automatically choose weights z_1, \dots, z_n
- Note setting z_j to zero eliminates this dimension altogether

see Moore and Lee [1994]

8

Locally Weighted Regression

Note k -NN forms local approximation to f for each query point x_q

Why not form an explicit approximation $\hat{f}(x)$ for region surrounding x_q ?

- Fit linear, quadratic, etc. function to k nearest neighbors
- Produces “piecewise approximation” to f
- Do this for **each** new query point x_q

Several choices of error to minimize:

- Squared error over k nearest neighbors

$$E_1(x_q) \equiv \frac{1}{2} \sum_{x \in k \text{ nearest nbrs of } x_q} (f(x) - \hat{f}(x))^2$$

- Distance-weighted squared error over all nbrs

$$E_2(x_q) \equiv \frac{1}{2} \sum_{x \in D} (f(x) - \hat{f}(x))^2 K(d(x_q, x))$$

(K is decreasing in its argument)

- Combine E_1 and E_2

9

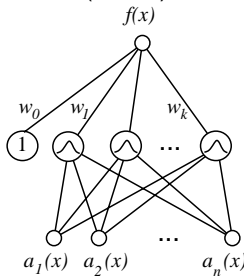
Radial Basis Function (RBF) Networks

- Global approximation to target function, in terms of linear combination of local approximations
- Used, e.g., for image classification
- A different kind of neural network
- Closely related to distance-weighted regression, but “eager” instead of “lazy”

10

RBF Networks

(cont'd)



where $a_i(x)$ are the attributes describing instance x , and

$$\hat{f}(x) = w_0 + \sum_{u=1}^k w_u K_u(d(x_u, x))$$

(Note no weights from input to hidden layer)

One common choice for $K_u(d(x_u, x))$ is

$$K_u(d(x_u, x)) = \exp\left(-\frac{1}{2\sigma_u^2} d^2(x_u, x)\right),$$

i.e. Gaussian with mean at x_u and variance σ_u^2 , all features independent

[note bug on p. 239]

11

Training Radial Basis Function Networks

1. Choose number of kernel functions (hidden units)
 - If = number training exs, can fit training data exactly by placing one center per ex
 - Using fewer \Rightarrow more efficient, less chance of overfitting
2. Choose center (= mean for Gaussian) x_u of kernel function $K_u(d(x_u, x))$
 - Use all training instances if enough kernels avail.
 - Use subset of training instances
 - Scatter uniformly throughout instance space
 - Can cluster data and assign one per cluster (helps answer step 1 also)
 - Can use EM to find means of mixture of Gaussians
 - Can also use e.g. EM to find σ_u 's (for Gaussian)
3. Hold kernels fixed and train weights to fit linear function (output layer), e.g. GD or EG

12

Case-Based Reasoning and CADET

Can apply instance-based learning even when X much more complex

Need different "distance" metric

Case-Based Reasoning is instance-based learning where instances have symbolic logic descriptions

```
((user-complaint error53-on-shutdown)
(cpu-model PowerPC) (operating-system Windows)
(memory 48meg)
(installed-apps Excel Netscape VirusScan)
(disk 1gig)
(likely-cause ???))
```

CADET: 75 stored examples of mechanical devices, e.g. water faucets

- Training ex: ⟨qualitative function, mech. structure⟩
- New query: desired function
- Target value: mechanical structure for this function

Distance metric: match qualitative function descriptions

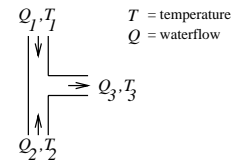
13

Case-Based Reasoning in CADET

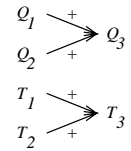
Example

A stored case: T-junction pipe

Structure:



Function:

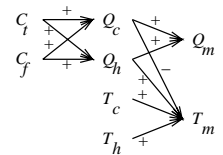


A problem specification: Water faucet

Structure:

?

Function:



E.g. distance measure = size of largest isomorphic subgraph

14

Case-Based Reasoning in CADET

(cont'd)

- Instances represented by rich structural (symbolic) descriptions, vs. e.g. points in \mathcal{R}^n for k -NN
- Multiple cases retrieved (and combined) to form solution to new problem: Similar to k -NN, except combination procedure can rely on knowledge-based reasoning (e.g. can two components be fit together?)
- Tight coupling between case retrieval, knowledge-based reasoning, and problem solving, e.g. application of rewrite rules in function graphs and backtracking in search space

Bottom line:

- Simple matching of cases useful for tasks such as answering help-desk queries
- Area of ongoing research, including improving indexing and search methods

15

Lazy and Eager Learning

Lazy: Wait for query before generalizing

- k -NN, locally weighted regression, Case based reasoning

Eager: Generalize before seeing query

- Radial basis function networks, ID3, Backpropagation, Naive Bayes

Does it matter?

- Computation time for training and generalization
- Eager learner must create global approximation, lazy learner can create many local approximations
- If they use same H , lazy can represent more complex functions (e.g. consider $H =$ linear functions) since it considers the query instance x_q before generalizing, i.e. lazy produces a new hypothesis for each new x_q

Topic Summary due in 1 week!

16