Chapter 8: Instance Based Learning

CS 536: Machine Learning

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Instance Based Learning

[Read Ch. 8]

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

Instance-Based Learning

Key idea: just store all training examples $<x_i, f(x_i)>$

Nearest neighbor:

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

Problem of noisy labels?

Adding Robustness

k-Nearest neighbor method:

- Given x_q, take vote among its k nearest neighbors (if discrete-valued target function)
- take mean of f values of k nearest neighbors (if real-valued)

$$\hat{f}(x_q) \leftarrow \Sigma_{i=1}^{k} f(x_n) \,/\, k$$

When To Consider kNN

- Instances map to points in $\Re^n$
- Fewer than 20 attributes per instance
- Lots of training data

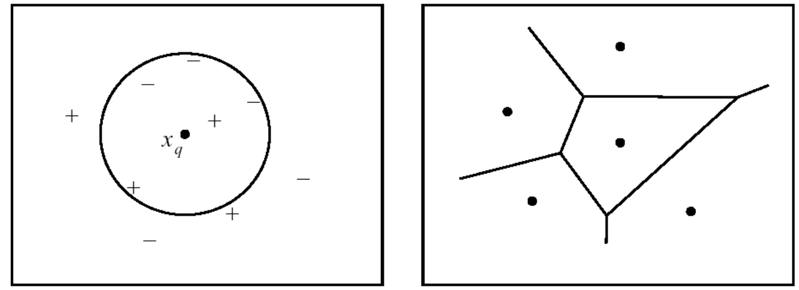
Advantages:

- Training is very fast
- Learn complex target functions
- Don't lose information

Disadvantages:

- Slow at query time
- Easily fooled by irrelevant attributes

Voronoi Diagram



Partition of space by nearness to instances.

Decision Rules

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

Gibbs Algorithm:

- with probability $p(x)$ predict 1, else 0

Bayes optimal decision rule:

- if $p(x) > .5$ then predict 1, else 0

Note Gibbs has at most twice the expected error of Bayes optimal.

(Look familiar?)

Behavior in the Limit

Nearest neighbor:

- As number of training examples grows, approaches Gibbs Algorithm

k–Nearest neighbor:

- As number of training examples grows and k gets large, approaches Bayes optimal

Distance-Weighted *k*NN

Might want weight nearer neighbors more heavily...

$$\hat{f}(x_q) \leftarrow \Sigma_{i=1}^{k} w_i f(x_n) \,/\, \Sigma_{i=1}^{k} w_i$$

where $w_i \equiv 1/\ d(x_q, x_i)^2$

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

Curse of Dimensionality

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

Curse of dimensionality: NN is easily misled in high-dimensional space

How do data requirements grow with dimensionality?

Attribute Weighting

One approach:

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

see Moore and Lee (1994)

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 function to k nearest neighbors
- Fit quadratic, ...
- Produces “piecewise approximation” to f

What to Minimize

Several choices of error to minimize:

- Squared error over k nearest neighbors

  $E_1(x_q) \equiv 1/2 \sum_{x \text{ in } k\text{NN}(xq)} (\hat{f}(x) - f(x))^2$

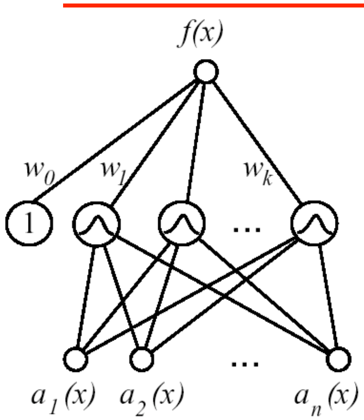
- Distance-weighted squared error over all neighbors

$E_2(x_q) \equiv {}^1/_2 \sum_{x \text{ in } D} (\hat{f}(x) - f(x))^2 \, K(d(x_q, x))$

Radial Basis Function Nets

- 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"

Radial Basis Function Nets



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

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

One common choice is

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

Training RBF Networks

Q1: What x_u to use for each kernel function $K_u(d(x_u, x))$

- Scatter uniformly throughout instance space
- Or use training instances (reflects instance distribution)

Q2: How to train weights (assume here Gaussian K_u)

- First choose variance (and perhaps mean) for each K_u
  - e.g., use EM
- Then hold K_u fixed, and train linear output layer
  - efficient methods to fit linear function

Case-Based Reasoning

Can apply instance-based learning even when $X \neq \Re^n$

- need different "distance" metric

Case-Based Reasoning is instance-based learning applied to instances with symbolic logic descriptions

CBR Example

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

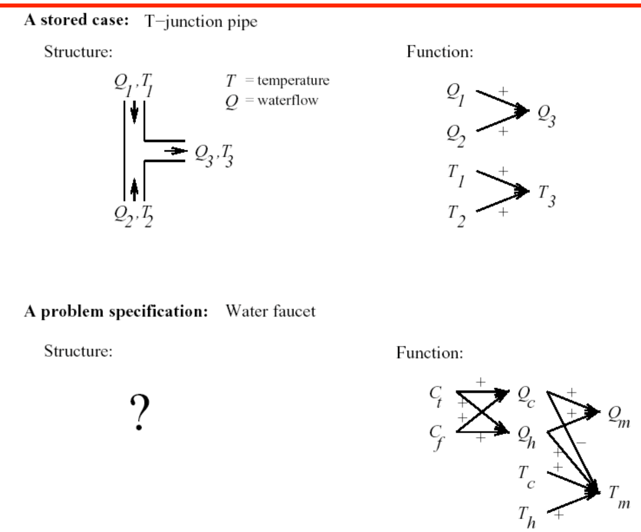
CBR in CADET

CADET: 75 stored examples of mechanical devices

- each training example: < qualitative function, mechanical structure >
- new query: desired function,
- target value: mechanical structure for this function

Distance metric: match qualitative function descriptions

CBR in CADET



CBR in CADET

- Instances represented by rich structural descriptions
- Multiple cases retrieved (and combined) to form solution to new problem
- Tight coupling between case retrieval and problem solving

Bottom line:

- Simple matching of cases useful for tasks such as answering help-desk queries
- Area of ongoing research

Lazy and Eager Learning

Lazy: wait for query before generalizing

- *k*-Nearest Neighbor, Case based reasoning

Eager: generalize before seeing query

- Radial basis function networks, ID3, Backpropagation, NaiveBayes, ...

Which is Better?

Does it matter?

- 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)