Instance Based Learning

- *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 (1 - Nearest neighbor) :

- Given query instance x_q, locate nearest example x_n, estimate

  $$\hat{f}(x_q) \leftarrow f(x_n)$$

k – Nearest neighbor :

- 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)

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

When to Consider Nearest Neighbor

- Instance map to points in R^n
- Less than 20 attributes per instance
- Lots of training data

Advantages

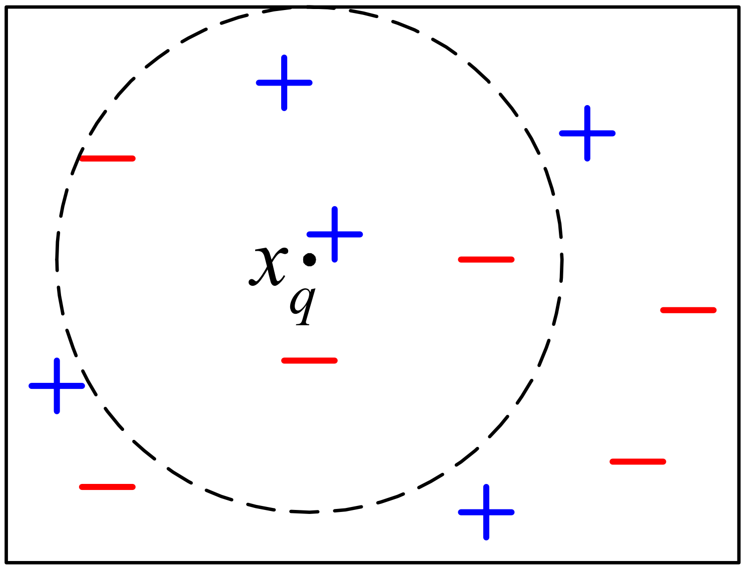
- Training is very fast
- Learn complex target functions
- Do not lose information

Disadvantages

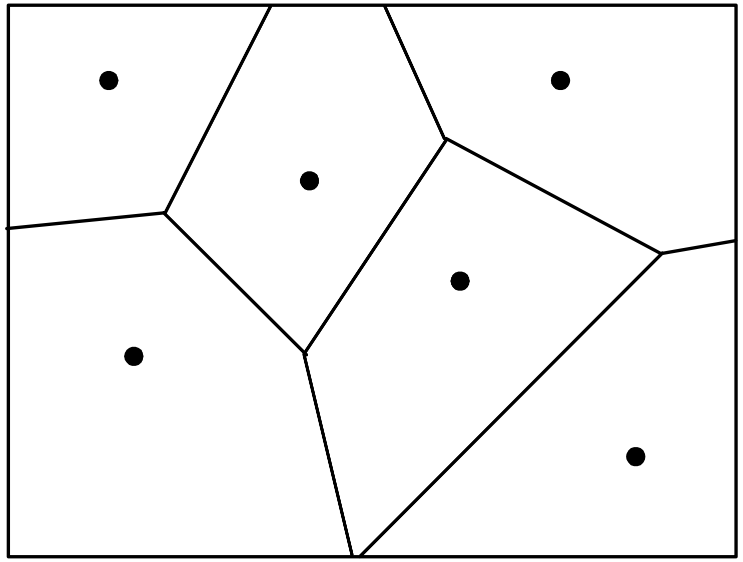
- Slow at query time
- Easily fooled by irrelevant attributes

k-NN Classification

5-Nearest Neighbor



1-NN Decision Surface



Behavior in the Limit

Define *p(x)* as probability that instance *x* will be labeled 1 (positive) versus 0 (negative)

Nearest Neighbor

- As number of training examples approaches infinity, approaches Gibbs Algorithm

  Gibbs: with probability *p(x)* predict 1, else 0

k-Nearest Neighbor:

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

  Bayes optimal: if *p(x)* > 0.5 then predict 1, else 0

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

Distance-Weighted *k*-NN

Might want to weight nearer neighbors more heavily ...

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

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*

$\rightarrow$ Shepard's method

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 when high-dimensional X

One approach:

- Stretch jth axis by weight z_j, where $z_1, z_2, \ldots, z_n$ chosen to minimize prediction error
- Use cross-validation to automatically choose weights $z_1, z_2, \ldots, z_n$
- Note setting z_j to zero eliminates dimension j altogether

see (Moore and Lee, 1994)

Locally Weighted Regression

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

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

- Fit linear function to k nearest neighbors
- Or fit quadratic, etc.
- Produces "piecewise approximation" to f

Several choices of error to minimize:

- Squared error over k nearest neighbors

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

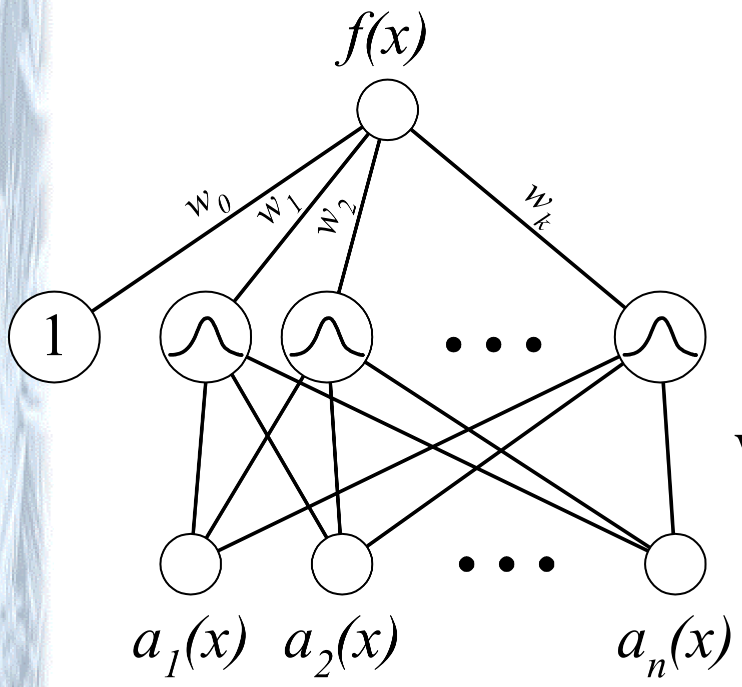
- Distance - weighted squared error over all neighbors

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

Radial Basis Function Networks

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

Radial Basis Function Networks



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 for $K_u(d(x_u,x))$ 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 kernel function $K_u(d(x_u,x))$?

- Scatter uniformly through 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 ❁ R^n

$\rightarrow$ need different “distance” metric

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

```
((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 ???))
```

Case-Based Reasoning in CADET

CADET: 75 stored examples of mechanical devices

- each training example:

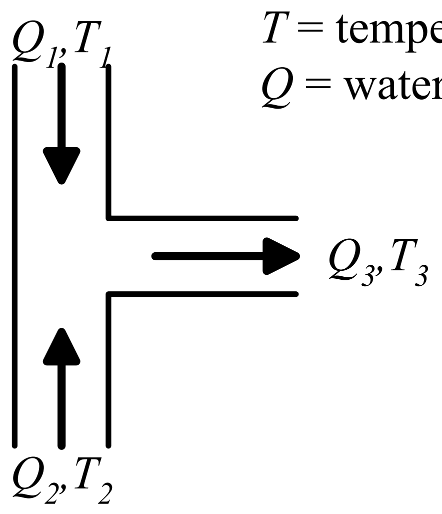
  <qualitative function, mechanical structure>
- new query: desired function
- target value: mechanical structure for this function

Distance metric: match qualitative function descriptions

Case-Based Reasoning in CADET

A stored case: T-junction pipe

Structure:



T = temperature
Q = waterflow

Function:

$$\begin{tikzcd} Q_1 \arrow[dr, "+"] & \\ & Q_3 \\ Q_2 \arrow[ur, "+"'] & \end{tikzcd}$$

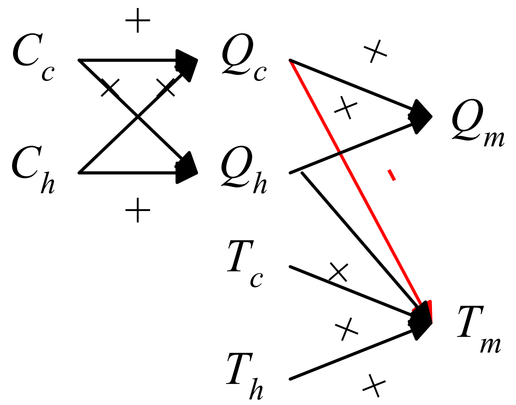
$$\begin{tikzcd} T_1 \arrow[dr, "+"] & \\ & T_3 \\ T_2 \arrow[ur, "+"'] & \end{tikzcd}$$

A problem specification: Water faucet

Structure:

?

Function:



Case-Based Reasoning 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, etc.

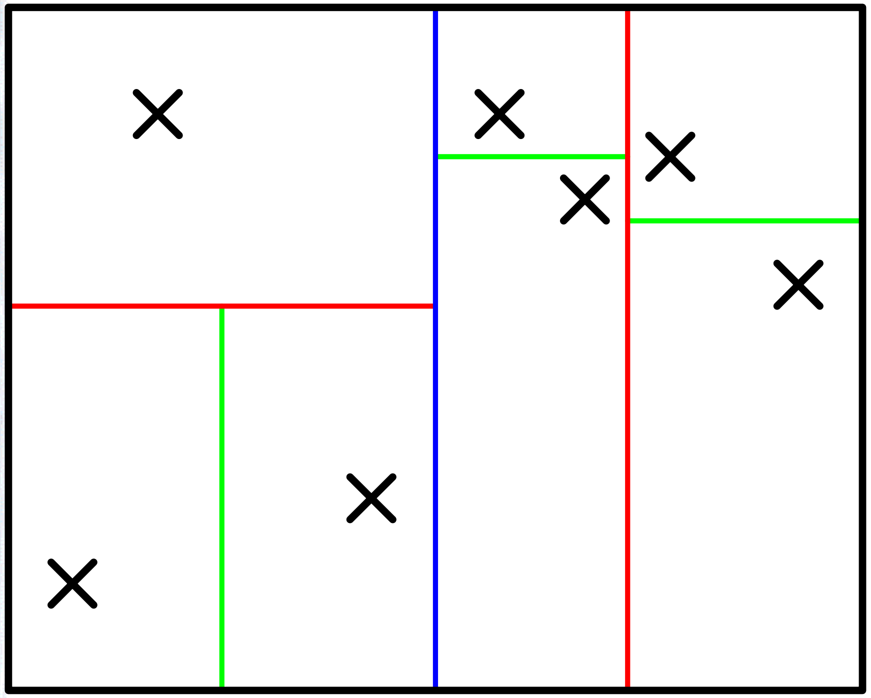
Does it matter?

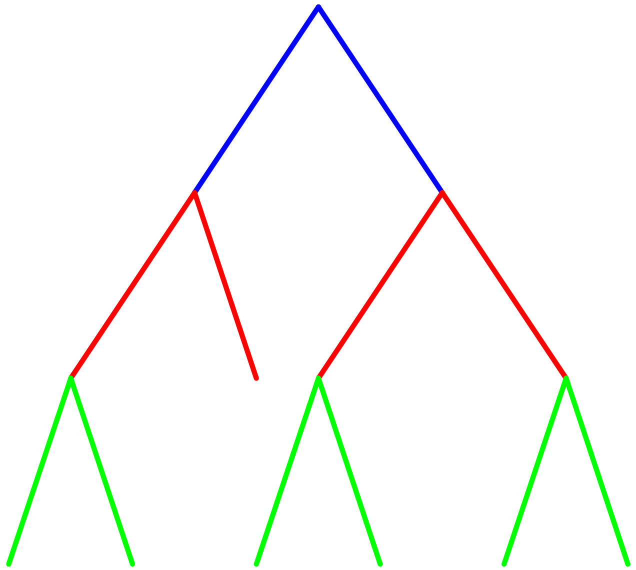
- Eager learner must create global approximation
- Lazy learner can create many local approximations
- If they use same *H*, lazy can represent more complex functions (e.g., consider *H*=linear functions)

*k*d-trees (Moore)

- *Eager* version of *k*-Nearest Neighbor
- Idea: decrease time to find neighbors
  - train by constructing a lookup (*k*d) tree
  - recursively subdivide space
    - ignore class of points
    - lots of possible mechanisms: grid, maximum variance, etc.
  - when looking for nearest neighbor search tree
  - nearest neighbor can be found in log(n) steps
  - k nearest neighbors can be found by generalizing process (still in log(n) steps if k is constant)
- Slower training but faster classification

*k*d Tree





Instance Based Learning Summary

- Lazy versus Eager learning
  - lazy - work done at testing time
  - eager -work done at training time
  - instance based sometimes lazy
- *k*-Nearest Neighbor (*k*-nn) lazy
  - classify based on k *nearest neighbors*
  - key: determining neighbors
  - variations:
    - distance weighted combination
    - locally weighted regression
  - limitation: curse of dimensionality
    - "stretching" dimensions

Instance Based Learning Summary

- *k*-d trees (eager version of *k*-nn)
  - structure built at train time to quickly find neighbors
- Radial Basis Function (RBF) networks (eager)
  - units active in region (sphere) of space
  - key: picking/training kernel functions
- Case-Based Reasoning (CBR) generally lazy
  - nearest neighbor when no continuos features
  - may have other types of features:
    - structural (graphs in CADET)