

# Instance Based Learning

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- ▶  $k$ -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  $\langle x_i, f(x_i) \rangle$

Nearest neighbor:

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

$k$ -Nearest neighbor:

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

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

# When To Consider Nearest Neighbor

- ▶ Instances map to points in  $\mathbb{R}^n$
- ▶ Less 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

# Behavior in the Limit

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

Nearest neighbor:

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

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

$k$ -Nearest neighbor:

- ▶ As number of training examples  $\rightarrow \infty$  and  $k$  gets large, approaches Bayes optimal

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

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

# Distance-Weighted $k$ NN

Might want 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  $k$

→ Shepard's method

# Curse of Dimensionality

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

*Curse of dimensionality*: nearest nbr is easily misled when 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]



# 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  $f$

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

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

▶ ...

# Radial Basis Function 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”

# 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 Radial Basis Function 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  $X \neq \mathbb{R}^n$

→ need different “distance” metric

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

# Case-Based Reasoning in CADET

CADET: 75 stored examples of mechanical devices

- ▶ each training example:  $\langle$  qualitative function, mechanical structure  $\rangle$
- ▶ new query: desired function,
- ▶ target value: mechanical structure for this function

Distance metric: match qualitative function descriptions

# Case-Based Reasoning in CADET

# 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

Neighbor , Case based reasoning

Eager: generalize before seeing query

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

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 fns (e.g., consider  $H =$  linear functions)