

Lecture 23

Instance-Based Learning (IBL): *k*-Nearest Neighbor and Radial Basis Functions

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Readings:

Chapter 8, Mitchell

Lecture Outline

- **Readings: Chapter 8, Mitchell**
- **Suggested Exercises: 8.3, Mitchell**
- **Next Week's Paper Review (Last One!)**
 - “An Approach to Combining Explanation-Based and Neural Network Algorithms”, Shavlik and Towell
 - Due Tuesday, 11/30/1999
- ***k*-Nearest Neighbor (*k*-NN)**
 - IBL framework
 - IBL and case-based reasoning
 - Prototypes
 - Distance-weighted *k*-NN
- **Locally-Weighted Regression**
- **Radial-Basis Functions**
- **Lazy and Eager Learning**
- **Next Lecture (Tuesday, 11/30/1999): Rule Learning and Extraction**

Instance-Based Learning (IBL)

- **Intuitive Idea**

- Store all instances $\langle x, c(x) \rangle$
- Given: query instance x_q
- Return: function (e.g., label) of closest instance in database of *prototypes*
- Rationale
 - Instance closest to x_q tends to have *target function* close to $f(x_q)$
 - Assumption can fail for deceptive hypothesis space or with too little data!

- **Nearest Neighbor**

- First locate nearest training example x_n to query x_q
- Then estimate $\hat{f}(x_q) \leftarrow f(x_n)$

- **k-Nearest Neighbor**

- Discrete-valued f : take vote among k nearest neighbors of x_q
- Continuous-valued f :

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

When to Consider Nearest Neighbor

- **Ideal Properties**
 - Instances map to points in \mathbb{R}^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*

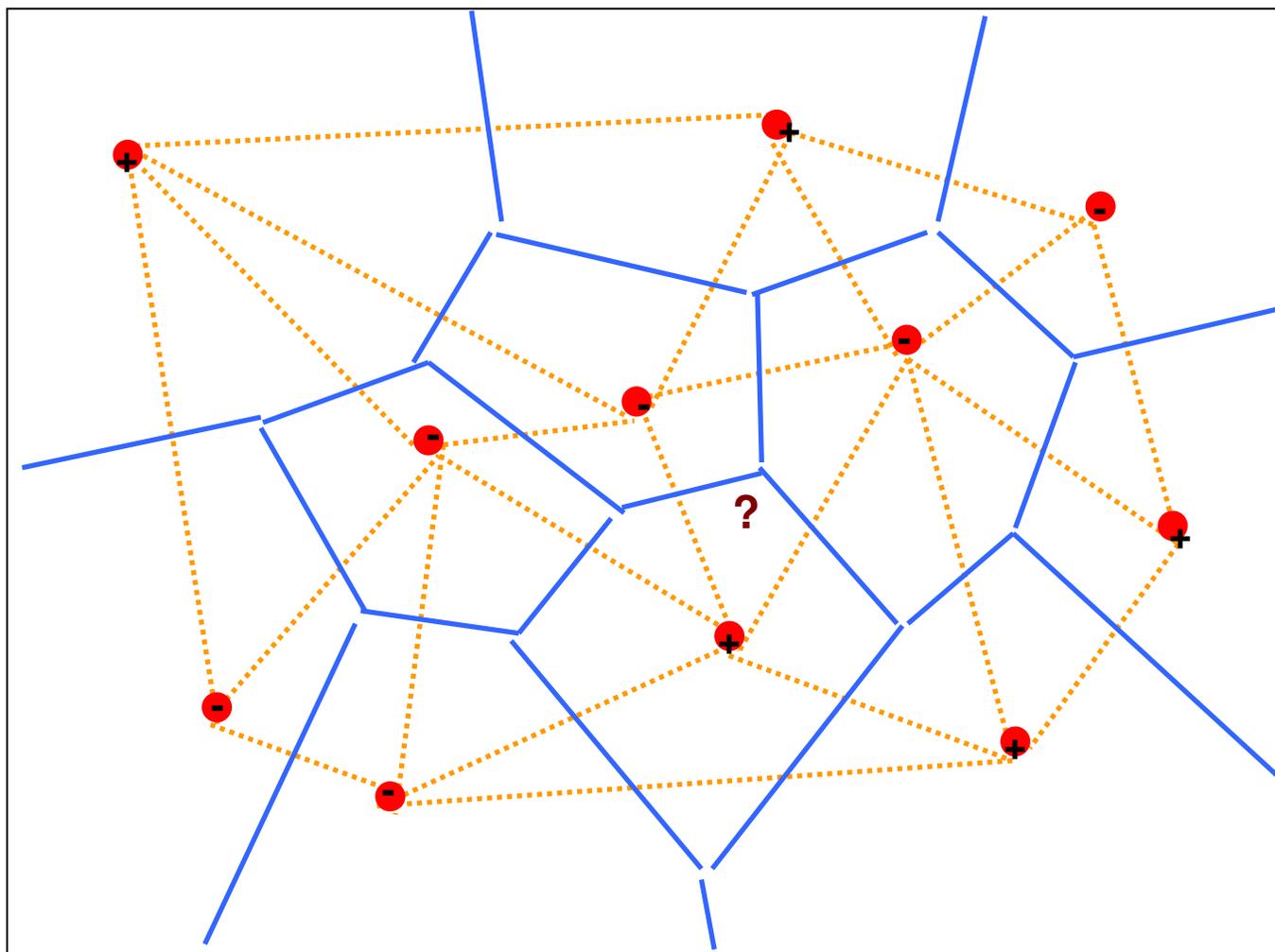
Voronoi Diagram

Training Data:
Labeled Instances

Delaunay
Triangulation

Voronoi
(Nearest Neighbor)
Diagram

Query Instance
 x_q



k -NN and Bayesian Learning: Behavior in the Limit

- **Consider: Probability Distribution over Labels**
 - Let p denote learning agent's *belief* in the distribution of labels
 - $p(x) \equiv$ probability that instance x will be labeled 1 (positive) versus 0 (negative)
 - Objectivist view: as more evidence is collected, approaches “true probability”
- **Nearest Neighbor**
 - As number of training examples $\rightarrow \infty$, approaches behavior of 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 $p(x) > 0.5$ then predict 1, else 0
- **Recall: Property of Gibbs Algorithm**
 - $E[\text{error}(h_{\text{Gibbs}})] \leq 2E[\text{error}(h_{\text{BayesOptimal}})]$
 - Expected error of Gibbs no worse than twice that of Bayes optimal

Distance-Weighted k -NN

- **Intuitive Idea**

- Might want to weight *nearer* neighbors more heavily
- Rationale
 - Instances closer to \mathbf{x}_q tend to have *target functions* closer to $f(\mathbf{x}_q)$
 - Want benefit of BOC over Gibbs (k -NN for large k over 1-NN)

- **Distance-Weighted Function**

$$\hat{f}(\mathbf{x}_q) \leftarrow \frac{\sum_{i=1}^k w_i \cdot f(\mathbf{x}_i)}{\sum_{i=1}^k w_i}$$

- Weights are proportional to distance: $w_i \equiv \frac{1}{d(\mathbf{x}_q, \mathbf{x}_i)^2}$
 - $d(\mathbf{x}_q, \mathbf{x}_i)$ is *Euclidean distance*
 - **NB:** now it makes sense to use *all* $\langle \mathbf{x}, f(\mathbf{x}) \rangle$ instead of just $k \rightarrow$ Shepard's method
- **Jargon from Statistical Pattern Recognition**
 - Regression: approximating a real-valued target function
 - Residual: error $\hat{f}(\mathbf{x}) - f(\mathbf{x})$
 - Kernel function: function K such that $w_i = K(d(\mathbf{x}_q, \mathbf{x}_i))$

Curse of Dimensionality

- **A Machine Learning Horror Story**

- **Suppose**

- Instances described by n attributes (x_1, x_2, \dots, x_n) , e.g., $n = 20$
- Only $n' \ll n$ are relevant, e.g., $n' = 2$

- **Horrors!** Real KDD problems usually *are* this bad or *worse*... (correlated, etc.)

- **Curse of dimensionality**: nearest neighbor learning algorithm is easily misled when n large (i.e., high-dimension X)

- **Solution Approaches**

- ***Dimensionality reducing transformations*** (e.g., SOM, PCA; see Lecture 15)

- **Attribute weighting and attribute subset selection**

- Stretch j th axis by weight z_j : (z_1, z_2, \dots, z_n) chosen to minimize prediction error
- Use cross-validation to automatically choose weights (z_1, z_2, \dots, z_n)
- **NB**: setting z_j to 0 eliminates this dimension altogether
- See [Moore and Lee, 1994; Kohavi and John, 1997]

Locally Weighted Regression

- **Global versus Local Methods**
 - Global: consider all training examples $\langle x, f(x) \rangle$ when estimating $f(x_q)$
 - Local: consider only examples within local neighborhood (e.g., k nearest)
- **Locally Weighted Regression**
 - Local method
 - Weighted: contribution of each training example is weighted by distance from x_q
 - Regression: approximating a real-valued target function
- **Intuitive Idea**
 - k -NN forms local approximation to $f(x)$ for each x_q
 - Explicit approximation to $f(x)$ for region surrounding x_q
 - Fit parametric function $\hat{f}(\bullet)$: e.g., linear, quadratic (piecewise approximation)
- **Choices of Error to Minimize**
 - Sum squared error (SSE) over k -NN
 - Distance-weighted SSE over *all* neighbors

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

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

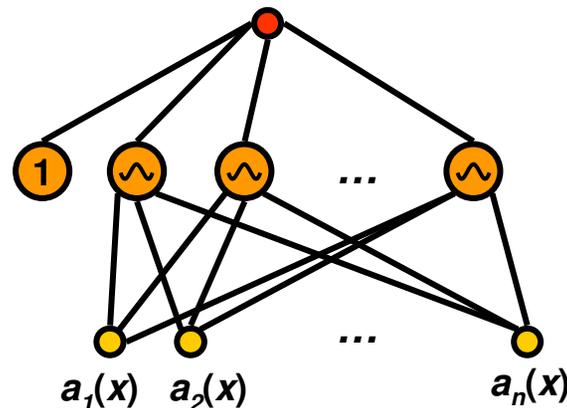


Radial Basis Function (RBF) Networks

- **What Are RBF Networks?**

- Global approximation to target function f , in terms of linear combination of local approximations
- Typical uses: image, signal classification
- Different kind of artificial neural network (ANN)
- Closely related to distance-weighted regression, but “eager” instead of “lazy”

- **Activation Function**



- where $a_i(x)$ are attributes describing instance x and $f(\mathbf{x}) = w_0 + \sum_{u=1}^k w_u \cdot K_u(d(x_u, \mathbf{x}))$
- Common choice for K_u : Gaussian kernel function $K_u(d(x_u, \mathbf{x})) = e^{-\frac{1}{2\sigma_u^2} d^2(x_u, \mathbf{x})}$

RBF Networks: Training

- **Issue 1: Selecting Prototypes**
 - What x_u should be used for each kernel function $K_u(d(x_u, x))$
 - Possible prototype distributions
 - Scatter uniformly throughout instance space
 - Use training instances (reflects instance distribution)
- **Issue 2: Training Weights**
 - Here, assume Gaussian K_u
 - First, choose hyperparameters
 - Guess variance, and perhaps mean, for each K_u
 - e.g., use EM
 - Then, hold K_u fixed and train parameters
 - Train weights in linear output layer
 - Efficient methods to fit linear function

Case-Based Reasoning (CBR)

- **Symbolic Analogue of Instance-Based Learning (IBL)**
 - Can apply IBL even when $X \neq \mathbb{R}^n$
 - Need different “distance” metric
 - Intuitive idea: *use symbolic (e.g., syntactic) measures of similarity*
- **Example**
 - Declarative knowledge base
 - Representation: symbolic, logical descriptions
 - ((user-complaint rundll-error-on-shutdown) (system-model thinkpad-600-E) (cpu-model mobile-pentium-2) (clock-speed 366) (network-connection PC-MCIA-100-base-T) (memory 128-meg) (operating-system windows-98) (installed-applications office-97 MSIE-5) (disk-capacity 6-gigabytes))
 - (likely-cause ?)

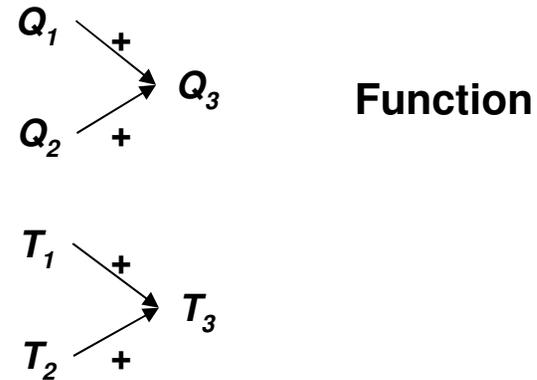
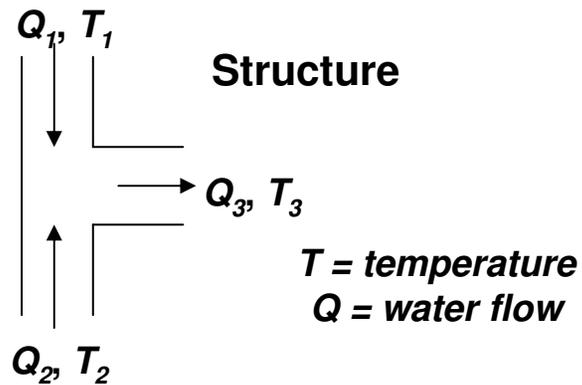
Case-Based Reasoning in CADET

- **CADET: CBR System for Functional Decision Support [Sycara *et al*, 1992]**
 - 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 functional descriptions
 - $X \neq \mathbb{R}^n$, so “distance” is not Euclidean even if it is quantitative

CADET: Example

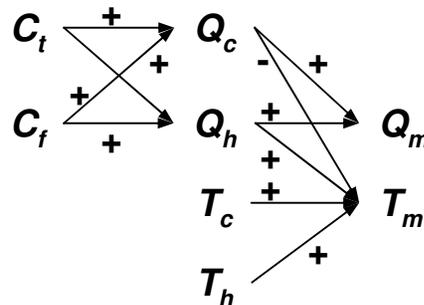
- **Stored Case: T-Junction Pipe**

- Diagrammatic knowledge
- Structure, function



- **Problem Specification: Water Faucet**

- Desired function:



- Structure: ?

CADET: Properties

- **Representation**
 - Instances represented by rich structural descriptions
 - Multiple instances retrieved (and combined) to form solution to new problem
 - Tight coupling between case retrieval and new problem
- **Bottom Line**
 - Simple matching of cases useful for tasks such as answering help-desk queries
 - Compare: technical support knowledge bases
 - Retrieval issues for natural language queries: not so simple...
 - User modeling in web IR, interactive help)
 - Area of continuing research

Lazy and Eager Learning

- **Lazy Learning**
 - Wait for query before generalizing
 - Examples of lazy learning algorithms
 - k -nearest neighbor (k -NN)
 - Case-based reasoning (CBR)
- **Eager Learning**
 - Generalize before seeing query
 - Examples of eager learning algorithms
 - Radial basis function (RBF) network training
 - ID3, backpropagation, simple (Naïve) Bayes, etc.
- **Does It Matter?**
 - Eager learner must create global approximation
 - Lazy learner can create many local approximations
 - If they use same H , lazy learner can represent more complex functions
 - e.g., consider $H \equiv$ linear functions

Terminology

- **Instance Based Learning (IBL): Classification Based On Distance Measure**
 - **k-Nearest Neighbor (k-NN)**
 - **Voronoi diagram** of order k : data structure that answers k -NN queries x_q
 - **Distance-weighted k -NN**: weight contribution of k neighbors by distance to x_q
 - **Locally-weighted regression**
 - **Function approximation method, generalizes k -NN**
 - **Construct explicit approximation to target function $f(\bullet)$ in neighborhood of x_q**
 - **Radial-Basis Function (RBF) networks**
 - **Global approximation algorithm**
 - **Estimates linear combination of local kernel functions**
- **Case-Based Reasoning (CBR)**
 - **Like IBL: lazy, classification based on similarity to prototypes**
 - **Unlike IBL: similarity measure not necessarily distance metric**
- **Lazy and Eager Learning**
 - **Lazy methods: may consider query instance x_q when generalizing over D**
 - **Eager methods: choose global approximation h before x_q observed**

Summary Points

- **Instance Based Learning (IBL)**
- *k*-Nearest Neighbor (*k*-NN) algorithms
 - When to consider: few continuous valued attributes (low dimensionality)
 - Variants: distance-weighted *k*-NN; *k*-NN with attribute subset selection
- Locally-weighted regression: function approximation method, generalizes *k*-NN
- Radial-Basis Function (RBF) networks
 - Different kind of artificial neural network (ANN)
 - Linear combination of local approximation → global approximation to $f(\bullet)$
- **Case-Based Reasoning (CBR) Case Study: CADET**
- Relation to IBL
- CBR online resource page: <http://www.ai-cbr.org>
- **Lazy and Eager Learning**
- **Next Week**
 - Rule learning and extraction
 - Inductive logic programming (ILP)