Machine Learning

Instance-based learning

(with slides/ideas from Bryan Pardo, Pedro Domingos, and Andrew Moore)

Nearest Neighbor Classifier

- Example of instance-based (a.k.a case-based) learning

- The basic idea:
  1. Get some example set of cases with known outputs

     e.g diagnoses of infectious diseases by experts
  2. When you see a new case, assign its output to be the same as the most similar known case.

     Your symptoms most resemble Mr X.

     Mr X had the flu.

     Ergo you have the flu.

General Learning Task

There is a set of possible examples $X = \{x_i\}$

Each example is an n-tuple of attribute values

$$\vec{x}_1 = < a_1, \ldots, a_k >$$

There is a target function that maps *X* onto some set *Y*

$$f : X \rightarrow Y$$

The DATA is a set of duples <example, target function values>

$$D = \{< \vec{x}_1, f(\vec{x}_1) >, \ldots < \vec{x}_m, f(\vec{x}_m) >\}$$

Find a hypothesis ***h*** such that...

$$\forall \vec{x}, h(\vec{x}) \approx f(\vec{x})$$

Nearest neighbor!

Task: Given some set of training data…

$$D = \{ < \vec{x}_1, f(\vec{x}_1) >, \ldots < \vec{x}_m, f(\vec{x}_m) > \}$$

…and query point $\vec{x}_q$, predict $f(\vec{x}_q)$

distance function

1. Find the nearest member of data set to the query

$$\vec{x}_{nn} = \arg\min_{x \in D} (\overset{\downarrow}{d}(\vec{x}, \vec{x}_q))$$

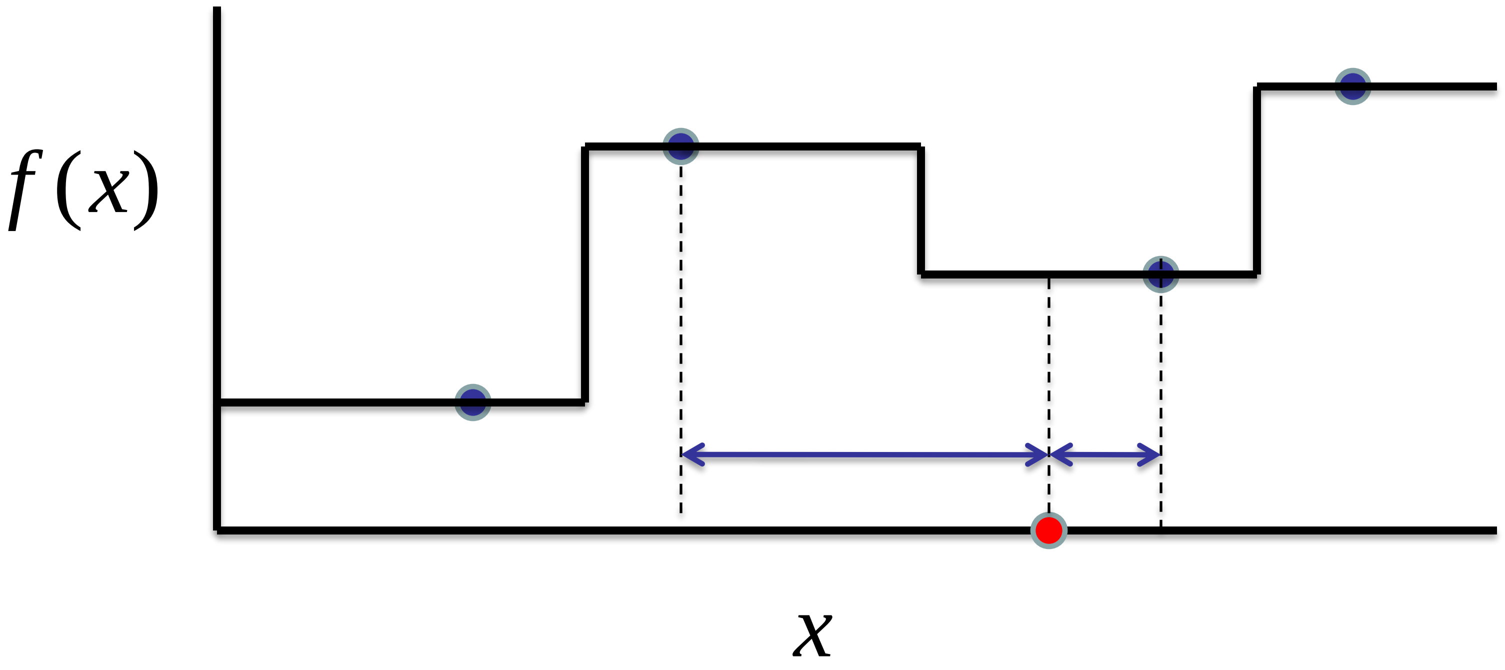
2. Assign the nearest neighbor's output to the query

$$\boxed{h(\vec{x}_q) = f(\vec{x}_{nn})}$$

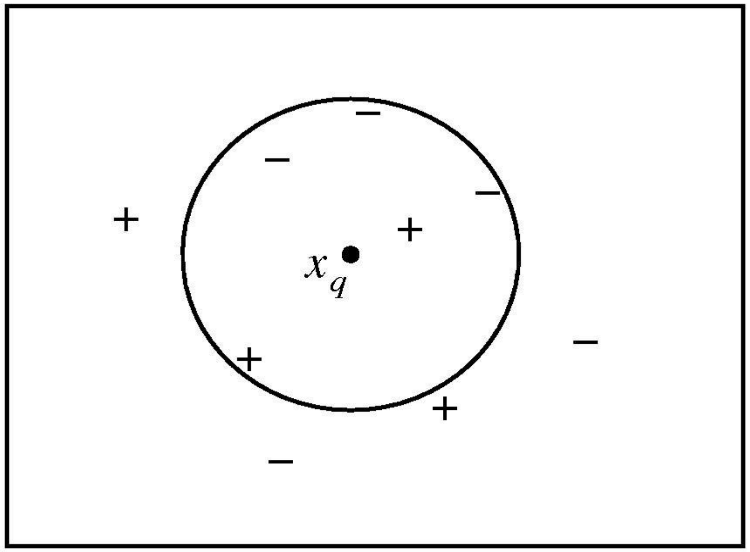
Our hypothesis

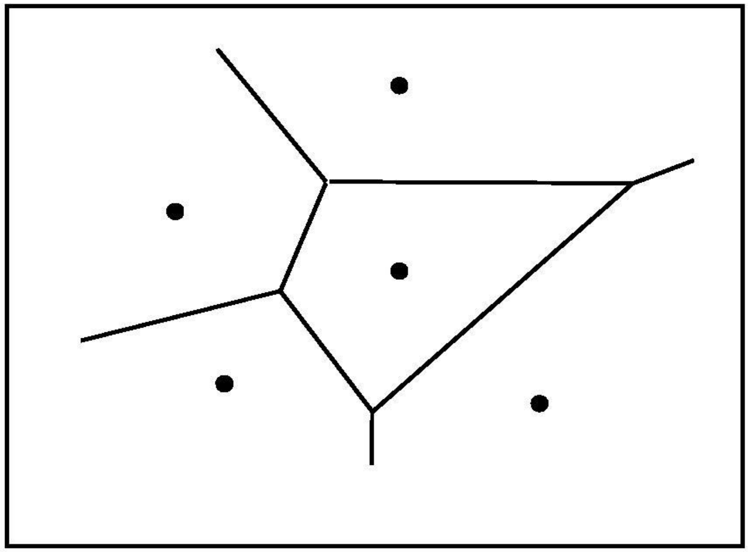
A Single-attribute Example

- Find closest point. $\vec{x}_{nn} = \arg\min_{x \in D}(d(\vec{x}, \vec{x}_q))$
- Give query its value $f(\vec{x}_q) = f(\vec{x}_{nn})$



Voronoi Diagram





S: Training set

Voronoi cell of $\mathbf{x} \in S$:
All points closer to $\mathbf{x}$ than to any other instance in S

Region of class C:
Union of Voronoi cells of instances of C in S

What makes an instance-based learner?

- A distance measure

  Nearest neighbor: typically Euclidean

- Number of neighbors to consider

  Nearest neighbor: One

- A weighting function (optional)

  Nearest neighbor: unused (equal weights)

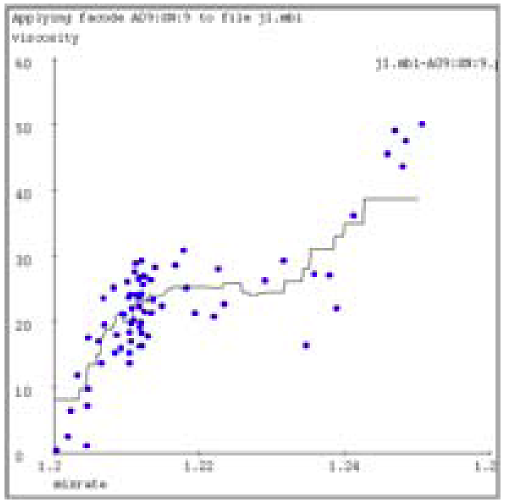
- How to fit with the neighbors

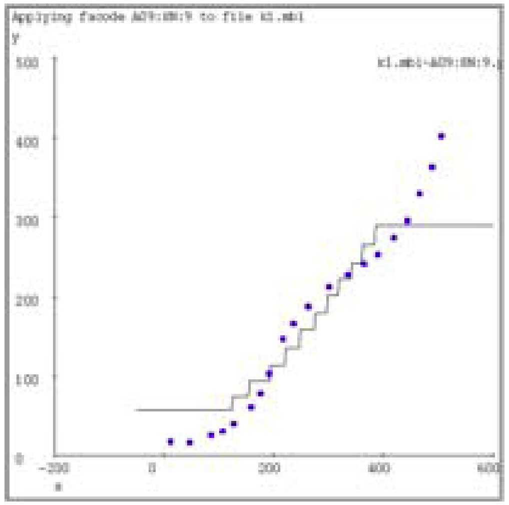
  Nearest neighbor: Same output as nearest neighbor

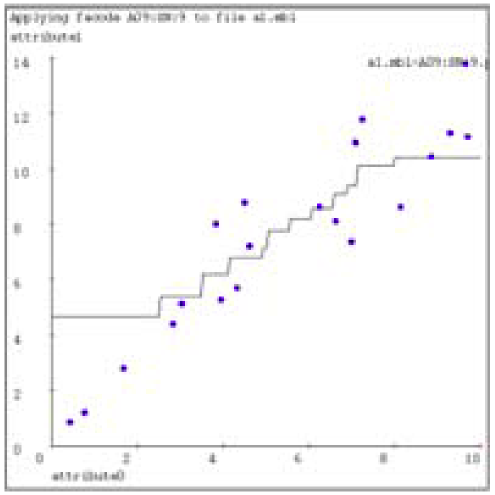
K-nearest neighbor

- A distance measure
  - ***Typically Euclidean***
- Number of neighbors to consider
  - ***K***
- A weighting function (optional)
  - ***Unused (i.e. equal weights)***
- How to fit with the neighbors
  - ***Vote using K nearest neighbors (or take average, for regression)***

Examples of KNN where K=9







Reasonable job
Did smooth noise

Screws up on the ends

OK, but problem on the ends again.

Pros and Cons

- Advantages
  - Fast training (a “lazy” method)
  - Learn complex functions easily
  - Don’t lose information
- Disadvantages
  - Slow at query time
  - Lots of storage
  - **Easily fooled by irrelevant attributes**

Irrelevant Attributes

- The Curse of Dimensionality
  - Nearest Neighbor easily misled when X high-dim
  - Low-dimensional intuitions don’t extend to high dim

- Example:
  - Uniform distribution on hypercube
  - Sphere approximation of cube
    - Exercise: prove that the maximal intersection of hypersphere of volume 1 and hypercube of volume 1 goes to zero as dim increases
      - (if it’s true)

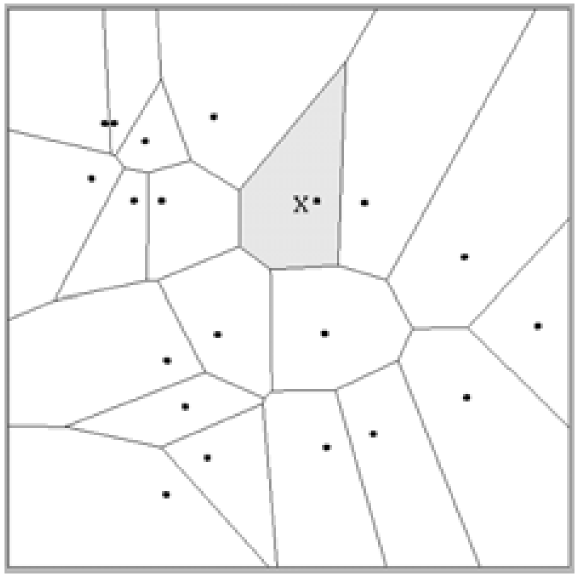
Feature Selection

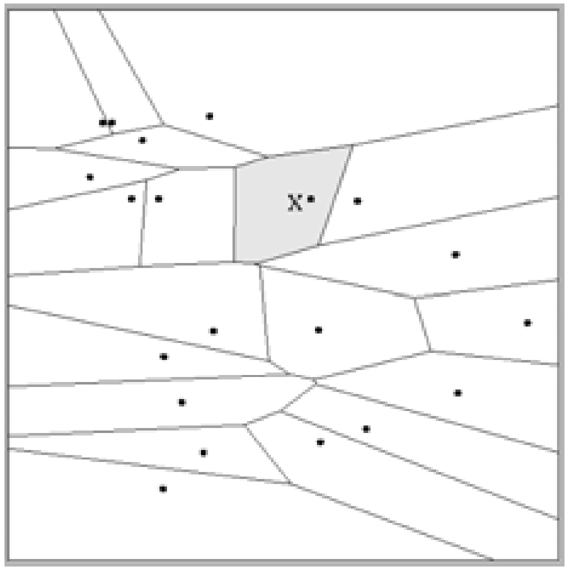
- Pre-selection
  - Identify a good set of *R* features
  - By e.g. information gain (as in decision trees)

- Wrapping
  - Starting with zero features, iterate:
    - greedily add a new feature based on NN performance

Weighting dimensions

- Suppose data points are two-dimensional
- Different dimensional weightings affect region shapes





$d(x,y)=(x_1-y_1)^2+(x_2-y_2)^2$ $d(x,y)=(x_1-y_1)^2+(3x_2-3y_2)^2$

Computational Cost?

- Optimized distance computations
  - Use cheap approximation to weed out most instances
  - Compute expensive measure on remainder
- Edited k-NN
  - For each x
    - If x correctly classified by $D - \{x\}$, remove x from D

Avoiding overfitting

- Choose *k* in *k*-nearest neighbor by
  - Cross validation
- Form prototypes
- Remove noisy instances

Kernel Regression

- A distance measure: ***Scaled Euclidean***
- Number of neighbors to consider: ***All of them***
- A weighting function (optional)

$$w_i = \exp\left(\frac{-d(x_i, x_q)^2}{K_W^2}\right)$$

Nearby points to the query are weighted strongly, far points weakly. The K_W parameter is the Kernel Width.

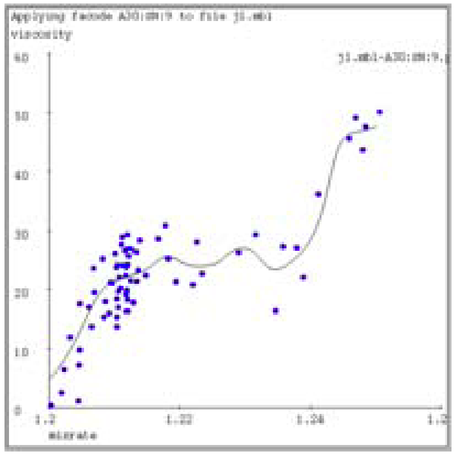
- How to fit with the neighbors

$$h(x_q) = \frac{\sum_i w_i \cdot f(x_i)}{\sum_i w_i}$$

A weighted average

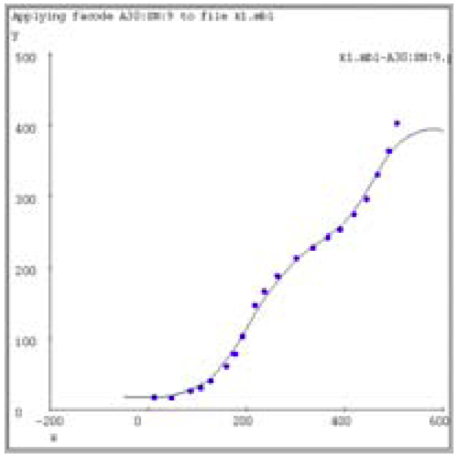
Kernel-weighted Regression

Kernel Weight = 1/32 of X-axis width



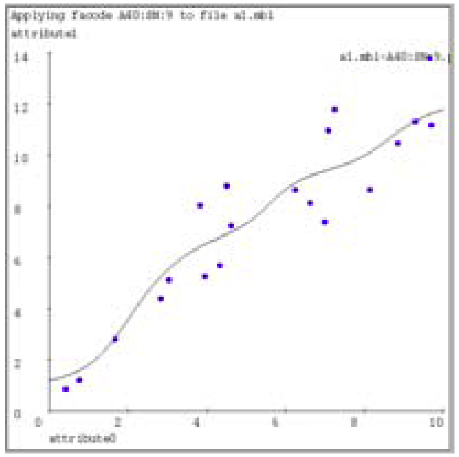
A better fit than KNN?

Kernel Weight = 1/32 of X-axis width



Definitely better than KNN! Catch: Had to play with kernel width to get This result

Kernel Weight = 1/16 of X-axis width



Nice and smooth, but are the bumps justified, or is this overfitting?

Discussion (related to hmwk 1)

- "Simply put, machine learning is the part of artificial intelligence that actually works."
  http://www.forbes.com/sites/anthonykosner/2013/12/29/why-is-machine-learning-cs-229-the-most-popular-course-at-stanford/

- "This is a world where massive amounts of data and applied mathematics replace every other tool that might be brought to bear. Out with every theory of human behavior, from linguistics to sociology. Forget taxonomy, ontology, and psychology…"
  http://www.wired.com/images/press/pdf/petaage.pdf

- Agree or Disagree?