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 $X = \{\vec{x}_i\}$

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

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

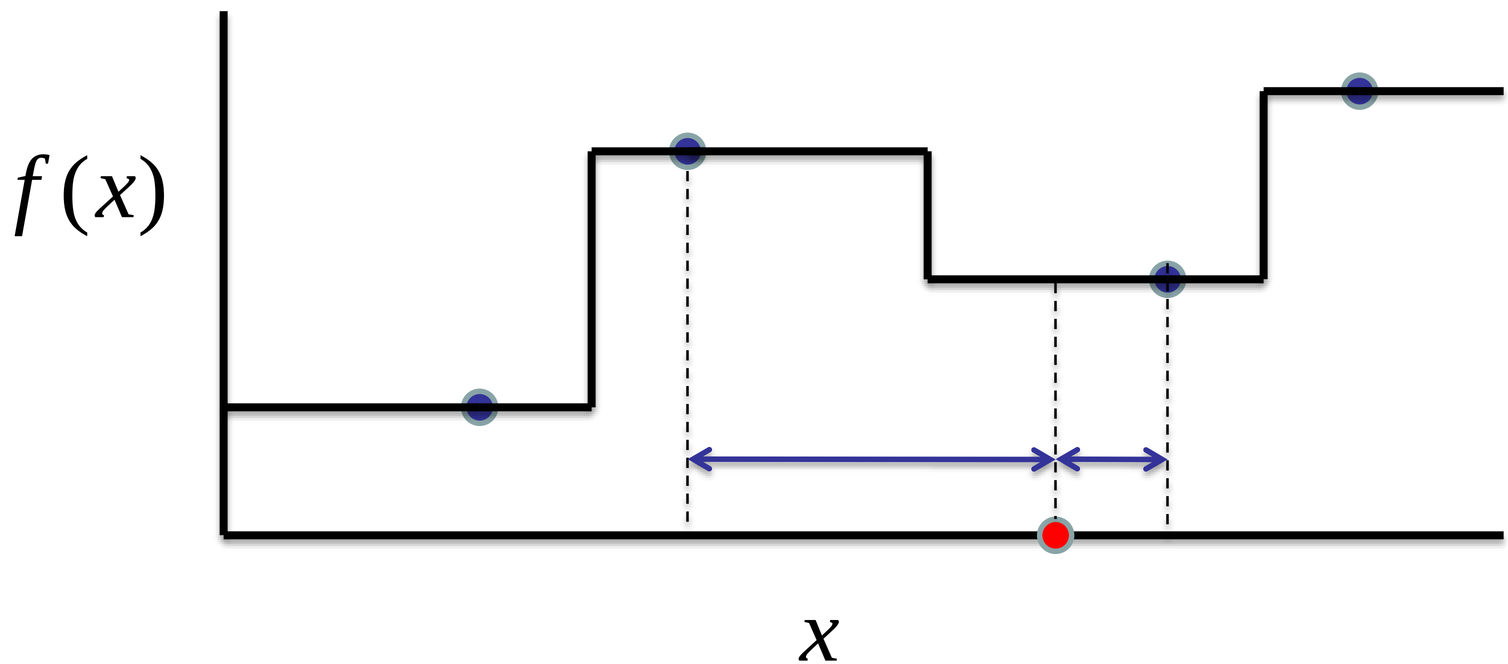
2. Assign the nearest neighbor's output to the query

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

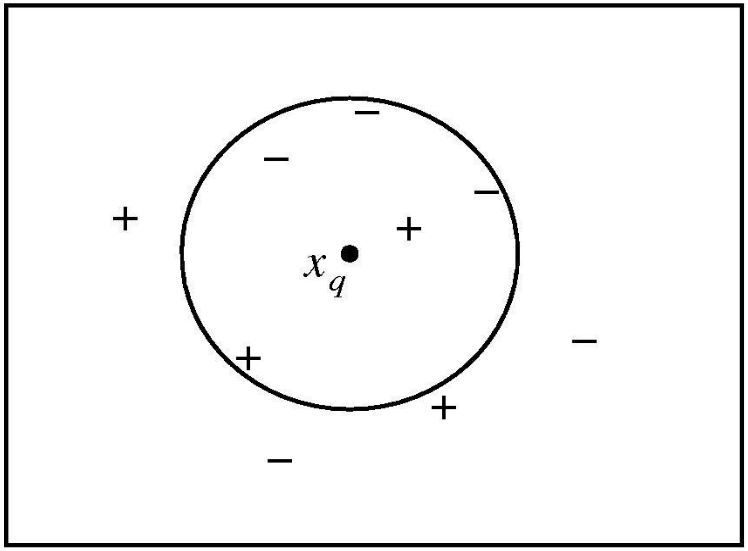
Our hypothesis

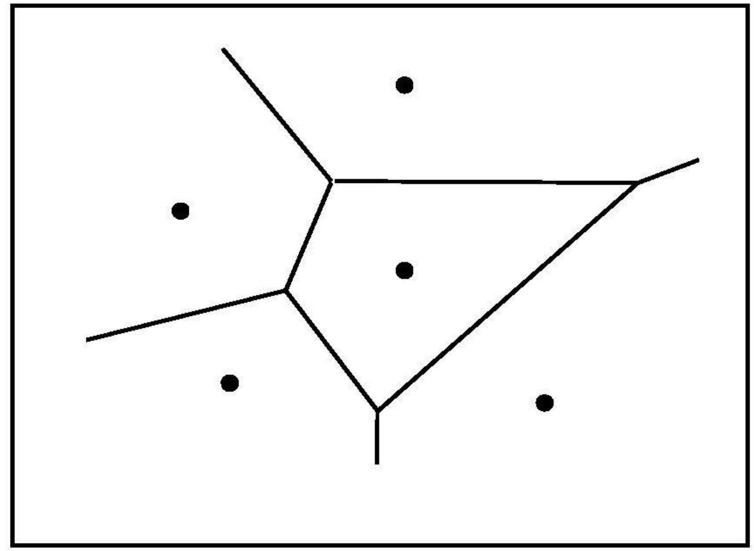
A Single-attribute Example

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



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)

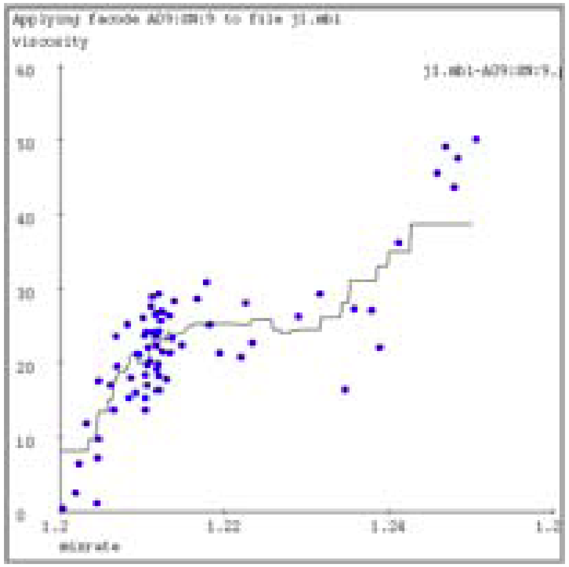
- How to fit with the neighbors

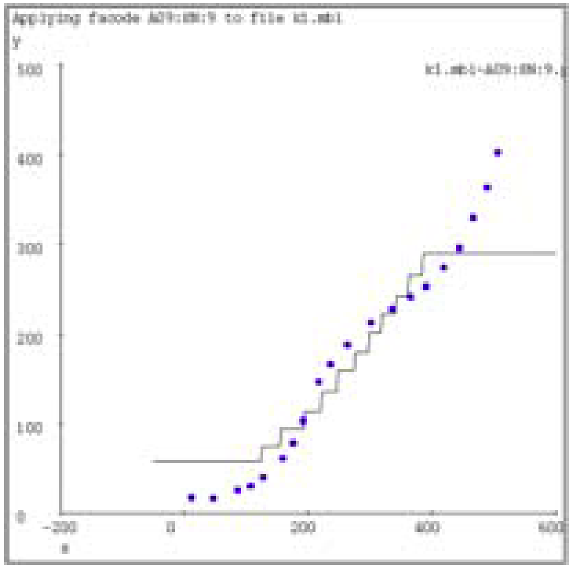
  Nearest neighbor: Same output as nearest neighbor

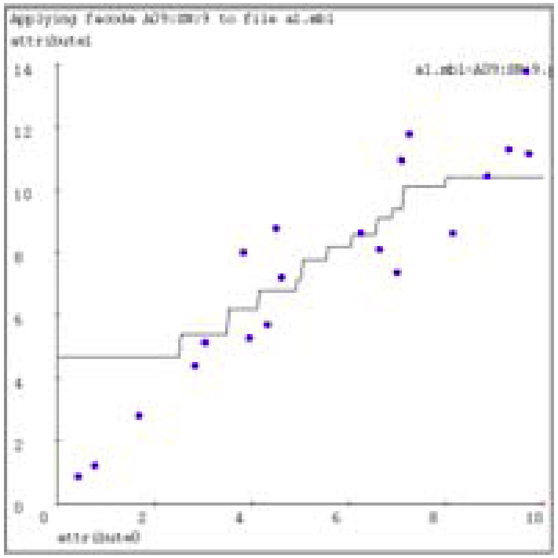
K-nearest neighbor

- 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.

Computational Complexity

- How does training time and testing time complexity compare between decision trees and nearest-neighbor?

Think/Pair/Share

How does training time and testing time complexity compare between decision trees and nearest-neighbor?

Think

Start

End

Think/Pair/Share

How does training time and testing time complexity compare between decision trees and nearest-neighbor?

Pair

Start

End

Think/Pair/Share

How does training time and testing time complexity compare between decision trees and nearest-neighbor?

Share

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
  - Can be fooled by irrelevant, redundant attributes

Irrelevant Attributes

- The Curse of Dimensionality
  - Low-dimensional intuitions don't extend to high dim
  - Nearest Neighbor can be misled when X high-dim
    - And lots of dims are irrelevant
- 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)

Think/Pair/Share

What can we do to combat the curse of dimensionality in nearest neighbor?

Think

Start

End

Think/Pair/Share

What can we do to combat the curse of dimensionality in nearest neighbor?

Pair

Start

End

Think/Pair/Share

What can we do to combat the curse of dimensionality in nearest neighbor?

Share

Feature Selection

- Pre-selection

  Take the top five, and that's totally reasonable

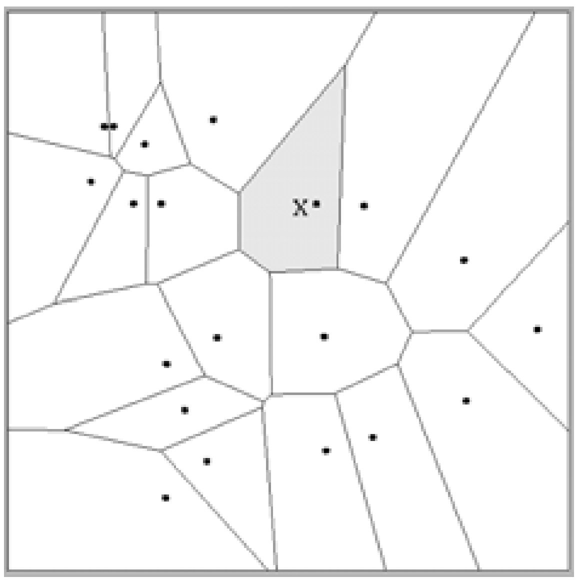
  - Identify a good set of *R* features
  - By e.g. information gain (as in decision trees)

Need a validation set and test each selection & features

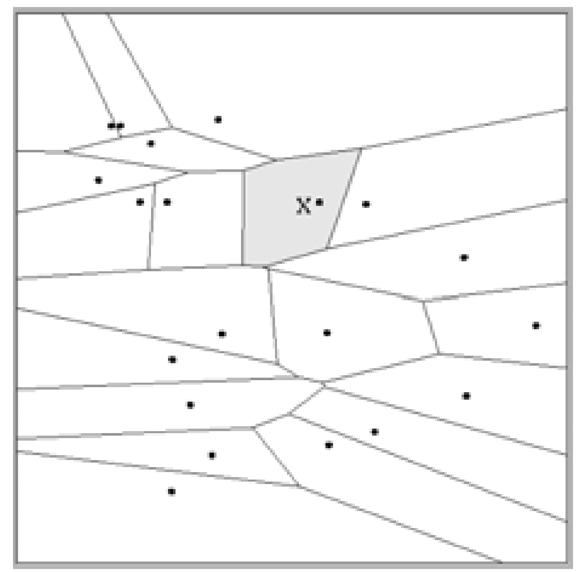
- Alternative approach: Wrapping
  - Starting with zero features, iterate:
    - greedily add a new feature based on NN performance

Weighting dimensions

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



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



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

vertical affected

Computational Cost?

“locality sensitive hashing”

- 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

If each example is unique, every example is its own NN
Training accuracy is then 100%

- Form prototypes

Obtained by merging similar instances in a way that does not decrease accuracy on a validation set

"What if we replaced those 2 instances with a single instance equal to the average?"
If it doesn't hurt our accuracy, we might want to do that

- 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

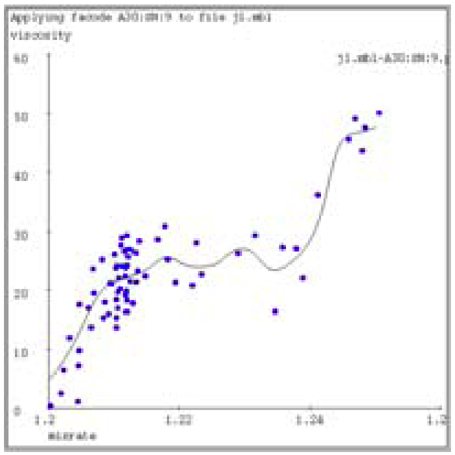
$$h(x_q) = \frac{\sum_i w_i \cdot f(x_i)}{\sum_i w_i}$$

A weighted average

Kernel-weighted Regression

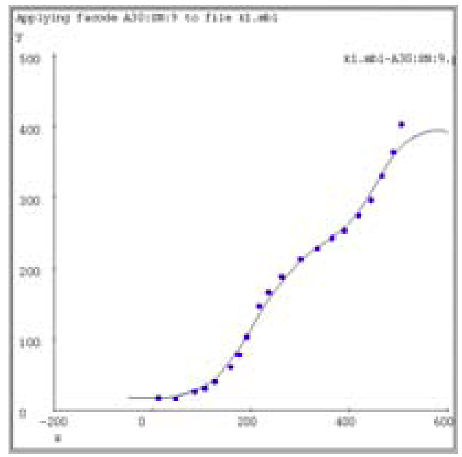
!!———————Should be “width” not weight———————!!

Kernel Weight = 1/32 of X-axis width



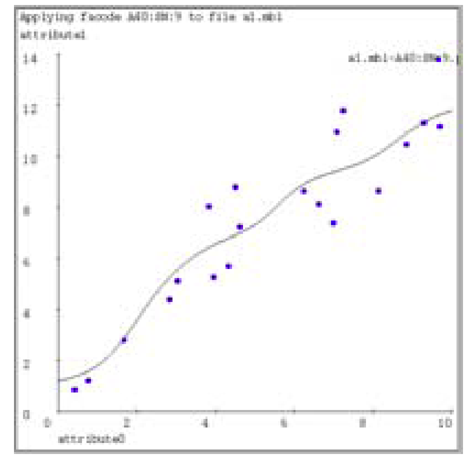
A better fit than KNN?

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?

Can be more expensive b/c averaging over all data points
(distance between points is the expense)

Realistically similar computation expense to NN

Discussion

- "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

INDUCTIVE BIAS

Can't learn all without inductive biases (use domain knowledge about a phenomenon to shape our inductive bias)

- Agree or Disagree?

So when we're choosing features, features are informed by our knowledge of the field

Reading

- Elements of Statistical Learning (2.3, 13.3)