Machine Learning

Topic 3: Memory based learning

Nearest Neighbor Classifier

- Example of memory-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 $X = \{\vec{x}_1, \ldots \vec{x}_n\}$

Each example is an k-tuple of attribute values

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

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

$$f : X \to Y$$

The DATA is a set of tuples <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...

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

Eager vs. Lazy

- Eager learning
  - Explicitly learn ***h*** from training data
  - E.g. decision tree, linear regression, svm, neural nets, etc.
- Lazy learning
  - Delay the learning process until a query example must be labeled
  - ***h*** *is implicity*
  - E.g. Nearest neighbor, kNN, locally weighted regression, etc.

Single Nearest Neighbor

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 the data set to the query

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

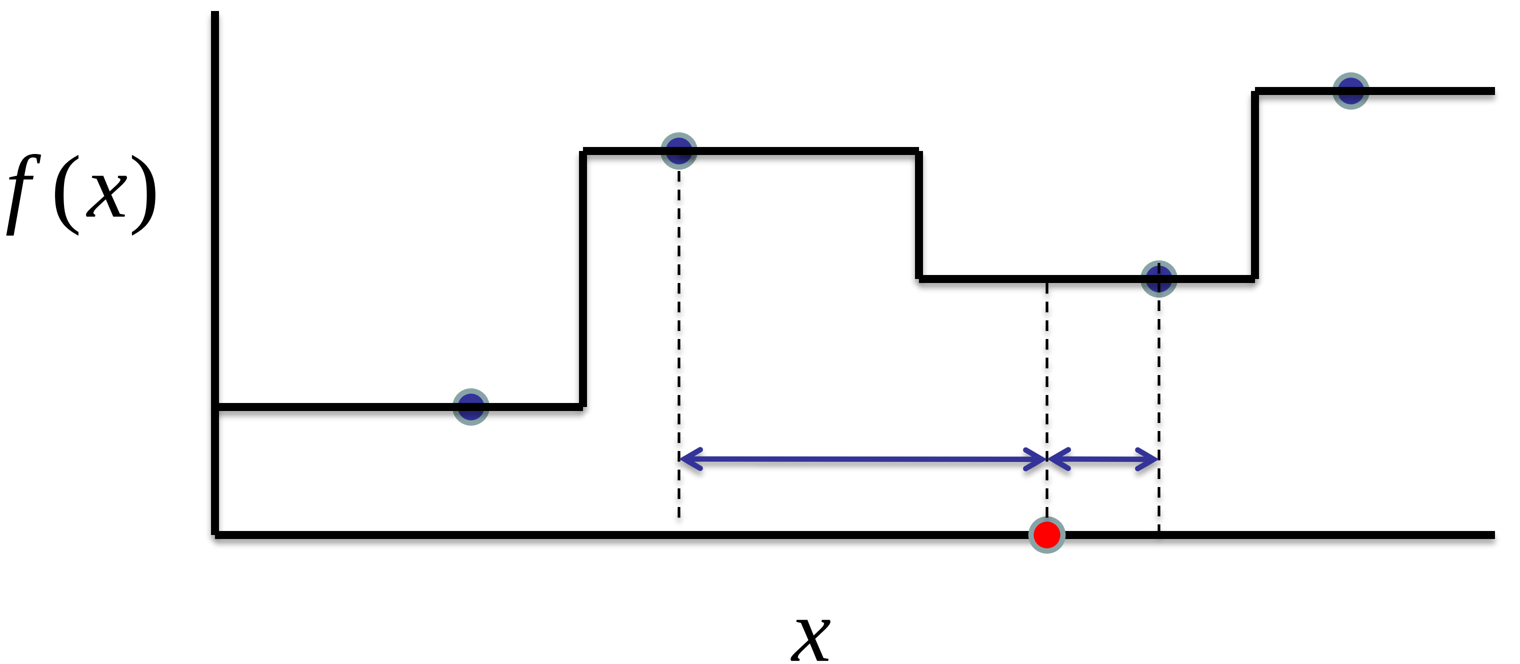
2. Assign the nearest neighbor's output to the query

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

Our hypothesis

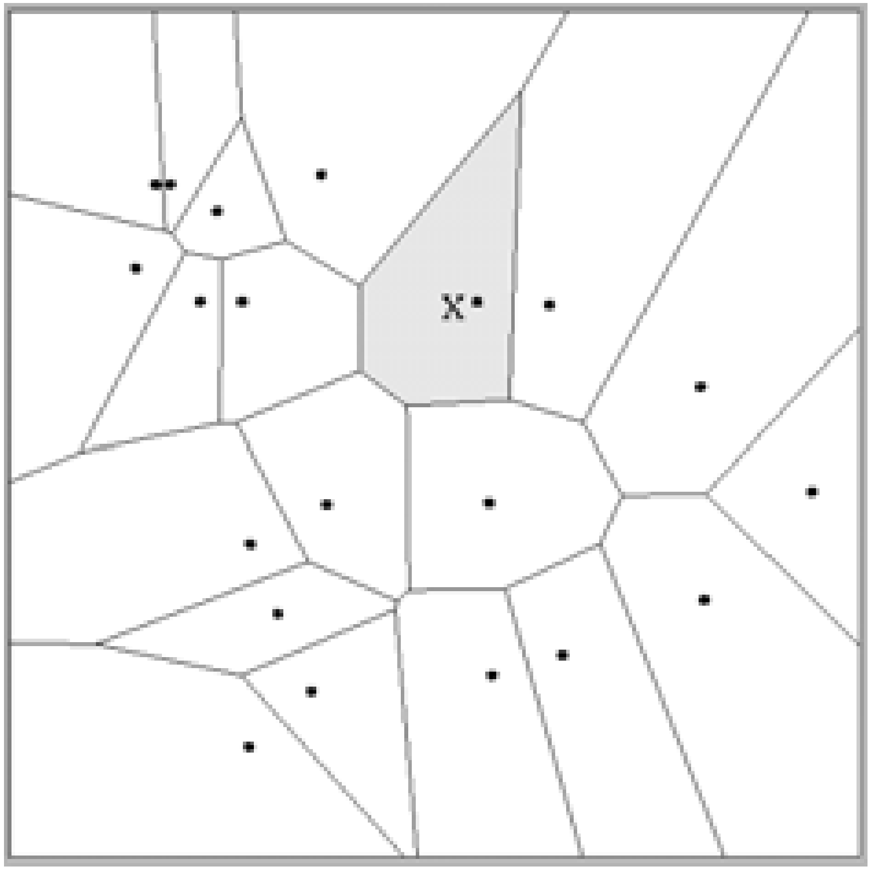
A Univariate Example

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



Two-dimensional

- Voronoi diagram



What makes a memory 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

  Euclidean

- Number of neighbors to consider

  K

- A weighting function (optional)

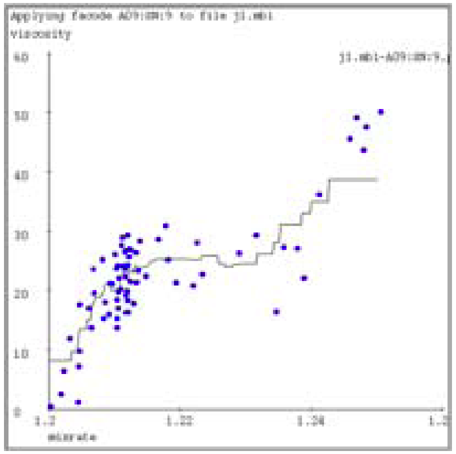
  Unused (i.e. equal weights)

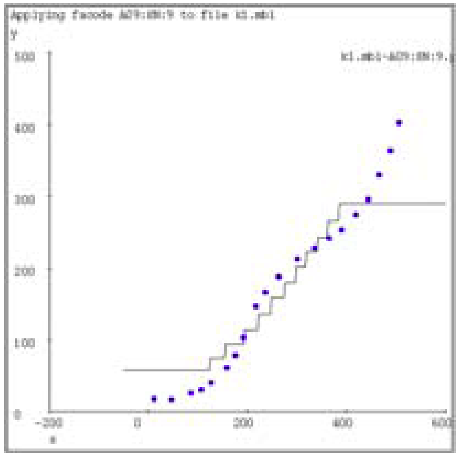
- How to fit with the neighbors

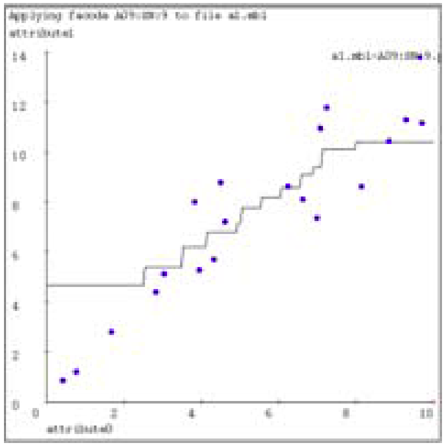
  regression: average output among K nearest neighbors.

  classification: most output among K nearest neighbors

Examples of KNN where K=9







Reasonable job
Did smooth noise

Screws up on the ends

OK, but problem on the ends again.

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.

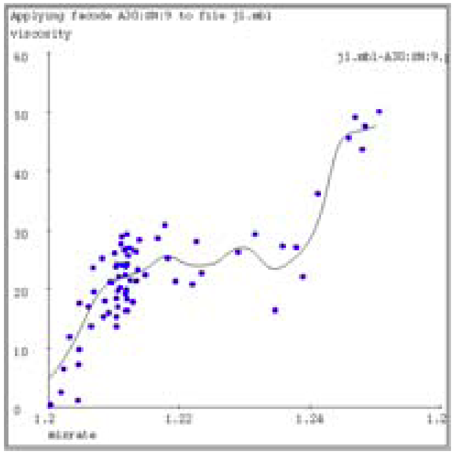
- How to fit with the neighbors

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

A weighted average

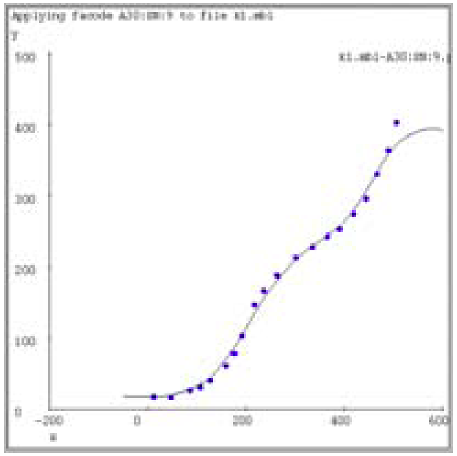
Kernel Regression

Kernel Weight = 1/32 of X-axis width



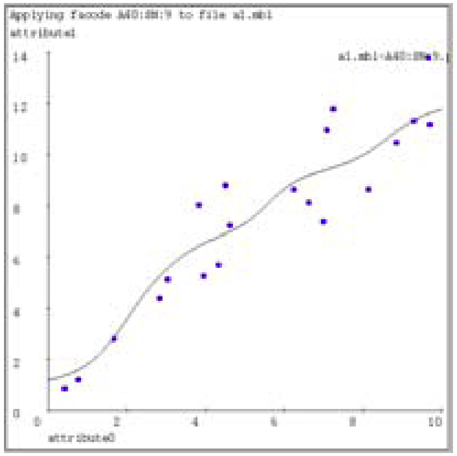
A better fit than KNN?

Kernel Weight = 1/32 of X-axis width



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

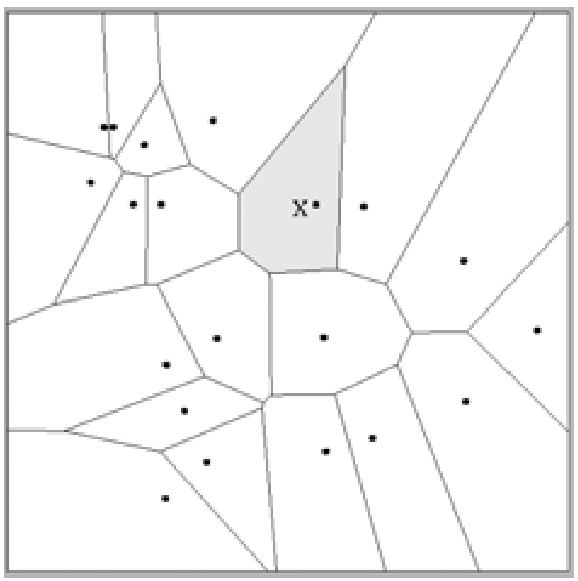
Kernel Weight = 1/16 of X-axis width



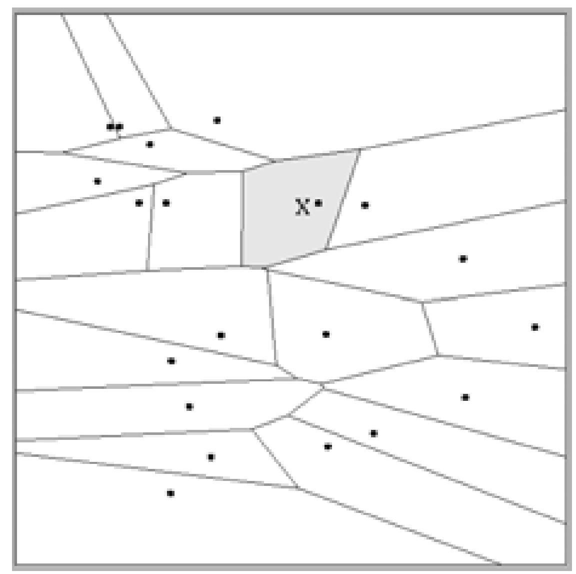
Nice and smooth, but are the bumps justified, or is this overfitting?

Weighting dimensions

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



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



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

kNN and Kernel Regression

- Pros
  - Robust to noise
  - Very effective when training data is sufficient
  - Customized to each query
- Cons
  - How to weight different dimensions?
  - Irrelevant dimensions
  - Computationally expensive to label a new query

Locally Weighted (Linear) Regression

- Linear regression: global, linear

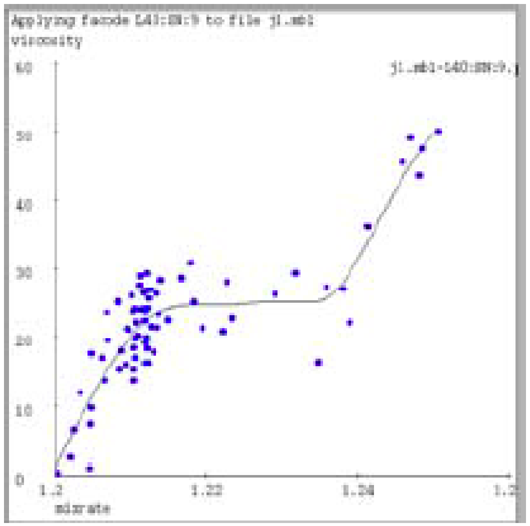
$$Err = \sum_{\vec{x} \in D} \frac{1}{2}\left(f(\vec{x}) - h(\vec{x})\right)^2 \qquad h(\vec{x}) = \vec{a}^T \vec{x} + \vec{b}$$

- kNN: local, constant
- LWR: local, linear

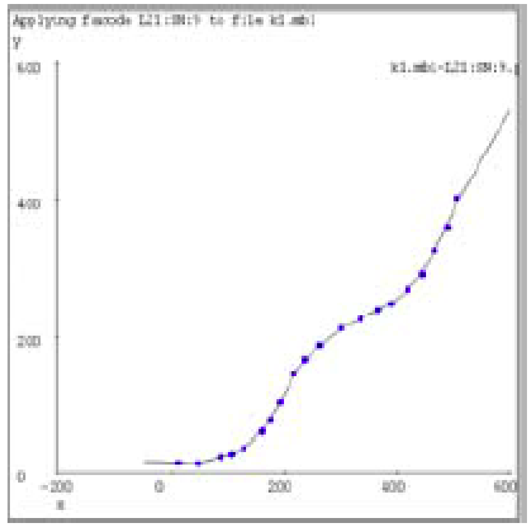
$$Err(x_q) = \sum_{x \in kNN(x_q)} \frac{1}{2}\left(f(x) - h(x)\right)^2$$

$$Err(x_q) = \sum_{x \in D} \frac{1}{2}\left(f(x) - h(x)\right)^2 \exp\left(\frac{-d(x, x_q)^2}{K_W^2}\right)$$

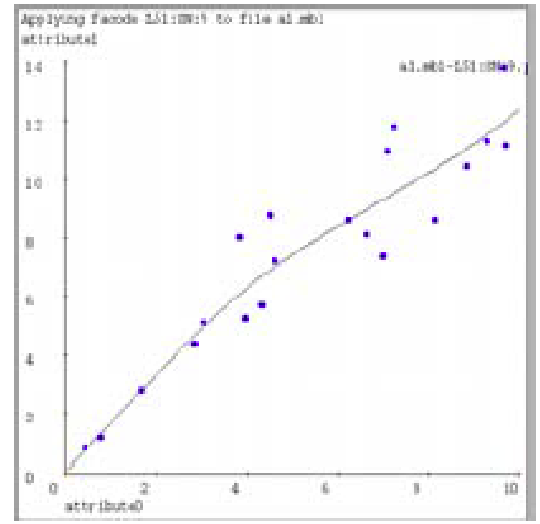
Locally Weighted (Linear) Regression



KW = 1/16 of x-axis width.



KW = 1/32 of x-axis width.

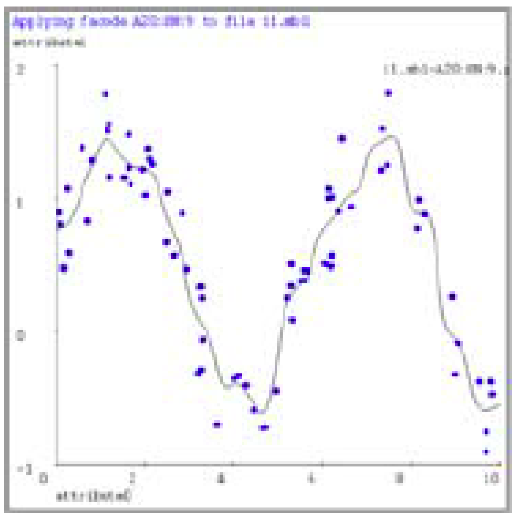


KW = 1/8 of x-axis width.

Nicer and smoother, but even now, are the bumps justified, or is this overfitting?

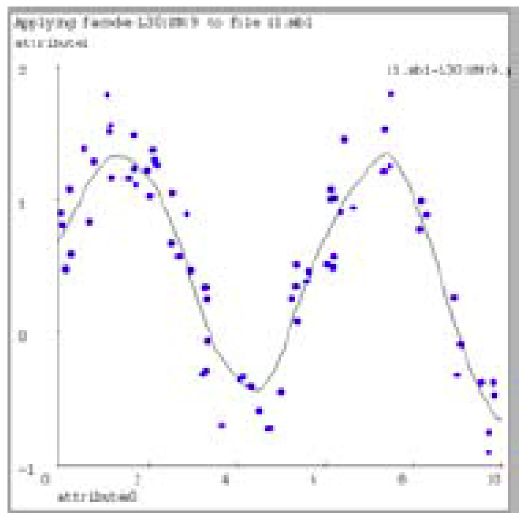
Locally Weighted Polynomial Regression

- Use a polynomial instead of a linear function to fit the data locally
  - Quadratic, cubic, etc.



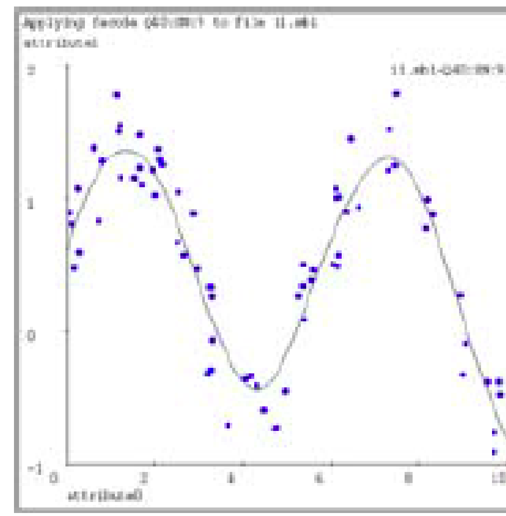
Kernel Regression
Kernel width K_W at optimal level.

KW = 1/100 x-axis



LW Linear Regression
Kernel width K_W at optimal level.

KW = 1/40 x-axis



LW Quadratic Regression
Kernel width K_W at optimal level.

KW = 1/15 x-axis

Summary

- Memory-based learning are “lazy”
  - Delay learning until receiving a query
- Local
  - Training data that localized around the query contribute more to the prediction label
- Robust to noise
- Curse of dimensionality
  - Irrelevant dimensions
  - How to scale dimensions

Summary

- Nearest neighbor
  – Output the nearest neighbor's label
- kNN
  – Output the average of the k NN's labels
- Kernel regression
  – Output weighted average of all training data's (or k NN's) labels
- Locally weighted (linear) regression
  – Fit a linear function locally