Neural Networks, cont.

Machine Learning – 10701/15781
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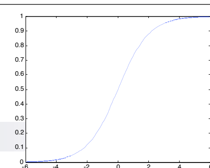
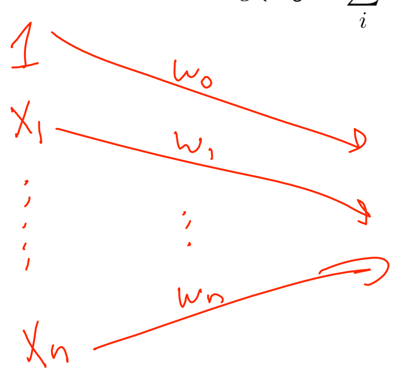
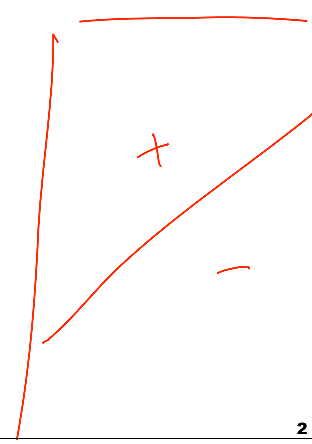
Perceptron as a graph



$$g(w_0 + \sum_i w_i x_i) = \frac{1}{1+e^{-(w_0+\sum_i w_i x_i)}}$$





The perceptron learning rule

Squared loss

learning rate

$$\boxed{w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta \sum_j x_i^j \delta^j}$$

$$\delta^j = [y^j - g(w_0 + \sum_i w_i x_i^j)] g^j (1 - g^j)$$

$$g^j = g(w_0 + \sum_i w_i x_i^j)$$

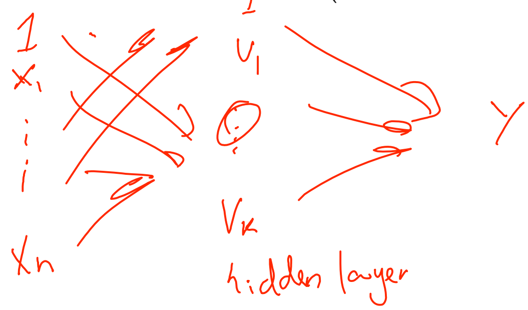
- Compare to MCLE:

$$\boxed{w_i \leftarrow w_i + \eta \sum_j x_i^j \delta^j} \qquad \delta^j = [y^j - g(w_0 + \sum_i w_i x_i^j)]$$

Hidden layer

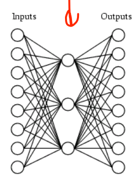
- Perceptron: $out(\mathbf{x}) = g(w_0 + \sum_i w_i x_i)$
- 1-hidden layer:

$$out(\mathbf{x}) = g\left(w_0 + \sum_k w_k \overbrace{g(w_0^k + \sum_i w_i^k x_i)}^{V_k}\right)$$



Example data for NN with hidden layer

hidden layer



A target function: x out (x)

dataset

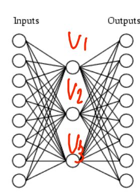
Input		Output
10000000	→	10000000
01000000	→	01000000
00100000	→	00100000
00010000	→	00010000
00001000	→	00001000
00000100	→	00000100
00000010	→	00000010
00000001	→	00000001

Can this be learned??

Learned weights for hidden layer

A network:

hidden layer

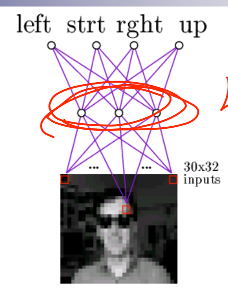


"learned" a lower dimensional encoding of the data

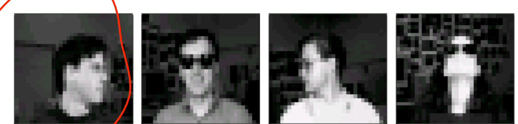
Learned hidden layer representation:

Input		Hidden Values				Output
		V_1	V_2	V_3		
10000000	→	.89	.04	.08	→	10000000
01000000	→	.01	.11	.88	→	01000000
00100000	→	.01	.97	.27	→	00100000
00010000	→	.99	.97	.71	→	00010000
00001000	→	.03	.05	.02	→	00001000
00000100	→	.22	.99	.99	→	00000100
00000010	→	.80	.01	.98	→	00000010
00000001	→	.60	.94	.01	→	00000001

NN for images



hidden layer

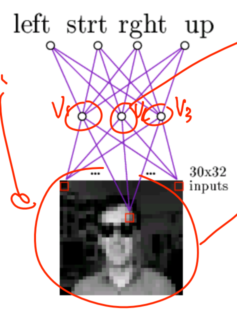


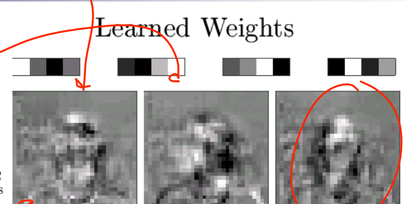
Typical input images

90% accurate learning head pose, and recognizing 1-of-20 faces

Weights in NN for images

$w_0 + \sum_i w_i x_i$





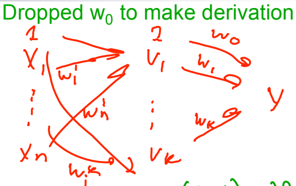
w_i^1 w_i^2 w_i^3

Typical input images

Gradient descent for 1-hidden layer – Back-propagation: Computing $\frac{\partial \ell(W)}{\partial w_k}$

initial w's usually random

Dropped w_0 to make derivation simpler



loss

doesn't depend on w_k

$$\ell(W) = \frac{1}{2}\sum_j [y^j - out(\mathbf{x}^j)]^2$$

$$out(\mathbf{x}) = g\left(\sum_{k'} w_{k'} \underbrace{g(\sum_{i'} w_{i'}^{k'} x_{i'})}_{V_{k'}}\right)$$

data point

$$\frac{\partial \ell(W)}{\partial w_k} = \sum_{j=1}^{m} -[y^j - out(\mathbf{x}^j)]\frac{\partial out(\mathbf{x}^j)}{\partial w_k}$$

$$\frac{\partial}{\partial w} g(f(w)) = \frac{\partial f}{\partial w} \cdot g'(f(w))$$

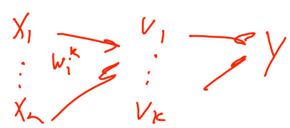
$$g' = g(1-g)$$

$$\frac{\partial out(x^j)}{\partial w_k} = V_k^j \cdot g'\left(\sum_{k'} w_{k'} g\left(\sum_{i'} w_{i'}^{k'} x_{i'}^j\right)\right)$$

$$= \underbrace{V_k^j \; g\left(\sum_{k'} w_{k'} V_{k'}^j\right)\left(1 - g\left(\sum_{k'} w_{k'} V_{k'}^j\right)\right)}_{\text{first compute } V_k\text{'s (forward sweep)}}$$

Gradient descent for 1-hidden layer – Back-propagation: Computing $\frac{\partial \ell(W)}{\partial w_i^k}$

Dropped w_0 to make derivation simpler



$$\ell(W) = \frac{1}{2}\sum_j [y^j - out(\mathbf{x}^j)]^2$$

$$out(\mathbf{x}) = g\left(\sum_{k'} w_{k'} g(\sum_{i'} w_{i'}^{k'} x_{i'})\right)$$

g, f, h

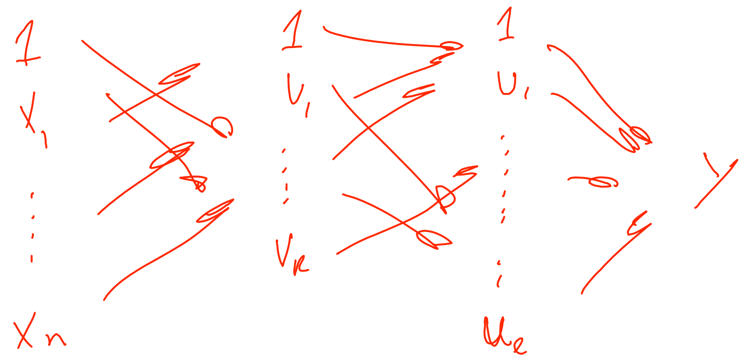
$$\frac{\partial \ell(W)}{\partial w_i^k} = \sum_{j=1}^{m} -[y - out(\mathbf{x}^j)]\boxed{\frac{\partial out(\mathbf{x}^j)}{\partial w_i^k}}$$

$$\frac{\partial}{\partial w} g(f(h(w))) = \frac{\partial g}{\partial f} \cdot \frac{\partial f}{\partial h} \cdot \frac{\partial h}{\partial w}$$

$$\frac{\partial out(x^j)}{\partial w_i^k} = x_i^j \, w_k g'\left(\sum_{i'} w_{i'}^k x_{i'}^j\right) \cdot \underbrace{g'\left(\sum_{k'} w_{k'} V_{k'}^j\right)}$$

$$= x_i^j \, w_k V_k^j (1 - V_k^j) \cdot \underbrace{g\left(\sum_{k'} w_{k'} V_{k'}^j\right)}_{out(x^j)} \underbrace{\left(1 - g\left(\sum_{k'} w_{k'} V_{k'}^j\right)\right)}_{(1 - out(x^j))}$$

Multilayer neural networks

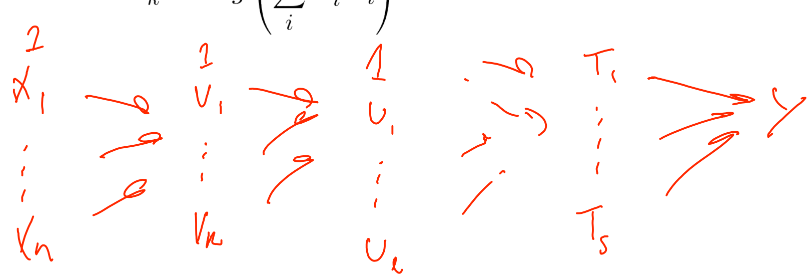


Forward propagation – prediction

recurrent NNs (cycles in graph)

- Recursive algorithm
- Start from input layer
- Output of node V_k with parents $U_1, U_2, \ldots$:

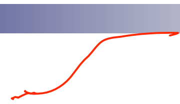
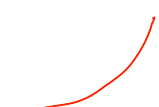
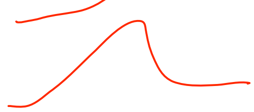
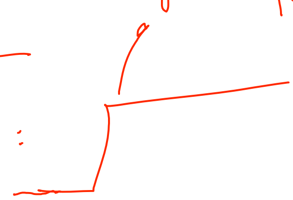
$$V_k = g\left(\sum_i w_i^k U_i\right)$$



Back-propagation – learning

- Just gradient descent!!!
- Recursive algorithm for computing gradient
- For each example
  - Perform forward propagation
  - Start from output layer
  - Compute gradient of node V_k with parents $U_1, U_2, \ldots$
  - Update weight w_i^k

Many possible response functions

- Sigmoid 
- Linear $g(w_0 + \sum_i w_i x_i) = w_0 + \sum_i w_i x_i$
- Exponential 
- Gaussian 
- … step/threshold : 

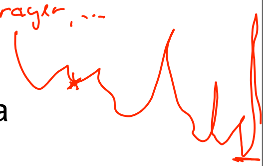
$g(z) = \begin{cases} 1 & \text{is } z > 0 \\ 0 & \text{otherwise} \end{cases}$

Convergence of backprop

- Perceptron leads to convex optimization
  - Gradient descent reaches **global minima**

→ simulated annealing, random restarts, prayer, ...

- Multilayer neural nets **not convex**
  - Gradient descent gets stuck in local minima
  - Hard to set learning rate
  - Selecting number of hidden units and layers = fuzzy process
  - NNs falling in disfavor in last few years
  - We'll see later in semester, *kernel trick* is a good alternative
  - Nonetheless, neural nets are one of the most used ML approaches



Overfitting?

- Neural nets represent complex functions
  - Output becomes more complex with gradient steps

more hidden units/layers

- regularized
- stop early
⋮

$\sum_j (y^j - out(x^j))^2 + \lambda_1 \sum_i w_i^2 + \lambda_2 \sum_i h_i^2$

Overfitting

- Output fits training data “too well”
  - Poor test set accuracy
- Overfitting the training data
  - Related to bias-variance tradeoff
  - One of central problems of ML
- Avoiding overfitting?
  - More training data
  - Regularization
  - Early stopping

What you need to know about neural networks

- Perceptron:
  - Representation
  - Perceptron learning rule
  - Derivation
- Multilayer neural nets
  - Representation
  - Derivation of backprop
  - Learning rule
- Overfitting
  - Definition
  - Training set versus test set
  - Learning curve

Announcements

- Recitation this week: Neural networks
- Project proposals due next Wednesday
  - Exciting data:
    - Swivel.com - user generated graphs
    - Recognizing Captchas
    - Election contributions
    - Activity recognition
    - …

ML & real data
the more, the better

Instance-based Learning

(non-parametric methods)

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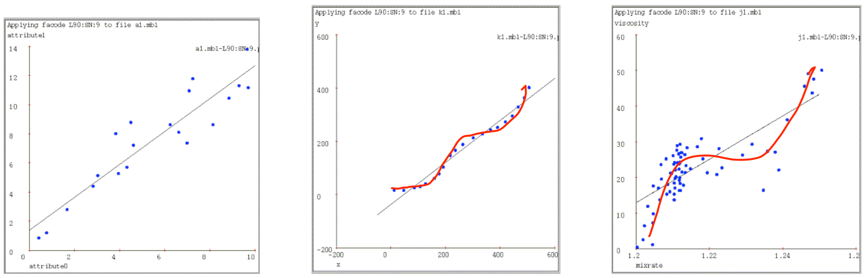
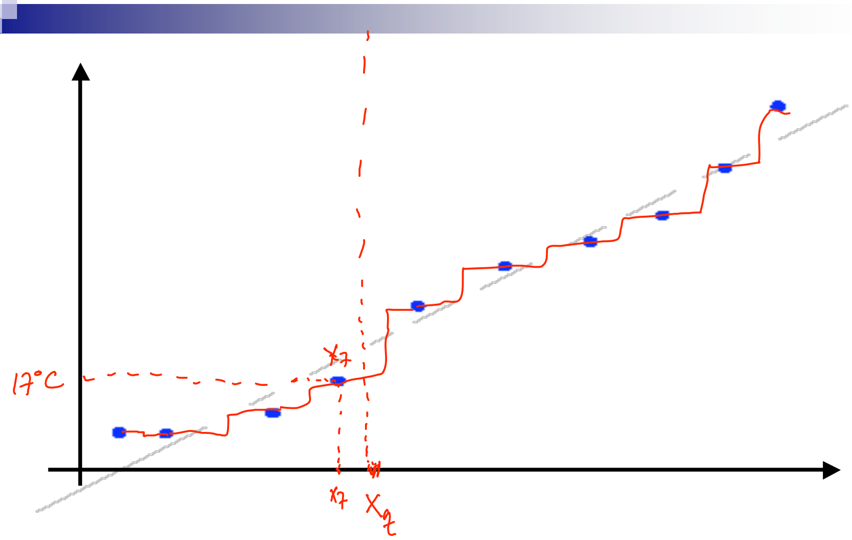
Why not just use Linear Regression?



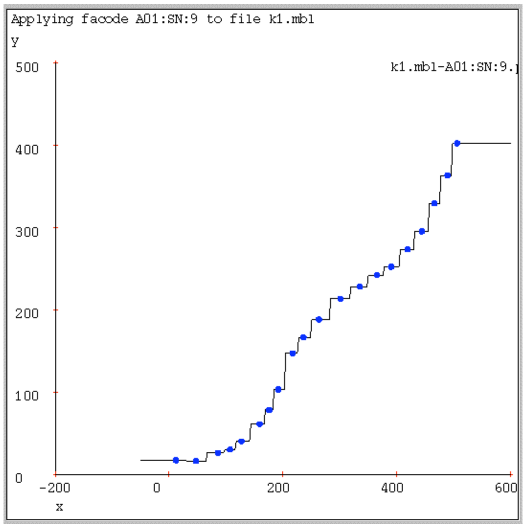
- use more basis functions

- non-parametric ...

Using data to predict new data



Nearest neighbor



works amazingly well with a lot of data

Univariate 1-Nearest Neighbor

Given datapoints (x_1,y_1) (x_2,y_2)..(x_N,y_N), where we assume $y_i=f(x_i)$ for some unknown function f.

Given query point x_q, your job is to predict $\hat{y} \approx f(x_q)$

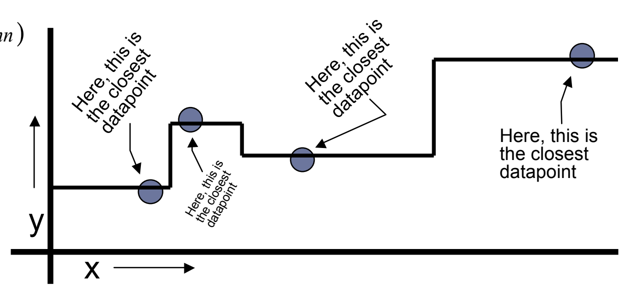
Nearest Neighbor:

1. Find the closest x_i in our set of datapoints

$$i(nn) = \underset{i}{\operatorname{argmin}} |x_i - x_q|$$

2. Predict $\hat{y} = y_{i(nn)}$

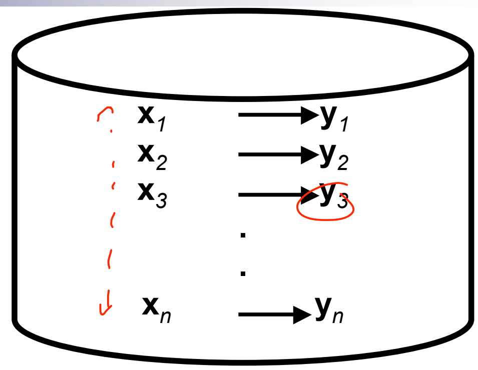
Here's a dataset with one input, one output and four datapoints.



1-Nearest Neighbor is an example of…. Instance-based learning

A function approximator that has been around since about 1910.

To make a prediction, search database for similar datapoints, and fit with the local points.



Four things make a memory based learner:

- A distance metric (what's near?)
- How many nearby neighbors to look at?
- A weighting function (optional)
- How to fit with the local points?

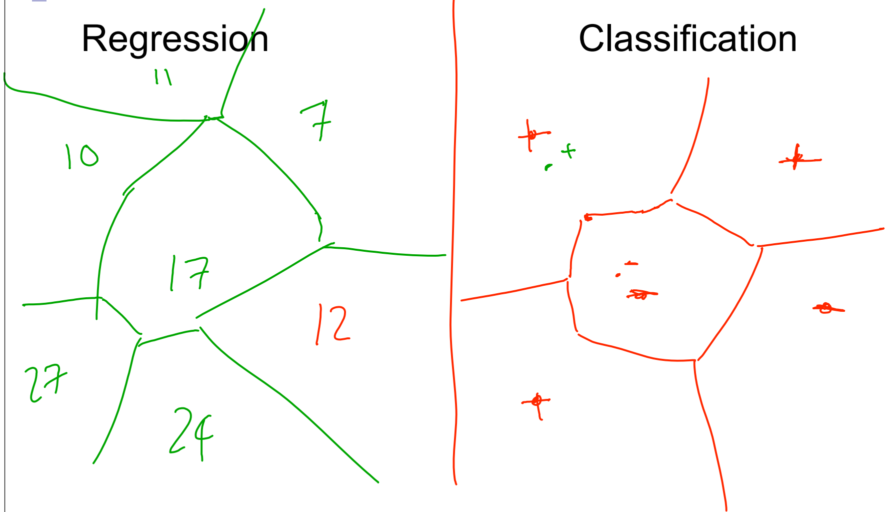
1-Nearest Neighbor

Four things make a memory based learner:

1. *A distance metric* $\|x_q - x_i\|_2$
   Euclidian (and many more)
2. *How many nearby neighbors to look at?*
   One
3. *A weighting function (optional)*
   Unused
4. *How to fit with the local points?*
   Just predict the same output as the nearest neighbor.

Multivariate 1-NN examples

Regression | Classification

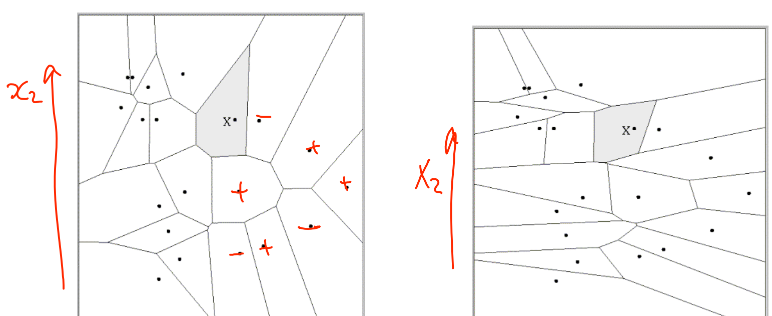


Multivariate distance metrics

Suppose the input vectors $x_1, x_2, \ldots x_n$ are two dimensional:

$\mathbf{x}_1 = (x_{11}, x_{12})$, $\mathbf{x}_2 = (x_{21}, x_{22})$, $\ldots \mathbf{x}_N = (x_{N1}, x_{N2})$.

One can draw the nearest-neighbor regions in input space.



$Dist(\mathbf{x}_i, \mathbf{x}_j) = (x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2$ $\quad$ $Dist(\mathbf{x}_i, \mathbf{x}_j) = (x_{i1} - x_{j1})^2 + (3x_{i2} - 3x_{j2})^2$

x_1 $\quad$ x_1

$\|x_i - x_j\|^2$

The relative scalings in the distance metric affect region shapes

Euclidean distance metric

Or equivalently,
$$D(\mathrm{x},\mathrm{x}') = \sqrt{\sum_i \sigma_i^2 (x_i - x'_i)^2}$$

where
$$D(\mathrm{x},\mathrm{x}') = \sqrt{(\mathrm{x}-\mathrm{x}')^T \sum (\mathrm{x}-\mathrm{x}')}$$

$\sigma_1 = \sigma_2$ $\qquad$ $\sigma_1 > \sigma_2$

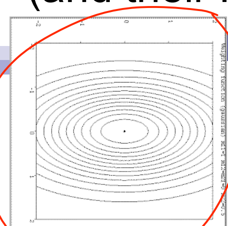
x_1

$$\Sigma = \begin{bmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & \sigma_N^2 \end{bmatrix}$$

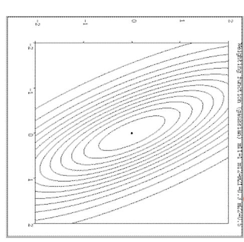
Other Metrics…

- Mahalanobis, Rank-based, Correlation-based,…

Notable distance metrics (and their level sets)



Scaled Euclidian (L_2)

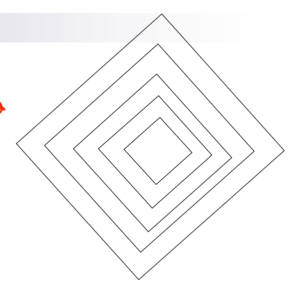


Mahalanobis (here, Σ on the previous slide is not necessarily diagonal, but is symmetric

$\Sigma = \begin{pmatrix} \diagdown & 0 \\ 0 & \end{pmatrix}$

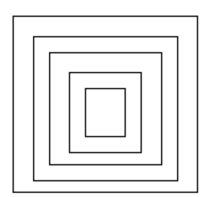
Σ

$\|x_1 - x_2\|_1 = \sum_i |x_{i1} - x_{i2}|$



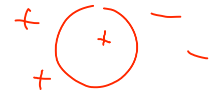
L_1 norm (absolute)

$\|x_1 - x_2\|_\infty = \max_i |x_{i1} - x_{i2}|$



L∞ *(max) norm*

Consistency of 1-NN



- Consider an estimator f_n trained on n examples
  - e.g., 1-NN, neural nets, regression,...
- Estimator is *consistent* if true error goes to zero as amount of data increases (i.i.d.)
  - e.g., for no noise data, consistent if:

$$\lim_{n \to \infty} MSE(f_n) = 0$$

- Regression is not consistent!
  - Representation bias
- **1-NN is consistent** (under some mild fineprint)

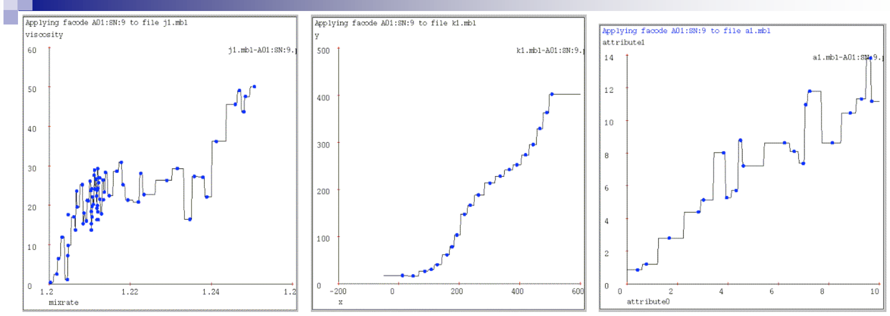
NN: Voronoi diag

DT: $X_1 > t$

$X_1 > t_3$ $X_2 > t_2$

What about variance???

1-NN overfits?

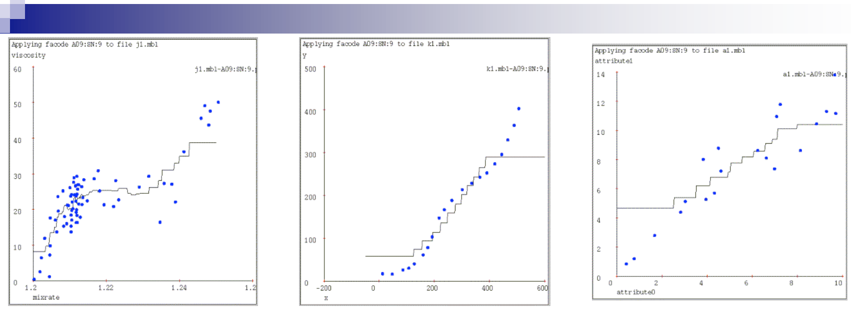


k-Nearest Neighbor

Four things make a memory based learner:

1. *A distance metric*
   Euclidian (and many more)
2. *How many nearby neighbors to look at?*
   k
1. *A weighting function (optional)*
   Unused
2. *How to fit with the local points?*
   Just predict the average output among the k nearest neighbors.

k-Nearest Neighbor (here k=9)



K-nearest neighbor for function fitting smoothes away noise, but there are clear deficiencies.

What can we do about all the discontinuities that k-NN gives us?

Weighted k-NNs

- Neighbors are not all the same

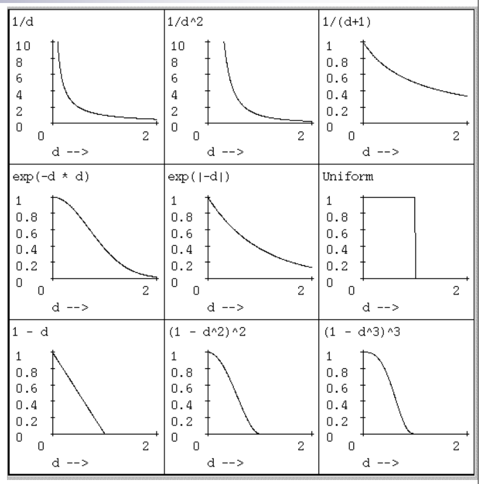
Kernel regression

Four things make a memory based learner:

1. *A distance metric*
   Euclidian (and many more)
2. *How many nearby neighbors to look at?*
   All of them
3. *A weighting function (optional)*
   $\boldsymbol{w_i = \exp(-D(x_i, query)^2 / K_w^2)}$
   Nearby points to the query are weighted strongly, far points weakly. The K_W parameter is the **Kernel Width**. Very important.
4. *How to fit with the local points?*
   Predict the weighted average of the outputs:
   predict = $\boldsymbol{\Sigma w_i y_i / \Sigma w_i}$

Weighting functions

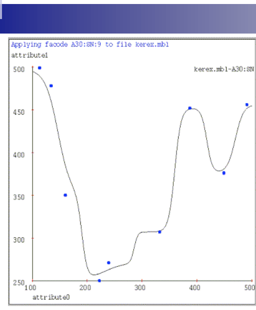
$w_i = \exp(-D(x_i, query)^2 / K_w^2)$



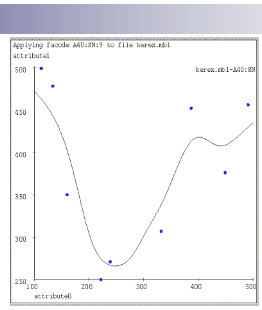
Typically optimize K_w using gradient descent

(Our examples use Gaussian)

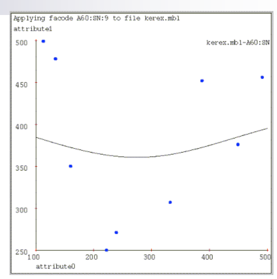
Kernel regression predictions



K_W=10



K_W=20

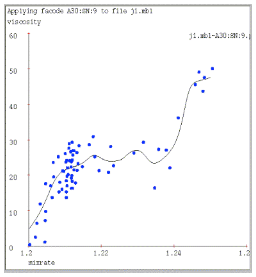


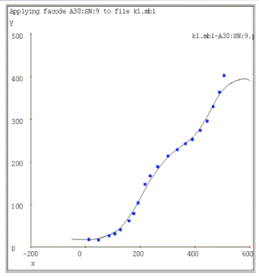
K_W=80

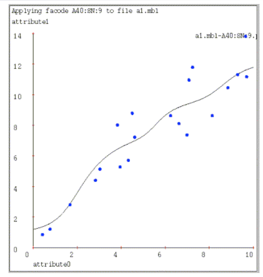
Increasing the kernel width K_w means further away points get an opportunity to influence you.

As $K_w \rightarrow \infty$, the prediction tends to the global average.

Kernel regression on our test cases



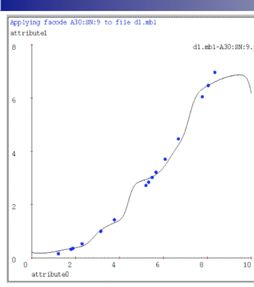


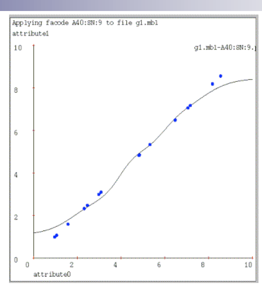


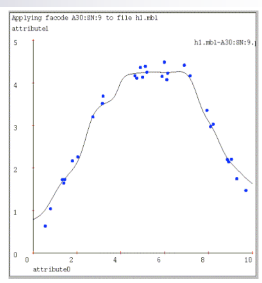
KW=1/32 of x-axis width. KW=1/32 of x-axis width. KW=1/16 axis width.

Choosing a good K_w is important. Not just for Kernel Regression, but for all the locally weighted learners we're about to see.

Kernel regression can look bad







KW = Best. KW = Best. KW = Best.

Time to try something more powerful…

Locally weighted regression

Kernel regression:

Take a very very conservative function approximator called AVERAGING. Locally weight it.

Locally weighted regression:

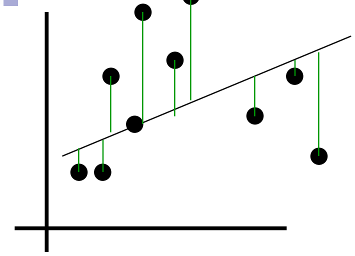
Take a conservative function approximator called LINEAR REGRESSION. Locally weight it.

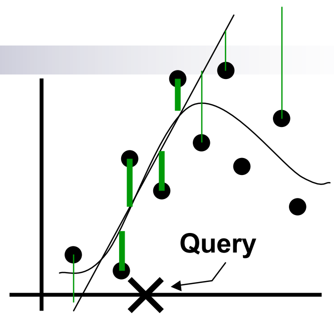
Locally weighted regression

- **Four things make a memory based learner:**
- *A distance metric*
  Any
- *How many nearby neighbors to look at?*
  All of them
- *A weighting function (optional)*
  Kernels
  - ***wi = exp(-D(xi, query)^2 / Kw^2)***
- *How to fit with the local points?*
  General weighted regression:

$$\hat{\mathrm{a}} = \underset{\hat{\mathrm{a}}}{\operatorname{argmin}} \sum_{k=1}^{N} w_k^{\,2} \left(\mathrm{y}_k - \hat{\mathrm{a}}^T \mathrm{x}_k \right)^2$$

How LWR works





Linear regression
- Same parameters for all queries

$$\hat{a} = \left(X^T X\right)^{-1} X^T Y$$

Locally weighted regression
- Solve weighted linear regression for each query

$$\beta = \left((WX)^T WX\right)^{-1} (WX)^T WY$$

$$W = \begin{pmatrix} w_1 & 0 & 0 & 0 \\ 0 & w_2 & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & w_n \end{pmatrix}$$

Another view of LWR

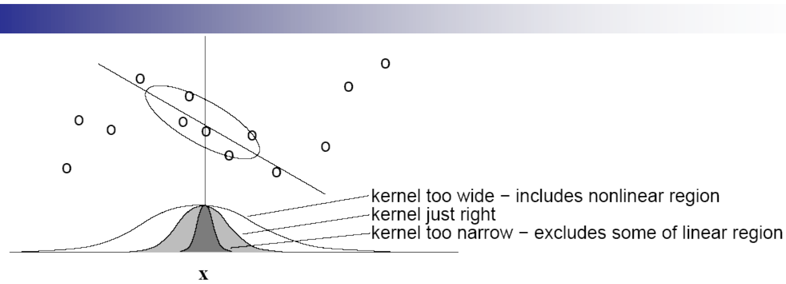
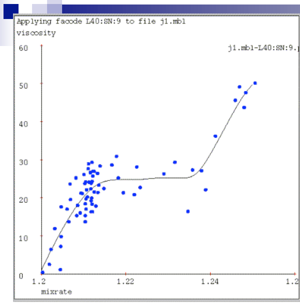
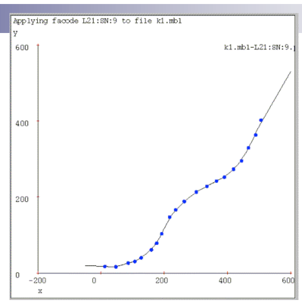


Image from Cohn, D.A., Ghahramani, Z., and Jordan, M.I. (1996), "Active Learning with Statistical Models", JAIR Volume 4, pages 129-145.

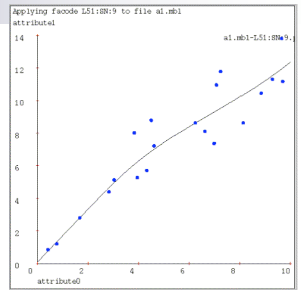
LWR on our test cases



KW = 1/16 of x-axis width.

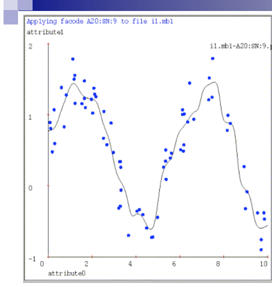


KW = 1/32 of x-axis width.



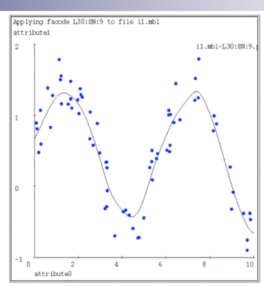
KW = 1/8 of x-axis width.

Locally weighted polynomial regression



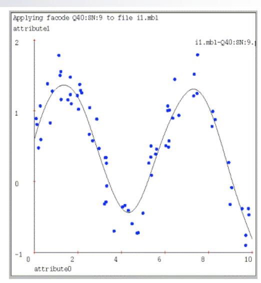
Kernel Regression
Kernel width K_W at optimal level.

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

Local quadratic regression is easy: just add quadratic terms to the WXTWX matrix. As the regression degree increases, the kernel width can increase without introducing bias.

Curse of dimensionality for instance-based learning

- Must store and retreve all data!
  - Most real work done during testing
  - For every test sample, must search through all dataset – very slow!
  - We'll see fast methods for dealing with large datasets
- Instance-based learning often poor with noisy or irrelevant features

Curse of the irrelevant feature

What you need to know about instance-based learning

- k-NN
  - Simplest learning algorithm
  - With sufficient data, very hard to beat “strawman” approach
  - Picking k?
- Kernel regression
  - Set k to n (number of data points) and optimize weights by gradient descent
  - Smoother than k-NN
- Locally weighted regression
  - Generalizes kernel regression, not just local average
- Curse of dimensionality
  - Must remember (very large) dataset for prediction
  - Irrelevant features often killers for instance-based approaches

Acknowledgment

- This lecture contains some material from Andrew Moore’s excellent collection of ML tutorials:
  - http://www.cs.cmu.edu/~awm/tutorials