Instance-based learning

(a.k.a. memory-based) (a.k.a. non-parametric regression) (a.k.a. case-based) (a.k.a kernel-based)

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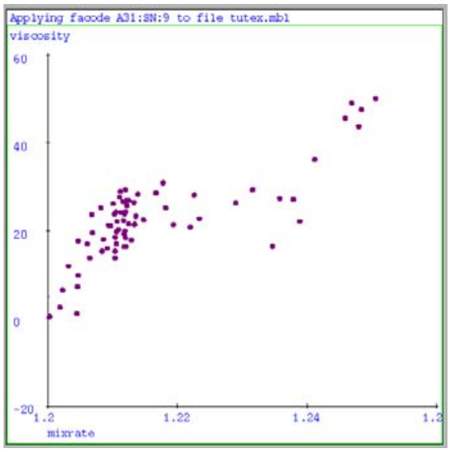
Software to play with the algorithms in this tutorial, and example data are available from: http://www.cs.cmu.edu/~awm/vizier . The example figures in this slide-set were created with the same software and data.

Overview

- What do we want a regressor to do?
- Why not stick with polynomial regression? Why not just "join the dots"?
- What's k-nearest-neighbor all about?
- And how about kernel regression, locally weighted regression?
- Hmm. But what about multivariate fitting?
- And how do you compute all that stuff? And why should I care?

This Tutorial's Starting Point



We've obtained some numeric data.

How do we exploit it?

Steel Temp	Line Speed	Slab Width	Temp Stage2	Cool Setpt	Cool Gain
-0.4788	0.3849	0.0357	0.8384	0.6620	-0.9512
0.3470	-0.6488	0.6629	-0.5087	0.6845	-0.0647
0.8622	-0.5367	-0.2459	-0.1438	-0.7267	-0.6119
-0.2099	-0.5975	0.0614	-0.7648	0.0222	-0.7623
-0.4627	0.6218	0.9254	0.6081	-0.8739	-0.6439
0.7341	0.0745	-0.2650	-0.4510	-0.4548	0.5753
0.4237	-0.5143	-0.0731	0.0385	-0.8068	0.3098
-0.1267	0.8105	-0.6619	-0.0768	-0.8738	-0.3367
0.0332	0.7754	0.7718	-0.5440	0.6237	0.5113
0.2668	0.8777	-0.5690	-0.5151	0.6493	0.7705
-0.5682	0.8457	0.5669	-0.7359	-0.3394	0.5880
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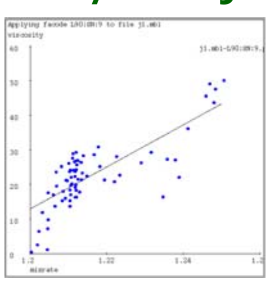
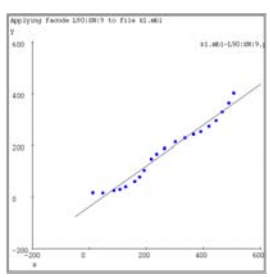
Simple, uni-variate case

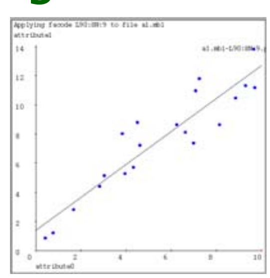
General, multi variate case

Software and data for the algorithms in this tutorial: http://www.cs.cmu.edu/~awm/vizier . The example figures in this slide-set were created with the same software and data.

Why not just use Linear Regression?







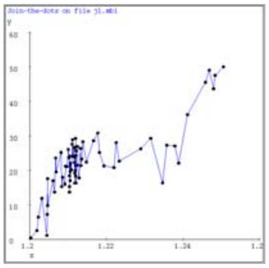
Here, linear regression manages to capture a significant trend in the data, but there is visual evidence of bias.

Here, linear regression appears to have a much better fit, but the bias is very clear.

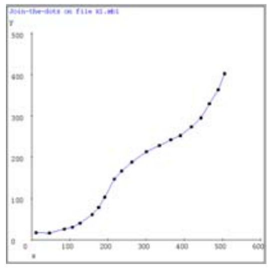
Here, linear regression may indeed be the right thing.

Bias: the underlying choice of model *(in this case, a line)* cannot, with any choice of parameters *(constant term and slope)* and with any amount of data *(the dots)* capture the full relationship.

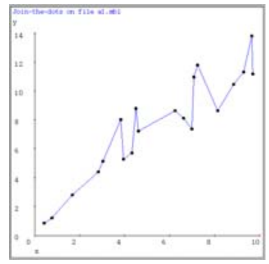
Why not just Join the Dots?



Here, joining the dots is clearly fitting noise.



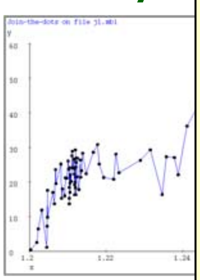
Here, joining the dots looks very sensible.



Again, a clear case of noise fitting.

Why is fitting the noise so bad?

Why



- You will tend to make somewhat bigger prediction errors on new data than if you filtered the noise perfectly.
- You don't get good gradient estimates or noise estimates.
- You can't make sensible confidence intervals.
- It's morally wrong.
- **Also:** Join the dots is *much harder* to implement for multivariate inputs.

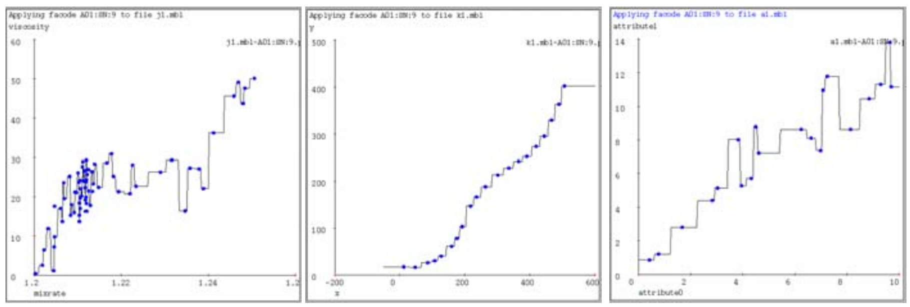
Here, joining the
clearly fitting noise.

noise fitting.

Why is fitting the noise so bad?

One-Nearest Neighbor

…One nearest neighbor for fitting is described shortly…



Similar to Join The Dots with two Pros and one Con.

- PRO: It is easy to implement with multivariate inputs.
- CON: It no longer interpolates locally.
- PRO: An excellent introduction to instance-based learning…

Univariate 1-Nearest Neighbor

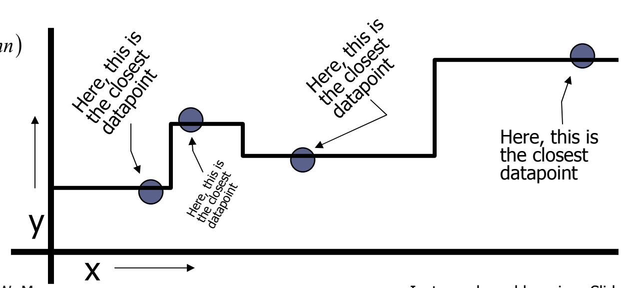
Given datapoints (x_1,y_1) (x_2,y_2)..(x_N,y_N),where we assume $y_i=f(s_i)$ for some unknown function f.
Given query point x_q, your job is to predict $\hat{y}=\hat{f}(x_q)$.
Nearest Neighbor:

1. Find the closest x_i in our set of datapoints

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

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

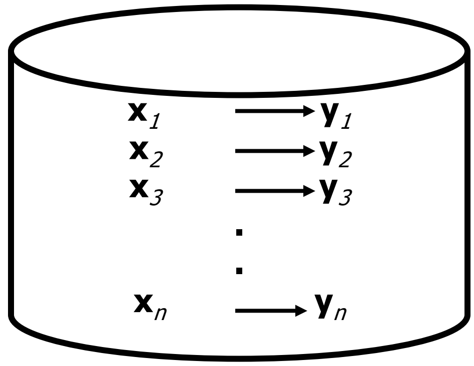
Here's a dataset with one input, one output and four datapoints.



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
- How many nearby neighbors to look at?
- A weighting function (optional)
- How to fit with the local points?

Nearest Neighbor

Four things make a memory based learner:

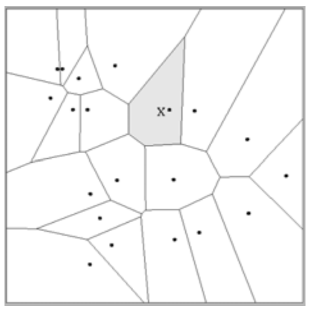
1. *A distance metric*
   Euclidian
2. *How many nearby neighbors to look at?*
   One
3. *A weighting function (optional)*
   Unused
4. *How to fit with the local points?*
   Just predict the same output as the nearest neighbor.

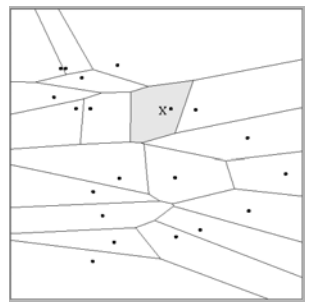
Multivariate Distance Metrics

Suppose the input vectors x1, x2, …xn are two dimensional:

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

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





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

The relative scalings in the distance metric affect region shapes.

Euclidean Distance Metric

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

Or equivalently,

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

where

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

Other Metrics…

- Mahalanobis, Rank-based, Correlation-based (Stanfill+Waltz, Maes' Ringo system…)

The Zen of Voronoi Diagrams

CNN Article

Mystery of renowned zen garden revealed

Thursday, September 26, 2002 Posted: 10:11 AM EDT (1411 GMT)

LONDON (Reuters) -- For centuries visitors to the renowned Ryoanji Temple garden in Kyoto, Japan have been entranced and mystified by the simple arrangement of rocks.

The five sparse clusters on a rectangle of raked gravel are said to be pleasing to the eyes of the hundreds of thousands of tourists who visit the garden each year.

Scientists in Japan said on Wednesday they now believe they have discovered its mysterious appeal.

"We have uncovered the implicit structure of the Ryoanji garden's visual ground and have shown that it includes an abstract, minimalist depiction of natural scenery," said Gert Van Tonder of Kyoto University.

The researchers discovered that the empty space of the garden evokes a hidden image of a branching tree that is sensed by the unconscious mind.

"We believe that the unconscious perception of this pattern contributes to the enigmatic appeal of the garden," Van Tonder added.

He and his colleagues believe that whoever created the garden during the Muromachi era between 1333-1573 knew exactly what they were doing and placed the rocks around the tree image.

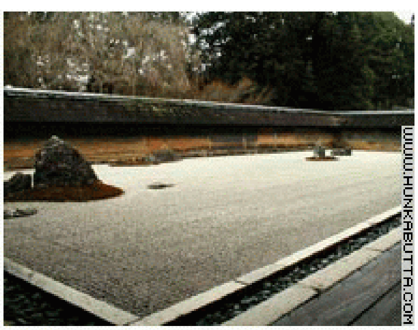
By using a concept called medial-axis transformation, the scientists showed that the hidden branched tree converges on the main area from which the garden is viewed.

The trunk leads to the prime viewing site in the ancient temple that once overlooked the garden.

It is thought that abstract art may have a similar impact.

"There is a growing realisation that scientific analysis can reveal unexpected structural features hidden in controversial abstract paintings," Van Tonder said

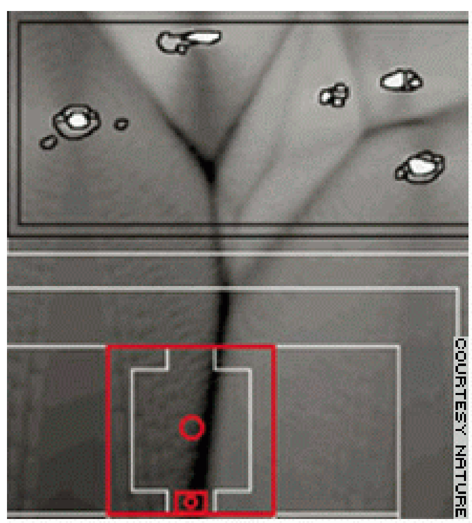
Zen Part Two



Ryoanji Temple garden in Kyoto

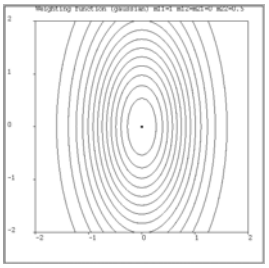
(Photos and article extracted from www.cnn.com)

Question: what set of five rocks placed at a distance would have *not* produced a tree-like voronoi diagram?



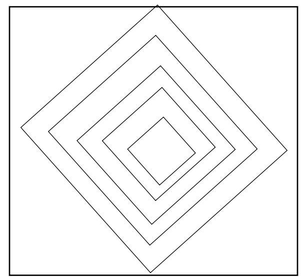
Layout shows the rock clusters (top) and the preferred viewing spot of the garden from the main hall (the circle in the middle of the square).

Notable Distance Metrics

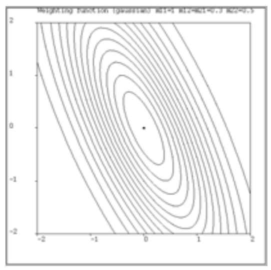


Scaled Euclidian (L_2)

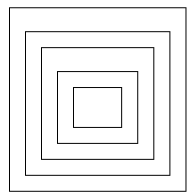
L_1 norm (absolute)



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

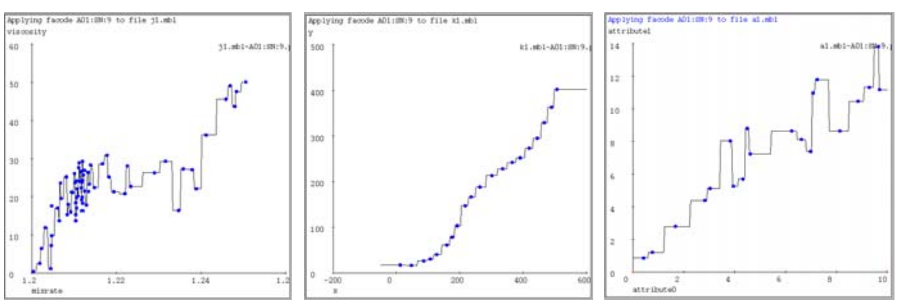


$L_{infinity}$ *(max) norm*



..let's leave distance metrics for now, and go back to….

One-Nearest Neighbor



Objection:

That noise-fitting is really objectionable.

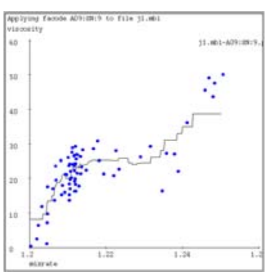
What's the most obvious way of dealing with it?

k-Nearest Neighbor

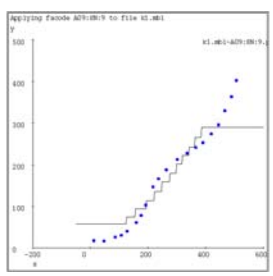
Four things make a memory based learner:

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

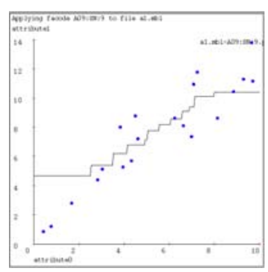
k-Nearest Neighbor (here k=9)



A magnificent job of noise-smoothing. Three cheers for 9-nearest-neighbor.
But the lack of gradients and the jerkiness isn't good.



Appalling behavior! Loses all the detail that join-the-dots and 1-nearest-neighbor gave us, yet smears the ends.



Fits much less of the noise, captures trends. But still, frankly, pathetic compared with linear regression.

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

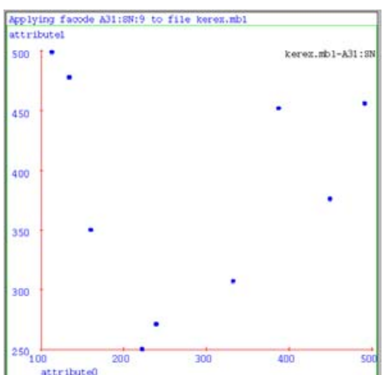
What can we do about all the discontinuities that k-NN gives us?

Kernel Regression

Four things make a memory based learner:

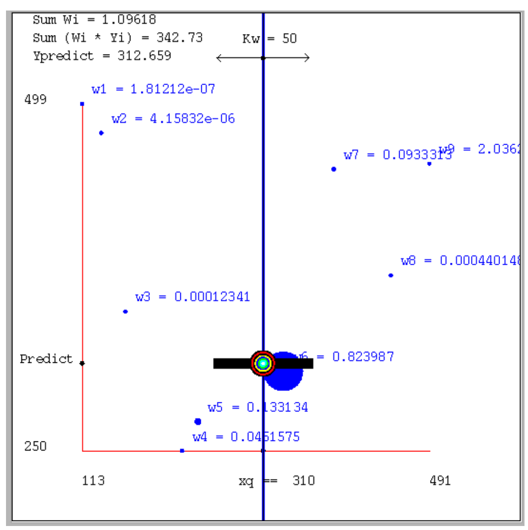
1. *A distance metric*
   Scaled Euclidian
2. *How many nearby neighbors to look at?*
   All of them
3. *A weighting function (optional)*
   $w_i = exp(-D(x_i, query)^2 / K_w^2)$
   Nearby points to the query are weighted strongly, far points weakly. The K_W parameter is the **Kernel Width**. Very important.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

Kernel Regression in Pictures

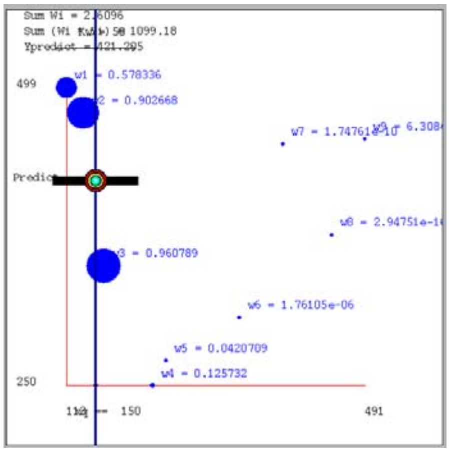


Take this dataset…

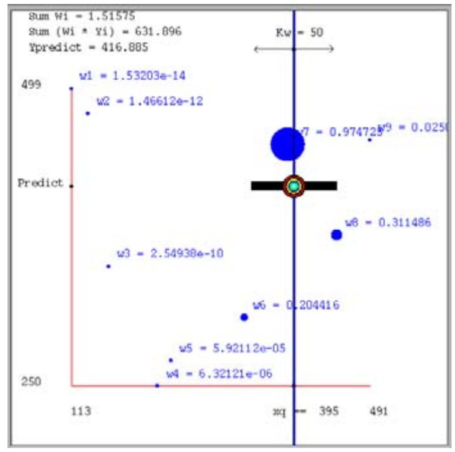
..and do a kernel prediction with x_q (query) = 310, K_w = 50.



Varying the Query

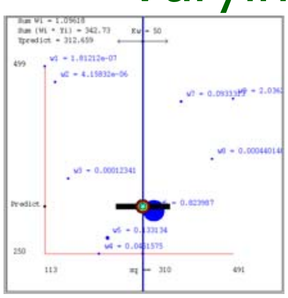


x_q = 150



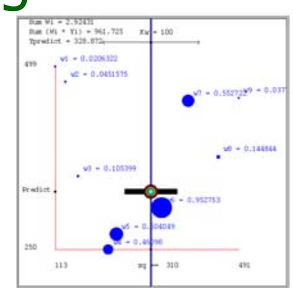
x_q = 395

Varying the kernel width



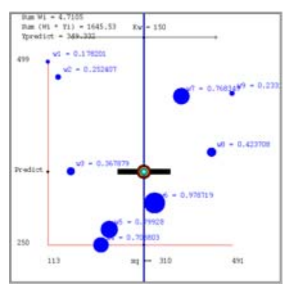
$x_q = 310$

K_W = 50 (see the double arrow at top of diagram)



$x_q = 310$ (the same)

K_W = 100



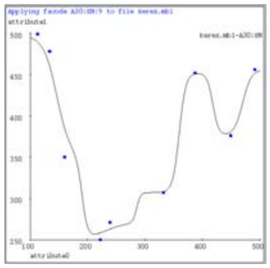
$x_q = 310$ (the same)

K_W = 150

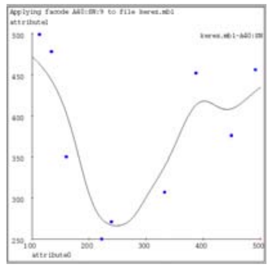
Increasing the kernel width K_w means further away points get an opportunity to influence you.

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

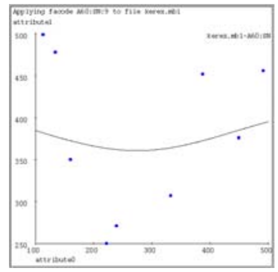
Kernel Regression Predictions



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

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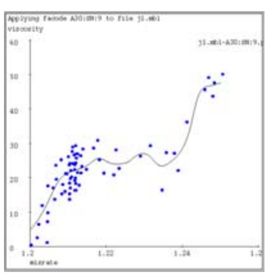
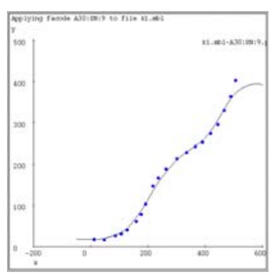
Kernel Regression on our test cases



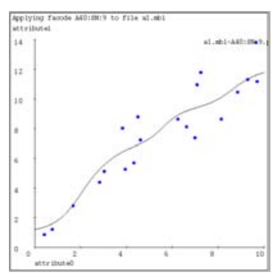
KW=1/32 of x-axis width.

It's nice to see a smooth curve at last. But rather bumpy. If Kw gets any higher, the fit is poor.



KW=1/32 of x-axis width.

Quite splendid. Well done, kernel regression. The author needed to choose the right K_W to achieve this.



KW=1/16 axis width.

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

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

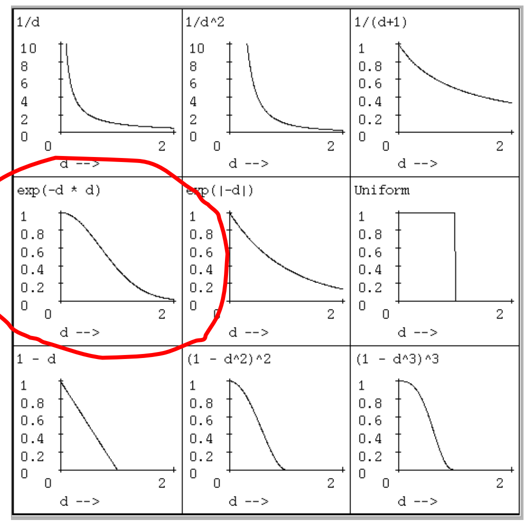
Weighting functions

Let

$d{=}D(x_i{,}x_{query})/K_W$

Then here are some commonly used weighting functions…

(we use a Gaussian)



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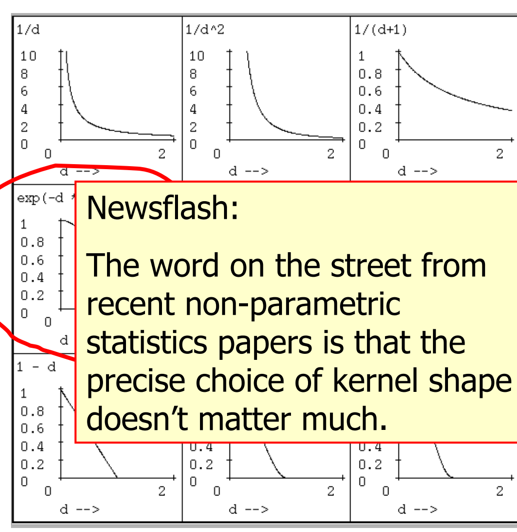
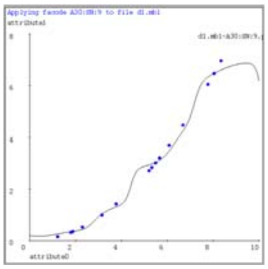


Newsflash:

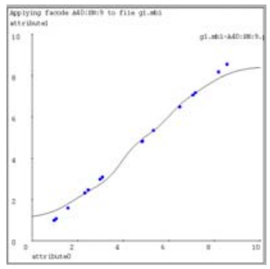
The word on the street from recent non-parametric statistics papers is that the precise choice of kernel shape doesn't matter much.

Kernel Regression can look bad



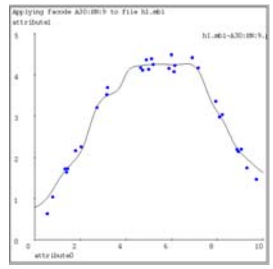
KW = Best.

Clearly not capturing the simple structure of the data.. Note the complete failure to extrapolate at edges.



KW = Best.

Also much too local. Why wouldn't increasing Kw help? Because then it would all be "smeared".



KW = Best.

Three noisy linear segments. But best kernel regression gives poor gradients.

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.

Let's Review Linear Regression….

Unweighted Linear Regression

You're lying asleep in bed. Then Nature wakes you.

YOU: "Oh. Hello, Nature!"

NATURE: "I have a coefficient β in mind. I took a bunch of real numbers called x_1, x_2 ..x_N thus: x_1=3.1,x_2=2, …x_N=4.5.

For each of them ($k=1,2,..N$), I generated $y_k = \beta x_k + \varepsilon_k$

where ε_k is a Gaussian (i.e. Normal) random variable with mean 0 and standard deviation σ. The ε_k's were generated independently of each other.

Here are the resulting y_i's: y_1=5.1 , y_2=4.2 , …y_N=10.2"

You: "Uh-huh."

Nature: "So what do you reckon β is then, eh?"

WHAT IS YOUR RESPONSE?

Global Linear Regression: $y_k=\beta x_k + \varepsilon_k$

$$\text{prob}(y_k \| x_k, \beta) \sim \text{Gaussian, mean } \beta x_k \text{, std. dev. } \sigma$$

$$\text{prob}(y_k \| x_k, \beta) = K \exp\left(\frac{-(y_k - \beta x_k)^2}{2\sigma^2}\right)$$

$$\text{prob}(y_1, y_2, \ldots y_N \| x_1, x_2, \ldots, x_N, \beta) = \prod_{k=1}^{N} K \exp\left(\frac{-(y_k - \beta x_k)^2}{2\sigma^2}\right)$$

Which value of β makes the y_1, y_2..y_N values most likely?

$$\hat{\beta} = \underset{\beta}{\arg\max}\ \text{prob}(y_1, y_2, \ldots y_N \| x_1, x_2, \ldots, x_N, \beta)$$

$$= \underset{\beta}{\arg\max}\ \log \text{prob}(y_1, y_2, \ldots y_N \| x_1, x_2, \ldots, x_N, \beta)$$

$$= \underset{\beta}{\arg\max}\ N \log K - \frac{1}{2\sigma^2} \sum_{k=1}^{N} (y_k - \beta x_k)^2$$

$$= \underset{\beta}{\arg\min} \sum_{k=1}^{N} (y_k - \beta x_k)^2$$

Least squares unweighted linear regression

Write $E(\beta)=\sum_k (y_k-\beta x_k)^2$, so $\hat{\beta}=\underset{\beta}{\arg\min}\, E(\beta)$

To minimize $E(\beta)$, set

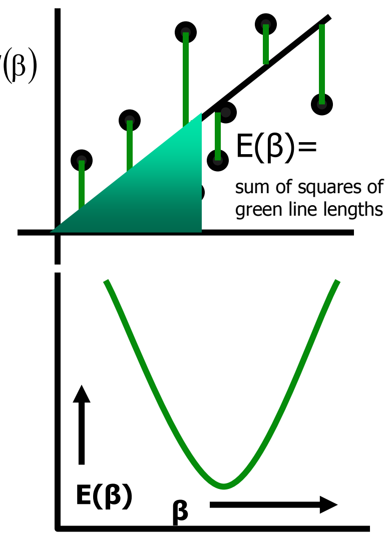
$$\frac{\partial}{\partial\beta}E(\beta)=0$$

so

$$0=\frac{\partial}{\partial\beta}E(\beta)=-2\sum_k x_k y_k+2\beta\sum_k x_k^2$$

giving

$$\hat{\beta}=\left(\sum_k x_k^2\right)^{-1}\sum_k x_k y_k$$



Multivariate unweighted linear regression

Nature supplies N input vectors. Each input vector x_k is D-dimensional: $\mathbf{x}_k = (x_{k1}, x_{k2} .. x_{kD})$. Nature also supplies N corresponding output values $y_1 .. y_N$.

$$X=\begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1D} \\ x_{21} & x_{22} & \cdots & x_{2D} \\ \vdots & \vdots & & \vdots \\ x_{N1} & x_{N2} & \cdots & x_{ND} \end{bmatrix} \quad Y=\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \quad \text{we are told } y_k=\left(\sum_{j=1}^{D}\beta_j x_{kj}\right)+\varepsilon_k$$

We must estimate $\beta = (\beta_1, \beta_2 \ldots \beta_D)$. It's easily shown using matrices instead of scalars on the previous slide that

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

Note that X^TX is a D x D positive definite symmetric matrix, and X^TY is a D x 1 vector:

$$\left(X^T X\right)_{ij}=\sum_{k=1}^{N}x_{ki}x_{kj} \qquad \left(X^T Y\right)_i=\sum_{k=1}^{N}x_{ki}y_i$$

The Pesky Constant Term

Now: Nature doesn't guarantee that the line/hyperplane passes through the origin.

In other words: Nature says

$$y_k = \beta_0 + \left(\sum_{j=1}^{D} \beta_j x_{kj} \right) + \varepsilon_k$$

"No problem," you reply. "Just add one extra input variable, x_{k0}, which is always 1"

$$\begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1D} \\ x_{21} & x_{22} & \cdots & x_{2D} \\ \vdots & \vdots & & \vdots \\ x_{N1} & x_{N2} & \cdots & x_{ND} \end{bmatrix} \rightarrow \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1D} \\ 1 & x_{21} & x_{22} & \cdots & x_{2D} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{N1} & x_{N2} & \cdots & x_{ND} \end{bmatrix}$$

Locally Weighted Regression

Four things make a memory-based learner:

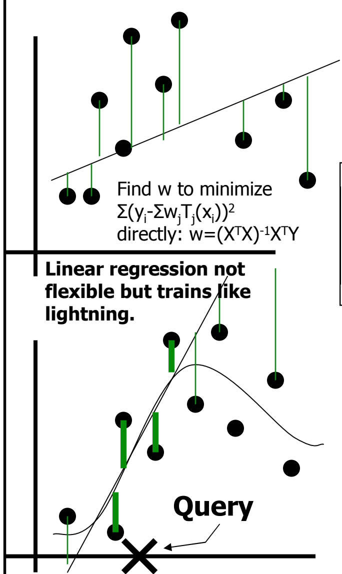
1. *A distance metric*
   Scaled Euclidian
2. *How many nearby neighbors to look at?*
   All of them
3. *A weighting function (optional)*
   $w_k = \exp(-D(x_k, x_{query})^2 / K_w^2)$

   Nearby points to the query are weighted strongly, far points weakly. The K_w parameter is the **Kernel Width**.
4. *How to fit with the local points?*
   First form a local linear model. Find the $\underline{\beta}$ that minimizes the locally weighted sum of squared residuals:

$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}} \sum_{k=1}^{N} w_k^{\,2} \left(y_k - \beta^T x_k \right)^2$$

Then predict $y_{predict} = \underline{\beta}^T x_{query}$

How LWR works



Locally weighted regression is very flexible and fast to train.

1. For each point $(\mathbf{x}_k, y_k)$ compute w_k.
2. Let $WX = Diag(w_1,..w_N)X$

$$\begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1D} \\ x_{21} & x_{22} & \cdots & x_{2D} \\ \vdots & \vdots & & \vdots \\ x_{N1} & x_{N2} & \cdots & x_{ND} \end{bmatrix} \rightarrow \begin{bmatrix} w_1 & w_1 x_{11} & w_1 x_{12} & \cdots & w_1 x_{1D} \\ w_2 & w_2 x_{21} & w_2 x_{22} & \cdots & w_2 x_{2D} \\ \vdots & \vdots & \vdots & & \vdots \\ w_N & w_N x_{N1} & w_N x_{N2} & \cdots & w_N x_{ND} \end{bmatrix}$$

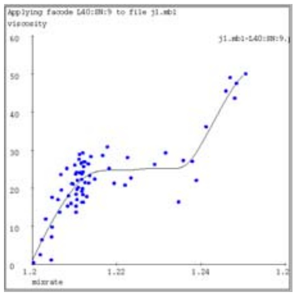
X **- - >** *WX*

3. Let $WY=Diag(w_1,..w_N)Y$, so that $y_k \rightarrow w_k y_k$
4. $\beta = (WX^T WX)^{-1}(WX^T WY)$

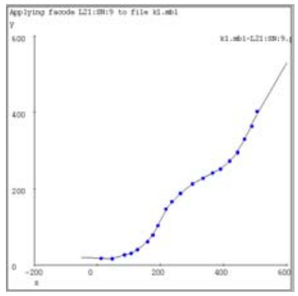

```
Input X matrix of inputs: X[k] [i] = i'th component of k'th input point.
Input Y matrix of outputs: Y[k] = k'th output value.
Input xq = query input.  Input kwidth.

WXTWX = empty (D+1) x (D+1) matrix
WXTWY = empty (D+1) x 1        matrix

for ( k = 1 ; k <= N ; k = k + 1 )
    /* Compute weight of kth point  */
    wk = weight_function( distance( xq , X[k] ) / kwidth )

    /* Add to (WX) ^T (WX) matrix */
     for ( i = 0 ; i <= D ; i = i + 1 )
           for ( j = 0 ; j <= D ; j = j + 1 )
                      if ( i == 0 ) xki = 1 else xki = X[k] [i]
                      if ( j == 0 ) xkj = 1 else xkj = X[k] [j]
                      WXTWX [i] [j] = WXTWX [i] [j] + wk * wk * xki * xkj

    /*  Add to (WX) ^T (WY) vector */
    for ( i = 0 ; i <= D ; i = i + 1 )
            if ( i == 0 ) xki = 1 else xki = X[k] [i]
            WXTWY [i] = WXTWY [i] + wk * wk * xki * Y[k]

/* Compute the local beta.  Call your favorite linear equation solver.  Recommend Cholesky
     Decomposition for speed.  Recommend Singular Val Decomp for Robustness. */
beta = (WXTWX)^-1 (WXTWY)
ypredict = beta[0] + beta[1]*xq[1] + beta[2]*xq[2] + … beta[D]*xq[D]
```

Software and data for the algorithms in this tutorial: http://www.cs.cmu.edu/~awm/vizier . The example figures in this slide-set were created with the same software and data.

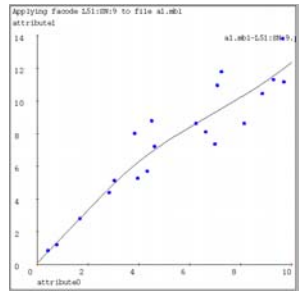
LWR on our test cases



KW = 1/16 of x-axis width.



KW = 1/32 of x-axis width.



KW = 1/8 of x-axis width.

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

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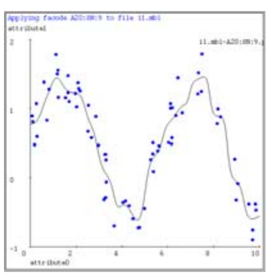
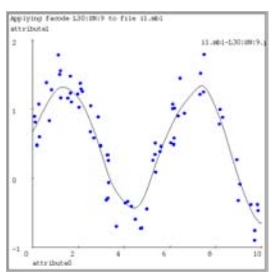
Locally weighted Polynomial regression



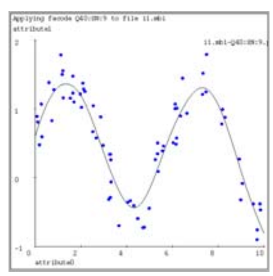
Kernel Regression
Kernel width K_W at optimal level.

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.

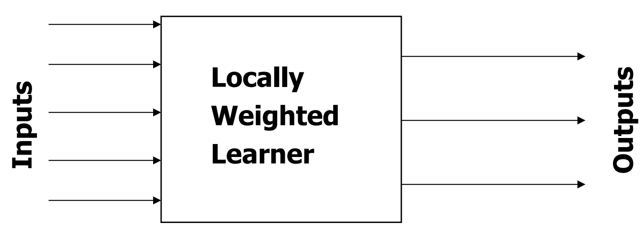
When's Quadratic better than Linear?

- It can let you use a wider kernel without introducing bias.
- Sometimes you want more than a prediction, you want an estimate of the local Hessian. Then quadratic is your friend!
- But in higher dimensions is appallingly expensive, and needs a lot of data. (Why?)
- Two "Part-way-between-linear-and-quadratic" polynomials:
  - "Ellipses": Add x_i^2 terms to the model, but not cross-terms (no $x_i x_j$ where $i=j$)
  - "Circles": Add only one extra term to the model:

$$x_{D+1} = \sum_{j=1}^{D} x_j^2$$

- Incremental insertion of polynomial terms is well established in conventional regression (GMDH,AIM): potentially useful here too

Multivariate Locally weighted learning



All the methods described so far can generalize to multivariate input and output. But new questions arise:

- What are good scalings for a Euclidean distance metric?
- What is a better Euclidean distance metric?
- Are all features relevant?
- Do some features have a global rather than local influence?

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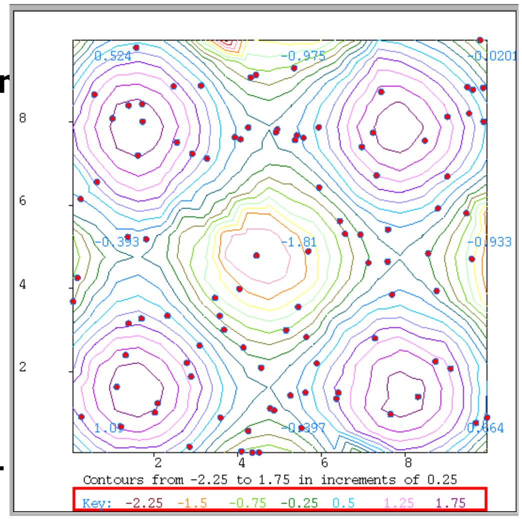
A Bivariate Fit Example

LWQ Regression

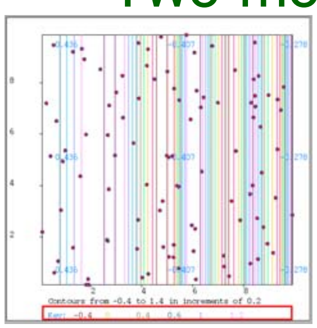
Let's graph the prediction surface given 100 noisy datapoints: each with 2 inputs, one output

Kernel Width, Number of fully weighted Neighbors, Distance Metric Scales all optimized.
Kw = 1/16 axis width
4 nearest neighs full weight
Distance metric scales each axis equally.

f(x,y) = sin(x) + sin(y) + noise



Two more bivariate fits



Kernel Regression.

KW, num neighs, metric scales all optimized.

KW=1/100 x-axis width. 1-NN fully weighted. y not included in distance metric.

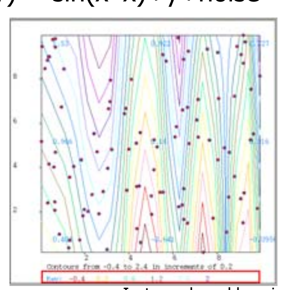
f(x,y) = sin(x*x)

Locally weighted linear regression.

KW, num neighs, metric scales all optimized.

KW=1/50 x-axis width. No neighbors fully weighted. y not included in distance metric, but is included in the regression.

f(x,y) = sin(x*x)+y+noise



Fabricated Example

f(x1,x2,x3,x4,x5,x6,x7,x8,x9) = noise + x2 + x4 + 4sin(0.3x6 + 0.3x8).

(Here we see the result of searching for the best metric, feature set, kernel width, polynomial type for a set of 300 examples generated from the above function)

Recommendation.

Based on the search results so far, the recommended function approximator encoding is L20:SN:-0-0-9-9. Let me explain the meaning:

Locally weighted regression. The following features define the distance metric:

x6 (full strength).
x8 (full strength).

A gaussian weighting function is used with kernel width 0.0441942 in scaled input space. We do a weighted least squares with the following terms:

Term 0 = 1
Term 1 = x2/10
Term 2 = x4/10
Term 3 = x6/10
Term 4 = x8/10

Locally Weighted Learning: Variants

- Range Searching: Average of all neighbors within a given range
- Range-based linear regression: Linear regression on all points within a given range
- Linear Regression on K-nearest-neighbors
- Weighting functions that decay to zero at the kth nearest neighbor
- Locally weighted Iteratively Reweighted Least Squares
- Locally weighted Logistic Regression
- Locally weighted classifiers

- Multilinear Interpolation
- Kuhn-Triangulation-based Interpolation
- Spline Smoothers

Using Locally Weighted Learning for Modeling

- "Hands-off" non-parametric relation finding
- Low Dimensional Supervised Learning
- Complex Function of a subset of inputs
- Simple function of most inputs but complex function of a few
- Complex function of a few features of many input variables

Use (1): "Hands-off" non-parametric relation finding.

You run an HMO (or a steel tempering process) (or a 7-dof dynamic robot arm)

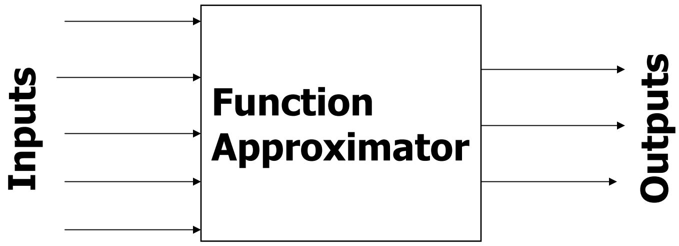
You want an intelligent assistant to spot patterns and regularities among pairs or triplets of variables in your database…

HMO variables:	Steel Variables:	Robot Variables:
Physician Age	Line Speed	Roll
Patient Age	Line Spd -10mins	DRoll
Charge/Day	Line Spd -20mins	DDRoll
Charge/Discharge	Slab width	Pitch
Discharges/100	Slab height	DPitch
ICD-9 Diagnosis	Slab Temp Stg1	DDPitch
Market Share	Slab Temp Stg2	SonarHeight
Mortality/100	CoolTunn2 Setp	LaserHeight
Patient ZIP	CoolTunn5 Sep	FlightTime
Zip Median Age	CoolTunn2 Temp	ThrustRate
….	….	….

You especially want to find more than just the linear correlations….

Use (2): Low Dimensional Supervised Learning

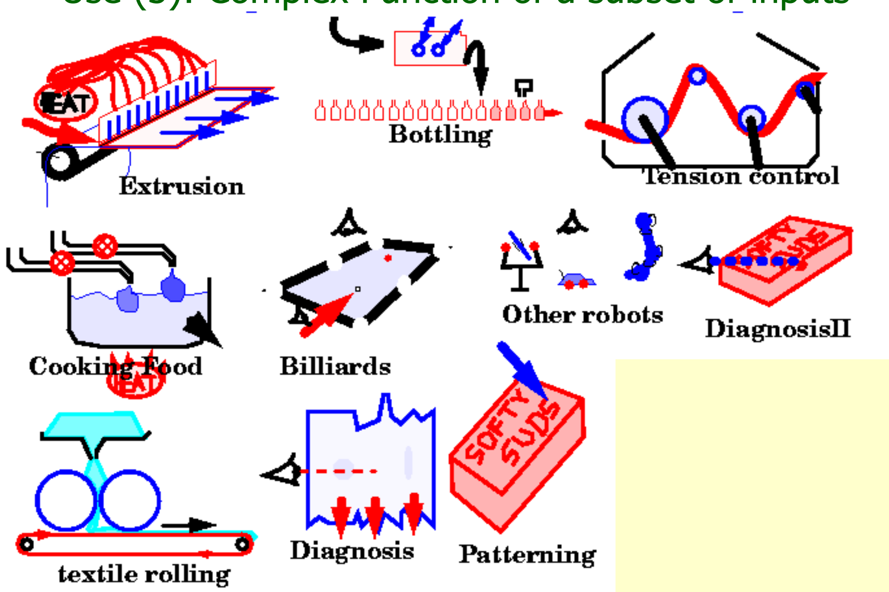
You have lots of data, not many input variables (less than 7, say) and you expect a very complex non-linear function of the data.



Examples:

- Skin Thickness vs τ,φ for face scanner
- Topographical Map
- Tumor density vs (x,y,z)
- Mean wasted Aspirin vs (fill-target, mean-weight, weight-sdev, rate) for an aspirin-bottle filler
- Object-ball collision-point vs (x,y,θ) in Pool

Use (3): Complex Function of a subset of inputs



Use (4): Simple function of most inputs but complex function of a few.

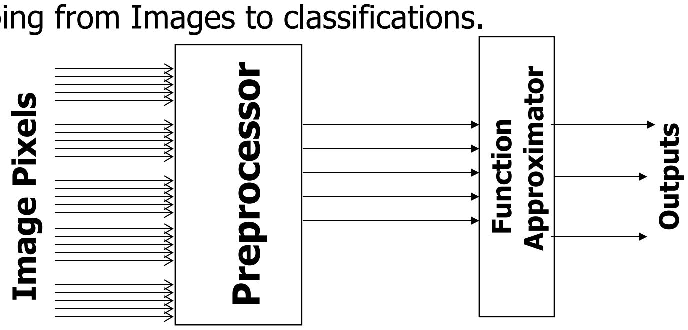
Examples:

- $f(x) = x_1 + 3x_2 - x_4 + sin(log(x_5)*x_6) - x_7^2 + x_8 - x_9 + 8x_{10}$
- Car Engine Emissions
- Food Cooling Tunnel

Use (5): Complex function of a few features of many input variables.

Examples:

- Mapping from acoustic signals to "Probability of Machine Breakdown".
- Time series data analysis.
- Mapping from Images to classifications.



- (e.g. Product inspection, Medical imagery, Thin Film imaging..)

Local Weighted Learning: Pros & Cons vs Neural Nets

Local weighted learning has some advantages:

- Can fit low dimensional, very complex, functions very accurately. Neural nets require considerable tweaking to do this.
- You can get meaningful confidence intervals, local gradients back, not merely a prediction.
- Training, adding new data, is almost free.
- "One-shot" learning---not incremental
- Variable resolution.
- Doesn't forget old training data unless statistics warrant.
- Cross-validation is cheap

Neural Nets have some advantages:

- With large datasets, MBL predictions are slow (although kdtree approximations, and newer cache approximations help a lot).
- Neural nets can be trained directly on problems with hundreds or thousands of inputs (e.g. from images). MBL would need someone to define a smaller set of image features instead.
- Nets learn incrementally.

What we have covered

- Problems of bias for unweighted regression, and noise-fitting for "join the dots" methods
- Nearest Neighbor and k-nearest neighbor
- Distance Metrics
- Kernel Regression
- Weighting functions
- Stable kernel regression
- Review of unweighted linear regression
- Locally weighted regression: concept and implementation
- Multivariate Issues
- Other Locally Weighted variants
- Where to use locally weighted learning for modeling?
- Locally weighted pros and cons

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