# Instance-based Learning

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

## Part II: Regression

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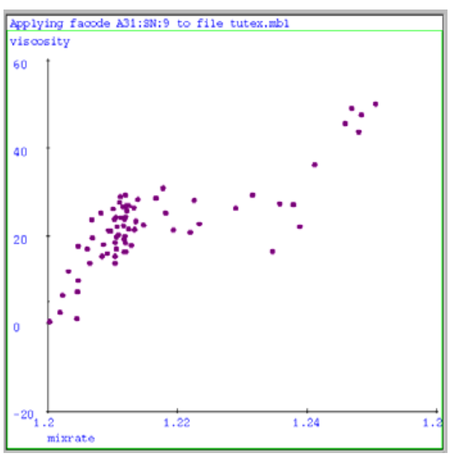
**CSG220**

**Spring 2007**

Adapted from parts of two Andrew Moore tutorials:
*Instance-Based Learning*
and
*Eight More Classic Machine Learning Algorithms*



# Starting Point




Simple, uni-variate case

***We've obtained some numeric data.***

***How do we exploit it?***

General, multi variate case

| 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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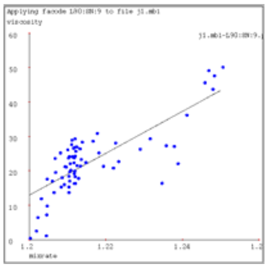
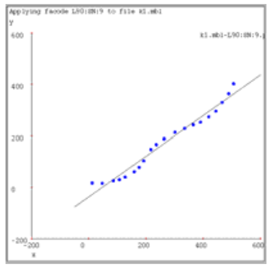
| . | . | . | . | . | . |

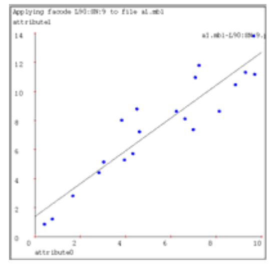
# Why not just use Linear Regression?



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.

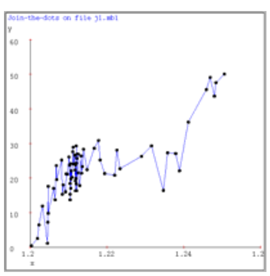


Here, linear regression may indeed be the right thing.

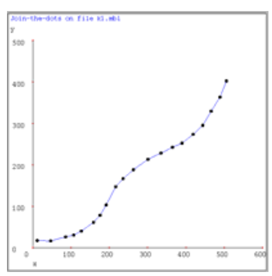
**Bias:** the underlying choice of model *(in this case, a line)* cannot, with any choice of parameters *(constant term and slope)* and with any amount of data *(the dots)* capture the full relationship.



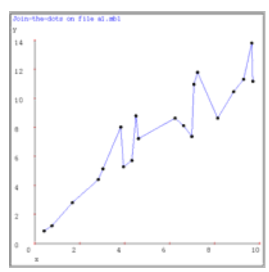
# Why not just Join the Dots?



Here, joining the dots is clearly fitting noise.



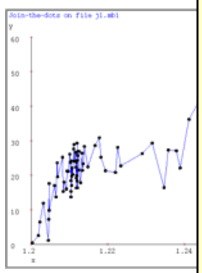
Here, joining the dots looks very sensible.



Again, a clear case of noise fitting.

Why is fitting the noise so bad?

# Why n



- 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.

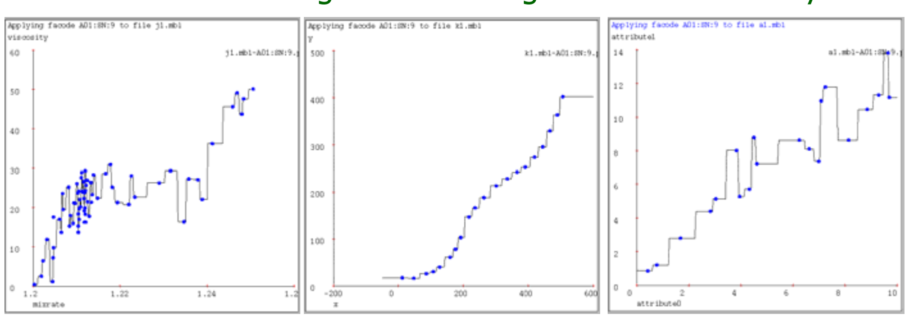
Here, joining the clearly fitting noise. l nsible. noise fitting.

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 $\hat{y}=\hat{f}(x_q)$.

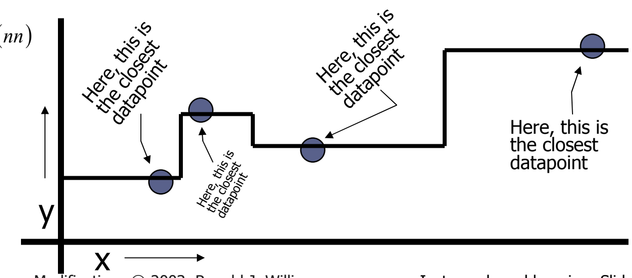
Nearest Neighbor:

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.



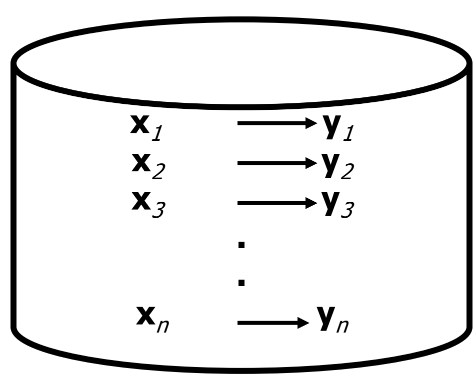




## *1-Nearest Neighbor is an example of….*
## **Instance-based learning**

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.**

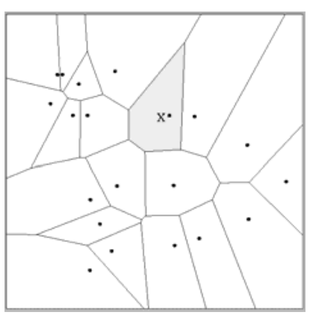
 

# Multivariate Distance Metrics

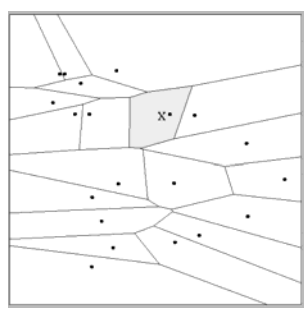
Suppose the input vectors x1, x2, …xn are two dimensional:

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

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




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




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

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

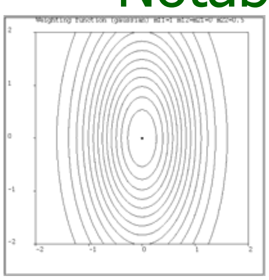
$$\sum = \begin{bmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & \sigma_N^2 \end{bmatrix}$$

Other Metrics…

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

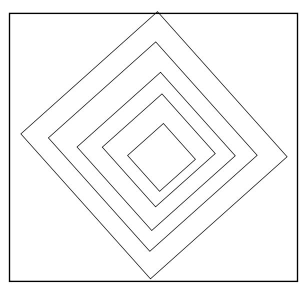


# Notable Distance Metrics

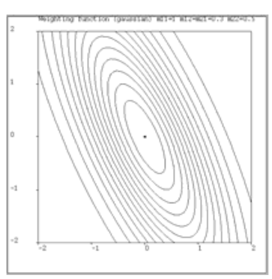


**Scaled Euclidian ($L_2$)**

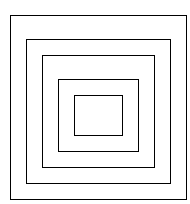
**$L_1$ norm (absolute)**



**Mahalanobis (here, $\Sigma$ on the previous slide is not necessarily diagonal, but is symmetric**

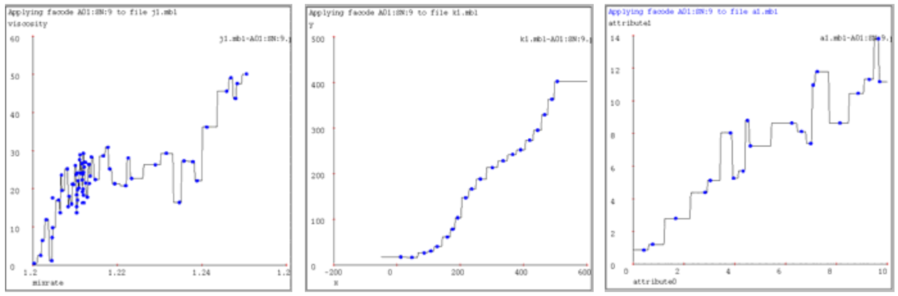


**$L_{infinity}$ *(max)* norm**



..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?

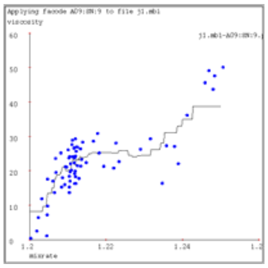



## k-Nearest Neighbor

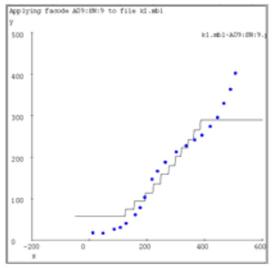
**Four things make a memory based learner:**

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.**

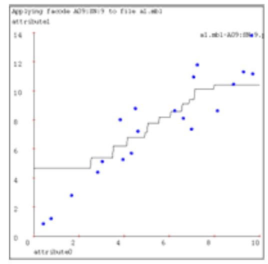
# k-Nearest Neighbor (here k=9)



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?

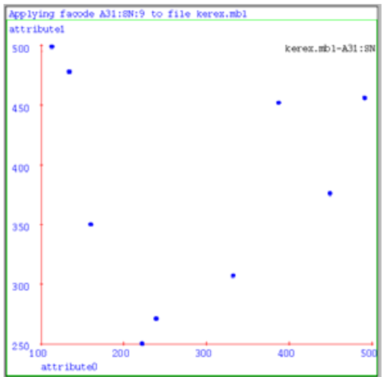



# Kernel Regression

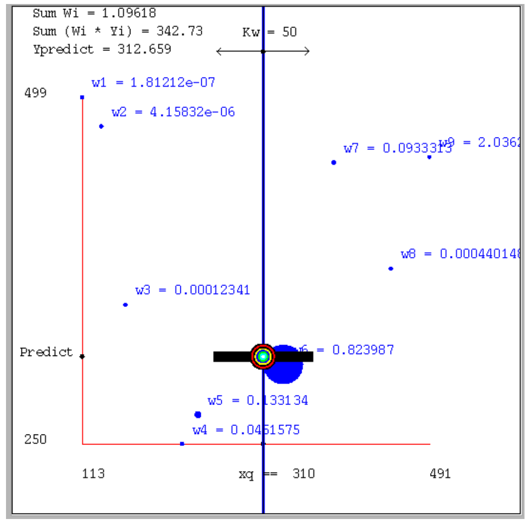
**Four things make a memory based learner:**

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



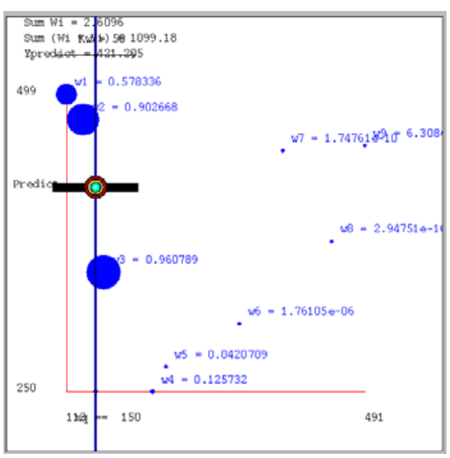
Take this dataset…

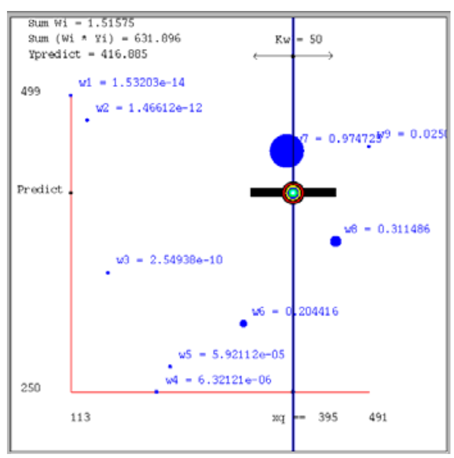



..and do a kernel prediction with $x_q$ (query) = 310, $K_w$ = 50.



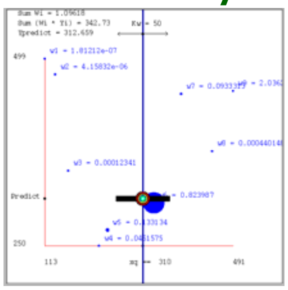
# Varying the Query



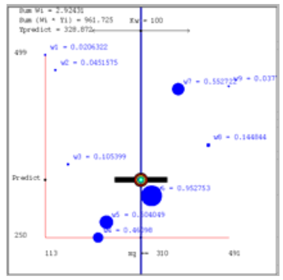

$x_q$ = 150    $x_q$ = 395

# Varying the kernel width



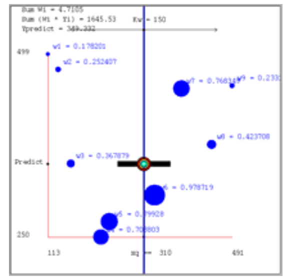
$x_q = 310$

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



$x_q = 310$ (the same)

$K_W = 100$



$x_q = 310$ (the same)

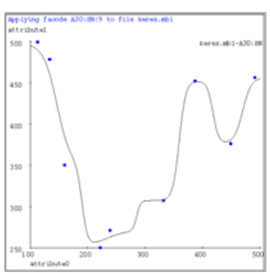
$K_W = 150$

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

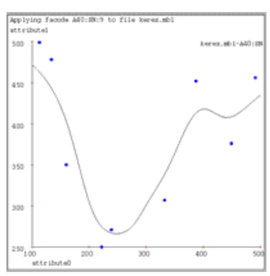
As $K_w \rightarrow$ infinity, the prediction tends to the global average.

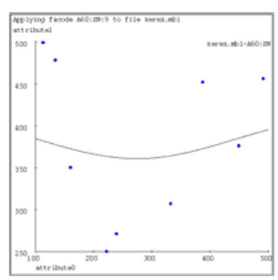
# Kernel Regression Predictions



$K_W$=10



$K_W$=20



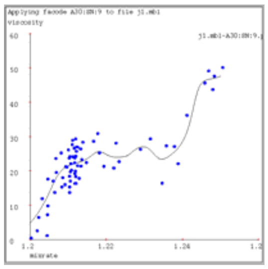
$K_W$=80

**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.

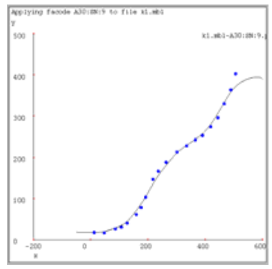
 

# Kernel Regression on our test cases



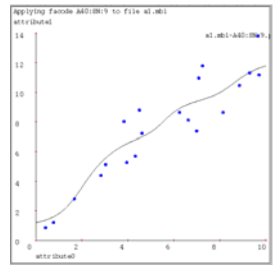
KW=1/32 of x-axis width.

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.



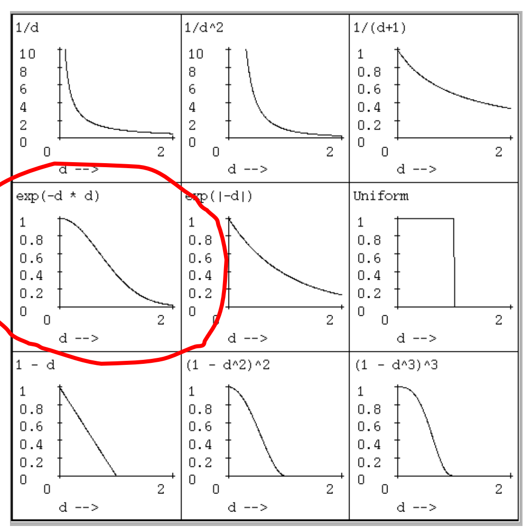
# Weighting functions

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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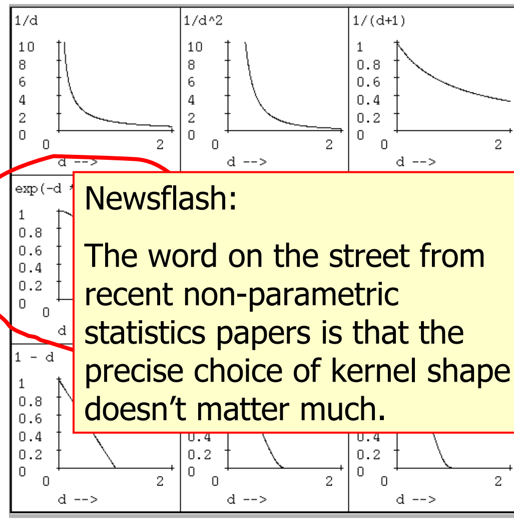
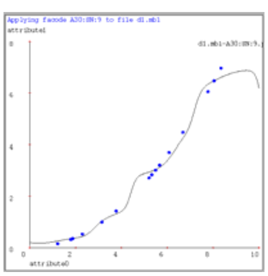



Newsflash:

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

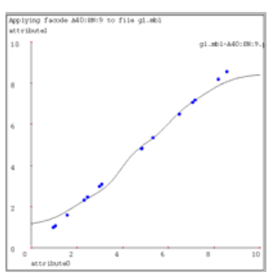



# Kernel Regression can look bad



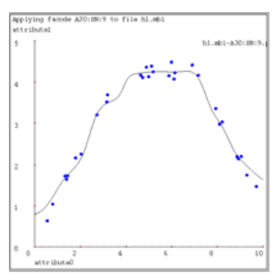
KW = Best.

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 $\varepsilon_k$ is a Gaussian (i.e. Normal) random variable with mean 0 and standard deviation σ. The $\varepsilon_k$'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

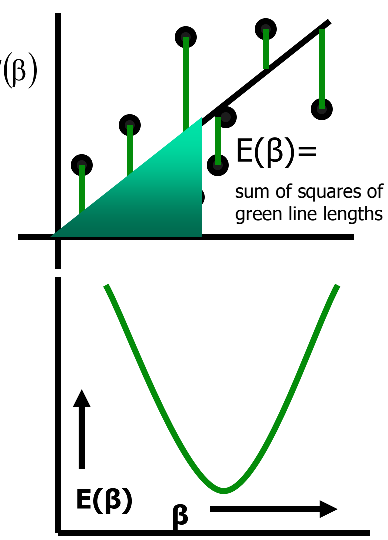
$$\frac{\partial}{\partial \beta} E(\beta) = 0$$

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 β = ($\beta_1$, $\beta_2$ … $\beta_D$). 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 $X^T X$ is a D x D positive definite symmetric matrix, and $X^T Y$ 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?*

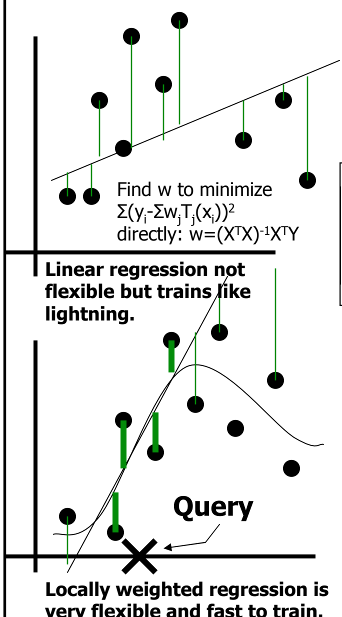
   First form a local linear model. Find the $\underline{\beta}$ that minimizes the locally weighted sum of squared residuals:

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

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



## How LWR works




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

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

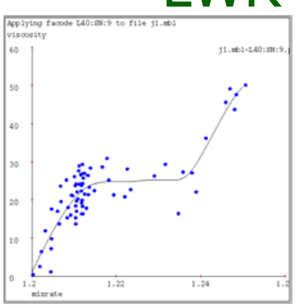
*X* **- - >** *WX*

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

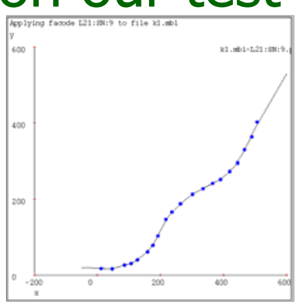
```
Input X matrix of inputs: X[k] [i] = i'th component of k'th input point.
Input Y matrix of outputs: Y[k] = k'th output value.
Input xq = query input.  Input kwidth.

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]
```

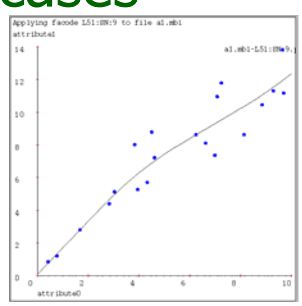
# LWR on our test cases



KW = 1/16 of x-axis width.



KW = 1/32 of x-axis width.

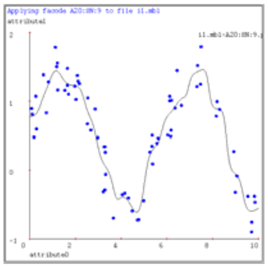


KW = 1/8 of x-axis width.

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

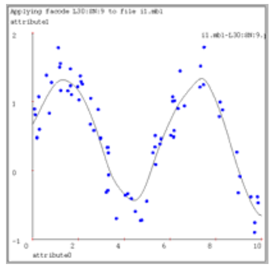
 

# Locally weighted Polynomial regression



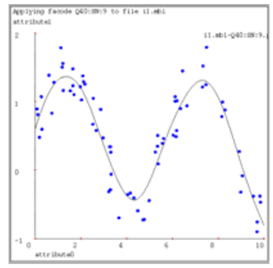
Kernel Regression
Kernel width $K_W$ at optimal level.

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

# 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

# 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.

# Radial Basis Functions (RBFs)

| $X_1$ | $X_2$ | $Y$ |
|---|---|---|
| 3 | 2 | 7 |
| 1 | 1 | 3 |
| : | : | : |

**X**=

| | |
|---|---|
| 3 | 2 |
| 1 | 1 |
| : | : |

**y**=

| |
|---|
| 7 |
| 3 |
| : |

Not necessarily instance-based, but can be.

Clearly related in any case.

**Z**=

| | | | | | |
|---|---|---|---|---|---|
| … | … | … | … | … | … |
| … | … | … | … | … | … |
| … | … | … | … | … | … |

**y**=

| |
|---|
| 7 |
| 3 |
| : |

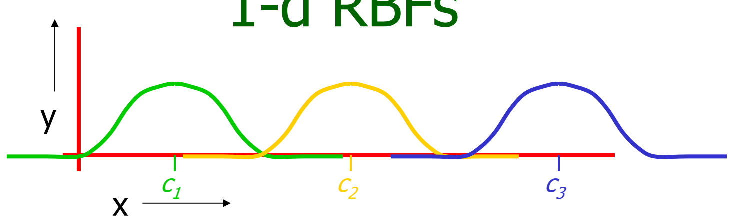
***z***=*(list of radial basis function evaluations)*

$\beta=(\mathbf{Z}^T\mathbf{Z})^{-1}(\mathbf{Z}^T\mathbf{y})$

$y^{est} = \beta_0 + \beta_1 x_1 + \ldots$



# 1-d RBFs

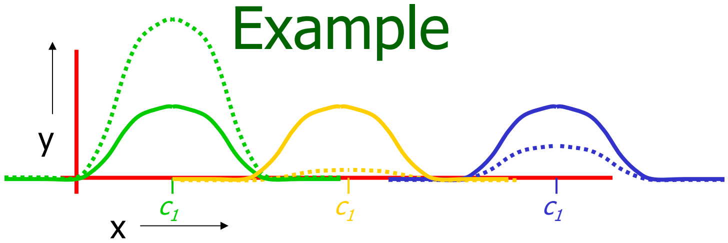



$y^{est} = \beta_1 \phi_1(x) + \beta_2 \phi_2(x) + \beta_3 \phi_3(x)$

where

$\phi_i(x) = KernelFunction( | x - c_i | / KW)$

# Example



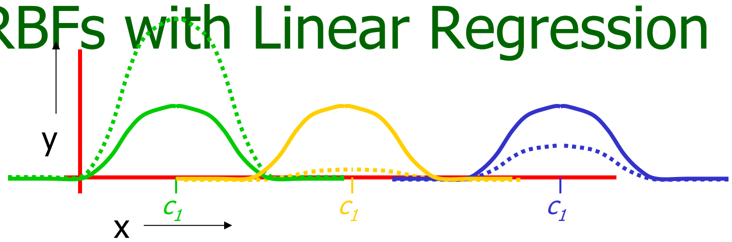

$y^{est} = 2\phi_1(x) + 0.05\phi_2(x) + 0.5\phi_3(x)$

where

$\phi_i(x) = KernelFunction(\,|\,x - c_i\,|\,/\,KW)$




# RBFs with Linear Regression




$y^{est} = 2\phi_1(x) + 0.05\phi_2(x) + 0.5\phi_3(x)$

where

$\phi_i(x) = KernelFunction(\,|\,x - c_i\,|\,/\,KW)$

# RBFs with Linear Regression

All $c_i$'s are held constant (initialized randomly or on a grid in m-dimensional input space)

*KW* also held constant (initialized to be large enough that there's decent overlap between basis functions*

*Usually much better than the crappy overlap on my diagram

$y^{est} = 2\phi_1(x) + 0.05\phi_2(x$ … $5\phi_3(x)$

where

$\phi_i(x) = KernelFunction(\,|\,x - c_i\,|\,/\,KW)$

then given $Q$ basis functions, define the matrix $Z$ such that $Z_{kj} = KernelFunction(\,|\,x_k - c_i\,|\,/\,KW)$ where $x_k$ is the kth vector of inputs

And as before, $\beta = (\mathbf{Z}^T\mathbf{Z})^{-1}(\mathbf{Z}^T\mathbf{y})$



# RBFs with NonLinear Regression

Allow the $c_i$'s to adapt to the data (initialized randomly or on a grid in m-dimensional input space)

*KW* allowed to adapt to the data. (Some folks even let each basis function have its own $KW_j$, permitting fine detail in dense regions of input space)

$y^{est} = 2\phi_1(x) + 0.05\phi_2(x$ … $5\phi_3(x)$

where

$\phi_i(x) = KernelFunction(\,|\,x - c_i\,|\,/\,KW)$

But how do we now find all the $\beta_j$'s, $c_i$'s and *KW*?

## RBFs with NonLinear Regression

Allow the $c_i$'s to adapt to the data (initialized randomly or on a grid in m-dimensional input space)

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$y^{est} = 2\phi_1(x) + 0.05\phi_2(x) \ldots 5\phi_3(x)$

where

$\phi_i(x) = KernelFunction(\,|\,x - c_i\,|\,/\,KW)$

But how do we now find all the $\beta_j$'s, $c_i$'s and $KW$?

Answer: Gradient Descent




## RBFs with NonLinear Regression

Allow the $c_i$'s to adapt to the data (initialized randomly or on a grid in m-dimensional input space)

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$y^{est} = 2\phi_1(x) + 0.05\phi_2(x) \ldots 5\phi_3(x)$

where

$\phi_i(x) = KernelFunction(\,|\,x - c_i\,|\,/\,KW)$

But how do we now find all the $\beta_j$'s, $c_i$'s and $KW$?

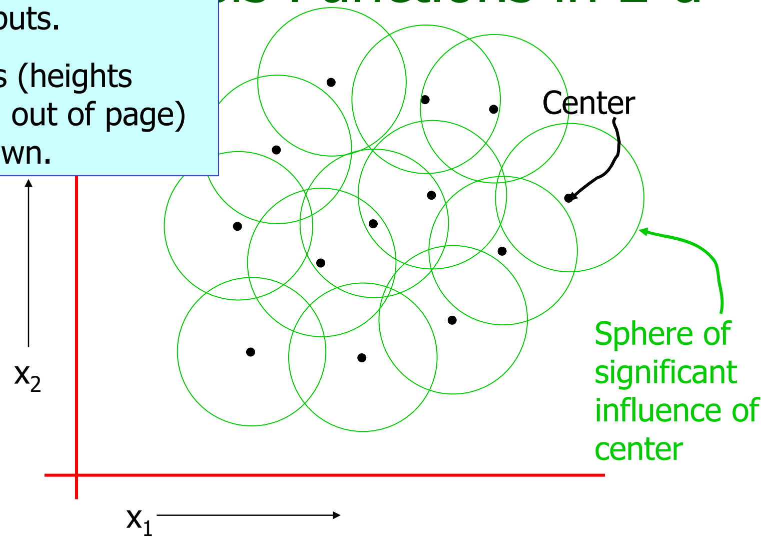
(But I'd like to see, or hope someone's already done, a hybrid, where the $c_i$'s and *KW* are updated with gradient descent while the $\beta_j$'s use matrix inversion)

Answer: Gradient Descent

# Radial Basis Functions in 2-d

Two inputs.

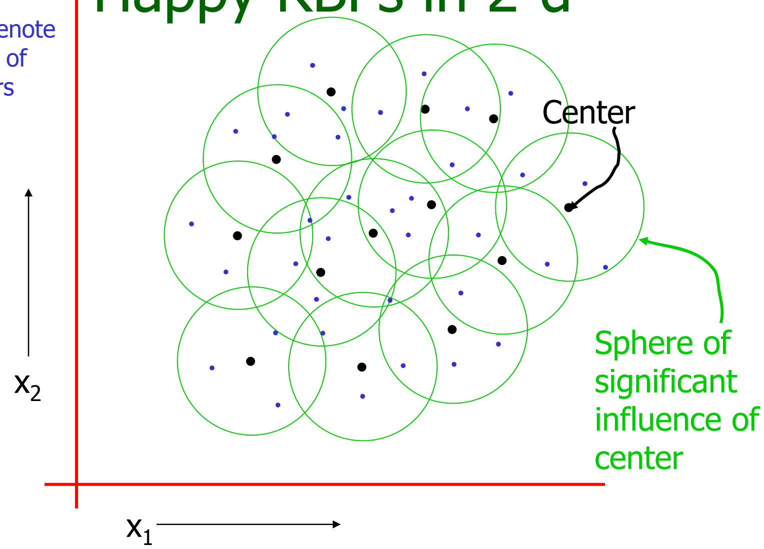
Outputs (heights sticking out of page) not shown.






# Happy RBFs in 2-d

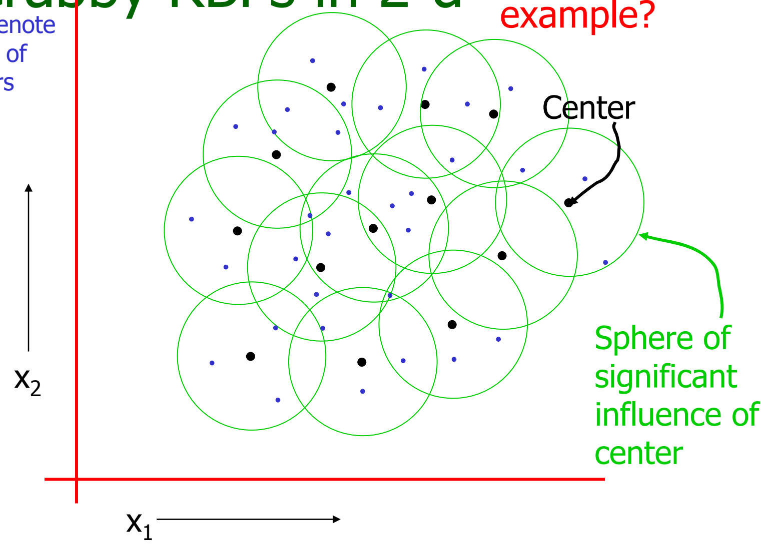
Blue dots denote coordinates of input vectors



What's the problem in this example?

# Crabby RBFs in 2-d

Blue dots denote coordinates of input vectors



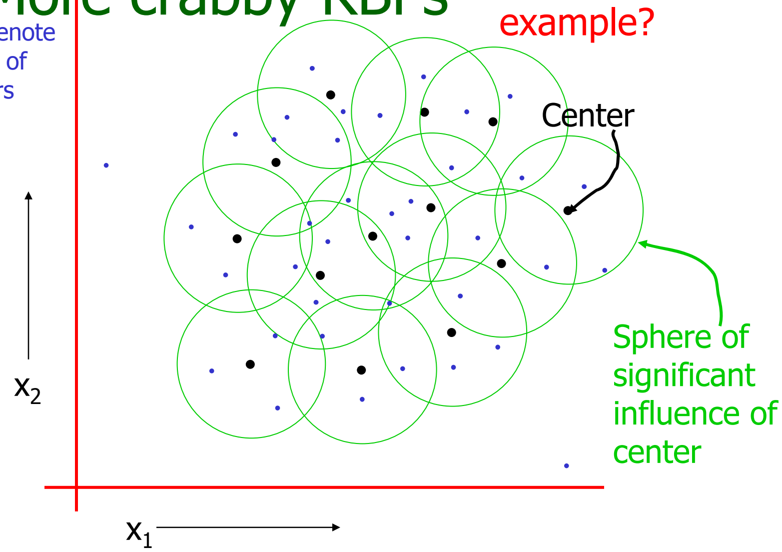


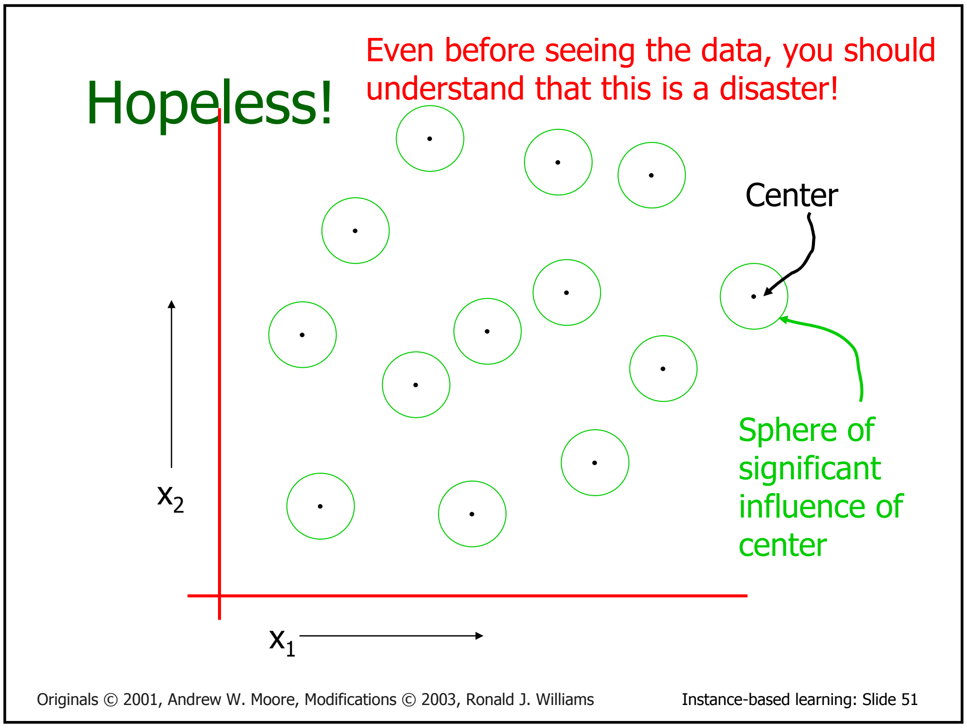


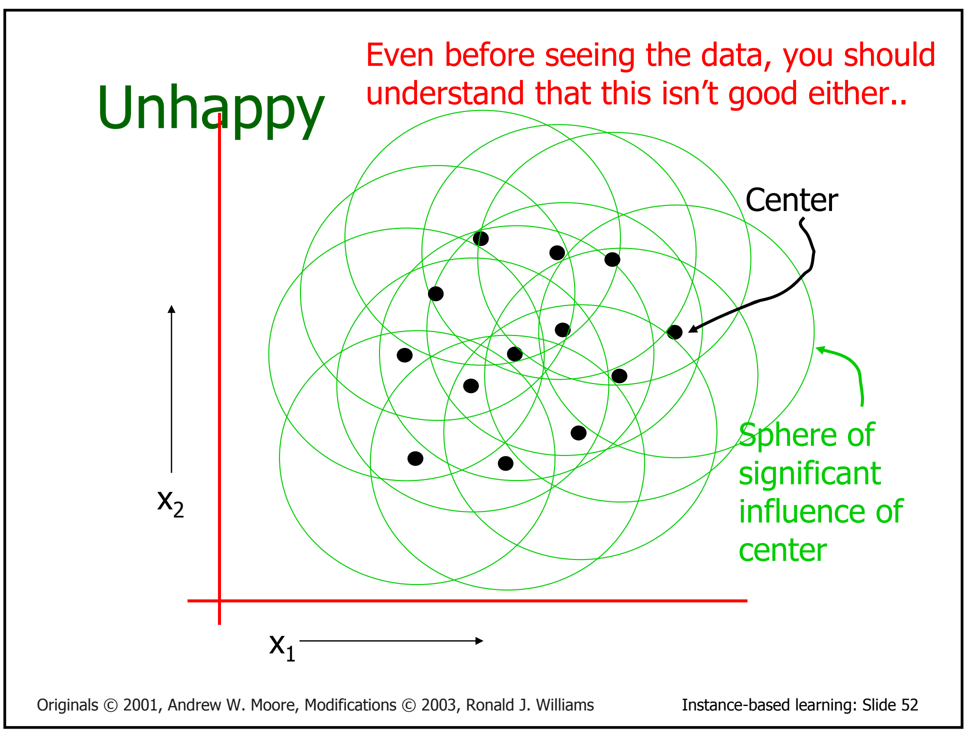

And what's the problem in this example?

# More crabby RBFs

Blue dots denote coordinates of input vectors




Hopeless!
Even before seeing the data, you should understand that this is a disaster!
Center
Sphere of significant influence of center
x2
x1
Originals © 2001, Andrew W. Moore, Modifications © 2003, Ronald J. Williams
Instance-based learning: Slide 51


Unhappy
Even before seeing the data, you should understand that this isn't good either..
Center
Sphere of significant influence of center
x2
x1
Originals © 2001, Andrew W. Moore, Modifications © 2003, Ronald J. Williams
Instance-based learning: Slide 52

## Instance-Based?

- Centers can be chosen to lie at data points
  - In that case almost like Kernel Regression, except no weight normalization
  - Sometimes choose centers to be a subset of the data points
- True instance-based considered *lazy method*
  - RBF is actually an *eager* method like
    - Decision Trees
    - Neural Nets
    - etc.



## What we have covered

- Problems of bias for unweighted regression, and noise-fitting for "join the dots" methods
- Nearest Neighbor and k-nearest neighbor regression
- Distance Metrics
- Kernel Regression
- Weighting functions
- 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
- Radial Basis Functions