

Machine Learning for Signal Processing Regression and Prediction

Instructor: Bhiksha Raj

1755/18797



Topics

- Nearest neighbor regression and classification
- Linear regression
 - With an application to glitch elimination in sound
 - And its relation to nearest-neighbor regression
- Regression in kernel spaces
- Kernel regression
- Regularization...



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The problems of classification and regression

- Classification: Given a feature X, determine the class Y
 - Given image features, classify if this is a face
- Regression: Given an input X, estimate another feature Y
 - Given height, age, gender, etc. of a person, estimate weight
- In reality both are the same problem:
 - The class is simply a categorical feature



Example-based estimation

Classification:

- Have seen one or more people who are exactly 160cm,
 50kg, and all are female
- Get a new test instance of a person who is exactly 160cm,
 50kg. Is this person..
 - Male?
 - Female?

Regression:

- Have seen one or more people who are exactly 160cm, female, and their weight is 50kg
- Get a new test instance of a 160cm female person. What is your best guess for her weight?



Example-based estimation

Classification:

- Have seen one or more people who are exactly 160cm, 50kg, and all are female
- BUT WHAT IF THE WEIGHT OF THE TEST SUBJECT IS 49 KG?

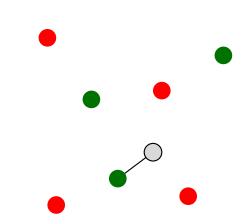
egression:

- Have seen one or more people who are exactly 160cm, female, and their weight is 50kg
- Get a new test instance of a 160cm female person. What is your best guess for her weight?



Example based prediction

 Problem: the gray circle is missing its color attribute.
 Predict it

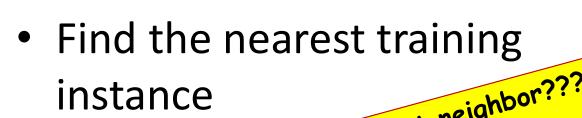


- Find the nearest training instance
 - Based on observed feature X
- Predict Y from it
 - Y may be a class value or a continuous valued estimator



Nearest-neighbor based prediction

 Problem: the gray circle is missing its color attribute. Predict it



What if the next-nearest neighbor is almost as close, but gives you Can you trust ONLY the nearest neighbor???

What it the answer?

a different answer?

a class value or a continuous valued estimator



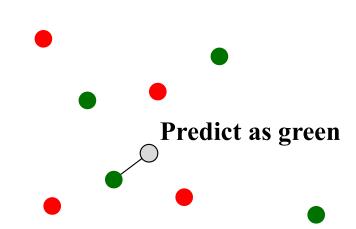
Nearest-neighbor prediction

- Alternately, find the k closest training instances
 - Called the k-nearest-neighbor method
- Predict desired attribute based on these k closest neighbors

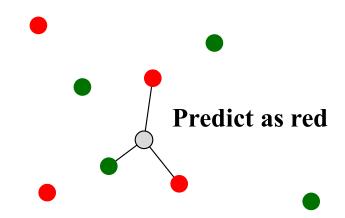


K-nearest neighbor prediction

- Problem: the gray circle is missing its color attribute. Predict it
- Nearest neighbor



- K-nearest neighbor
 - Example for k=3



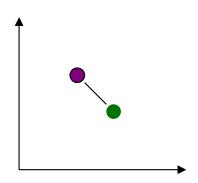


Distance functions

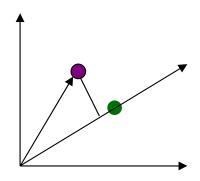
- How does one define the distance between two instances?
 - Some attributes may be numeric
 - Other attributes may nominal
- Numeric attributes: Usually the Euclidean distance between attribute values is used
- Nominal attributes: Usually a binary distance function –
 distance is set to 1 if attribute values are different, 0 if
 they are the same
- Will assume numeric attributes for our signals...



Distance on numeric features



$$d(x_1, x_2) = \|x_1 - x_2\|^2$$

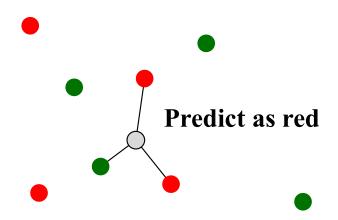


$$w(x_1, x_2) = x_1^T x_2$$
$$d(x_1, x_2) = \frac{1}{x_1^T x_2}$$



K-nearest neighbor prediction

- Find the K nearest neighbors
- Predict as the majority opinion
 - But should we also consider the actual distance
 - Is a farther neighbor as important as a closer one?
 - What about numeric prediction?
 - No notion of "majority"
 - No two neighbors may have the same value for Y





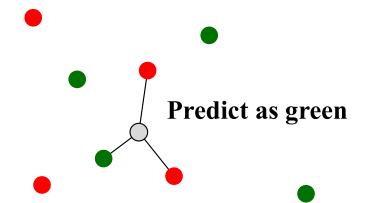
Weighted K-nearest neighbor prediction

Classification

- Score(class) = $\sum_{i:(i \in KNN) \& class(i) = class} w(x, x_i)$
- $class(x) = \underset{class}{\operatorname{argmax}} Score(class)$
- Regression:

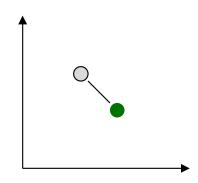
$$-Y(x) = \sum_{i \in KNN} w(x, x_i) Y_i$$

- The weight $w(x, x_i)$ is inversely related to $d(x, x_i)$
 - If $d(x, x_i)$ increases, $w(x, x_i)$ decreases

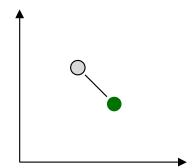




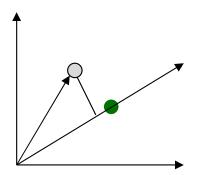
Weights of neighbors...



$$d(x_1, x_2) = \|x_1 - x_2\|^2 \qquad w(x, y) = \frac{1}{d(x, y)}$$



$$w(x_1, x_2) = exp(-\alpha d(x_1, x_2))$$



$$w(x_1, x_2) = x_1, x_2 = x_1^T x_2$$



Poll 1

- KNN uses the labels of the nearest neighbor, as defined under a given distance measure, to make predictions
 - True
 - False
- The K closest data points to a given testing instance (in the KNN algorithm) always have the same weight
 - True
 - False



Poll 1

- KNN uses the labels of the nearest neighbor, as defined under a given distance measure, to make predictions
 - True
 - False
- The K closest data points to a given testing instance (in the KNN algorithm) always have the same weight
 - True
 - False

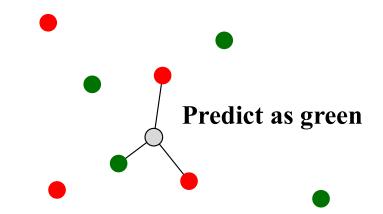


Weighted K-nearest neighbor prediction

- Classification
 - Score(class) = $\sum_{i:(i \in KNN)\& \ class(i) = class} w(x, x_i)$
 - $class(x) = \underset{class}{\operatorname{argmax}} Score(class)$
- Regression:

$$-Y(x) = \sum_{i \in KNN} w(x, x_i) Y_i$$

- The weight $w(x, x_i)$ is inversely related to $d(x, x_i)$
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WHY RESTRICT TO K
NEAREST NEIGHBORS?
Considering that distant
examples carry less weight

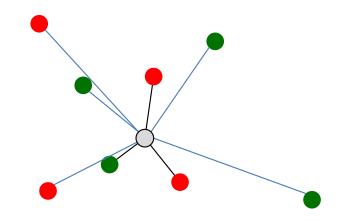


Weighted example-based prediction

- Classification
 - -Score(class) =

$$\sum_{i:class(i)=class} w(x,x_i)$$

 $- class(x) = \underset{class}{\operatorname{argmax}} Score(class)$



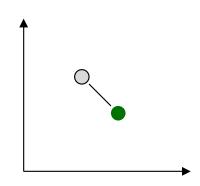
Regression:

$$-Y(x) = \sum_{i} w(x, x_i) Y_i$$

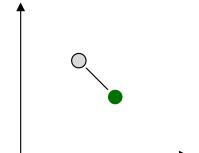
All training instances invoked!



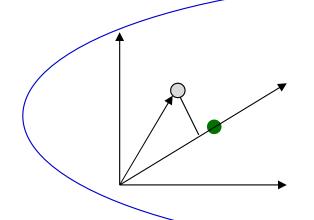
Weights of cohort



$$d(x_1, x_2) = \|x_1 - x_2\|^2 \qquad w(x, y) = \frac{1}{d(x, y)}$$

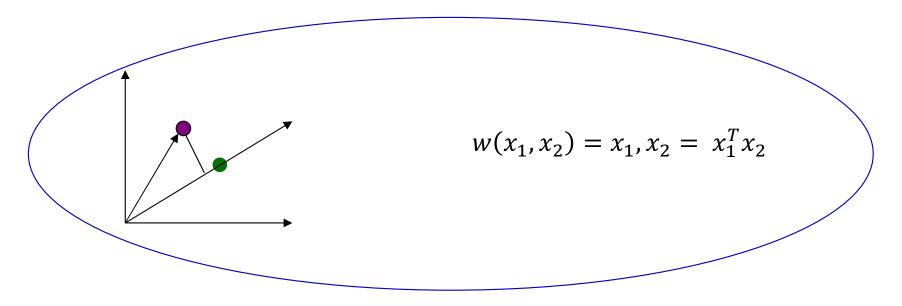


$$w(x_1, x_2) = exp(-\alpha d(x_1, x_2))$$



$$w(x_1, x_2) = x_1, x_2 = x_1^T x_2$$

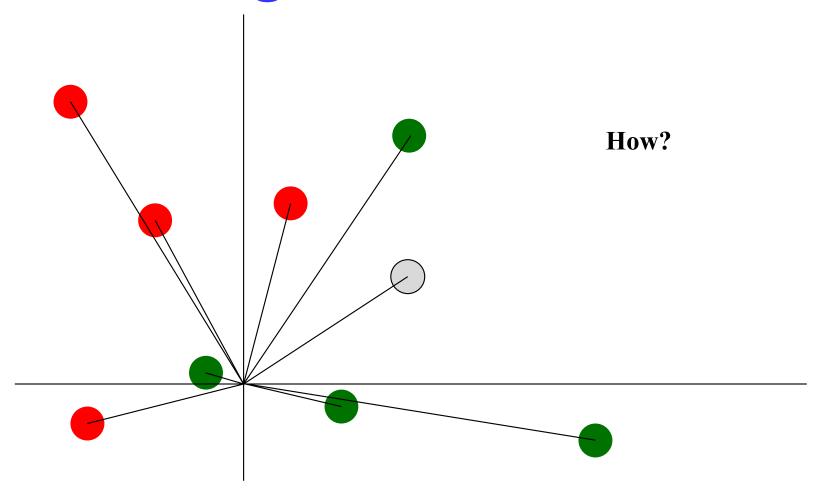
NN prediction with inner-product weights



$$Y_{test} = \sum_{i \in training \ set} (x_{test}^T x_i) Y_i$$



Nearest Neighbor Classification



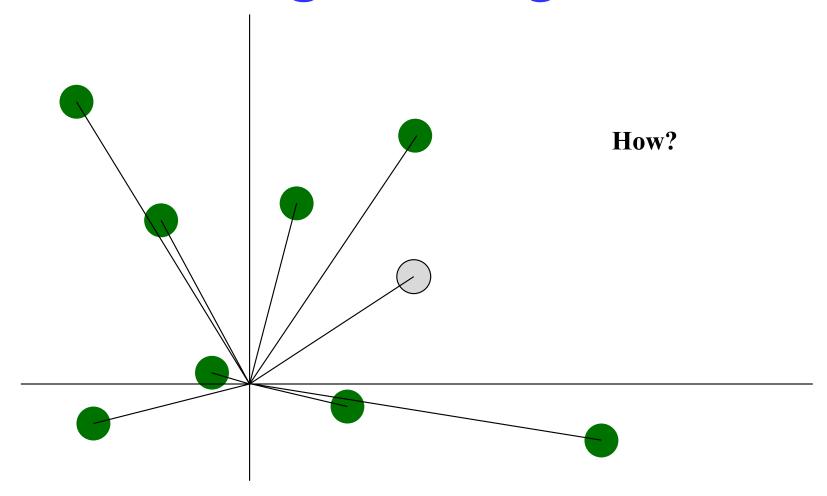
$$Score_{green} = \sum_{i \in green} (x_{test}^T x_i)$$

$$Score_{red} = \sum_{i \in red} (x_{test}^T x_i)$$

$$Y_{test} = Score_{green} > Score_{red}$$
? Green,
else Red



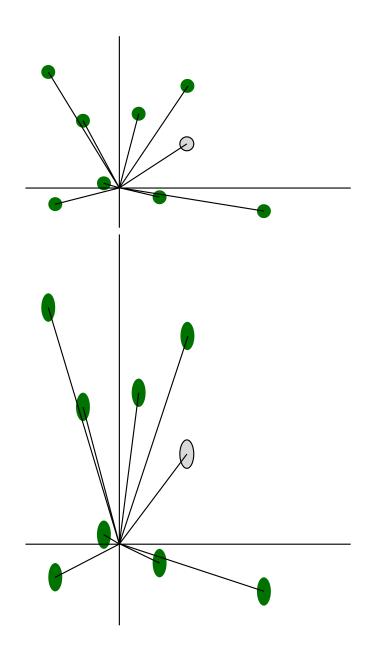
Nearest Neighbor Regression

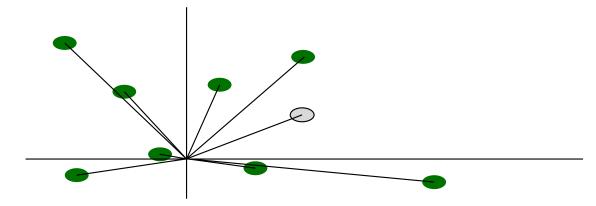


$$Y_{test} = \sum_{i \in training \ set} (x_{test}^T x_i) Y_i$$



Nearest Neighbor Regression





$$Y_{test} = \sum_{i \in training \ set} (x_{test}^T x_i) Y_i$$

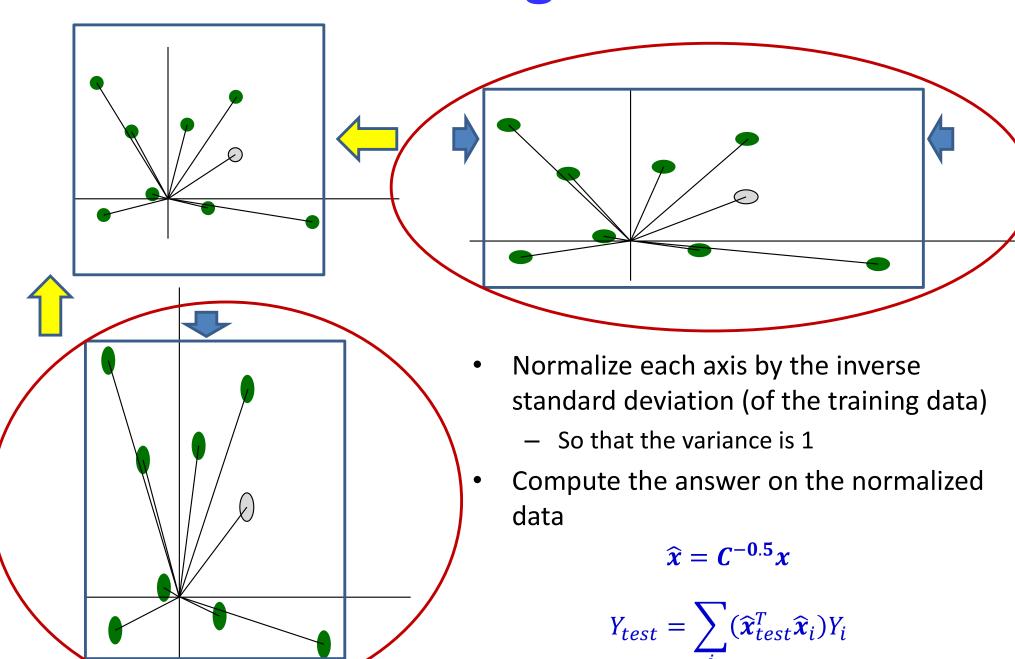
Simply stretching any axis changes the inner products and, as a result, the relative weights of the training instances.

Stretching an axis can change the answer!

How do we fix this?



Normalizing the axes





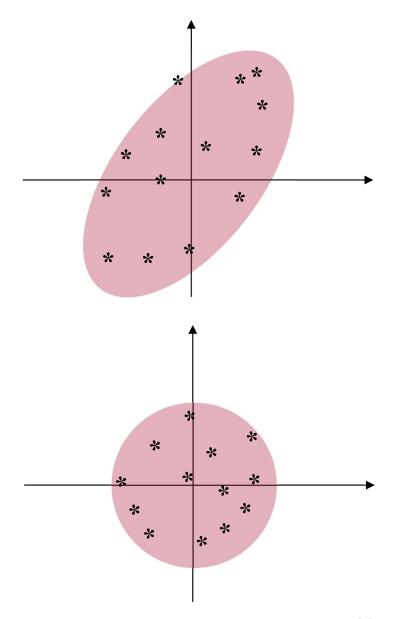
The whitening matrix

 Top: Skewed natural scatter of a data set

Bottom: Scatter after whitening via

$$\hat{\mathbf{x}} = \mathbf{C}^{-\frac{1}{2}} \mathbf{x}$$

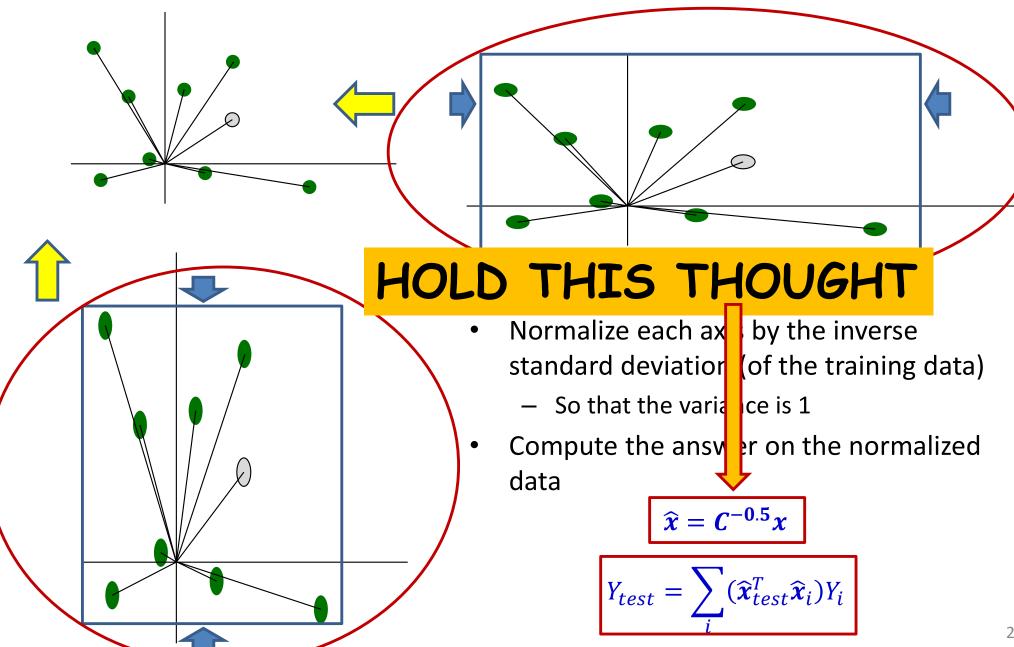
 Rotates and rescales the axes to make scatter circular (spherical)



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Normalizing the axes





Poll 2

- Mark all that are true
 - The order of the distance among data points is invariant to scaling an axis
 - The inner product is a good measure of weight, as closer points have larger inner products
 - Whitening is an essential step for the KNN algorithm
 - KNN can only be used for classification and not regression



Poll 2

- Mark all that are true
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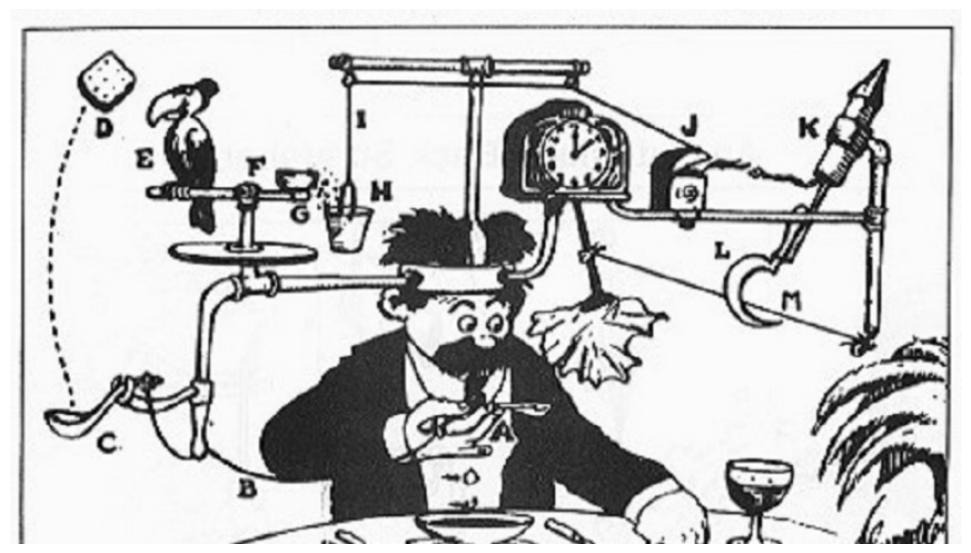


Lessons

- Classification are regression are two versions of the same problem
 - Predicting an attribute of a data instance based on other attributes
- Nearest-neighbor based prediction: Predict the weighted average value of desired attribute from all the training instances
- Amazing fact they never told you: Every form of prediction/classification/regression is actually just a variant of weighted nearest-neighbor prediction



Changing Gears



Rube Goldberg

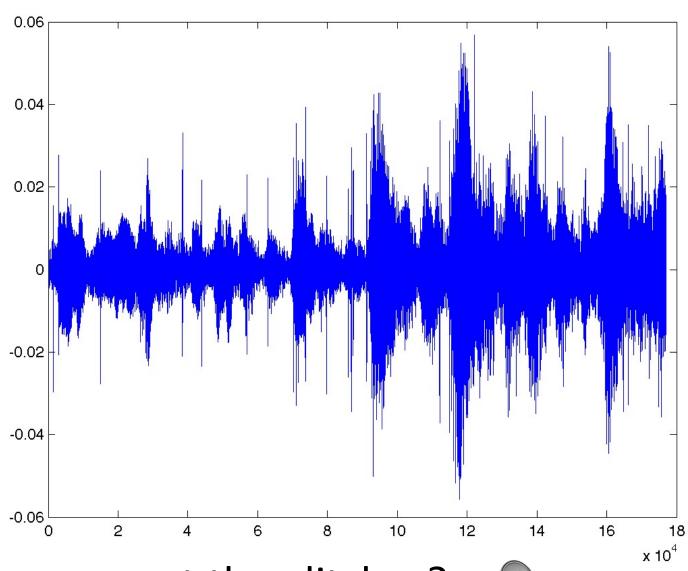


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- Regularization...



A Common Problem



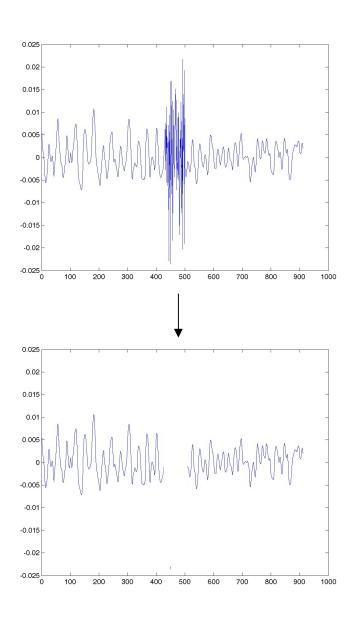
Can you spot the glitches?





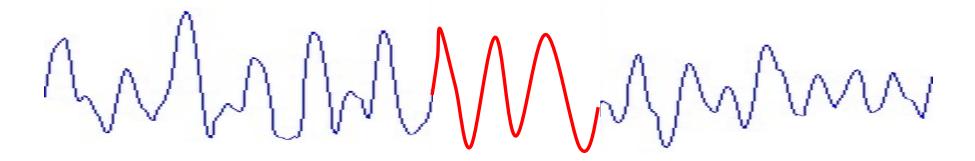
How to fix this problem?

- "Glitches" in audio
 - Must be detected
 - How?
- Then what?
- Glitches must be "fixed"
 - Delete the glitch
 - Results in a "hole"
 - Fill in the hole
 - How?





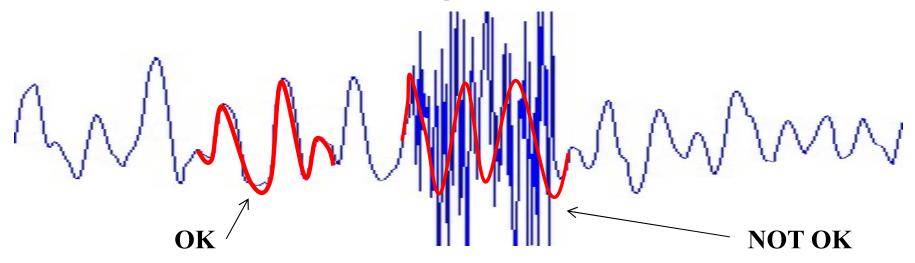
Interpolation..



- "Extend" the curve on the left to "predict" the values in the "blank" region
 - Forward prediction
- Extend the blue curve on the right leftwards to predict the blank region
 - Backward prediction
- How?
 - Regression analysis...



Detecting the Glitch



- Regression-based reconstruction can be done anywhere
- Reconstructed value will not match actual value
- Large error of reconstruction identifies glitches

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What is a regression

- Analyzing relationship between variables
- Expressed in many forms
- Wikipedia
 - Linear regression, Simple regression, Ordinary least squares, Polynomial regression, General linear model, Generalized linear model, Discrete choice, Logistic regression, Multinomial logit, Mixed logit, Probit, Multinomial probit,
- Generally a tool to predict variables

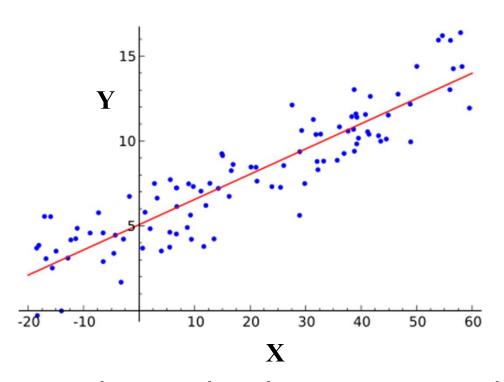


Regressions for prediction

- $y = f(x; \Theta) + e$
- Different possibilities
 - -y is a scalar
 - y is real
 - y is categorical (classification)
 - y is a vector
 - x is a vector
 - x is a set of real valued variables
 - x is a set of categorical variables
 - x is a combination of the two
 - f(.) is a linear or affine function
 - f(.) is a non-linear function
 - f(.) is a *time-series* model



A linear regression

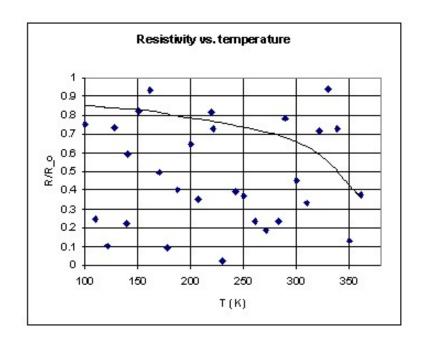


- Assumption: relationship between variables is linear
 - A linear *trend* may be found relating \mathbf{x} and \mathbf{y}
 - y = dependent variable
 - $\mathbf{x} = explanatory variable$
 - Given x, y can be predicted as an affine function of x



An imaginary regression...

- http://pages.cs.wisc.edu/~kovar/hall.html
- Check this shit out (Fig. 1).
 That's bonafide, 100%-real data, my friends. I took it myself over the course of two weeks. And this was not a leisurely two weeks, either; I busted my ass day and night in order to provide you with nothing but the best data possible. Now, let's look a bit more closely at this data, remembering



that it is absolutely first-rate. Do you see the exponential dependence? I sure don't. I see a bunch of crap.

Christ, this was such a waste of my time.

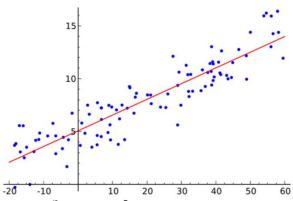
Banking on my hopes that whoever grades this will just look at the pictures, I drew an exponential through my noise. I believe the apparent legitimacy is enhanced by the fact that I used a complicated computer program to make the fit. I understand this is the same process by which the top quark was discovered.



Linear Regressions

•
$$\mathbf{y} = \mathbf{a}^{T}\mathbf{x} + \mathbf{b} + \mathbf{e}$$

- \mathbf{e} = prediction error



• Given a "training" set of $\{x, y\}$ values: estimate a and b

$$-\mathbf{y}_1 = \mathbf{a}^T \mathbf{x}_1 + \mathbf{b} + \mathbf{e}_1$$

 $-\mathbf{y}_2 = \mathbf{a}^T \mathbf{x}_2 + \mathbf{b} + \mathbf{e}_2$
 $-\mathbf{y}_3 = \mathbf{a}^T \mathbf{x}_3 + \mathbf{b} + \mathbf{e}_3$

 If a and b are well estimated, prediction error will be small



Linear Regression to a scalar

$$y_1 = a^T x_1 + b + e_1$$

 $y_2 = a^T x_2 + b + e_2$
 $y_3 = a^T x_3 + b + e_3$

Define:

$$\mathbf{y} = \begin{bmatrix} y_1 & y_2 & y_3 \dots \end{bmatrix} \qquad \mathbf{X} = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 \\ 1 & 1 & 1 \end{bmatrix} \qquad \mathbf{a} = \begin{bmatrix} \boldsymbol{a}^T & b \end{bmatrix}$$
$$\mathbf{e} = \begin{bmatrix} e_1 & e_2 & e_3 \dots \end{bmatrix}$$

Rewrite

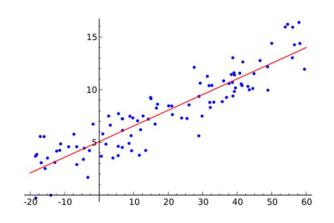
$$y = aX + e$$



Learning the parameters

$$y = aX + e$$

$$\hat{\mathbf{v}} = \mathbf{a}\mathbf{X}$$
 Assuming no error



- Given training data: several \mathbf{x}, \mathbf{y}
- Can define a "divergence": $D(y, \hat{y})$
 - Measures how much $\hat{\mathbf{y}}$ differs from \mathbf{y}
 - Ideally, if the model is accurate this should be small
- Estimate a to minimize $D(y, \hat{y})$



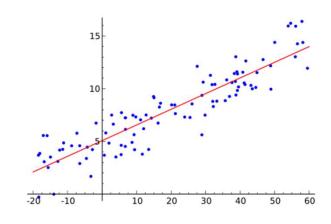
The prediction error as divergence

$$y_1 = \mathbf{a}^{T} \mathbf{x_1} + b + e_1$$

$$y_2 = \mathbf{a}^{T} \mathbf{x_2} + b + e_2$$

$$y_3 = \mathbf{a}^{T} \mathbf{x_3} + b + e_3$$

$$y = aX + e$$



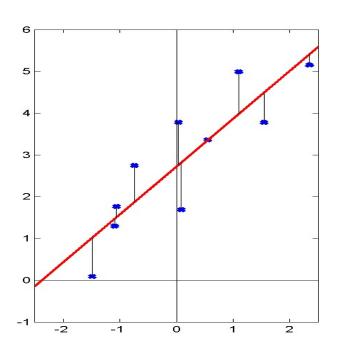
$$\mathbf{D}(\mathbf{y}, \hat{\mathbf{y}}) = \mathbf{E} = e_1^2 + e_2^2 + e_3^2 + \dots$$

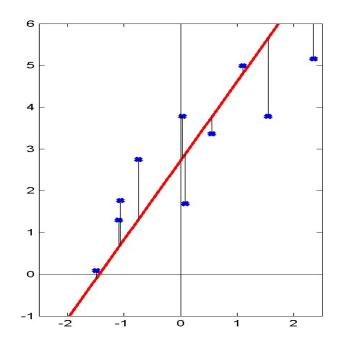
$$\mathbf{E} = \|\mathbf{y} - \mathbf{a}\mathbf{X}\|^2$$

Define divergence as sum of the squared error in predicting y



Prediction error as divergence





- $y = \mathbf{a}\mathbf{x} + e$
 - -e = prediction error
 - Find the "slope" a such that the total squared length of the error lines is minimized



Solving a linear regression

$$y = aX + e$$

Minimize squared error

$$\mathbf{E} = \|\mathbf{y} - \mathbf{a}\mathbf{X}\|^2$$

$$\mathbf{a} = \mathbf{y}pinv(\mathbf{X})$$



More Explicitly

$$\mathbf{y} = \begin{bmatrix} y_1 & y_2 & y_3 \dots \end{bmatrix} \qquad \mathbf{X} = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 \\ 1 & 1 & 1 \end{bmatrix}$$

$$\mathbf{A} = \mathbf{y} \mathbf{X}^T \left(\mathbf{X} \mathbf{X}^T \right)^{-1}$$

$$\mathbf{a} = \mathbf{y}pinv(\mathbf{X})$$

X is wider than it is tall

$$pinv(\mathbf{X}) = \mathbf{X}^T (\mathbf{X} \mathbf{X}^T)^{-1}$$

$$\mathbf{a} = \mathbf{y} \mathbf{X}^T (\mathbf{X} \mathbf{X}^T)^{-1}$$



Regression in multiple dimensions

$$y_1 = Ax_1 + b + e_1$$

 $y_2 = Ax_2 + b + e_2$
 $y_3 = Ax_3 + b + e_3$

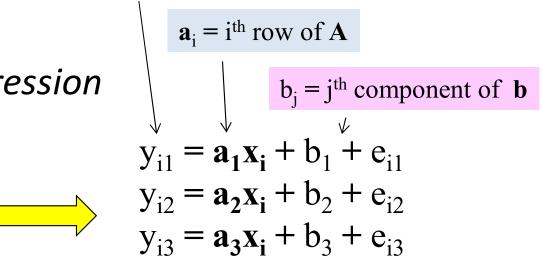
y_i is a vector

 $y_{ij} = j^{th}$ component of vector y_i

- Also called multiple regression
- Equivalent of saying:

$$\mathbf{y}_{i} = \mathbf{A}\mathbf{x}_{i} + \mathbf{b} + \mathbf{e}_{i}$$





- Fundamentally no different from N separate single regressions
 - But we can use the relationship between ys to our benefit

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Multiple Regression

$$\mathbf{Y} = [\mathbf{y}_1 \ \mathbf{y}_2 \ \mathbf{y}_3...] \qquad \mathbf{X} = \begin{bmatrix} \mathbf{x}_1 \ \mathbf{x}_2 \ \mathbf{x}_3 \end{bmatrix} ...$$

$$\hat{\mathbf{A}} = [\mathbf{A} \ \mathbf{b}]$$

$$\mathbf{E} = [\mathbf{e}_1 \ \mathbf{e}_2 \ \mathbf{e}_3...]$$

$$\mathbf{Y} = \hat{\mathbf{A}}\mathbf{X} + \mathbf{E}$$
 Frobenius norm
$$DIV = \sum_{i} \left\| \mathbf{y}_{i} - \hat{\mathbf{A}}\overline{\mathbf{x}}_{i} \right\|^{2} = \left\| \mathbf{Y} - \hat{\mathbf{A}}\mathbf{X} \right\|_{F}^{2}$$

Minimizing

$$\hat{\mathbf{A}} = \mathbf{Y}pinv(\mathbf{X}) = \mathbf{Y}\mathbf{X}^T (\mathbf{X}\mathbf{X}^T)^{-1}$$



Aside: The Frobenius norm

 The Frobenius norm is the square root of the sum of the squares of all the components of the matrix

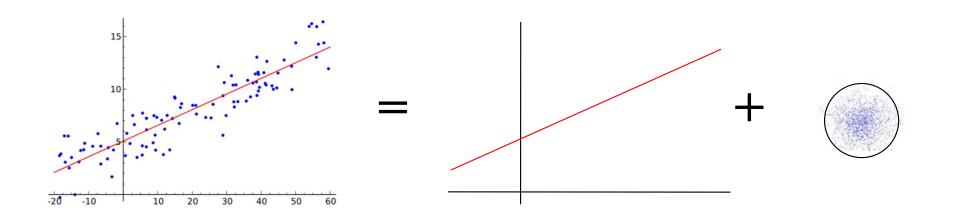
$$\|\mathbf{E}\|_F = \sqrt{\sum_{i,j} e_{i,j}^2}$$

The derivative of the squared Frobenius norm:

$$\nabla_A \|\mathbf{Y} - \mathbf{A}\mathbf{X}\|_F^2 = 0 \Rightarrow \mathbf{A} = \mathbf{Y}\mathbf{X}(\mathbf{X}\mathbf{X}^T)^{-1}$$



A Different Perspective



• y is a noisy reading of Ax

$$y = Ax + e$$

Error e is Gaussian

$$\mathbf{e} \sim N(\mathbf{0}, \sigma^2 \mathbf{I})$$

• Estimate A from $\mathbf{Y} = [\mathbf{y}_1 \ \mathbf{y}_2...\mathbf{y}_N] \ \mathbf{X} = [\mathbf{x}_1 \ \mathbf{x}_2...\mathbf{x}_N]$



The Likelihood of the data

$$\mathbf{y} = \mathbf{A}\mathbf{x} + \mathbf{e}$$
 $\mathbf{e} \sim N(0, \sigma^2 \mathbf{I})$

• Probability of observing a specific y, given x, for a particular matrix A

$$P(\mathbf{y} \mid \mathbf{x}; \mathbf{A}) = N(\mathbf{y}; \mathbf{A}\mathbf{x}, \sigma^2 \mathbf{I})$$

Probability of collection:

$$P(\mathbf{Y} \mid \mathbf{X}; \mathbf{A}) = \prod_{i} N(\mathbf{y}_{i}; \mathbf{A}\mathbf{x}_{i}, \sigma^{2}\mathbf{I})$$

Assuming IID for convenience (not necessary)



A Maximum Likelihood Estimate

$$\mathbf{y} = \mathbf{A}^{T} \mathbf{x} + \mathbf{e} \quad \mathbf{e} \sim N(0, \sigma^{2} \mathbf{I}) \quad \mathbf{Y} = [\mathbf{y}_{1} \quad \mathbf{y}_{2} ... \mathbf{y}_{N}] \quad \mathbf{X} = [\mathbf{x}_{1} \quad \mathbf{x}_{2} ... \mathbf{x}_{N}]$$

$$P(\mathbf{Y} \mid \mathbf{X}) = \prod_{i} \frac{1}{\sqrt{(2\pi\sigma^{2})^{D}}} \exp\left(\frac{-1}{2\sigma^{2}} \|\mathbf{y}_{i} - \mathbf{A}^{T} \mathbf{x}_{i}\|^{2}\right)$$

$$\log P(\mathbf{Y} \mid \mathbf{X}; \mathbf{A}) = C - \sum_{i} \frac{1}{2\sigma^{2}} \|\mathbf{y}_{i} - \mathbf{A} \mathbf{x}_{i}\|^{2}$$

- Maximizing the log probability is identical to minimizing the error
 - Identical to the least squares solution

$$\mathbf{A} = \mathbf{Y}\mathbf{X}^T (\mathbf{X}\mathbf{X}^T)^{-1} = \mathbf{Y}pinv(\mathbf{X})$$



Returning to Multiple Regression

$$\mathbf{Y} = [\mathbf{y}_1 \ \mathbf{y}_2 \ \mathbf{y}_3...] \qquad \mathbf{X} = \begin{bmatrix} \mathbf{x}_1 \ \mathbf{x}_2 \ \mathbf{x}_3 \\ \mathbf{1} \ \mathbf{1} \ \mathbf{1} \end{bmatrix} \qquad \hat{\mathbf{A}} = [\mathbf{A} \quad \mathbf{b}]$$

$$\mathbf{E} = [\mathbf{e}_1 \ \mathbf{e}_2 \ \mathbf{e}_3...]$$

$$\mathbf{Y} = \hat{\mathbf{A}}\mathbf{X} + \mathbf{E}$$

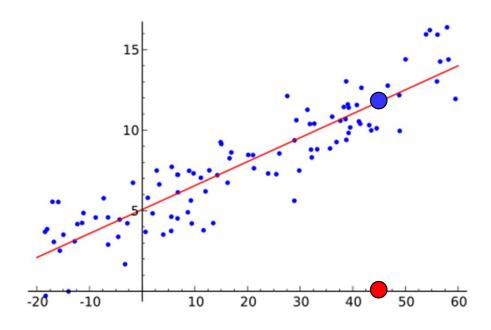
$$DIV = \sum_{i} \left\| \mathbf{y}_{i} - \hat{\mathbf{A}} \overline{\mathbf{x}}_{i} \right\|^{2} = \left\| \mathbf{Y} - \hat{\mathbf{A}} \mathbf{X} \right\|_{F}^{2}$$

Minimizing

$$\hat{\mathbf{A}} = \mathbf{Y}pinv(\mathbf{X}) = \mathbf{Y}\mathbf{X}^T (\mathbf{X}\mathbf{X}^T)^{-1}$$



Predicting an output



- From a collection of training data, have learned A
- Given x for a new instance, but not y, what is y?
- Simple solution:

$$\hat{\mathbf{y}} = \mathbf{A}\mathbf{x} + \mathbf{b}$$



Applying it to our problem

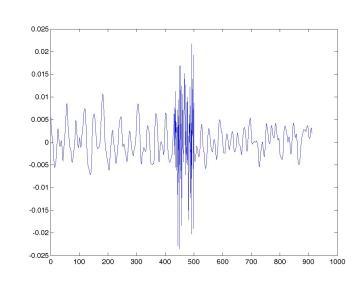
Prediction by regression

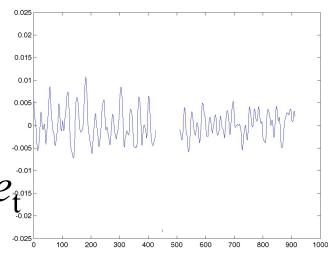
Forward regression

•
$$x_t = a_1 x_{t-1} + a_2 x_{t-2} \dots a_k x_{t-k} + e_t$$



•
$$x_{t} = b_{1}x_{t+1} + b_{2}x_{t+2} ... b_{k}x_{t+k} + e_{t_{00}}$$





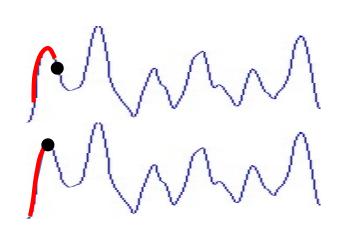


Applying it to our problem

Forward prediction

$$\begin{bmatrix} x_{t} \\ x_{t-1} \\ ... \\ x_{K+1} \end{bmatrix} = \begin{bmatrix} x_{t-1} & x_{t-2} & ... & x_{t-K} \\ x_{t-2} & x_{t-3} & ... & x_{t-K-1} \\ ... & ... & ... & ... \\ x_{K} & x_{K-1} & ... & x_{1} \end{bmatrix} \mathbf{a}_{t} + \begin{bmatrix} e_{t} \\ e_{t-1} \\ ... \\ e_{K+1} \end{bmatrix}$$





$$\mathbf{x} = \mathbf{X}\mathbf{a}_t + \mathbf{e}$$

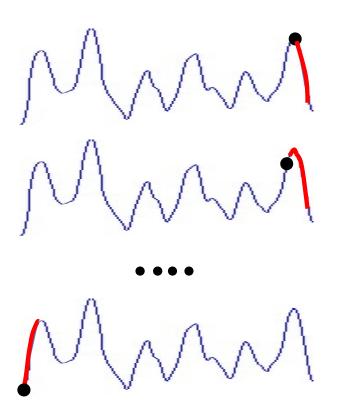
$$pinv(\mathbf{X})\mathbf{x} = \mathbf{a}_{t}$$



Applying it to our problem

Backward prediction

$$\begin{bmatrix} x_{t-K-1} \\ x_{t-K-2} \\ ... \\ x_1 \end{bmatrix} = \begin{bmatrix} x_t & x_{t-1} & ... & x_{t-K} \\ x_{t-1} & x_{t-2} & ... & x_{t-K-1} \\ ... & ... & ... & ... \\ x_{K+1} & x_K & ... & x_2 \end{bmatrix} \mathbf{b}_t + \begin{bmatrix} e_{t-K-1} \\ e_{t-K-2} \\ ... \\ e_1 \end{bmatrix}$$

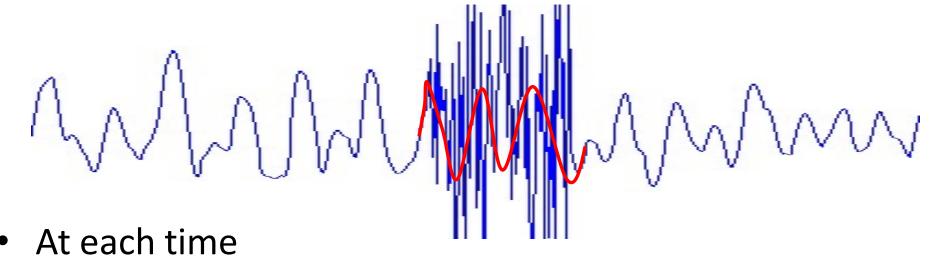


$$\overline{\mathbf{x}} = \overline{\mathbf{X}}\mathbf{b}_t + \mathbf{e}$$

$$pinv(\overline{\mathbf{X}})\overline{\mathbf{x}} = \mathbf{b}_t$$



Finding the burst

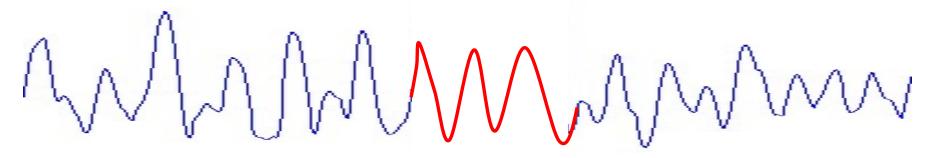


- Learn a "forward" predictor \mathbf{a}_{t}
- At each time, predict next sample $x_t^{\text{est}} = \sum_i a_{t,k} x_{t-k}$
- Compute error: $ferr_t = |x_t x_t^{\text{est}}|^2$
- Learn a "backward" predict and compute backward error
 - berr_t
- Compute average prediction error over window, threshold
- If the error exceeds a threshold, identify burst

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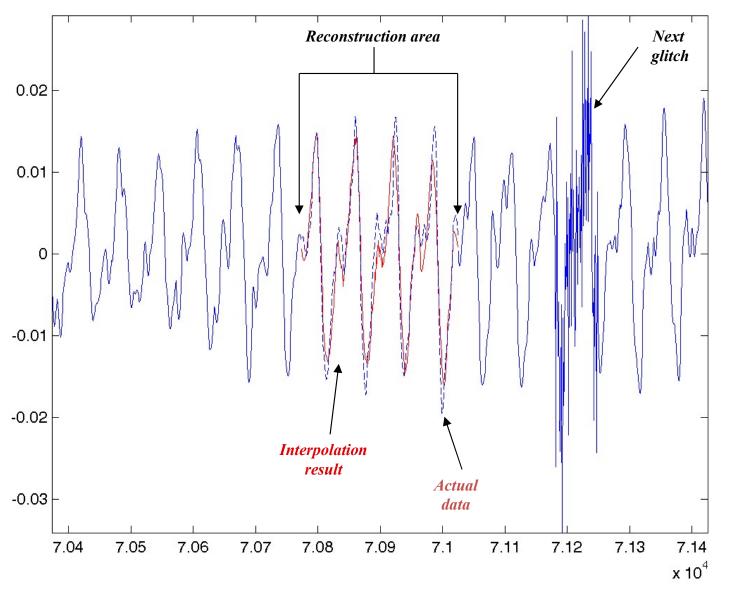
Filling the hole



- Learn "forward" predictor at left edge of "hole"
 - For each missing sample
 - At each time, predict next sample $x_t^{\text{est}} = \sum_i a_{t,k} x_{t-k}$
 - Use estimated samples if real samples are not available
- Learn "backward" predictor at left edge of "hole"
 - For each missing sample
 - At each time, predict next sample $x_t^{\text{est}} = \sum_i b_{t,k} x_{t+k}$
 - Use estimated samples if real samples are not available
- Average forward and backward predictions



Reconstruction zoom in





Distorted signal



Recovered signal



Incrementally learning the regression

$$\mathbf{A} = \mathbf{Y}\mathbf{X}^T \left(\mathbf{X}\mathbf{X}^T\right)^{\mathbf{1}}$$

Requires knowledge of all (x,y) pairs

- Can we learn A incrementally instead?
 - As data comes in?

The Widrow Hoff rule

Scalar prediction version

$$\mathbf{a}^{t+1} = \mathbf{a}^t + \eta (y_t - \hat{y}_t) \mathbf{x}_t \qquad \hat{y}_t = (\mathbf{a}^t)^T \mathbf{x}_t$$

- Note the structure error
 - Can also be done in batch mode!



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Predicting a value

$$\mathbf{A} = \mathbf{Y}\mathbf{X}^T \left(\mathbf{X}\mathbf{X}^T\right)^{-1}$$

$$\mathbf{A} = \mathbf{Y}\mathbf{X}^{T} \left(\mathbf{X}\mathbf{X}^{T}\right)^{-1} \mathbf{y} = \mathbf{A}\mathbf{x} = \mathbf{Y}\mathbf{X}^{T} \left(\mathbf{X}\mathbf{X}^{T}\right)^{-1} \mathbf{x}$$

- What are we doing exactly?
 - For the explanation we are assuming no " \mathbf{b} " (\mathbf{X} is 0 mean)
 - Explanation generalizes easily even otherwise

$$\mathbf{C} = \mathbf{X}\mathbf{X}^T$$

Let
$$\hat{\mathbf{x}} = \mathbf{C}^{-\frac{1}{2}}\mathbf{x}$$
 and $\hat{\mathbf{X}} = \mathbf{C}^{-\frac{1}{2}}\mathbf{X}$

- Whitening **x**
- $N^{-0.5}$ C^{-0.5} is the *whitening* matrix for **x**

$$\hat{\mathbf{y}} = \mathbf{Y}\mathbf{X}^T\mathbf{C}^{-\frac{1}{2}}\mathbf{C}^{-\frac{1}{2}}\mathbf{x} = \mathbf{Y}\hat{\mathbf{X}}^T\hat{\mathbf{x}}_i$$

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Predicting a value

$$\hat{\mathbf{y}} = \mathbf{Y}\hat{\mathbf{X}}^T\hat{\mathbf{x}} = \sum_i \mathbf{y}_i \hat{\mathbf{x}}_i^T \hat{\mathbf{x}}$$

$$\hat{\mathbf{y}} = \mathbf{Y}\hat{\mathbf{X}}^T\hat{\mathbf{x}} = \begin{bmatrix} \mathbf{y}_1 & \dots & \mathbf{y}_N \end{bmatrix} \begin{bmatrix} \hat{\mathbf{x}}_1^T \\ \vdots \\ \hat{\mathbf{x}}_N^T \end{bmatrix} \hat{\mathbf{x}} = \sum_i \mathbf{y}_i (\hat{\mathbf{x}}_i^T \hat{\mathbf{x}})$$

What are we doing exactly?



Predicting a value

$$\hat{\mathbf{y}} = \sum_{i} \mathbf{y}_{i} \left(\hat{\mathbf{x}}_{i}^{T} \hat{\mathbf{x}} \right)$$

- Given training instances $(\mathbf{x}_i, \mathbf{y}_i)$ for i = 1..N, estimate \mathbf{y} for a new test instance of \mathbf{x} with unknown \mathbf{y} :
- ${\bf y}$ is simply a weighted sum of the ${\bf y}_i$ instances from the training data
- The weight of any y_i is simply the inner product between its corresponding x_i and the new x
 - With due whitening and scaling..



Poll 3

- Mark all true statements
 - Every form of prediction/classification/regression is just a variant of weighted nearest-neighbor prediction
 - We can regard classification as a special kind of regression where the scalar prediction is not a real regression but a categorical value
 - Besides pseudo-inverse, we can use maximum-likelihood estimation (MLE) to solve some of the linear regression problems by assuming that the data is produced by a linear model with Gaussian noise with unknown parameters
 - Linear prediction can be applied on time series to detect every glitch in a signal, no matter how large the error is, and reconstruct the original signal perfectly



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What are we doing: A different perspective

$$\hat{\mathbf{y}} = \mathbf{A}\mathbf{x} = \mathbf{Y}\mathbf{X}^T \left(\mathbf{X}\mathbf{X}^T\right)^{-1}\mathbf{x}$$

- Assumes XX^T is invertible
- What if it is not
 - Dimensionality of X is greater than number of observations?
 - Underdetermined
- In this case X^TX will generally be invertible

$$\mathbf{A} = \mathbf{Y} \left(\mathbf{X}^T \mathbf{X} \right)^{-1} \mathbf{X}^T$$

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



High-dimensional regression

$$\hat{\mathbf{y}} = \mathbf{Y} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{x}$$

X^TX is the "Gram Matrix"

$$\mathbf{G} = \begin{bmatrix} \mathbf{x}_1^T \mathbf{x}_1 & \mathbf{x}_1^T \mathbf{x}_2 & \dots & \mathbf{x}_1^T \mathbf{x}_N \\ \mathbf{x}_2^T \mathbf{x}_1 & \mathbf{x}_2^T \mathbf{x}_2 & \dots & \mathbf{x}_2^T \mathbf{x}_N \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{x}_N^T \mathbf{x}_1 & \mathbf{x}_N^T \mathbf{x}_2 & \dots & \mathbf{x}_N^T \mathbf{x}_N \end{bmatrix}$$

$$\hat{\mathbf{y}} = \mathbf{Y}\mathbf{G}^{-1}\mathbf{X}^T\mathbf{x}$$



High-dimensional regression

$$\hat{\mathbf{y}} = \mathbf{Y}\mathbf{G}^{-1}\mathbf{X}^T\mathbf{x}$$

Normalize Y by the inverse of the gram matrix

$$\ddot{\mathbf{Y}} = \mathbf{Y}\mathbf{G}^{-1}$$

Working our way down..

$$\hat{\mathbf{y}} = \ddot{\mathbf{Y}}\mathbf{X}^T\mathbf{x}$$

$$\hat{\mathbf{y}} = \sum_{i} \ddot{\mathbf{y}}_{i} \mathbf{x}_{i}^{T} \mathbf{x}$$

Linear Regression in High-dimensional **Spaces**

$$\hat{\mathbf{y}} = \sum_{i} \ddot{\mathbf{y}}_{i} \mathbf{x}_{i}^{T} \mathbf{x}$$

$$\ddot{\mathbf{Y}} = \mathbf{Y}\mathbf{G}^{-1}$$

- Given training instances $(\mathbf{x}_i, \mathbf{y}_i)$ for i = 1..N, estimate \mathbf{y} for a new test instance of x with unknown y:
- y is simply a weighted sum of the normalized y_i instances from the training data
 - The normalization is done via the Gram Matrix
- The weight of any y_i is simply the inner product between its corresponding \mathbf{x}_i and the new \mathbf{x}

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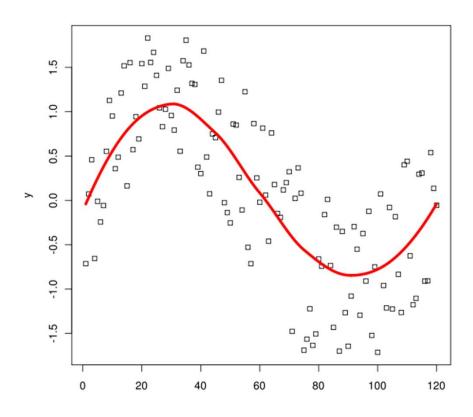


Topics

- Nearest neighbor regression and classification
- Linear regression
 - With an application to glitch elimination in sound
 - And its relation to nearest-neighbor regression
- Regression in kernel spaces
- Kernel regression
- Regularization...



Relationships are not always linear



- How do we model these?
- Multiple solutions

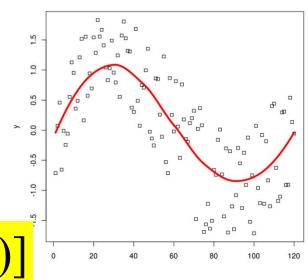


Non-linear regression

•
$$y = A\phi(x) + e$$

$$x \to \phi(x)$$

$$\mathbf{X} \to \Phi(\mathbf{X}) = [\boldsymbol{\varphi}(\mathbf{x}_1) \ \boldsymbol{\varphi}(\mathbf{x}_2) ... \boldsymbol{\varphi}(\mathbf{x}_K)]$$



- $Y = A\Phi(X) + e$
- Replace X with $\Phi(X)$ in earlier equations for solution

$$\mathbf{A} = \mathbf{Y} \left(\Phi(\mathbf{X}) \Phi(\mathbf{X})^T \right)^{-1} \Phi(\mathbf{X})^T$$

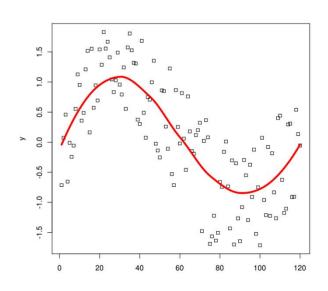


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Problem

- $Y = A\Phi(X) + e$
- Replace X with $\Phi(X)$ in earlier equations for solution

$$\mathbf{A} = \mathbf{Y} \left(\Phi(\mathbf{X}) \Phi(\mathbf{X})^T \right)^{-1} \Phi(\mathbf{X})^T$$



- $lackbox\Phi(\mathbf{X})$ may be in a very high-dimensional space
- The high-dimensional space (or the transform $\Phi(\mathbf{X})$) may be unknown..
 - Note: For any new instance x:

$$\hat{\mathbf{y}} = \mathbf{A}\Phi(\mathbf{x}) = \mathbf{Y}(\Phi(\mathbf{X})\Phi(\mathbf{X})^T)^{-1}\Phi(\mathbf{X})^T\Phi(\mathbf{x}) = \mathbf{Y}\mathbf{G}^{-1}\Phi(\mathbf{X})^T\Phi(\mathbf{x})$$



The regression is in high dimensions

• Linear regression: $\hat{\mathbf{y}} = \sum \ddot{\mathbf{y}}_i \mathbf{x}_i^T \mathbf{x}$ $\ddot{\mathbf{Y}} = \mathbf{Y} \mathbf{G}^{-1}$

$$\hat{\mathbf{y}} = \sum_{i} \ddot{\mathbf{y}}_{i} \mathbf{x}_{i}^{T} \mathbf{x}$$

$$\ddot{\mathbf{Y}} = \mathbf{Y}\mathbf{G}^{-1}$$

High-dimensional regression

$$\mathbf{G} = \begin{bmatrix} \Phi(\mathbf{x}_1)^T \Phi(\mathbf{x}_1) & \Phi(\mathbf{x}_2)^T \Phi(\mathbf{x}_2) & \dots & \Phi(\mathbf{x}_1)^T \Phi(\mathbf{x}_N) \\ \Phi(\mathbf{x}_2)^T \Phi(\mathbf{x}_1) & \Phi(\mathbf{x}_2)^T \Phi(\mathbf{x}_2) & \dots & \Phi(\mathbf{x}_2)^T \Phi(\mathbf{x}_N) \\ \vdots & \vdots & \ddots & \vdots \\ \Phi(\mathbf{x}_1)^T \Phi(\mathbf{x}_1) & \Phi(\mathbf{x}_N)^T \Phi(\mathbf{x}_2) & \dots & \Phi(\mathbf{x}_N)^T \Phi(\mathbf{x}_N) \end{bmatrix}$$

$$\ddot{\mathbf{Y}} = \mathbf{Y}\mathbf{G}^{-1}$$

$$\hat{\mathbf{y}} = \sum_{i} \ddot{\mathbf{y}}_{i} \Phi(\mathbf{x}_{i})^{T} \Phi(\mathbf{x})$$



Doing it with Kernels

High-dimensional regression with Kernels:

$$K(\mathbf{x},\mathbf{y}) = \Phi(\mathbf{x})^T \Phi(\mathbf{y})$$

$$\mathbf{G} = \begin{bmatrix} K(\mathbf{x}_1, \mathbf{x}_1) & K(\mathbf{x}_1, \mathbf{x}_1) & \dots & K(\mathbf{x}_1, \mathbf{x}_N) \\ K(\mathbf{x}_2, \mathbf{x}_1) & K(\mathbf{x}_2, \mathbf{x}_2) & \dots & K(\mathbf{x}_2, \mathbf{x}_N) \\ \vdots & \vdots & \ddots & \vdots \\ K(\mathbf{x}_N, \mathbf{x}_1) & K(\mathbf{x}_N, \mathbf{x}_2) & \dots & K(\mathbf{x}_N, \mathbf{x}_N) \end{bmatrix}$$

Regression in Kernel Hilbert Space...

$$\ddot{\mathbf{Y}} = \mathbf{Y}\mathbf{G}^{-1}$$

$$\hat{\mathbf{y}} = \sum_{i} \ddot{\mathbf{y}}_{i} K(\mathbf{x}_{i}, \mathbf{x})$$



Poll 4

- We can carry out non-linear regression by applying a Kernel function to linear regression
 - True
 - False
- The Gram matrix X^TX will always be full rank, where X is the data matrix
 - True
 - False



Poll 4

- We can carry out non-linear regression by applying a Kernel function to linear regression
 - True
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 - True
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Topics

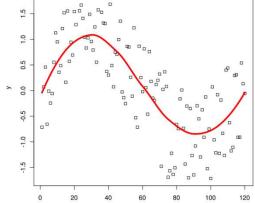
- Nearest neighbor regression and classification
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 - And its relation to nearest-neighbor regression
- Regression in kernel spaces
- Kernel regression
- Regularization...

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- Previous discussion: Regression parameters are optimized over the entire training set
- Minimize

$$\mathbf{E} = \sum_{all\ i} \left\| \mathbf{y}_i - \mathbf{A}^T \mathbf{x}_i - \mathbf{b} \right\|^2$$



- Single global regression is estimated and applied to all future ${\bf x}$
- Alternative: Local regression
- Learn a regression that is specific to x

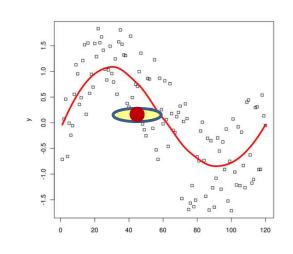
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Being non-committal: Local Regression

 Estimate the regression to be applied to any x using training instances near x

$$\mathbf{E} = \sum_{\mathbf{x}_{j} \in neighborhood(\mathbf{x})} \left\| \mathbf{y}_{i} - \mathbf{A}^{T} \mathbf{x}_{i} - \mathbf{b} \right\|^{2}$$



The resultant regression has the form

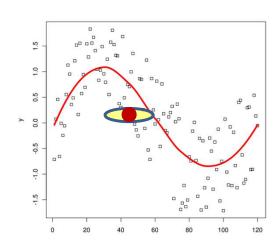
$$\mathbf{y} = \sum_{\mathbf{x}_j \in neighborhood(\mathbf{x})} w(\mathbf{x}, \mathbf{x}_j) \mathbf{y}_j + \mathbf{e}$$

- Note: this regression is specific to x
 - A separate regression must be learned for every x



Local Regression

$$\mathbf{y} = \sum_{\mathbf{x}_j \in neighborhood(\mathbf{x})} w(\mathbf{x}, \mathbf{x}_j) \mathbf{y}_j + \mathbf{e}$$



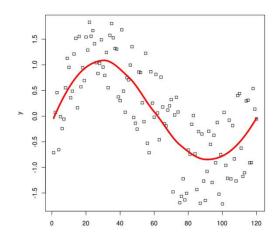
- But what is w()?
 - For linear regression d() is an inner product
- More generic form: Choose d() as a function of the distance between \mathbf{x} and \mathbf{x}_{j}
- If w() falls off rapidly with $|\mathbf{x}|$ and \mathbf{x}_j the "neighbhorhood" requirement can be relaxed

$$\mathbf{y} = \sum_{all} w(\mathbf{x}, \mathbf{x}_j) \mathbf{y}_j + \mathbf{e}$$



Kernel Regression: d() = K()

$$\hat{\mathbf{y}} = \frac{\sum_{i} K_h(\mathbf{x} - \mathbf{x}_i) \mathbf{y}_i}{\sum_{i} K_h(\mathbf{x} - \mathbf{x}_i)}$$



- Typical Kernel functions: Gaussian, Laplacian, other density functions
 - Must fall off rapidly with increasing distance between \boldsymbol{x} and \boldsymbol{x}_i
- Regression is *local* to every x : Local regression
- Actually a non-parametric MAP estimator of y
 - But first.. MAP estimators 1/18797



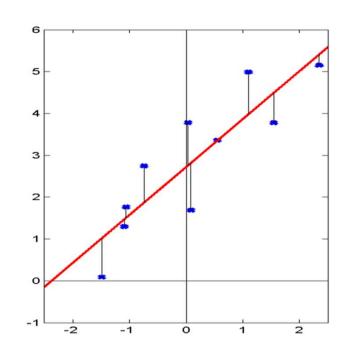
Topics

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Returning to Linear Regression

Model: $y = \widehat{A}x + \widehat{b}$ $\widehat{A}, \widehat{b} = \operatorname{argmin}(Y - (Ax + b))^2$



Without outliers

- The problem with fitting a linear model to minimize L2 error
 - Highly sensitive to outliers

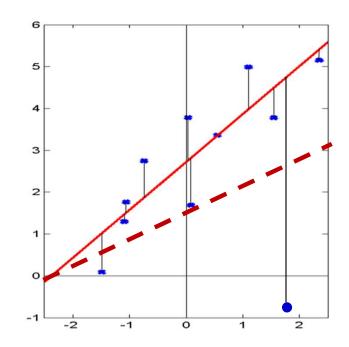


Returning to Linear Regression

Model:

$$y = \widehat{A}x + \widehat{b}$$

 $\widehat{A}, \widehat{b} = \underset{A,b}{\operatorname{argmin}} (Y - (Ax + b))^2$

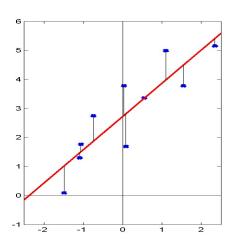


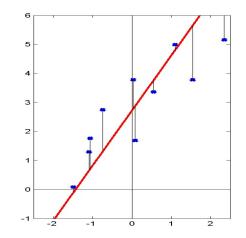
With a single outlier

- The problem with fitting a linear model to minimize L2 error
 - Highly sensitive to outliers



A problem with regressions





$$\mathbf{A} = \mathbf{Y}\mathbf{X}^T \left(\mathbf{X}\mathbf{X}^T\right)^{-1}$$

- Least-squares fit is sensitive
 - Error is squared
 - Small variations in data → large variations in weights
 - Outliers affect it adversely
- Unstable
 - If dimension of $X \ge no.$ of instances
 - (XX^T) is not invertible

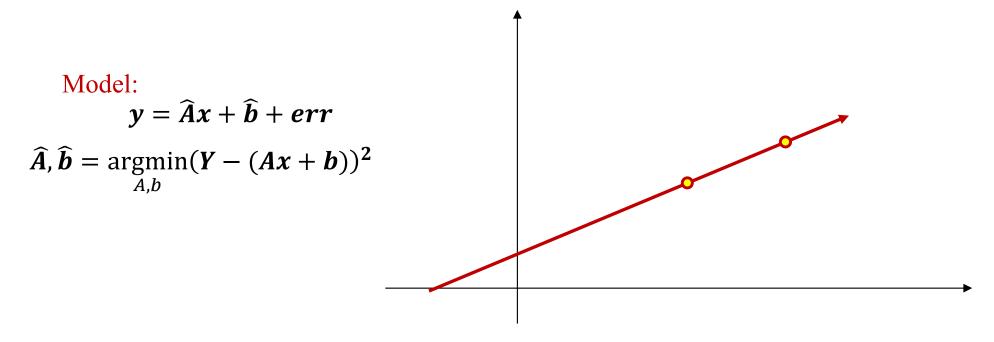


Conservative solution

- Default: Y is extremely sensitive to X
 - Results in large changes in regression estimate in response to small changes in input
- Alternate default assumption: Y does not depend on X
 - Prediction is just a horizontal line at Y = 0
 - Useless
- Conservative Compromise: Y is weakly related to X
 - Large increments in X result in small increments in Y
 - Willing to change opinion if we see a large number of instances where a large increment in X resulted in a large change in Y
 - Seeing just a few instances will not satisfy us
 - Reduced sensitivity to outliers



The Believer's Linear Regression



- Response of standard regression given only two training instances
 - Belief: Observed data tell the entire truth
 - Model completely fit to trends in data
 - A single point is a trend



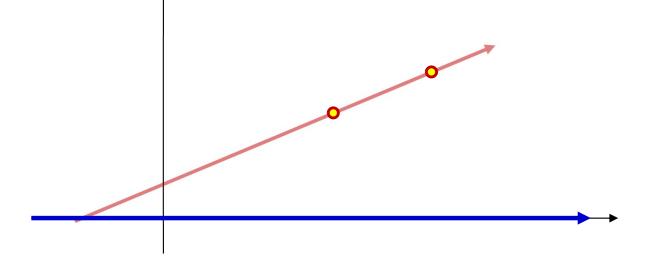
The Disbeliever's Linear Regression

Model:

$$y = err$$

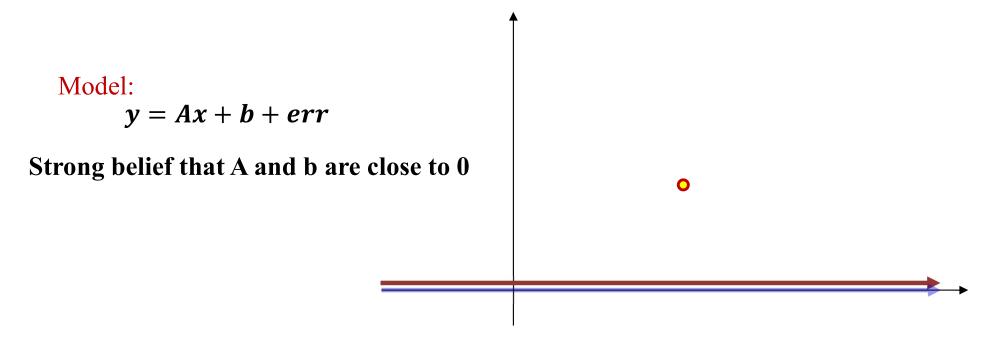
Alternately stated:

$$y = Ax + b + err$$
$$A = b = 0$$



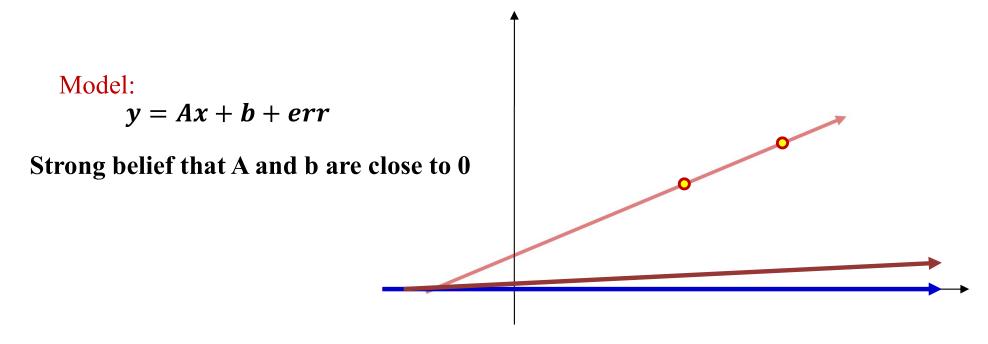
- All data are noise
 - The truth is that Y is a zero-mean random variable
 - The observed data are outcomes of noise variations





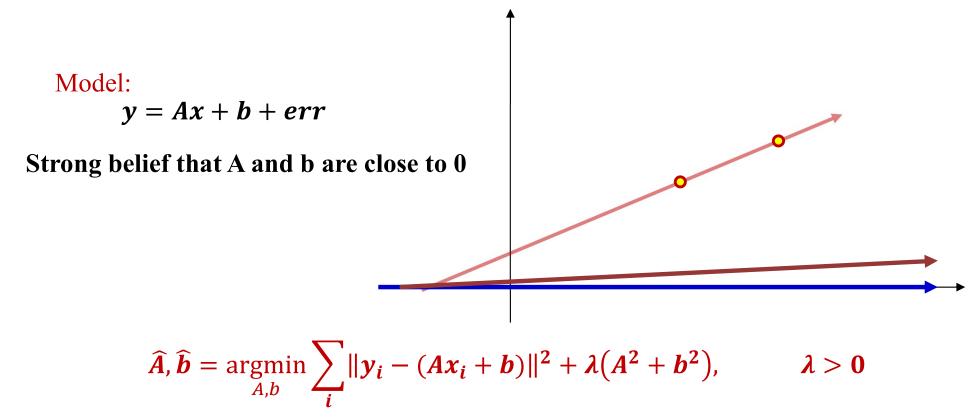
After seeing only one point...





The data provide evidence, but belief in the default is strong





- Minimize the error of prediction by the model
- But also insist that A and b be as small as possible
 - $-\lambda$ gives measure of "insistence" that A and b be small
 - Externally set

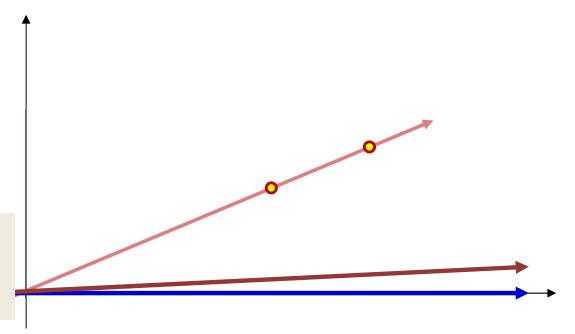


Model:

$$y = A\widehat{x} + err$$

Strong belief that A is close to 0

Using the augmented x notation (padding x with a 1) to include bias term



$$\widehat{A} = \underset{A}{\operatorname{argmin}} \sum_{i} ||y_i - A\widehat{x}_i||^2 + \lambda ||A||_F^2, \qquad \lambda > 0$$

- Minimize the error of prediction by the model
- But also insist that A should be as small as possible
 - $-\lambda$ gives measure of "insistence" that A must be small
 - Externally set



Simple solution

Conventional solution:

$$\widehat{A} = \underset{A}{\operatorname{argmin}} \| Y - A \widehat{X} \|_{F}^{2}$$

$$\widehat{A} = Y \widehat{X} (\widehat{X} \widehat{X}^{T})^{-1}$$

With regularization

$$\widehat{A} = \underset{A}{\operatorname{argmin}} \| Y - A \widehat{X} \|_F^2 + \lambda \| A \|_F^2$$

- Also called Tikhonov Regularization or Ridge regression
- Minmization gives us

$$\widehat{A} = Y\widehat{X}\big(\widehat{X}\widehat{X}^T + \lambda I\big)^{-1}$$

- This is exactly the same as conventional estimation, with additional diagonal loading of the correlation matrix of \widehat{X}
 - Can be alternately explained as "stabilizing" the correlation matrix, for inversion

Other forms of regularization: L1 regularization

An alternate regularization

$$\widehat{A} = \underset{A}{\operatorname{argmin}} \|Y - A\widehat{X}\|_F^2 + \lambda |A|_1$$

- The one-norm A_1 sums the magnitude of components of A
 - The minimization causes A to be sparse
- No closed form solution
 - Quadratic programming solutions required
- Dual formulation

$$\widehat{A} = \underset{A}{\operatorname{argmin}} \| Y - A \widehat{X} \|_F^2 \quad \text{subject to } |A|_1 \le t$$

"LASSO" – Least absolute shrinkage and selection operator



Regularization

$$E = \|\mathbf{y} - \mathbf{a}^T X\|^2 + \Omega(\mathbf{a})$$

$$\downarrow$$
Constraints

$$\Omega(\mathbf{a}) = \sigma \|\mathbf{a}\|_2^2$$



Map Estimation

A Maximum Likelihood Estimator maximizes

 $\mathbb{P}(\text{data} \mid \text{parameters})$

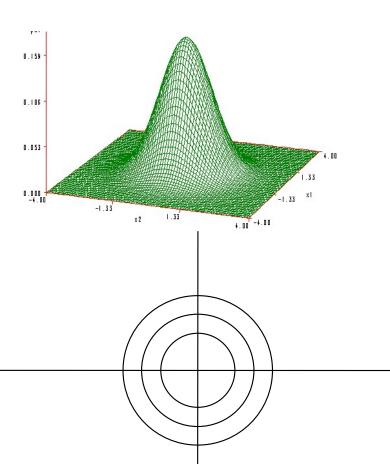
A Maximum A Posteriori Estimator maximizes

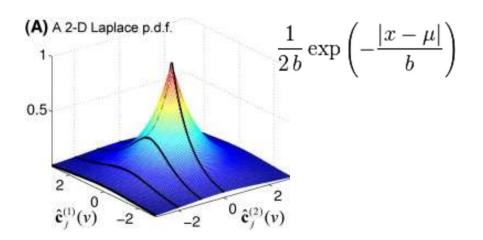
 $\mathbb{P}(\text{parameters} \mid \text{data})$

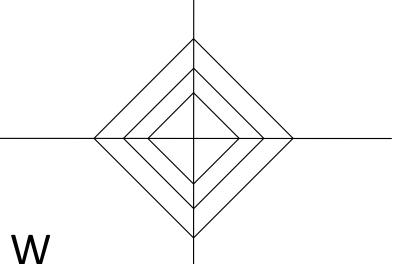
$$\mathbb{P}(\text{parameters} \mid \text{data}) = \frac{\mathbb{P}(\text{data} \mid \text{parameters}) \cdot \mathbb{P}(\text{parameters})}{\mathbb{P}(\text{data})}$$



MAP estimate priors







- Left: Gaussian Prior on W
- Right: Laplacian Prior



MAP estimate of weights

$$dL = (2\mathbf{a}^T \mathbf{X} \mathbf{X}^T + 2\mathbf{y} \mathbf{X}^T + 2\sigma \mathbf{I})d\mathbf{a} = 0$$

$$\mathbf{a} = \left(\mathbf{X}\mathbf{X}^T + \boldsymbol{\sigma}\mathbf{I}\right)^{-1}\mathbf{X}\mathbf{Y}^T$$

- Equivalent to diagonal loading of correlation matrix
 - Improves condition number of correlation matrix
 - Can be inverted with greater stability
 - Will not affect the estimation from well-conditioned data
 - Also called Tikhonov Regularization
 - Dual form: Ridge regression
- MAP estimate of weights
 - Not to be confused with MAP estimate of Y



MAP estimation of weights with Laplacian prior

- Assume weights drawn from a Laplacian
 - $-P(\mathbf{a}) = \lambda^{-1} \exp(-\lambda^{-1}|\mathbf{a}|_1)$
- Maximum *a posteriori* estimate

$$\hat{\mathbf{a}} = \arg\max_{\mathbf{A}} C' - (\mathbf{y} - \mathbf{a}^T \mathbf{X})^T (\mathbf{y} - \mathbf{a}^T \mathbf{X})^T - \lambda^{-1} |\mathbf{a}|_1$$

- No closed form solution
 - Quadratic programming solution required
 - Non-trivial



MAP estimation of weights with Laplacian prior

Assume weights drawn from a Laplacian

$$-P(\mathbf{a}) = \lambda^{-1} \exp(-\lambda^{-1}|\mathbf{a}|_1)$$

• Maximum *a posteriori* estimate

$$\hat{\mathbf{a}} = \operatorname{arg\,max}_{\mathbf{A}} C' - (\mathbf{y} - \mathbf{a}^T \mathbf{X})^T (\mathbf{y} - \mathbf{a}^T \mathbf{X})^T - \lambda^{-1} |\mathbf{a}|_1$$

Identical to L₁ regularized least-squares estimation



L₁-regularized LSE

$$\hat{\mathbf{a}} = \arg\max_{\mathbf{A}} C' - (\mathbf{y} - \mathbf{a}^T \mathbf{X})^T (\mathbf{y} - \mathbf{a}^T \mathbf{X})^T - \lambda^{-1} |\mathbf{a}|_1$$

- No closed form solution
 - Quadratic programming solutions required
- Dual formulation

$$\hat{\mathbf{a}} = \arg\max_{\mathbf{A}} C' - (\mathbf{y} - \mathbf{a}^T \mathbf{X})^T (\mathbf{y} - \mathbf{a}^T \mathbf{X})^T$$
 subject to $|\mathbf{a}|_1 \le t$

 "LASSO" – Least absolute shrinkage and selection operator



LASSO Algorithms

Various convex optimization algorithms

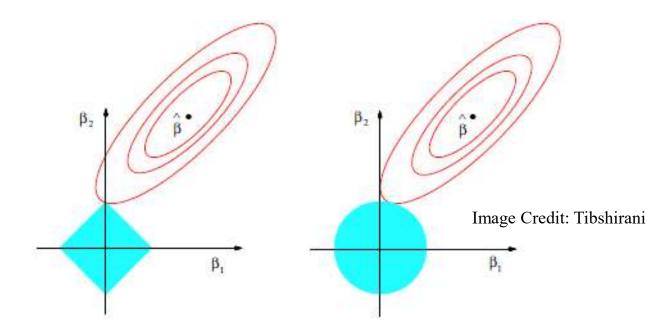
LARS: Least angle regression

• Pathwise coordinate descent..

Matlab code available from web



Regularized least squares



- Regularization results in selection of suboptimal (in least-squares sense) solution
 - One of the loci outside center
- Tikhonov regularization selects shortest solution
- L₁ regularization selects sparsest solution

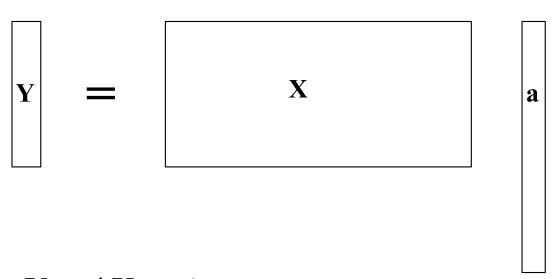


Next up...

- Classification with linear regression models
 - AKA linear classifiers



LASSO and Compressive Sensing



- Given \mathbf{Y} and \mathbf{X} , estimate sparse \mathbf{a}
- LASSO:
 - X = explanatory variable
 - Y = dependent variable
 - -a = weights of regression
- CS:
 - X = measurement matrix
 - Y = measurement
 - -a = data



An interesting problem: Predicting War!

- Economists measure a number of social indicators for countries weekly
 - Happiness index
 - Hunger index
 - Freedom index
 - Twitter records
 - **—** ...
- Question: Will there be a revolution or war next week?



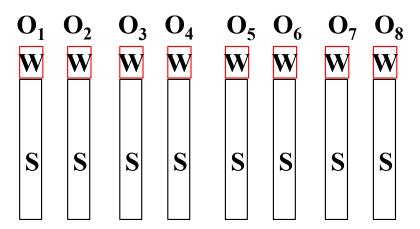
An interesting problem: Predicting War!

Issues:

- Dissatisfaction builds up not an instantaneous phenomenon
 - Usually
- War / rebellion build up much faster
 - Often in hours
- Important to predict
 - Preparedness for security
 - Economic impact



Predicting War



Given

wk1 wk2 wk3 wk4 wk5wk6 wk7wk8

- Sequence of economic indicators for each week
- Sequence of unrest markers for each week
 - At the end of each week we know if war happened or not that week
- Predict probability of unrest next week
 - This could be a new unrest or persistence of a current one



Predicting Time Series

Need time-series models

• HMMs – later in the course

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