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## Machine Learning for Signal Processing Regression and Prediction

Instructor: Bhiksha Raj



# **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..



# **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..

# 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 more or less 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
- emale2 emale2 BUT WHAT IF THE WEIGHT OF THE TEST SUBJECT IS 49 KG?

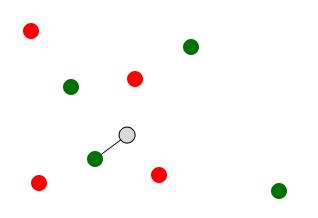
*Legression*:

- 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

Find the nearest training instance
Based only the nearest neighbor???
Based only the nearest neighbor is almost as close, but gives you trust ONLY the nearest neighbor is almost as close, but gives you trust on you trust only the nearest neighbor is almost as close, but gives you what if the next-nearest neighbor is almost as close, but gives you what if the next-nearest neighbor is almost as close, but gives you what if the next-nearest neighbor is almost as close, but gives you what if the next-nearest neighbor is almost as close, but gives you what if the next-nearest neighbor is almost as close, but gives you what if the next-nearest neighbor is almost as close, but gives you a different answer?



## **Nearest-neighbor prediction**

• Alternately, find the k closest training instances

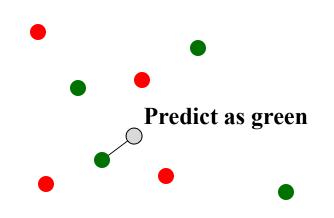
Called the k-nearest-neighbor method

 Predict desired attribute based on these k closest neighbors

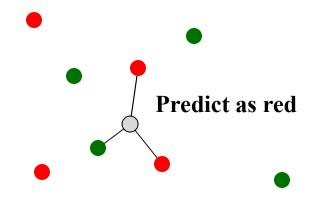


### **K-nearest neighbor prediction**

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



K-nearest neighbor
 Example for k=3



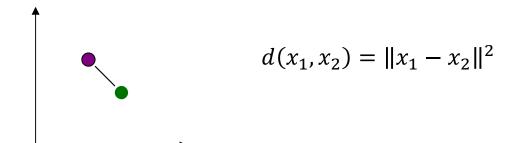


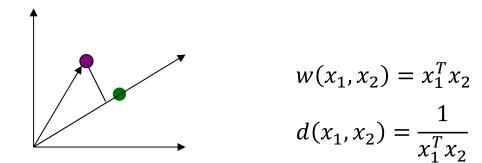
### **Distance functions**

- 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**

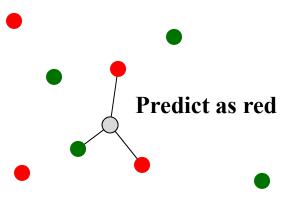






### **K-nearest neighbor prediction**

- 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



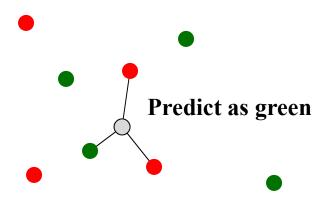


# Weighted K-nearest neighbor prediction

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

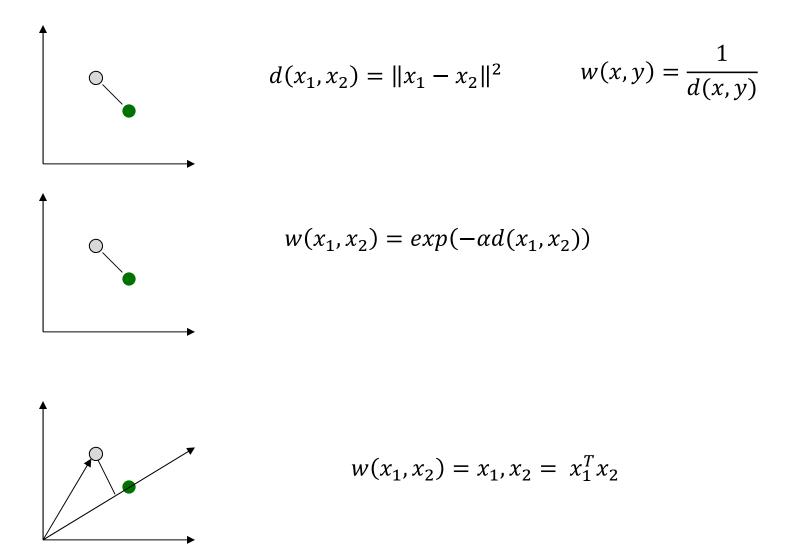
 $-Y(x) = \sum_{i \in KNN} w(x, x_i) Y_i$ 

- The weight w(x, x<sub>i</sub>) is inversely related to d(x, x<sub>i</sub>)
  - If  $d(x, x_i)$  increases,  $w(x, x_i)$  decreases





### Weights of neighbors..



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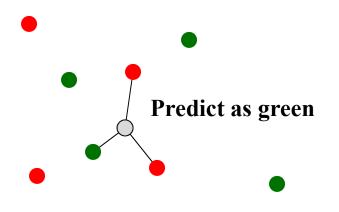


# Weighted K-nearest neighbor prediction

- 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



WHY RESTRICT TO K NEAREST NEIGHBORS? Considering that distant examples carry less weight

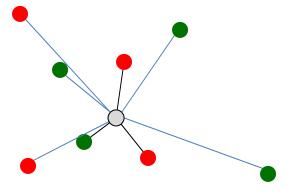


# Weighted example-based prediction

Classification

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

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



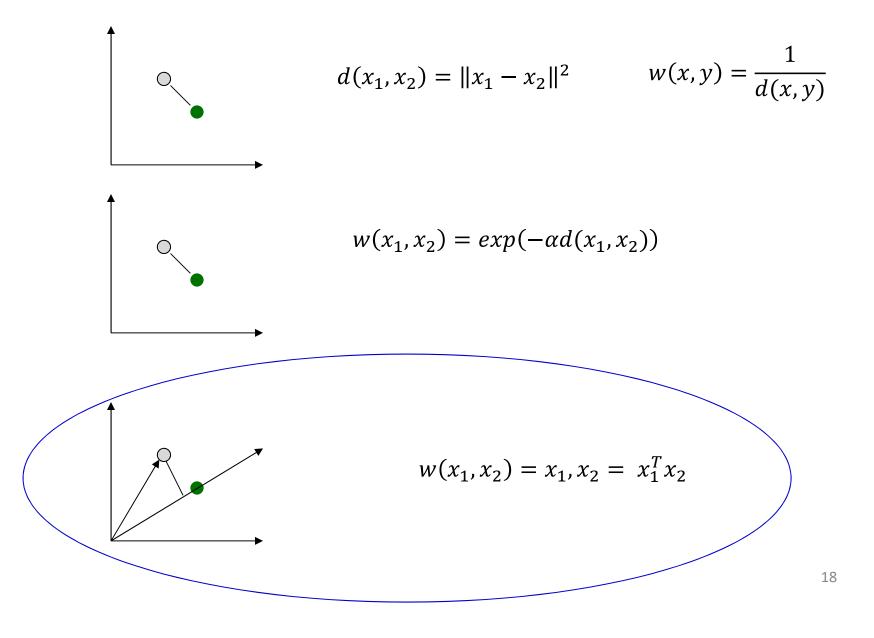
• Regression:

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

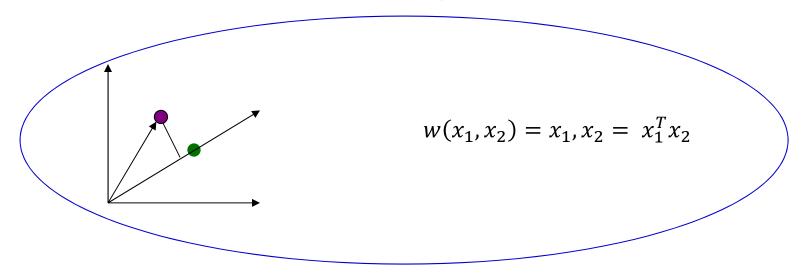
• All training instances invoked!



### Weights from numeric features



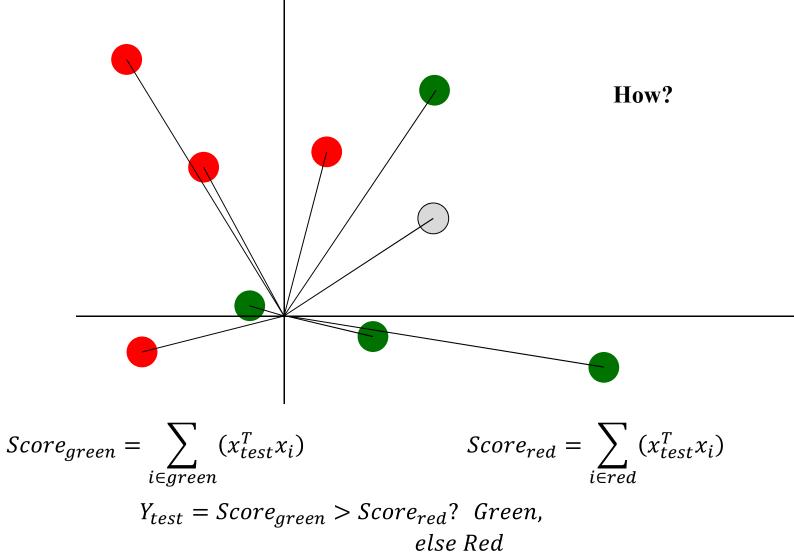
# NN prediction with inner-product weights



 $Y_{test} = \sum_{i=1}^{n} (x_{test}^T x_i) Y_i$ i∈training set

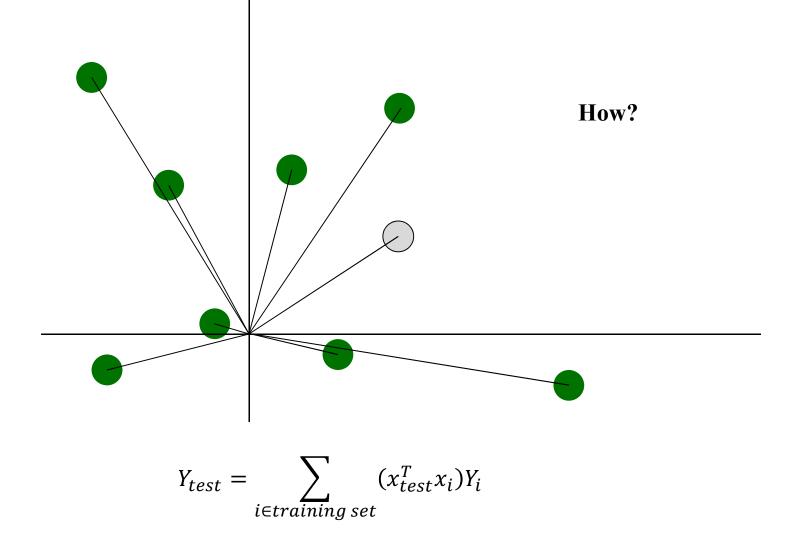


### **Nearest Neighbor Classification**



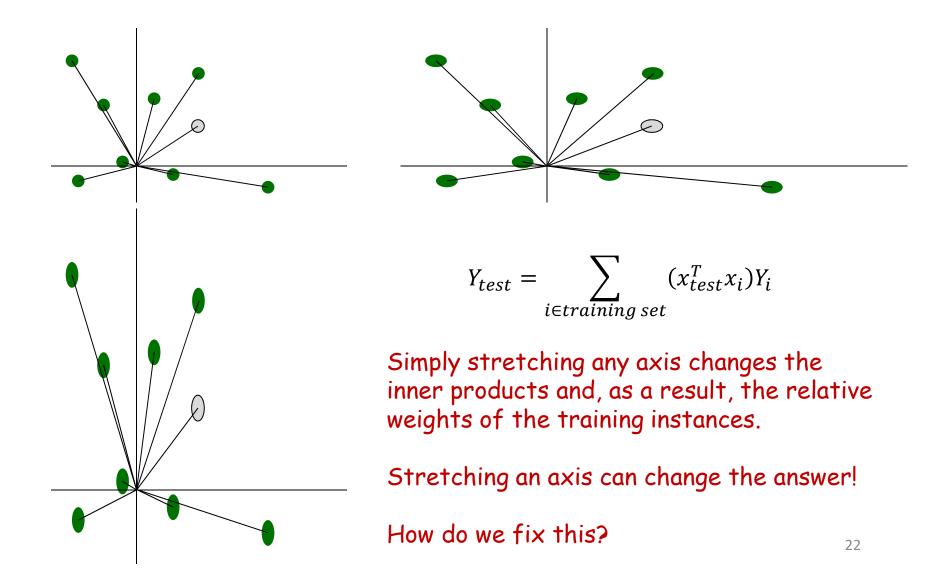


### **Nearest Neighbor** *Regression*



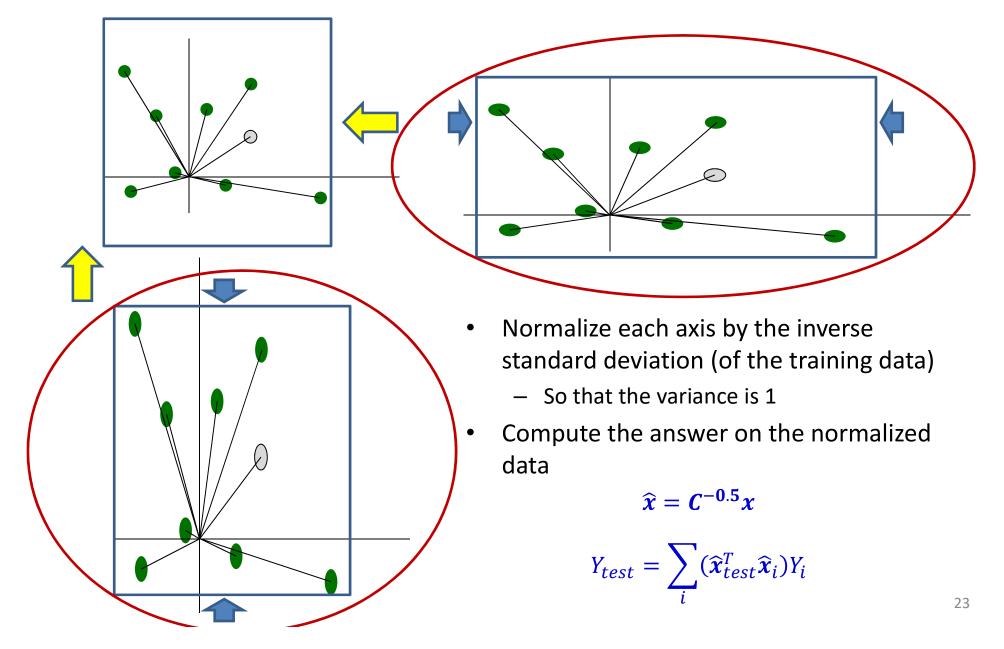


### **Nearest Neighbor** *Regression*





### **Normalizing the axes**



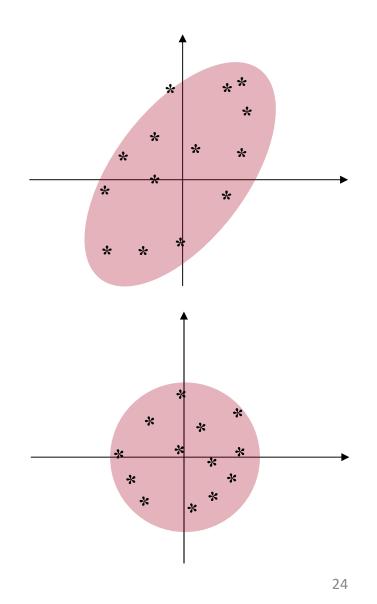


# The whitening matrix

- Top: Skewed natural scatter of a data set
- Bottom: Scatter after whitening via

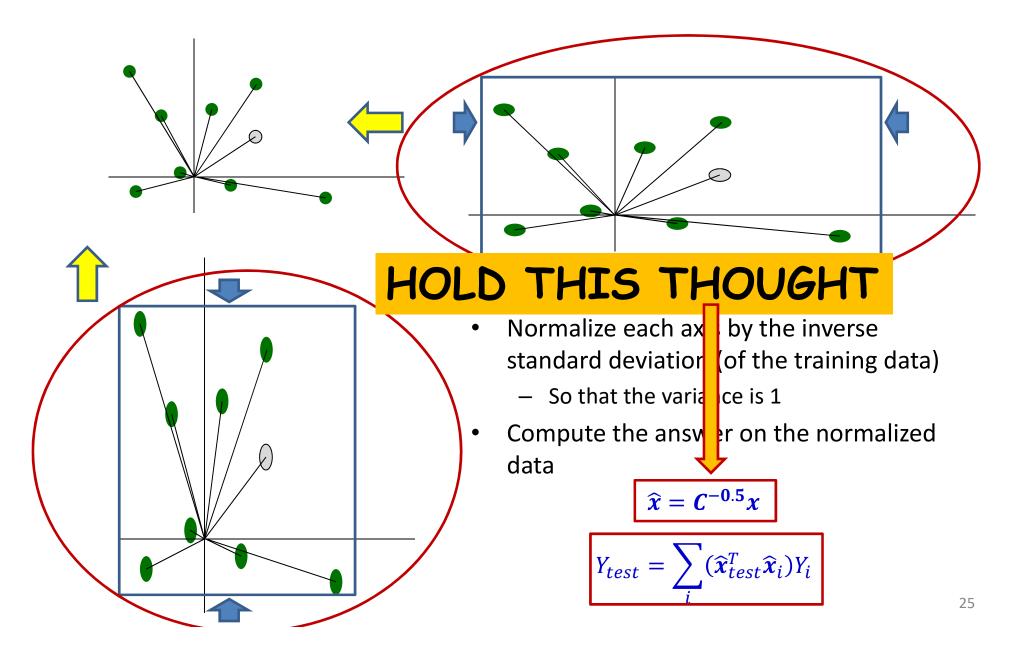
 $\hat{\mathbf{x}} = \mathbf{C}^{-\frac{1}{2}}\mathbf{x}$ 

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





### **Normalizing the axes**



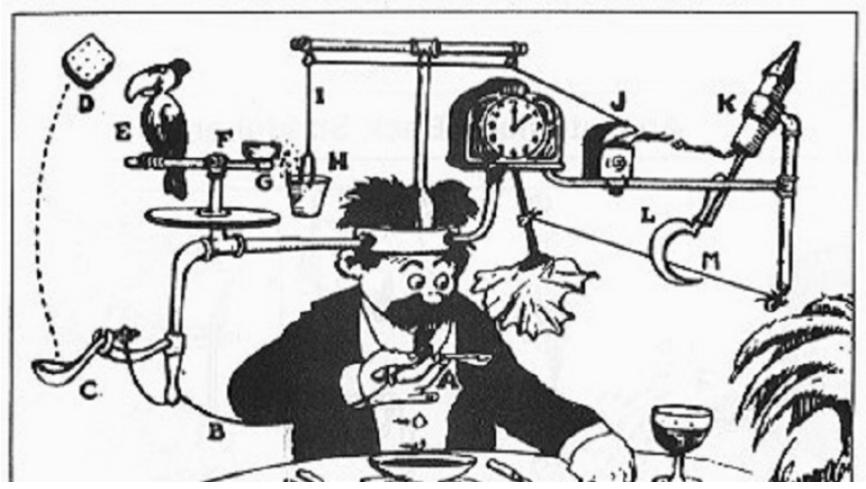




- Classification are regression are two versions of the same problem
  - Predicting an attribute of a data instance based on other attributes
- Nearest-neighbor based prediction: Predict the weighted average value of desired attribute from all the training instances
- Amazing fact they never told you: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



## **Changing Gears**



Rube Goldberg

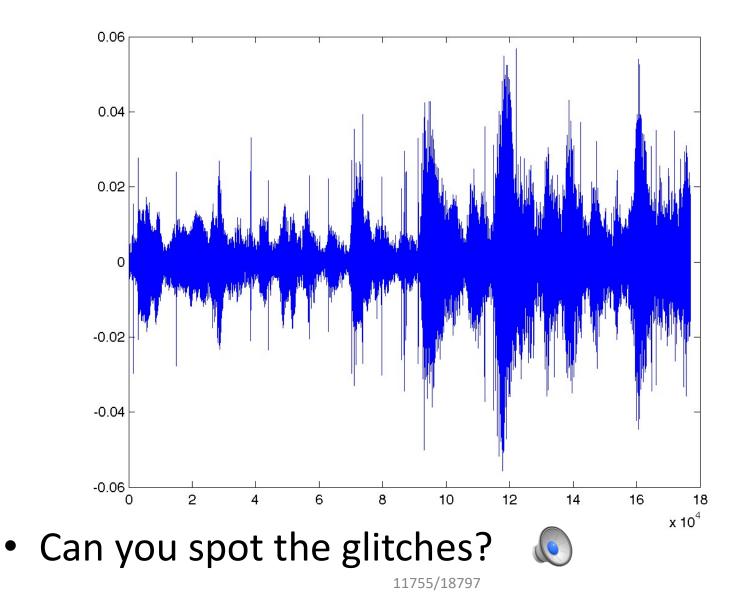


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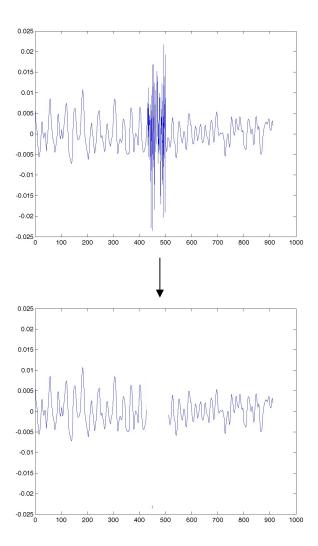
## **A Common Problem**





# 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?



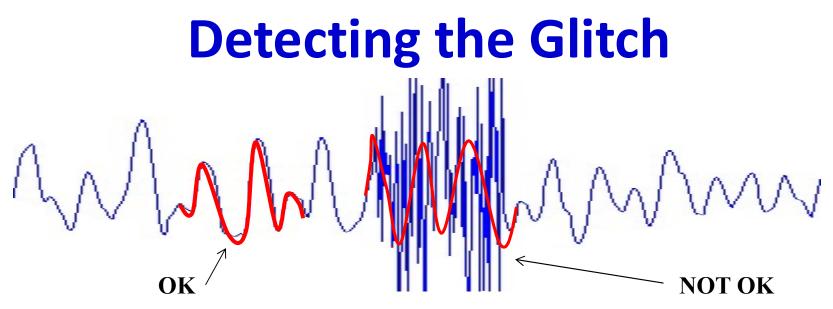


# Interpolation..

MAMMAM

- "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..





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



# 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

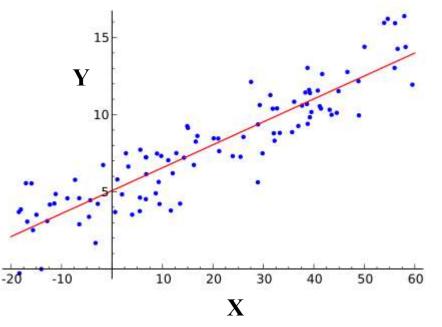


# **Regressions for prediction**

- $\mathbf{y} = \mathbf{f}(\mathbf{x}; \boldsymbol{\Theta}) + \mathbf{e}$
- Different possibilities
  - $-\mathbf{y}$  is a scalar
    - y is real
    - y is categorical (classification)
  - $-\mathbf{y}$  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

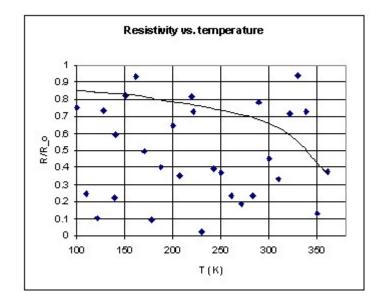


- Assumption: relationship between variables is linear
  - A linear *trend* may be found relating x and y
  - y = dependent variable
  - x = explanatory variable
  - Given x, y can be predicted as an affine function of x



# An imaginary regression..

- <u>http://pages.cs.wisc.edu/~kovar/hall.html</u>
- 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.

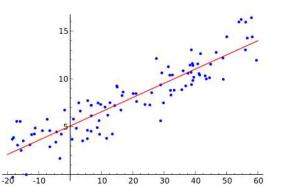
Christ, this was such a waste of my time.

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**

•  $\mathbf{y} = \mathbf{a}^{\mathrm{T}}\mathbf{x} + \mathbf{b} + \mathbf{e}$ -  $\mathbf{e}$  = prediction error



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

$$- y_{1} = a^{T}x_{1} + b + e_{1}$$
  
- y\_{2} = a^{T}x\_{2} + b + e\_{2}  
- y\_{3} = a^{T}x\_{3} + b + e\_{3}

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



#### Linear Regression to a scalar

$$y_1 = \mathbf{a}^{\mathrm{T}}\mathbf{x_1} + \mathbf{b} + \mathbf{e}_1$$
  

$$y_2 = \mathbf{a}^{\mathrm{T}}\mathbf{x_2} + \mathbf{b} + \mathbf{e}_2$$
  

$$y_3 = \mathbf{a}^{\mathrm{T}}\mathbf{x_3} + \mathbf{b} + \mathbf{e}_3$$

Define:

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

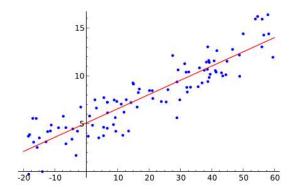
• Rewrite

$$\mathbf{y} = \mathbf{A}\mathbf{X} + \mathbf{e}$$



# Learning the parameters

$$\mathbf{y} = \mathbf{A}\mathbf{X} + \mathbf{e}$$

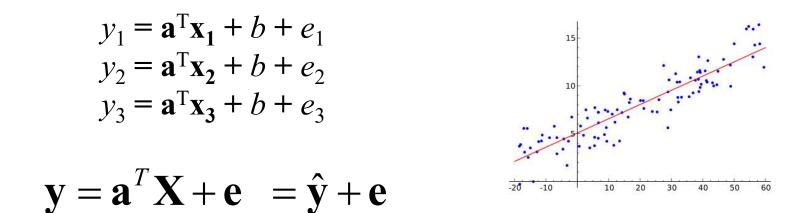


 $\hat{\mathbf{y}} = \mathbf{A}\mathbf{X}$  Assuming no error

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



#### The prediction error as divergence



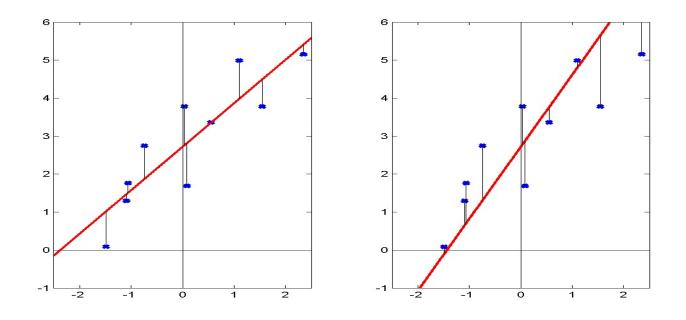
$$\mathbf{D}(\mathbf{y}, \hat{\mathbf{y}}) = \mathbf{E} = e_1^2 + e_2^2 + e_3^2 + \dots$$
  
=  $(y_1 - \mathbf{a}^T \mathbf{x}_1 - b)^2 + (y_2 - \mathbf{a}^T \mathbf{x}_2 - b)^2 + (y_3 - \mathbf{a}^T \mathbf{x}_3 - b)^2 + \dots$ 

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

• 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

$$\mathbf{E} = \parallel \mathbf{y} - \mathbf{A}\mathbf{X} \parallel^2$$

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



#### **More Explicitly**

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

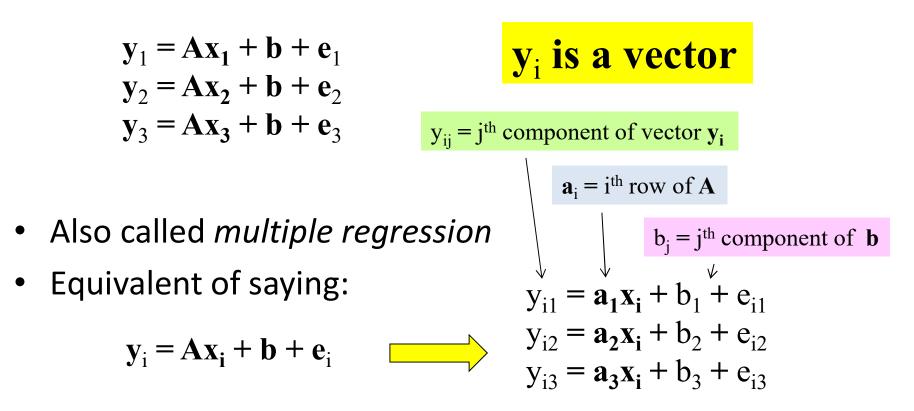
$$\mathbf{A} = \mathbf{y} pinv(\mathbf{X})$$

• X is wider than it is tall  $pinv(\mathbf{X}) = \mathbf{X}^T (\mathbf{X}\mathbf{X}^T)^{-1}$ 

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



#### **Regression in multiple dimensions**



- Fundamentally no different from *N* separate single regressions
  - But we can use the relationship between  $\mathbf{y}$ s to our benefit



#### **Multiple Regression**

• Minimizing

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



#### Aside: The Frobenius norm

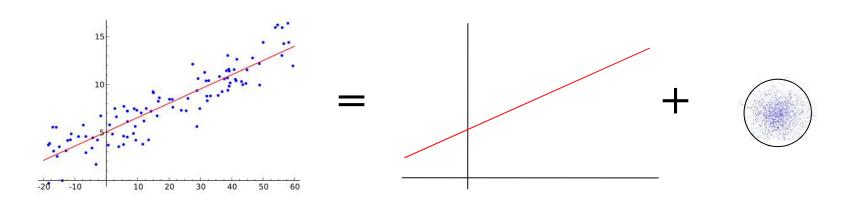
 The Frobenius norm is the square root of the sum of the squares of all the components of the matrix

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

• 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

$$\mathbf{y} = \mathbf{A}\mathbf{x} + \mathbf{e}$$

• Error e is Gaussian

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

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



#### The Likelihood of the data

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

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

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

Probability of collection:

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

• Assuming IID for convenience (not necessary)



#### A Maximum Likelihood Estimate

$$\mathbf{y} = \mathbf{A}^{T}\mathbf{x} + \mathbf{e} \quad \mathbf{e} \sim N(0, \sigma^{2}\mathbf{I}) \quad \mathbf{Y} = [\mathbf{y}_{1} \ \mathbf{y}_{2}...\mathbf{y}_{N}] \quad \mathbf{X} = [\mathbf{x}_{1} \ \mathbf{x}_{2}...\mathbf{x}_{N}]$$
$$P(\mathbf{Y} \mid \mathbf{X}) = \prod_{i} \frac{1}{\sqrt{(2\pi\sigma^{2})^{D}}} \exp\left(\frac{-1}{2\sigma^{2}} \left\|\mathbf{y}_{i} - \mathbf{A}^{T}\mathbf{x}_{i}\right\|^{2}\right)$$
$$\log P(\mathbf{Y} \mid \mathbf{X}; \mathbf{A}) = C - \sum_{i} \frac{1}{2\sigma^{2}} \left\|\mathbf{y}_{i} - \mathbf{A}\mathbf{x}_{i}\right\|^{2}$$

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

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



#### **Returning to Multiple Regression**

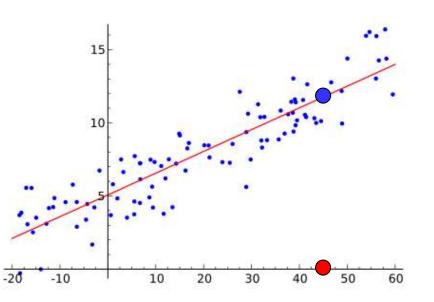
$$\mathbf{Y} = \begin{bmatrix} \mathbf{y}_1 \ \mathbf{y}_2 \ \mathbf{y}_3 \dots \end{bmatrix} \qquad \mathbf{X} = \begin{bmatrix} \mathbf{x}_1 \ \mathbf{x}_2 \ \mathbf{x}_3 \\ \mathbf{1} \ \mathbf{1} \ \mathbf{1} \ \mathbf{1} \end{bmatrix} \qquad \hat{\mathbf{A}} = \begin{bmatrix} \mathbf{A} & \mathbf{b} \end{bmatrix}$$
$$\mathbf{E} = \begin{bmatrix} \mathbf{e}_1 \ \mathbf{e}_2 \ \mathbf{e}_3 \dots \end{bmatrix} \qquad \mathbf{Y} = \hat{\mathbf{A}} \mathbf{X} + \mathbf{E}$$
$$DIV = \sum_i \left\| \mathbf{y}_i - \hat{\mathbf{A}} \overline{\mathbf{x}}_i \right\|^2 = \left\| \mathbf{Y} - \hat{\mathbf{A}} \mathbf{X} \right\|_F^2$$

• Minimizing

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



#### **Predicting an output**



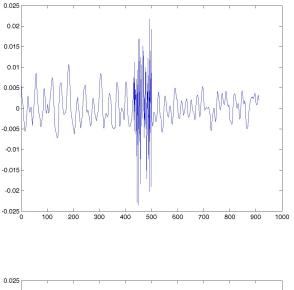
- From a collection of training data, have learned A
- Given **x** for a new instance, but not **y**, what is **y**?
- Simple solution:

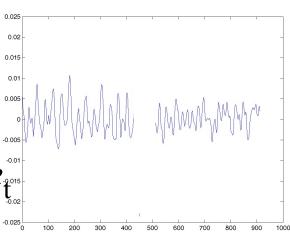
$$\hat{\mathbf{y}} = \mathbf{A}\mathbf{x} + \mathbf{b}$$



#### Applying it to our problem

- Prediction by regression
- Forward regression
- $x_t = a_1 x_{t-1} + a_2 x_{t-2} \dots a_k x_{t-k} + e_t$
- Backward regression
- $x_{t} = b_{1}x_{t+1} + b_{2}x_{t+2} \dots b_{k}x_{t+k} + e_{t}^{\text{OUT}}$







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#### Applying it to our problem

Forward prediction

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

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



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#### Applying it to our problem

Backward prediction

$$\begin{bmatrix} x_{t-K-1} \\ x_{t-K-2} \\ \vdots \\ x_{1} \end{bmatrix} = \begin{bmatrix} x_{t} & x_{t-1} & \vdots & x_{t-K} \\ x_{t-1} & x_{t-2} & \vdots & x_{t-K-1} \\ \vdots & \vdots & \vdots & \vdots \\ x_{K+1} & x_{K} & \vdots & x_{2} \end{bmatrix} \mathbf{b}_{t} + \begin{bmatrix} e_{t-K-1} \\ e_{t-K-2} \\ \vdots \\ e_{1} \end{bmatrix}$$

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

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



# Finding the burst

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



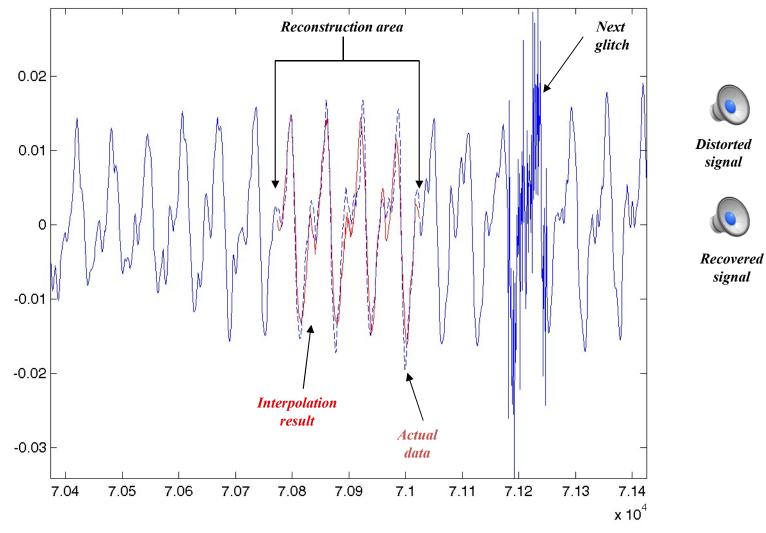
#### Filling the hole

MAMMM

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



#### **Reconstruction zoom in**



11/00/10/0/



#### **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

 $\hat{y}_t = (\mathbf{a}^t)$ 

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

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



#### **Predicting a value**

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

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

- What are we doing exactly?
  - For the explanation we are assuming no "b" (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
- $N^{-0.5} \mathbf{C}^{-0.5}$  is the *whitening* matrix for  $\mathbf{x}$

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



#### **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 (x<sub>i</sub>,y<sub>i</sub>) for *i* = 1..N, estimate y for a new test instance of x with unknown y :
- $\mathbf{y}$  is simply a weighted sum of the  $\mathbf{y}_i$  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..



# 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**<sup>T</sup> is invertible
- What if it is not
  - Dimensionality of X is greater than number of observations?
  - Underdetermined
- In this case  $\mathbf{X}^{\mathrm{T}}\mathbf{X}$  will generally be invertible

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



#### **High-dimensional regression**

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

• **X**<sup>T</sup>**X** 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  ${\bf Y}$  by the inverse of the gram matrix

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

• Working our way down..

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

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

#### Linear Regression in High-dimensional Spaces $\hat{\mathbf{y}} = \sum \ddot{\mathbf{y}}_i \mathbf{x}_i^T \mathbf{x}$ $\ddot{\mathbf{Y}} = \mathbf{Y} \mathbf{G}^{-1}$

- Given training instances (x<sub>i</sub>,y<sub>i</sub>) for *i* = 1..N, estimate y for a new test instance of x with unknown y :
- $\mathbf{y}$  is simply a weighted sum of the normalized  $\mathbf{y}_i$  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  $x_i$  and the new x

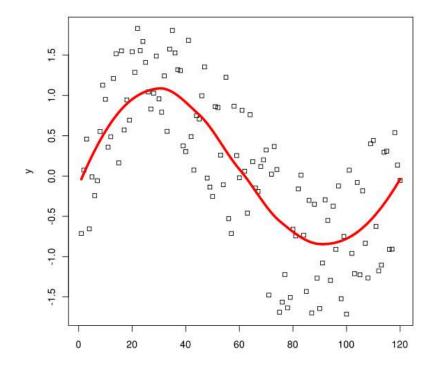


# **Topics**

- 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



0 0

#### **Non-linear regression**

• 
$$y = A\phi(x) + e$$
  
 $x \to \phi(x) = [\phi_1(x) \ \phi_2(x) \dots \phi_N(x)]$   
 $X \to \Phi(X) = [\phi(x_1) \ \phi(x_2) \dots \phi(x_K)]$ 

• 
$$\mathbf{Y} = \mathbf{A}\Phi(\mathbf{X}) + \mathbf{e}$$

Replace X with  $\Phi(X)$  in earlier equations for solution

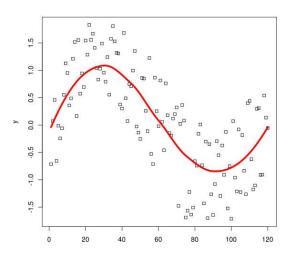
$$\mathbf{A} = \mathbf{Y} \Big( \Phi(\mathbf{X}) \Phi(\mathbf{X})^T \Big)^{\mathbf{1}} \Phi(\mathbf{X})^T$$



## Problem

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

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



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

$$\hat{\mathbf{y}} = \mathbf{A}\Phi(\mathbf{x}) = \mathbf{Y}(\Phi(\mathbf{X})\Phi(\mathbf{X})^T)^{-1}\Phi(\mathbf{X})^T\Phi(\mathbf{x}) = \mathbf{Y}\mathbf{G}^{-1}\Phi(\mathbf{X})^T\Phi(\mathbf{x})$$
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#### The regression is in high dimensions

• Linear regression:

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

• High-dimensional regression

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

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

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



### **Doing it with Kernels**

• High-dimensional regression with Kernels:

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

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

• Regression in Kernel Hilbert Space..

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

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



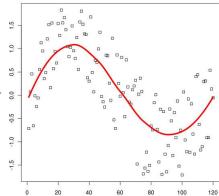
# **Topics**

- 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..

## A different way of finding nonlinear relationships: Locally linear regression

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

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



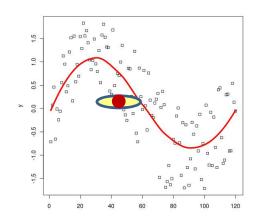
- Single global regression is estimated and applied to all future x
- Alternative: *Local regression*
- Learn a regression that is specific to **x**



#### 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

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

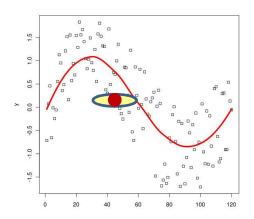
- Note : this regression is specific to x
  - A separate regression must be learned for every **x**



#### **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 x and x<sub>i</sub>
- If w() falls off rapidly with |x and x<sub>j</sub>| the "neighbhorhood" requirement can be relaxed

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



# $\hat{\mathbf{y}} = \frac{\sum_{i} K_{h}(\mathbf{x} - \mathbf{x}_{i}) \mathbf{y}_{i}}{\sum_{i} K_{h}(\mathbf{x} - \mathbf{x}_{i})}$

- 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 5/18797

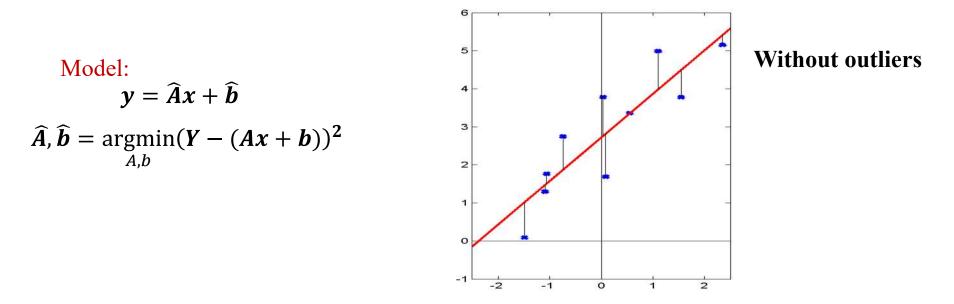


#### **Topics**

- 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..



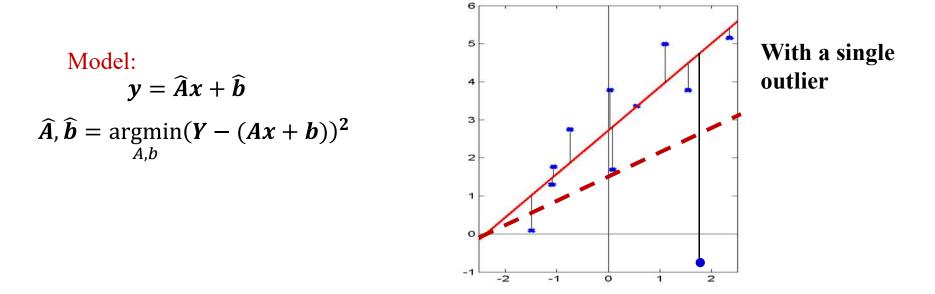
#### **Returning to Linear Regression**



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



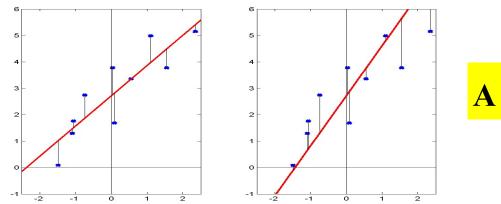
#### **Returning to Linear Regression**



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



#### A problem with regressions





- Least-squares fit is sensitive
  - Error is squared
  - Small variations in data  $\rightarrow$  large variations in weights
  - Outliers affect it adversely
- Unstable
  - If dimension of X >= no. of instances
    - (XX<sup>T</sup>) is not invertible

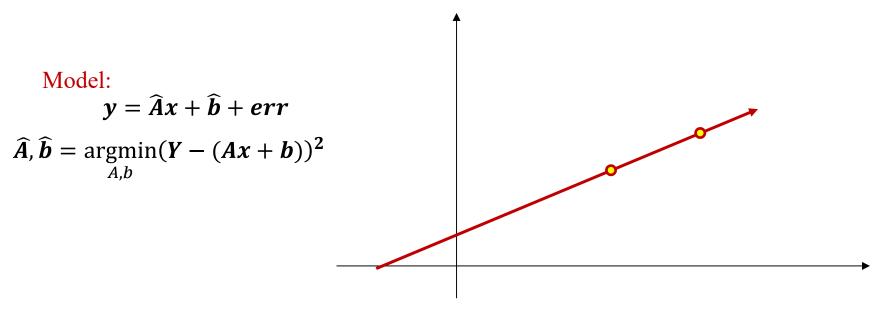


#### **Conservative solution**

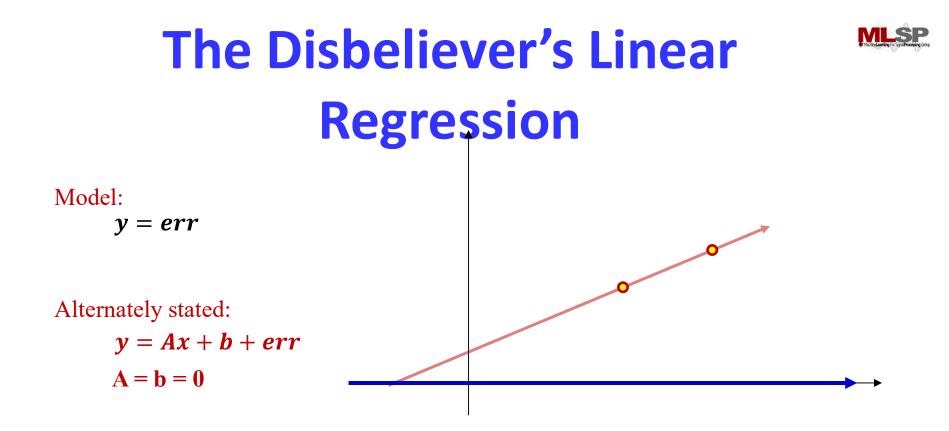
- Default: *Y* is extremely sensitive to *X* 
  - Results in large changes in regression estimate in response to small changes in input
- Alternate default assumption: *Y* does not depend on *X* 
  - Prediction is just a horizontal line at Y = 0
  - Useless
- Conservative Compromise: *Y* is *weakly* 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**

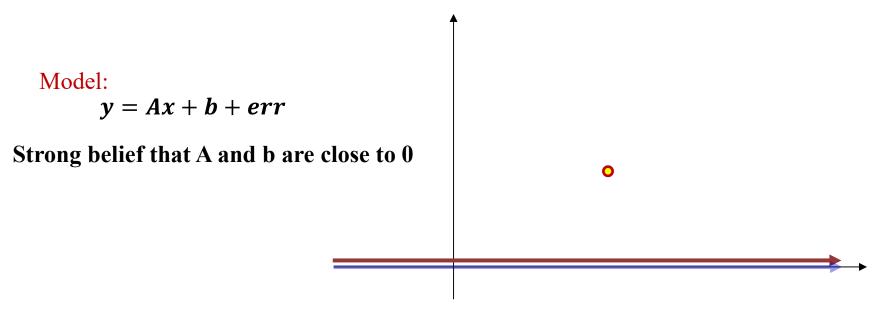


- Response of standard regression given only two training instances
  - Belief: Observed data tell the entire truth
    - Model completely fit to trends in data
    - A single point is a trend



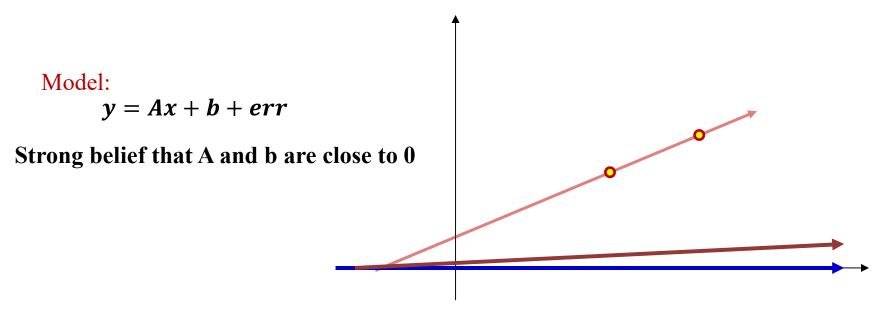
- All data are noise
  - The truth is that Y is a zero-mean random variable
  - The observed data are outcomes of noise variations





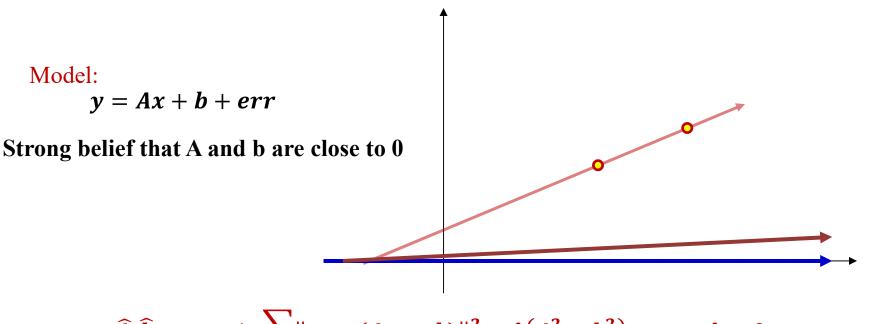
• After seeing only one point..





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

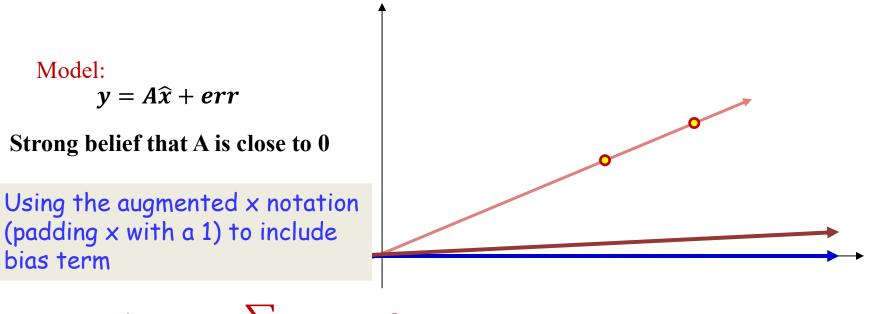




 $\widehat{A}, \widehat{b} = \underset{A,b}{\operatorname{argmin}} \sum_{i} ||y_i - (Ax_i + b)||^2 + \lambda (A^2 + b^2), \qquad \lambda > 0$ 

- 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





$$\widehat{A} = \underset{A}{\operatorname{argmin}} \sum_{i} ||y_{i} - A\widehat{x}_{i}||^{2} + \lambda ||A||_{F}^{2}, \qquad \lambda > 0$$

- 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

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

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

#### Other forms of regularization: L1 regularization

• An alternate regularization

$$\widehat{A} = \underset{A}{\operatorname{argmin}} \| Y - A \widehat{X} \|_{F}^{2} + \lambda |A|_{1}$$

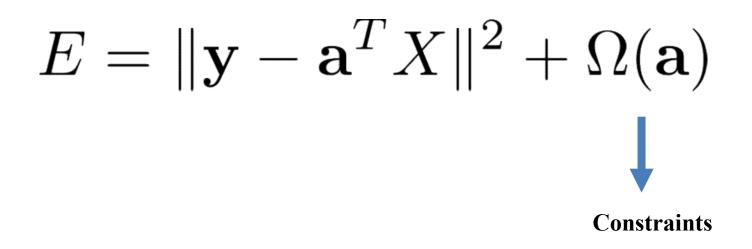
- The one-norm A<sub>1</sub> sums the magnitude of components of A
  - The minimization causes *A* to be *sparse*
- No closed form solution
  - Quadratic programming solutions required
- Dual formulation

$$\widehat{A} = \underset{A}{\operatorname{argmin}} \| Y - A \widehat{X} \|_{F}^{2}$$
 subject to  $|A|_{1} \leq t$ 

• "LASSO" – Least absolute shrinkage and selection operator



#### Regularization



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



#### **Map Estimation**

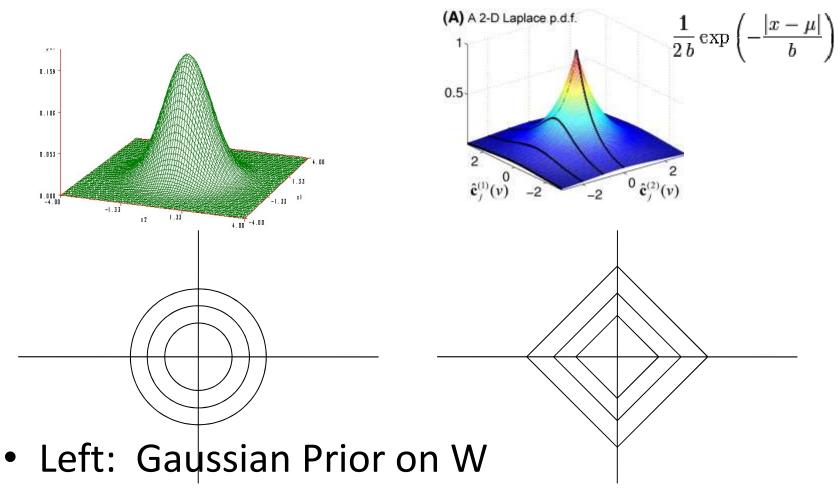
#### A Maximum Likelihood Estimator maximizes $\mathbb{P}(\text{data} \mid \text{parameters})$

#### 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**



• Right: Laplacian Prior



## **MAP estimate of weights** $dL = (2\mathbf{a}^T \mathbf{X} \mathbf{X}^T + 2\mathbf{y} \mathbf{X}^T + 2\mathbf{\sigma} \mathbf{I}) d\mathbf{a} = 0$ $\mathbf{a} = (\mathbf{X} \mathbf{X}^T + \mathbf{\sigma} \mathbf{I})^{-1} \mathbf{X} \mathbf{Y}^T$

- 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

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

Identical to L<sub>1</sub> regularized least-squares estimation



#### L<sub>1</sub>-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  $|\mathbf{a}|_1 \leq C'$ 

"LASSO" – Least absolute shrinkage and selection operator

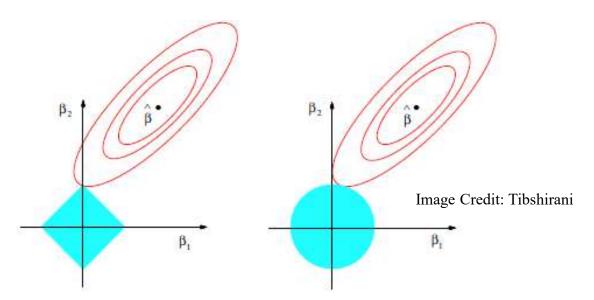


#### **LASSO Algorithms**

- 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
- L<sub>1</sub> regularization selects *sparsest* solution

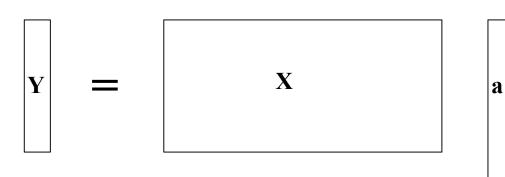


#### Next up..

Classification with linear regression models
 – AKA linear classifiers



#### LASSO and Compressive Sensing



- Given Y and X, estimate sparse 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?

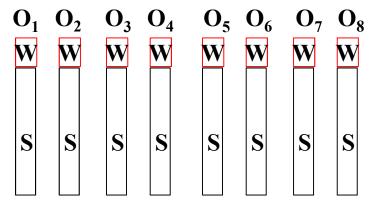


#### An interesting problem: Predicting War!

- 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