# **MLE & Regression**

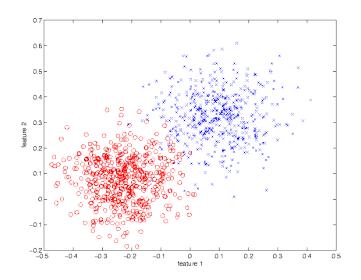
Nuno Vasconcelos (Ken Kreutz-Delgado)

**UCSD** 

# **Statistical Learning from Data**

• **Goal:** Given a relationship between a feature vector x and a vector y, and iid data samples  $(x_i, y_i)$ , find an approximating function  $f(x) \approx y$ 

$$f(\cdot) \qquad \hat{y} = f(x) \approx y$$



- This is called training or learning.
- Two major types of learning:
  - Unsupervised (aka Clustering) : only X is known.
  - Supervised (Classification or Regression): both X and target value Y are known during training, only X is known at test time.

# **Supervised Learning**

 Feature Vector X can be anything, but the type of Y dictates the type of supervised learning problem

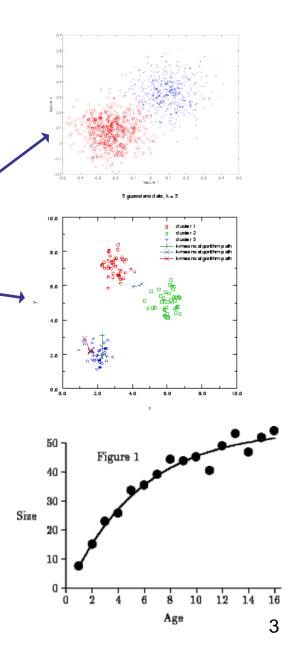
Y in {0,1} is referred to as detection

 Y in {0, ..., M-1} is referred to as (M-ary) classification

Y continuous is referred to as regression

 We have been dealing mostly with classification, now we will emphasize regression

 The regression problem provides a relatively easy setting to explain non-trivial MLE problems



# **The Standard Regression Model**

- The regression problem is usually modeled as follow:
  - The are two random vectors. The independent (regressor) variable
     X and the dependent (regressed) variable Y.
  - An iid dataset of training examples  $\mathcal{D} = \{(x_1, y_1), \dots, (x_n, y_n)\}$
  - An additive noise parametric model of the form

$$Y = f(X; \theta) + E$$

where  $\theta \in \Theta \subset \mathbb{R}^p$  is a deterministic parameter vector, and E is an iid additive random vector that accounts for noise and model error.

- Two fundamental types of regression problems
  - Linear regression, where f(.) is linear in  $\theta$
  - Nonlinear regression, otherwise
  - What matters is *linearity in the parameter*  $\theta$ , not in the data X!

# **Example Regression Models**

- Linear Regression:
  - Line Fitting

$$f(x;\theta) = \theta_1 x + \theta_0$$

Polynomial Fitting

$$f(x;\theta) = \sum_{i=0}^{k} \theta_i x^i$$

Truncated Fourier Series

$$f(x;\theta) = \sum_{i=0}^{k} \theta_i \cos(ix)$$

- Nonlinear Regression:
  - Neural Networks

$$f(x;\theta) = \frac{1}{1 + e^{-\theta_1 x - \theta_0}}$$

- Sinusoidal Decompositions

$$f(x;\theta) = \sum_{i=0}^{k} \cos(\theta_i x)$$

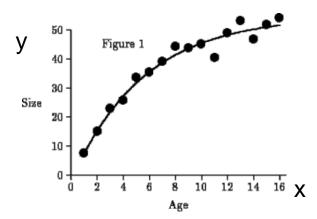
- Etc.
- We often assume that E is additive white Gaussian noise (AWGN)
- We always assume that E and X are independent

### Probabilistic Model of Y Conditioned on X

• A realization is X = x,  $E = \varepsilon$ , Y = y:

$$y = f(x; \theta) + \varepsilon$$

 x is always known, the goal is to predict y given x



- Thus, for each x,  $f(x,\theta)$  is treated like a constant
- The realization  $E = \varepsilon$  is added to  $f(x, \theta)$  to form Y = y
- Hence, Y is conditionally distributed as E but with a constant added
- This only changes the mean of the distribution of E,  $P_E(\varepsilon;\theta)$ , yielding

$$P_{Y|X}(y \mid x;\theta) = P_{E}(y - f(x;\theta);\theta)$$

- The conditional probability model for Y|X is determined from the distribution of the noise,  $P_E(\varepsilon;\theta)$ !

# The (Conditional) Likelihood Function

- Consider a collection of iid training points  $\mathcal{D} = \{(x_1, y_1), \dots, (x_n, y_n)\}$ . If we define  $\mathcal{X} = \{x_1, \dots, x_n\}$   $\mathcal{Y} = \{y_1, \dots, y_n\}$ , we have  $\mathcal{D} = \mathcal{X} \times \mathcal{Y}$ .
- Conditioned on X, the likelihood of  $\theta$  given  $\mathcal{D}$  is

$$\begin{aligned} P_{D|X}\left(\mathsf{D}\mid\mathsf{X};\theta\right) &= P_{\mathsf{Y}|X}\left(\mathsf{Y}\mid\mathsf{X};\theta\right) = \prod_{i=1}^{n} P_{\mathsf{Y}|X}\left(y_{i}\mid\mathsf{X};\theta\right) \\ &= \prod_{i=1}^{n} P_{\mathsf{Y}|X}\left(y_{i}\mid x_{i};\theta\right) = \prod_{i=1}^{n} P_{\mathsf{E}}\left(y_{i} - f(x_{i};\theta);\theta\right) \end{aligned}$$

- This is also the X-conditional likelihood of  $\theta$  given Y
- Note: we have used the facts that  $y_i$  is conditionally iid and depends only on  $x_i$  (both facts being a consequence of our modeling assumptions).

#### **Maximum Likelihood Estimation**

- This suggests that
  - Given a collection of iid training points  $\mathcal{D} = \{(x_1, y_1), ..., (x_n, y_n)\}$ , the natural procedure to estimate the parameter  $\theta$  is ML estimation:

$$\hat{\theta}_{\text{ML}} = \arg \max_{\theta \in \Theta} \prod_{i} P_{Y|X} (y_i | x_i; \theta)$$

$$= \arg \max_{\theta \in \Theta} \prod_{i} P_{E} (y_i - f(x_i; \theta); \theta)$$

#### Equivalently,

$$\begin{split} \hat{\theta}_{\text{ML}} &= \arg\max_{\theta \in \Theta} \sum_{i} \log P_{Y|X} \left( y_{i} \mid x_{i}; \theta \right) \\ &= \arg\max_{\theta \in \Theta} \sum_{i} \log P_{E} \left( y_{i} - f(x_{i}; \theta); \theta \right) \end{split}$$

### **AWGN MLE**

• One frequently used model is the *scalar AWGN* case where the noise is zero-mean with variance  $\sigma^2$ 

$$P_{\rm E}(\varepsilon) = \frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{\varepsilon^2}{2\sigma^2}}$$

• In this case the conditional pdf for Y|X is a Gaussian of mean  $f(x;\theta)$  and variance  $\sigma^2$ 

$$P_{Y|X}(y \mid x; \theta) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{\left(y - f(x; \theta)\right)^2}{2\sigma^2}\right\}$$

• If the variance  $\sigma^2$  is unknown, it is included in  $\theta$ 

#### **AWGN MLE**

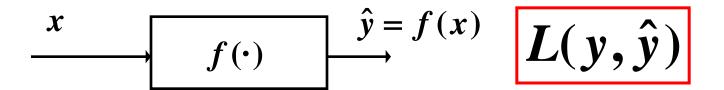
• Assume the variance  $\sigma^2$  is known. Then the MLE is:

$$\begin{split} \hat{\theta}_{\text{ML}} &= \arg\max_{\theta \in \Theta} \sum_{i} \log P_{\text{E}} \left( y_{i} - f(x_{i}; \theta) \right) \\ &= \arg\min_{\theta \in \Theta} \sum_{i} \frac{\left( y_{i} - f(x_{i}; \theta) \right)^{2}}{2\sigma^{2}} + \frac{1}{2} \log(2\pi\sigma^{2}) \\ &= \arg\min_{\theta \in \Theta} \sum_{i} \left( y_{i} - f(x_{i}; \theta) \right)^{2} \end{split}$$

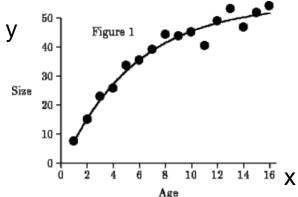
 Since this minimizes the squared Euclidean distance of the estimation error (or prediction error), it is also known as least squares curve fitting

# **MLE & Optimal Regression**

 The above development can be framed in our initial formulation of optimizing the loss of the learning system



- For a regression problem this still applies
  - the interpretation of f (.) as a predictor even becomes more intuitive
- Solving by ML is equivalent to picking a loss identical to the negative of the log of the noise probability density



### Loss for Scalar Noise with Known PDF

- Additive Error PDF:
  - Gaussian (AWGN case)

$$P_{\rm E}(\varepsilon) = \frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{\varepsilon^2}{2\sigma^2}}$$

Laplacian

$$P_{\rm E}(\varepsilon) = \frac{1}{2\sigma}e^{-\frac{|\varepsilon|}{\sigma}}$$

Rayleigh

$$P_{\rm E}(\varepsilon) = \frac{\varepsilon}{\sigma^2} e^{-\frac{\varepsilon^2}{2\sigma^2}}$$

• Loss,  $\varepsilon = (y - f(x; \theta))$ :

L<sub>2</sub> Distance

$$L(f(x;\theta),y) = (y - f(x;\theta))^2$$

− L₁ Distance

$$L(f(x;\theta),y) = |y-f(x;\theta)|$$

Rayleigh Distance

$$L(f(x;\theta),y) = (y - f(x;\theta))^{2}$$
$$-\log(y - f(x;\theta))$$

### **Maximum Likelihood Estimation**

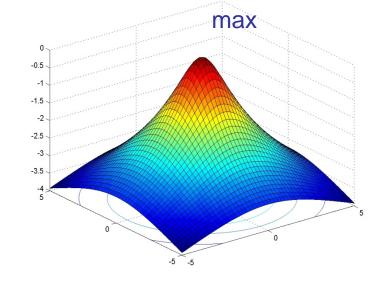
- How do we find the optimal parameters?
- Recall that to obtain the MLE we need to solve

$$\theta^* = \arg\max_{\theta \in \Theta} P_D(D;\theta)$$

 The unique local solutions are the parameter values such that

$$\frac{\partial}{\partial \theta} P_{D}(\mathsf{D}; \hat{\theta}) = \mathbf{0}$$

$$\theta^T H(D, \hat{\theta}) \theta < 0, \quad \forall \theta \neq 0$$



 Note that you always have to check the second-order Hessian condition!

### **Maximum likelihood Estimation**

#### Recall some important results

- FACT: each of the following is a necessary and sufficient condition for a real symmetric matrix A to be (strictly) positive definite:
  - i)  $x^T A x > 0, \forall x \neq 0$
  - ii) All eigenvalues of A are real and satisfy  $\lambda_i > 0$
  - iii) All upper-left submatrices  $A_k$  have strictly positive determinant. (strictly positive leading principal minors).
  - iv) There exists a matrix R with independent rows such that  $A = RR^T$ . Equivalently, there exists a matrix Q with independent columns such that  $A = Q^TQ$
- Definition of upper left submatrices:

$$A_1 = a_{1,1} \qquad A_2 = \begin{bmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{bmatrix} \qquad A_3 = \begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} \\ a_{2,1} & a_{2,2} & a_{2,3} \\ a_{3,1} & a_{3,2} & a_{3,3} \end{bmatrix} \qquad \cdots$$

### Matrix derivatives

- to compute the gradient and Hessian it is useful to rely on matrix derivatives
- some examples that we will use

$$\nabla_{\Theta}(A\Theta) = A^{T}$$

$$\nabla_{\Theta} (\Theta^T A \Theta) = (A + A^T) \Theta$$

$$\nabla_{\Theta} ||b - A\Theta||^2 = -2A^T (b - A\Theta)$$

- there are various lists of the most popular formulas
- one example is http://www.ee.ic.ac.uk/hp/staff/dmb/matrix/calculus.html

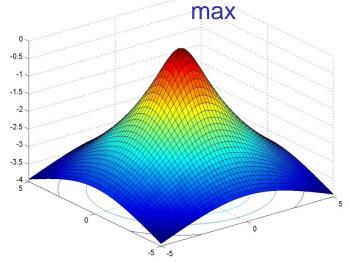
### Maximum likelihood

- returning to our problem
- to obtain ML estimate we need to solve

$$\Theta^* = \arg\max_{\Theta} P_X(D;\Theta)$$

 the solutions are the parameters such that

$$\nabla_{\Theta} P_{\chi}(\mathbf{X}; \mathbf{\Theta}) = 0$$



$$\theta^t \nabla_{\Theta}^2 P_X(x;\theta) \theta \le 0, \quad \forall \theta \in \mathbb{R}^n$$

note that you always have to check the second-order condition

### Maximum likelihood

for regression this becomes

$$\Theta^* = \underset{\Theta}{\operatorname{arg\,max}} \sum_{i} \log P_{Y|X}(y_i \mid x_i; \Theta)$$
$$= \underset{\Theta}{\operatorname{arg\,min}} \sum_{i} L(y_i, x_i; \Theta)$$

and the solution is given by

$$\nabla_{\Theta} \left[ \sum_{i} L(y_{i}, x_{i}; \Theta) \right] = 0$$

$$\theta^T \nabla_{\Theta}^2 \left[ \sum_i L(y_i, x_i; \Theta) \right] \theta \ge 0, \quad \forall \theta$$

### Maximum likelihood

- noting that the gradient and Hessian are linear operators (derivatives are linear)
- these can be written as

$$\sum_{i} \nabla_{\Theta} \big[ L(y_i, x_i; \Theta) \big] = 0$$

and

$$\theta^{T} \left[ \sum_{i} \nabla_{\Theta}^{2} L(y_{i}, x_{i}; \Theta) \right] \theta \geq 0, \quad \forall \theta$$

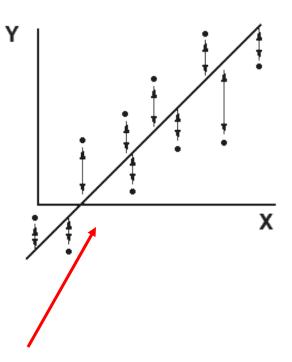
- Consider the problem of 2-D line fitting
  - The model is

$$y = f(x; \theta) + \varepsilon = \theta_1 x + \theta_0 + \varepsilon$$

where is  $\varepsilon$  is scalar AWGN of known variance

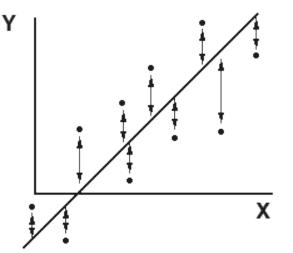
- The (effective) loss function is

$$\mathbf{L} = \sum_{i} (y_i - \theta_1 x_i - \theta_0)^2$$



- We are looking for the line that makes the square of these vertical distances as small as possible in an averaged sense.
- Our first step is to compute the zeros of the gradient
  - this amounts to solving a system of linear equations

$$\begin{cases} \frac{\partial L}{\partial \theta_0} = -2\sum_{i} (y_i - \theta_1 x_i - \theta_0) = 0 \\ \frac{\partial L}{\partial \theta_0} = -2\sum_{i} (y_i - \theta_1 x_i - \theta_0) x_i = 0 \end{cases}$$



$$\begin{cases} \sum_{i} y_{i} = \theta_{1} \sum_{i} x_{i} + n\theta_{0} \\ \sum_{i} y_{i} x_{i} = \theta_{1} \sum_{i} x_{i}^{2} + \theta_{0} \sum_{i} x_{i} \end{cases}$$

This can be written in matrix form as

$$\begin{bmatrix} \frac{1}{n} \sum_{i} y_{i} \\ \frac{1}{n} \sum_{i} y_{i} x_{i} \end{bmatrix} = \begin{bmatrix} 1 & \frac{1}{n} \sum_{i} x_{i} \\ \frac{1}{n} \sum_{i} x_{i} & \frac{1}{n} \sum_{i} x_{i}^{2} \end{bmatrix} \begin{bmatrix} \theta_{0} \\ \theta_{1} \end{bmatrix}$$

Defining the sample averaged quantities:

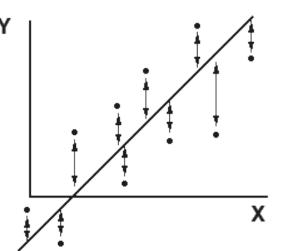
$$\overline{y} = \langle y \rangle = \frac{1}{n} \sum_{i} y_{i}, \quad \langle x^{k} \rangle = \frac{1}{n} \sum_{i} x_{i}^{k}, \quad \langle yx \rangle = \frac{1}{n} \sum_{i} y_{i} x_{i}$$

we get

$$\begin{bmatrix} \langle y \rangle \\ \langle xy \rangle \end{bmatrix} = \begin{bmatrix} 1 & \langle x \rangle \\ \langle x \rangle & \langle x^2 \rangle \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}$$

The solution is

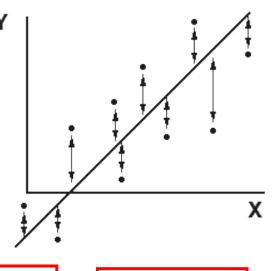
$$\begin{bmatrix} \hat{\theta}_{0} \\ \hat{\theta}_{1} \end{bmatrix}_{ML} = \begin{bmatrix} 1 & \langle x \rangle \\ \langle x \rangle & \langle x^{2} \rangle \end{bmatrix}^{-1} \begin{bmatrix} \langle y \rangle \\ \langle xy \rangle \end{bmatrix} \\
= \frac{1}{\langle x^{2} \rangle - \langle x \rangle^{2}} \begin{bmatrix} \langle x^{2} \rangle & -\langle x \rangle \\ -\langle x \rangle & 1 \end{bmatrix} \begin{bmatrix} \langle y \rangle \\ \langle xy \rangle \end{bmatrix} \\
= \frac{1}{\langle x^{2} \rangle - \langle x \rangle^{2}} \begin{bmatrix} \langle x^{2} \rangle \langle y \rangle - \langle x \rangle \langle xy \rangle \\ \langle xy \rangle - \langle x \rangle \langle y \rangle \end{bmatrix}$$



or, in a form that may be more familiar

$$\hat{\theta}_0 = \frac{1}{n} \sum_i y_i - \hat{\theta}_1 \frac{1}{n} \sum_i x_i$$

$$\hat{\theta}_1 = \frac{n\sum_i x_i y_i - \sum_i x_i \sum_j y_j}{n\sum_i x_i^2 - \left(\sum_i x_i\right)^2}$$



$$\hat{\theta}_1 = \frac{\overline{\text{cov}(x,y)}}{\overline{\text{var}(x)}}$$

$$\hat{\theta}_0 = \overline{y} - \hat{\theta}_1 \overline{x}$$

we also need to check that we have a minimum

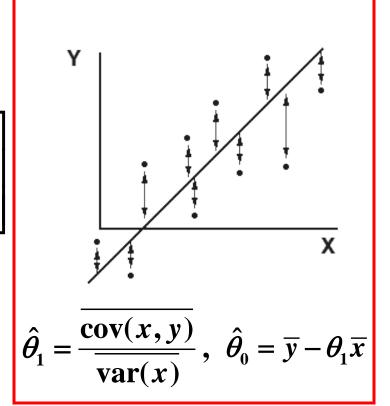
$$\frac{\partial L}{\partial \theta_0} = -2\sum_{i} (y_i - \theta_1 x_i - \theta_0) 
\frac{\partial L}{\partial \theta_1} = -2\sum_{i} (y_i - \theta_1 x_i - \theta_0) x_i \Rightarrow \frac{\partial^2}{\partial \theta^2} L = 2n \begin{bmatrix} 1 & \langle x \rangle \\ \langle x \rangle & \langle x^2 \rangle \end{bmatrix}$$
23

The Hessian

$$H(\hat{\theta}) = \frac{\partial^2}{\partial \theta^2} \mathbf{L}(\hat{\theta}) = 2n \begin{bmatrix} 1 & \langle x \rangle \\ \langle x \rangle & \langle x^2 \rangle \end{bmatrix}$$

has to be positive definite

 Recall that one of the criteria is for the leading principal minors to be strictly positive



$$-1>0$$

$$- \langle x^2 \rangle - \langle x \rangle^2 = \overline{\text{var}(x)} = \text{sample variance of } x > 0$$



### **Least Squares in General**

- What if I have other models?
- Can we solve this more generally?
  - Note that we can write the model

$$f(x;\theta) = \theta_1 x + \theta_0$$

as

$$f(x;\theta) = \gamma(x)^T \theta \qquad \gamma(x) = \begin{vmatrix} 1 \\ x \end{vmatrix} \qquad \theta = \begin{vmatrix} \theta_0 \\ \theta_1 \end{vmatrix}$$

$$\theta = \begin{bmatrix} \theta_0 \end{bmatrix}$$

• This can be generalized to any model if we exploit the assumption of linearity in the (k+1)-vector  $\theta$  to form

$$\gamma(x) = \begin{bmatrix} \gamma_0(x) \\ \vdots \\ \gamma_k(x) \end{bmatrix}, \quad \theta = \begin{bmatrix} \theta_0 \\ \vdots \\ \theta_k \end{bmatrix}$$

- Elements of  $\gamma(x)$  can be arbitrary non-linear functions of x
  - Line Fitting

$$f(x;\theta) = \theta_1 x + \theta_0$$

Polynomial Fitting

$$\gamma(x)^T = [1 \quad x]$$

$$f(x;\theta) = \sum_{i=0}^{k} \theta_i x^i$$

$$\gamma(x)^T = \begin{bmatrix} 1 & \cdots & x^k \end{bmatrix}$$

Truncated Fourier Series

$$f(x;\theta) = \sum_{i=0}^{k} \theta_i \cos(ix) \qquad \boxed{\gamma(x)^T = \begin{bmatrix} 1 & \cdots & \cos(kx) \end{bmatrix}}$$

$$\gamma(x)^T = \begin{bmatrix} 1 & \cdots & \cos(kx) \end{bmatrix}$$

# **Least Squares Parameter Estimation**

 For scalar iid AWGN of known variance, we have the (unweighted) least squares loss function

$$L = \sum_{i} (y_i - \theta_1 x_i - \theta_0)^2$$

which we can write as

$$\mathbf{L} = \sum_{i} \left( y_{i} - \gamma (x_{i})^{T} \theta \right)^{2}$$

• or

$$\mathbf{L} = \|\mathbf{y} - \mathbf{\Gamma}(\mathbf{x})\boldsymbol{\theta}\|^2$$

X

where

$$y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \qquad \Gamma(x) = \begin{bmatrix} \gamma(x_1)^T \\ \vdots \\ \gamma(x_n)^T \end{bmatrix} \qquad \theta = \begin{bmatrix} \theta_0 \\ \vdots \\ \theta_k \end{bmatrix}$$

- The most important component is the matrix  $\Gamma(x)$ 
  - Line Fitting

$$\Gamma(x) = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}$$

- Polynomial Fitting

$$\Gamma(x) = \begin{bmatrix} 1 & \cdots & x_1^k \\ \vdots & \ddots & \vdots \\ 1 & \cdots & x_n^k \end{bmatrix}$$

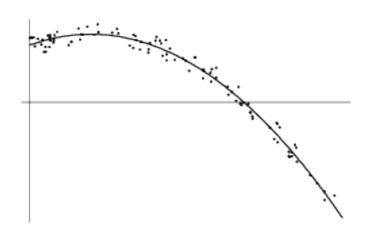
Truncated Fourier Series

$$\Gamma(x) = \begin{bmatrix} 1 & \cdots & \cos(k x_1) \\ \vdots & \ddots & \vdots \\ 1 & \cdots & \cos(k x_n) \end{bmatrix}$$

## Least squares

in summary, we always have

$$L = \|y - \Gamma(x)\Theta\|^2$$



 to minimize this we simply have to find x such that

$$\nabla_{\Theta} L = -2\Gamma(x)^T [y - \Gamma(x)\Theta] = 0$$

or

$$\Gamma(x)^T \Gamma(x) \Theta = \Gamma(x)^T y$$

from which, as long as  $\Gamma(x)^T\Gamma(X)$  is invertible,

$$\Theta^* = \left[ \Gamma(x)^T \Gamma(x) \right]^{-1} \Gamma(x)^T y$$

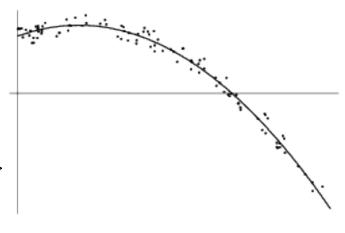
### Least squares

we next check the Hessian

$$\nabla_{\Theta}^{2} L = \nabla_{\Theta} (\nabla_{\Theta} L)$$

$$= -2\nabla_{\Theta} \{ \Gamma(x)^{T} [y - \Gamma(x)\Theta] \}$$

$$= 2\Gamma(x)^{T} \Gamma(x)$$

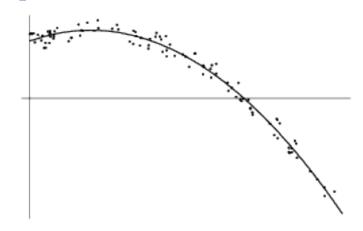


- this is positive definite if the rows of  $\Gamma(x)$  are independent
- which turns out to be
  - the condition for  $\Gamma(x)^T\Gamma(X)$  to be invertible,
  - which is the necessary condition for the solution to be feasible
- note that we design  $\Gamma(x)$ , so we can always make this happen
- usually we only have to make sure all the x<sub>i</sub> are different

# (Unweighted) Least Squares

- In summary
  - A problem of the type

$$\min_{\theta} \mathbf{L}(\theta) = \|y - \Gamma(x)\theta\|^2$$



has a least squares solution

$$\hat{\theta}_{LS} = \left[ \Gamma(x)^T \Gamma(x) \right]^{-1} \Gamma(x)^T y = \Gamma(x)^+ y$$

iff  $\Gamma(x)$  has full column rank.

The matrix

$$\Gamma(x)^{+} = \left[\Gamma(x)^{T} \Gamma(x)\right]^{-1} \Gamma(x)^{T}$$

# (Unweighted) Least Squares

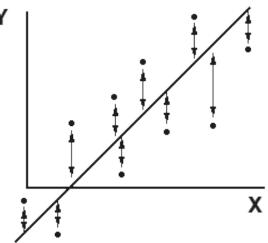
- Here is a way of thinking about this
  - we have an inconsistent system of equations

$$y \approx \Gamma(x)\theta$$

This can't be solved because although  $\Gamma(x)$  has full (column) rank, it is "tall" (has more rows than columns) and thus is not invertible

E.g. consider the line

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \approx \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}$$



- To make a consistent system, we multiply both sides by  $\Gamma(x)^T$ 

$$\Gamma(x)^T y = \Gamma(x)^T \Gamma(x) \theta$$

# (Unweighted) Least Squares

This is now a solvable system. E.g.,

$$\begin{bmatrix} 1 & \dots & 1 \\ x_1 & \dots & x_n \end{bmatrix} \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & \dots & 1 \\ x_1 & \dots & x_n \end{bmatrix} \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}$$

whose solution is given by the pseudo-inverse

$$\hat{\theta}_{LS} = \Gamma^{+}(x)y = \left[\Gamma(x)^{T}\Gamma(x)\right]^{-1}\Gamma(x)^{T}y$$

We have just seen that this is the best approximate solution to the original problem in the (unweighted) least squares sense

$$\hat{\theta}_{LS} = \arg\min_{\theta \in \Theta} ||y - \Gamma(x)\theta||^2$$

## (Unweighted) Least squares

- In principle, assuming that the matrix  $\Gamma(x)$  has full column rank, the least squares solution is straightforward to compute
- For example, let's redo the line example

$$\Gamma(x)^{T} \Gamma(x) = \begin{bmatrix} 1 & \dots & 1 \\ x_{1} & \dots & x_{n} \end{bmatrix} \begin{bmatrix} 1 & x_{1} \\ \vdots & \vdots \\ 1 & x_{n} \end{bmatrix} = n \begin{bmatrix} 1 & \langle x \rangle \\ \langle x \rangle & \langle x^{2} \rangle \end{bmatrix}$$

$$\Gamma(x)^{T} y = \begin{bmatrix} 1 & \dots & 1 \\ x_{1} & \dots & x_{n} \end{bmatrix} \begin{vmatrix} y_{1} \\ \vdots \\ y_{n} \end{vmatrix} = n \begin{bmatrix} \langle y \rangle \\ \langle xy \rangle \end{bmatrix}$$

# (Unweighted) Least squares

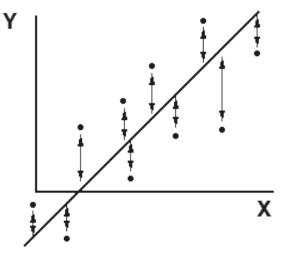
So that

$$\hat{\theta}_{LS} = \Gamma^{+}(x) = \left[\Gamma(x)^{T} \Gamma(x)\right]^{-1} \Gamma(x)^{T} y$$

leads to

$$\begin{bmatrix}
\hat{\theta}_{0} \\
\hat{\theta}_{1}
\end{bmatrix}_{LS} = \begin{bmatrix}
1 & \langle x \rangle \\
\langle x \rangle & \langle x^{2} \rangle
\end{bmatrix}^{-1} \begin{bmatrix} \langle y \rangle \\
\langle xy \rangle
\end{bmatrix}$$

$$= \frac{1}{\langle x^{2} \rangle - \langle x \rangle^{2}} \begin{bmatrix} \langle x^{2} \rangle \langle y \rangle - \langle x \rangle \langle xy \rangle \\
\langle xy \rangle - \langle x \rangle \langle y \rangle
\end{bmatrix}$$

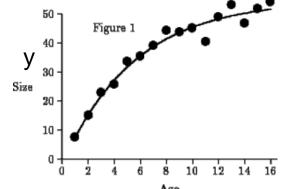


which is the solution that we had obtained before, but now with less work. Of course, we know from ECE174 that there is a deep geometric formalism at play here.

# Relationship to Probabilistic Model

- The (unweighted) least square solution
  - Estimates the function  $f(x; \theta)$  of maximum likelihood for the scalar model

$$y = f(x;\theta) + \varepsilon$$



- where  $\varepsilon$  is a scalar iid zero-mean Gaussian error (AWGN) of known variance,

$$P_{\rm E}(\varepsilon) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{\varepsilon^2}{2\sigma^2}}$$

- The method is general
- Other models  $f(x,\theta)$  will lead to other least squares problems
- If variance is unknown, we don't have a pure LS problem
- If we have a vector model, in general we have weighted LS
- If the error is not Gaussian, problem is not least squares.

X

# **END**