ELEC2146

Electrical Engineering Modelling and Simulation

Least Squares

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Least Squares

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Lecture notes written by Dr Julien Epps

Overview

- Motivation
- Error minimisation
- Polynomial form for LS
- General form for LS
- Linearization
- Multivariate LS
- Nonlinear LS
- Gradient descent

Motivation

- Consider:

  $y = c_1 x$

x	$y = f(x)$
-1	-3
2	6
3	9

- An exact solution exists: $c_1 = 3$

- What about:

x	$y = f(x)$
-1	-4
2	3
3	7

- No exact solution exists
  - Overdetermined
  - What kind of approximate solution should we look for ?

Motivation

- Common problem in modelling:
  - Have data from an experiment
    - Maybe inputs and outputs at different times, or for different conditions
    - Often have a reasonable amount of data $\rightarrow$ overdetermined equations
  - Have some hypothesis about the model structure
    - e.g. polynomial, sum of sinusoids, mixture of Gaussians etc
  - Want to use the data and assumed model structure to estimate the model parameters
  - More later on…
    - Model structure
    - Parameter estimation

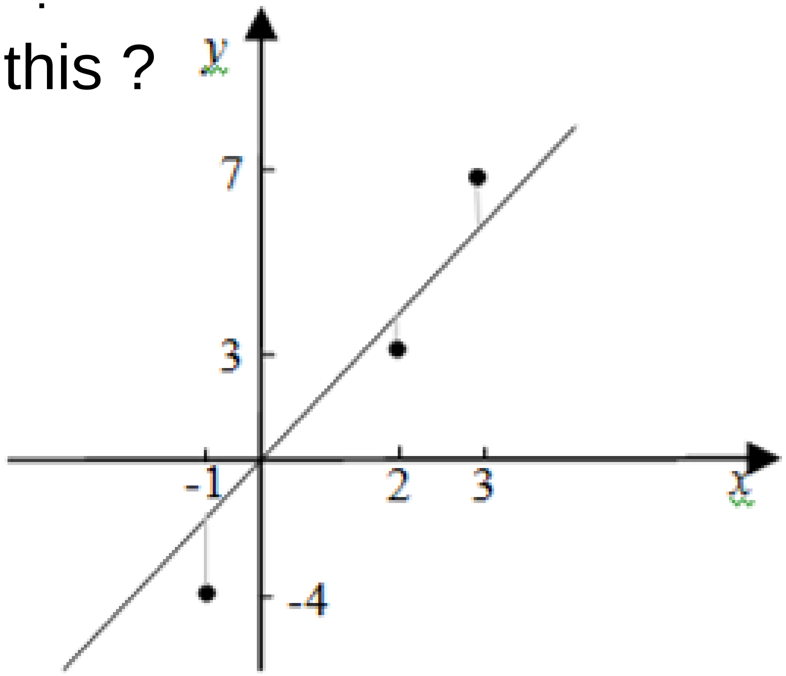
Error Minimisation

- Look for a solution to

$$y = c_1 x + \varepsilon$$

  - ε : error
  - "Smaller" $\varepsilon \Rightarrow$ better solution
    - But what do we mean by "small" ?
  - Also, how do we minimise this ?
  - From our example,

$$\boldsymbol{\varepsilon} = \begin{bmatrix} -4 \\ 3 \\ 7 \end{bmatrix} - c_1 \begin{bmatrix} -1 \\ 2 \\ 3 \end{bmatrix}$$



Error Minimisation

- Could try to minimise

$$|\boldsymbol{\varepsilon}| = \sum_{i=1}^{3} |\varepsilon_i| = \sum_{i=1}^{3} |y_i - c_1 x_i|$$

  - Sum of absolute errors

  - Introduces a nonlinearity in ε
    - Not very convenient
    - Piecewise linear

Error Minimisation

- Could try to minimise $\|\boldsymbol{\varepsilon}\|$ or $\|\boldsymbol{\varepsilon}\|^2$

$$\|\boldsymbol{\varepsilon}\|^2 = \sum_{i=1}^{3} \varepsilon_i^2 = \sum_{i=1}^{3} (y_i - c_1 x_i)^2 = (-4 + c_1)^2 + (3 - 2c_1)^2 + (7 - 3c_1)^2$$

  – Sum of squared errors
    - Larger errors are weighted more heavily than small ones

  – Conveniently, $\|\boldsymbol{\varepsilon}\|^2$ is a quadratic function of c_1, with a unique minimum

Error Minimisation

- Let's find the minimum:

$$\frac{d\|\boldsymbol{\varepsilon}\|^2}{dc_1} = 0$$

$$\frac{d\|\boldsymbol{\varepsilon}\|^2}{dc_1} = -8 + 2c_1 - 12 + 8c_1 - 42 + 18c_1$$

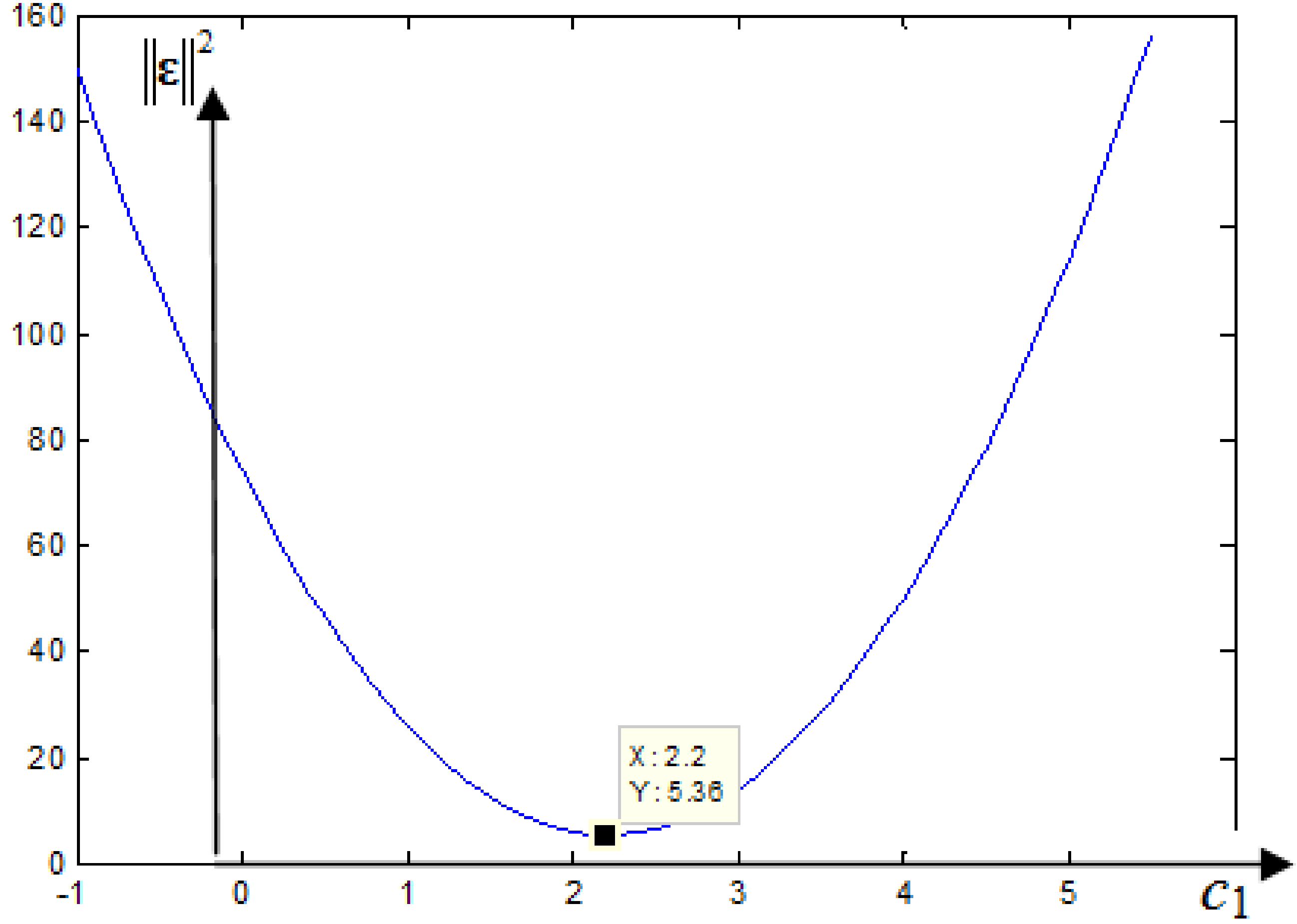
$$= -62 + 28c_1 = 0$$

$$c_1 = \frac{31}{14}$$

  - Error at this point is $\|\boldsymbol{\varepsilon}\|^2 = 5.357$

Error Minimisation

- Graphically:



LS: Polynomial Form

- Consider fitting:

$$y = c_n x^n + c_{n-1} x^{n-1} + \ldots + c_0$$

  - To some data $\{x_1, x_2, \ldots, x_m\}, \{y_1, y_2, \ldots, y_m\}$

$$y_1 = c_n x_1^n + c_{n-1} x_1^{n-1} + \ldots + c_0 + \varepsilon_1$$
$$y_2 = c_n x_2^n + c_{n-1} x_2^{n-1} + \ldots + c_0 + \varepsilon_2$$
$$\vdots$$
$$y_m = c_n x_m^n + c_{n-1} x_m^{n-1} + \ldots + c_0 + \varepsilon_m$$

LS: Polynomial Form

- Matrix-Vector form:

$$\mathbf{y} = \mathbf{X}\mathbf{c} + \boldsymbol{\varepsilon}$$

$$\mathbf{y} = \begin{bmatrix} y_1 & y_2 & \cdots & y_m \end{bmatrix}^T, \quad \mathbf{X} = \begin{bmatrix} x_1^n & x_1^{n-1} & \dots & 1 \\ x_2^n & x_2^{n-1} & \dots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ x_m^n & x_m^{n-1} & \dots & 1 \end{bmatrix},$$

$$\mathbf{c} = \begin{bmatrix} c_n & c_{n-1} & \cdots & c_0 \end{bmatrix}^T, \quad \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_1 & \varepsilon_2 & \cdots & \varepsilon_m \end{bmatrix}^T$$

  – $\mathbf{y} = \mathbf{X}\mathbf{c}$ is a model for the data, **c** are the parameters and $\boldsymbol{\varepsilon}$ are the model errors

LS: Polynomial Form

- Rearranging:

$$\boldsymbol{\varepsilon} = \mathbf{y} - \mathbf{X}\mathbf{c},$$

- In matrix-vector form,

$$\|\boldsymbol{\varepsilon}\|^2 = \boldsymbol{\varepsilon}^T \boldsymbol{\varepsilon}$$

  – so

$$\begin{aligned}\|\boldsymbol{\varepsilon}\|^2 &= \boldsymbol{\varepsilon}^T \boldsymbol{\varepsilon} = (\mathbf{y} - \mathbf{X}\mathbf{c})^T (\mathbf{y} - \mathbf{X}\mathbf{c}) \\ &= \mathbf{y}^T \mathbf{y} - (\mathbf{X}\mathbf{c})^T \mathbf{y} - \mathbf{y}^T \mathbf{X}\mathbf{c} + (\mathbf{X}\mathbf{c})^T (\mathbf{X}\mathbf{c})\end{aligned}$$

LS: Polynomial Form

- Derivative wrt c_n:

$$\frac{\partial \|\boldsymbol{\varepsilon}\|^2}{\partial c_n} = -\begin{bmatrix} x_1^n & x_2^n & \dots & x_m^n \end{bmatrix}\mathbf{y} - \mathbf{y}^T \begin{bmatrix} x_1^n \\ x_2^n \\ \vdots \\ x_m^n \end{bmatrix} + 2\sum_{i=1}^{m} (x_i^n)^2 c_n$$

$$= -2\begin{bmatrix} x_1^n & x_2^n & \dots & x_m^n \end{bmatrix}\mathbf{y} + 2\begin{bmatrix} x_1^n & x_2^n & \dots & x_m^n \end{bmatrix} \begin{bmatrix} x_1^n \\ x_2^n \\ \vdots \\ x_m^n \end{bmatrix} c_n$$

LS: Polynomial Form

- Set derivative of error vector to zero:

$$\begin{bmatrix} \dfrac{\partial\|\boldsymbol{\varepsilon}\|^2}{\partial c_n} \\ \dfrac{\partial\|\boldsymbol{\varepsilon}\|^2}{\partial c_{n-1}} \\ \vdots \\ \dfrac{\partial\|\boldsymbol{\varepsilon}\|^2}{\partial c_0} \end{bmatrix} = -2\mathbf{X}^T\mathbf{y} + 2\mathbf{X}^T\mathbf{X}\mathbf{c} = \mathbf{0}$$

$$\hat{\mathbf{c}} = [\mathbf{X}^T\mathbf{X}]^{-1}\mathbf{X}^T\mathbf{y}$$

  – General least squares estimate of **c**
    - Vector of polynomial coefficients

LS: Polynomial Form

- Some notes:
  - Using $\hat{\mathbf{c}}$, we can estimate *y* values for given *x* values

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\mathbf{c}}$$

    - Prediction
  - LS assumes a Gaussian distribution of the data

$$\{y_1, y_2, \ldots, y_m\}$$

    about the true *y*-values at the respective points
    - Not often true in practise
  - LS is a very popular method
    - Leads to a simple and optimal (sum of squared error) solution

MSE and SSE

- Important quantities:
  - The mean-square error (MSE):

$$MSE = \frac{1}{m}\sum_{i=1}^{m}(\hat{y}_i - y_i)^2$$

    - Average of squared errors between original y_i and estimated $\hat{y}_i$

  - The sum of squared errors (SSE):

$$SSE = \sum_{i=1}^{m}(\hat{y}_i - y_i)^2$$

Linear Regression

- Special case: n = 1

$$\mathbf{c} = [\mathbf{X}^T \mathbf{X}]^{-1} \mathbf{X}^T \mathbf{y}$$

$$= \left[\begin{bmatrix} x_1 & x_2 & \cdots & x_m \\ 1 & 1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_m & 1 \end{bmatrix} \right]^{-1} \begin{bmatrix} x_1 & x_2 & \cdots & x_m \\ 1 & 1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}^T$$

$$= \begin{bmatrix} \sum_{i=1}^{m} x_i^2 & \sum_{i=1}^{m} x_i \\ \sum_{i=1}^{m} x_i & m \end{bmatrix}^{-1} \begin{bmatrix} \sum_{i=1}^{m} x_i y_i \\ \sum_{i=1}^{m} y_i \end{bmatrix}$$

Linear Regression

- Special case: $n = 1$

$$= \frac{1}{m\sum_{i=1}^{m} x_i^2 - \left(\sum_{i=1}^{m} x_i\right)^2} \begin{bmatrix} m & -\sum_{i=1}^{m} x_i \\ -\sum_{i=1}^{m} x_i & \sum_{i=1}^{m} x_i^2 \end{bmatrix} \begin{bmatrix} \sum_{i=1}^{m} x_i y_i \\ \sum_{i=1}^{m} y_i \end{bmatrix}$$

$$\begin{bmatrix} c_1 \\ c_0 \end{bmatrix} = \frac{1}{m\sum_{i=1}^{m} x_i^2 - \left(\sum_{i=1}^{m} x_i\right)^2} \begin{bmatrix} m\sum_{i=1}^{m} x_i y_i - \sum_{i=1}^{m} x_i \sum_{i=1}^{m} y_i \\ \sum_{i=1}^{m} x_i^2 \sum_{i=1}^{m} y_i - \sum_{i=1}^{m} x_i \sum_{i=1}^{m} x_i y_i \end{bmatrix}$$

LS General Form

- So far:
  - We looked at polynomial fitting
  - LS is applicable to fitting data of the form

$$y(x) = c_0 f_0(x) + c_1 f_1(x) + \ldots + c_n f_n(x)$$

  - Much more general
    - Many models have this form
  - LS useful in a huge range of applications

LS General Form

- Matrix-Vector form:

$$\mathbf{y} = \mathbf{X}\mathbf{c} + \boldsymbol{\varepsilon}$$

$$\mathbf{y} = \begin{bmatrix} y_1 & y_2 & \cdots & y_m \end{bmatrix}^T, \quad \mathbf{X} = \begin{bmatrix} f_0(x_1) & f_1(x_1) & \dots & f_n(x_1) \\ f_0(x_2) & f_1(x_2) & \dots & f_n(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ f_0(x_m) & f_1(x_m) & \dots & f_n(x_m) \end{bmatrix},$$

$$\mathbf{c} = \begin{bmatrix} c_0 & c_1 & \cdots & c_n \end{bmatrix}^T, \quad \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_1 & \varepsilon_2 & \cdots & \varepsilon_m \end{bmatrix}^T$$

$$\hat{\mathbf{c}} = [\mathbf{X}^T\mathbf{X}]^{-1}\mathbf{X}^T\mathbf{y}$$

LS General Form

- Sum form:
  - Sum of squared errors:

$$\|\boldsymbol{\varepsilon}\|^2 = \sum_{i=1}^{m} \left(\sum_{j=0}^{n} c_j f_j(x_i) - y_i \right)^2$$

$$\frac{\partial \|\boldsymbol{\varepsilon}\|^2}{\partial c_k} = 2 \sum_{i=1}^{m} f_k(x_i) \left(\sum_{j=0}^{n} c_j f_j(x_i) - y_i \right) = 0, \quad k = 0,1,\ldots,n$$

$$\sum_{j=0}^{n} c_j \left(\sum_{i=1}^{m} f_j(x_i) f_k(x_i) \right) = \sum_{i=1}^{m} f_k(x_i) y_i, \quad k = 0,1,\ldots,n$$

  - The normal equations

Weighted LS

- Possible to weight contribution of data:
  – Sum of squared errors becomes:

$$\|\boldsymbol{\varepsilon}\|^2 = \sum_{i=1}^{m} w_i \left(\sum_{j=0}^{n} c_j f_j(x_i) - y_i \right)^2$$

  – Derivation is similar
  – Normal equations similar, but include weight terms

Linearisation

- LS general form is great, but . . .
  - What if the equation (model) is not linear in c_j ?
  - Make it linear in terms of some other constants

$$y = ax^b \quad \rightarrow \quad \ln y = \ln a + b \ln x$$

$$y = ae^{bx} \quad \rightarrow \quad \ln y = \ln a + bx$$

$$y = \frac{ax}{b+x} \quad \rightarrow \quad \frac{1}{y} = \frac{b}{ax} + \frac{1}{a}$$

$$y = \frac{a}{b+x} \quad \rightarrow \quad \frac{1}{y} = \frac{b}{a} + \frac{x}{a}$$

LS General Form

- So far:
  - Only functions of one variable (*x*)
  - LS is applicable to linear combination of several variables

$$y(x_1,\ldots,x_n) = c_0 + c_1 x_1 + \ldots + c_n x_n$$

    - e.g. matrix multiplication, where matrix is unknown
  - Or linear combinations of functions of multiple variables

$$y(x_1,\ldots,x_p) = c_0 f_0(x_1,\ldots,x_p) + c_1 f_1(x_1,\ldots,x_p) + \ldots + c_n f_n(x_1,\ldots,x_p)$$

Nonlinear Least Squares

- So far:
  - Forms that are linear in the c_k, or could be linearised
  - What if the model is nonlinear in the parameters (c_k) ?
  - Nonlinear relations of the form

$$y = f(x, c_0, c_1, ..., c_n)$$

  - Start with an initial estimate of c_k: $\tilde{c}_k$
  - Evaluate

$$\hat{y}_i = f(x_i, \tilde{c}_0, \tilde{c}_1, ..., \tilde{c}_n)$$

Nonlinear Least Squares

– Define the error between true value and estimates as

$$\Delta\beta_i = y_i - \hat{y}_i$$

– Model the variation of $y = f(x, c_0, c_1, \ldots, c_n)$ about each data point due to each c_k using a first-order Taylor Series:

$$f(x_i, c_0, c_1, \ldots, c_n) \approx f(x_i, \tilde{c}_0, \tilde{c}_1, \ldots, \tilde{c}_n) + \sum_{k=0}^{n} \frac{\partial f(x_i, \tilde{c}_0, \tilde{c}_1, \ldots, \tilde{c}_n)}{\partial c_k} \Delta c_k$$

$$y_i \approx \hat{y}_i + \sum_{k=0}^{n} \frac{\partial f(x_i, \tilde{c}_0, \tilde{c}_1, \ldots, \tilde{c}_n)}{\partial c_k} \Delta c_k$$

– Δc_k is a small change in c_k $\quad \Delta c_k = c_k - \tilde{c}_k$

Nonlinear Least Squares

- So

$$\Delta\beta_i = y_i - \hat{y}_i = \sum_{k=0}^{n} \frac{\partial f}{\partial c_k} \Delta c_k \bigg|_{x_i,\tilde{\mathbf{c}}}, \quad i = 1,2,\ldots,m$$

$$\mathbf{\Delta\beta} = \begin{bmatrix} \left.\dfrac{\partial f}{\partial c_0}\right|_{x_1,\tilde{\mathbf{c}}} & \left.\dfrac{\partial f}{\partial c_1}\right|_{x_1,\tilde{\mathbf{c}}} & \cdots & \left.\dfrac{\partial f}{\partial c_n}\right|_{x_1,\tilde{\mathbf{c}}} \\ \left.\dfrac{\partial f}{\partial c_0}\right|_{x_2,\tilde{\mathbf{c}}} & \left.\dfrac{\partial f}{\partial c_1}\right|_{x_2,\tilde{\mathbf{c}}} & \cdots & \left.\dfrac{\partial f}{\partial c_n}\right|_{x_2,\tilde{\mathbf{c}}} \\ \vdots & \vdots & & \vdots \\ \left.\dfrac{\partial f}{\partial c_0}\right|_{x_m,\tilde{\mathbf{c}}} & \left.\dfrac{\partial f}{\partial c_1}\right|_{x_m,\tilde{\mathbf{c}}} & \cdots & \left.\dfrac{\partial f}{\partial c_n}\right|_{x_m,\tilde{\mathbf{c}}} \end{bmatrix} \mathbf{\Delta c} = \mathbf{X\Delta c}$$

Nonlinear Least Squares

- Now have a linear set of equations in Δc_k
  - Overdetermined ($m > n$)
- Solve as before:

$$\mathbf{\Delta c} = \left[\mathbf{X}^T \mathbf{X}\right]^{-1} \mathbf{X}^T \mathbf{\Delta \beta}$$

- Algorithm:
  - Start with initial estimates $\tilde{c}_k$
  - Calculate **X**, $\mathbf{\Delta\beta}$ and hence $\mathbf{\Delta c} = \left[\mathbf{X}^T \mathbf{X}\right]^{-1} \mathbf{X}^T \mathbf{\Delta \beta}$
  - Update the c_k using $\tilde{\tilde{c}}_k = \tilde{c}_k + \Delta c_k$

Nonlinear Least Squares

- Example
  - Original data: {(-1,-1), (2,3), (3,7)}
  - Initial estimate: $\tilde{c}_1 = 3$
- 1st iteration:

$$\mathbf{\Delta\beta} = \begin{bmatrix} -1 - -3 \\ 3 - 6 \\ 7 - 9 \end{bmatrix} = \begin{bmatrix} 2 \\ -3 \\ -2 \end{bmatrix}$$

$$\mathbf{X} = \begin{bmatrix} \left.\dfrac{dy}{dc_1}\right|_{x_1,\tilde{c}_1} \\ \left.\dfrac{dy}{dc_1}\right|_{x_2,\tilde{c}_1} \\ \left.\dfrac{dy}{dc_1}\right|_{x_3,\tilde{c}_1} \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ 2 \\ 3 \end{bmatrix}$$

$$\mathbf{\Delta\beta} = \mathbf{X}c_1, \quad \begin{bmatrix} 2 \\ -3 \\ -2 \end{bmatrix} = \begin{bmatrix} -1 \\ 2 \\ 3 \end{bmatrix} c_1$$

$$\mathbf{\Delta c} = \left[\mathbf{X}^T\mathbf{X}\right]^{-1}\mathbf{X}^T\mathbf{\Delta\beta} = [14]^{-1}\begin{bmatrix} -1 & 2 & 3 \end{bmatrix}\begin{bmatrix} 2 \\ -3 \\ -2 \end{bmatrix} = -1$$

Nonlinear Least Squares

- Example
  - Original data: {(-1,-1), (2,3), (3,7)}
  - New estimate: $\tilde{\tilde{c}}_1 = \tilde{c}_1 + \mathbf{\Delta c} = 3 - 1 = 2$

Close to optimum value 31/14

- 2nd iteration:

$$\mathbf{\Delta\beta} = \begin{bmatrix} -1 - -2 \\ 3 - 4 \\ 7 - 6 \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix}$$

$$\mathbf{X} = \begin{bmatrix} \left.\dfrac{dy}{dc_1}\right|_{x_1, \tilde{c}_1} \\ \left.\dfrac{dy}{dc_1}\right|_{x_2, \tilde{c}_1} \\ \left.\dfrac{dy}{dc_1}\right|_{x_3, \tilde{c}_1} \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ 2 \\ 3 \end{bmatrix}$$

$$\mathbf{\Delta\beta} = \mathbf{X}c_1, \quad \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix} = \begin{bmatrix} -1 \\ 2 \\ 3 \end{bmatrix} c_1$$

$$\mathbf{\Delta c} = \left[\mathbf{X}^T\mathbf{X}\right]^{-1}\mathbf{X}^T\mathbf{\Delta\beta} = [14]^{-1}\begin{bmatrix} -1 & 2 & 3 \end{bmatrix}\begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix} = 0$$

Gradient Descent

- LS solutions keep looking like:

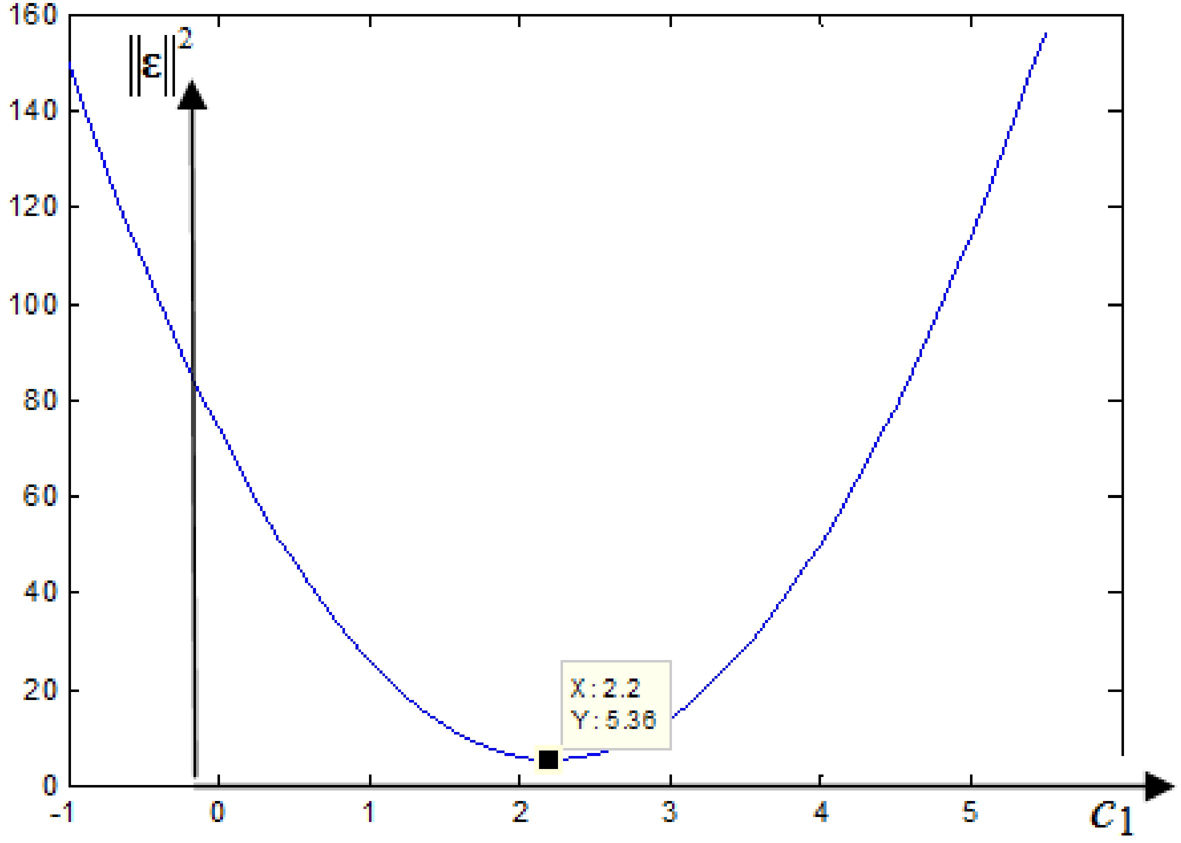
$$\mathbf{c} = [\mathbf{X}^T \mathbf{X}]^{-1} \mathbf{X}^T \mathbf{y}$$

  – Matrix inversion is not what we want to do
    - What if we have to do LS lots of times, or very fast, or we have lots of parameters (large $\mathbf{X}^T\mathbf{X}$) ?

  – Can we solve this some other way ?

Gradient Descent

- Previous example:
  - Gradient at every position on this error surface ‘points away’ from minimum



Gradient Descent

- Still on the original example:

$$\|\boldsymbol{\varepsilon}\|^2 = \sum_{i=1}^{3} \varepsilon_i^2 = (-4 + c_1)^2 + (3 - 2c_1)^2 + (7 - 3c_1)^2$$

$$= 14c_1^2 - 62c_1 + 74$$

  – Suppose we guess that c_1 is $c_1^0 = 5$
    - Can actually safely make any guess for c_1, because error surface is quadratic
  – What is the gradient of the error surface at this point ?

$$\left.\frac{d\|\boldsymbol{\varepsilon}\|^2}{dc_1}\right|_{c_1=5} = 28c_1 - 62\Big|_{c_1=5} = 28(5) - 62 = 78$$

Gradient Descent

- Still on the previous example:
  - Suppose we subtract some small proportion of the gradient, say 2%, from our initial guess of c_1
    - Pushes c_1 closer to optimum
    - Produces a new estimate of c_1

$$c_1^1 = c_1^0 - 0.02 \cdot 78 = 3.44$$

  - Now what is the gradient of the error surface at this new estimate c_1^1 ?

$$\left. \frac{d\|\boldsymbol{\varepsilon}\|^2}{dc_1} \right|_{c_1=3.44} = 28(3.44) - 62 = 34.32$$

Gradient Descent

- Still on the previous example:
  - Suppose we do it again: subtract 2% of this new gradient from our latest estimate of c_1

$$c_1^2 = c_1^1 - 0.02 \cdot 34.32 = 2.75$$

  - Now what is the gradient of the error surface at this new estimate c_1^2 ?

$$\left.\frac{d\|\boldsymbol{\varepsilon}\|^2}{dc_1}\right|_{c_1=2.75} = 28(2.75) - 62 = 15$$

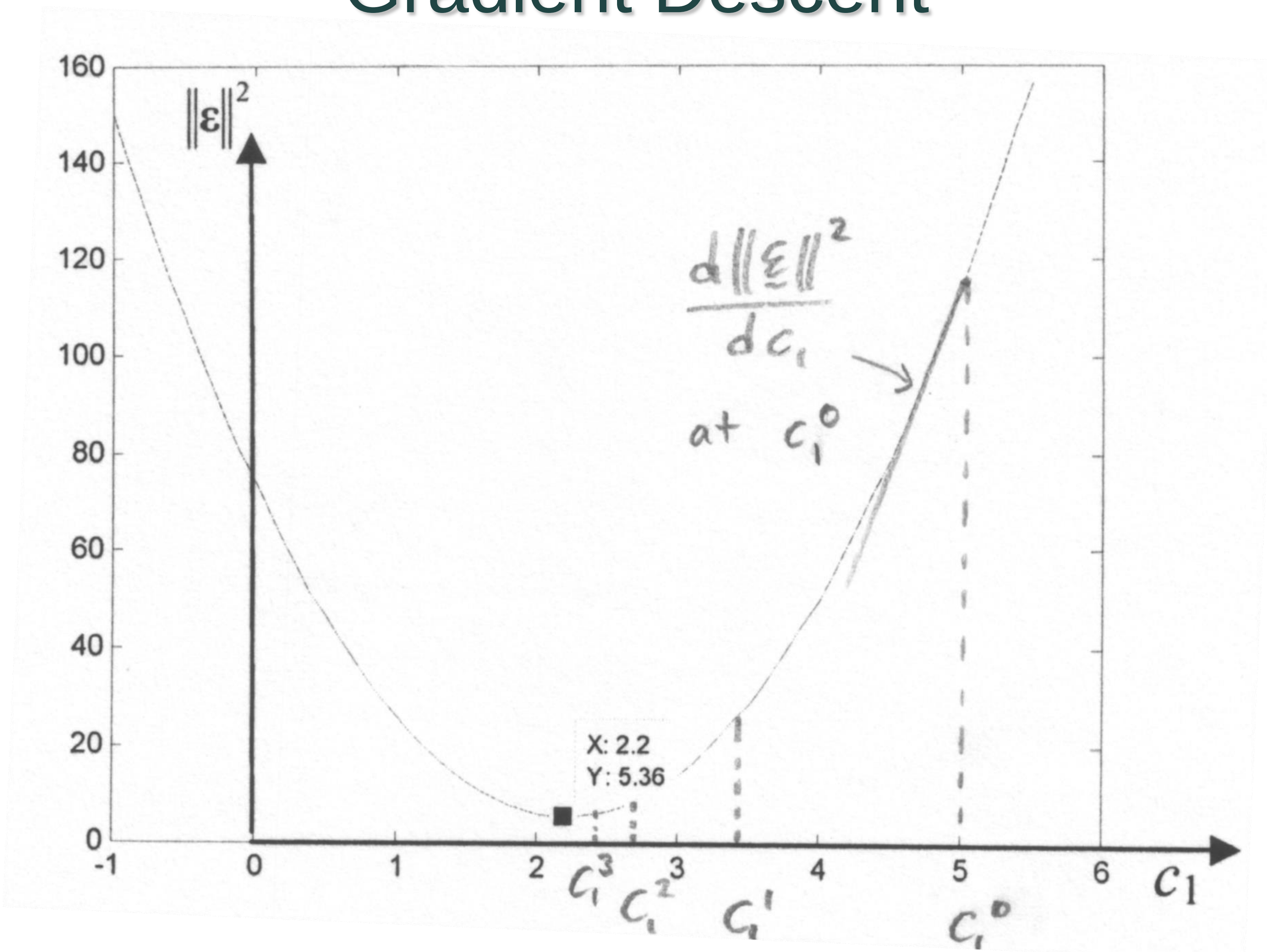
Gradient Descent

- Still on the previous example:
  - And again: subtract 2% of this new gradient from our latest estimate of c_1

$$c_1^3 = c_1^2 - 0.02 \cdot 15 = 2.45$$

  - Where are we now ?

Gradient Descent



Gradient Descent

- Algorithm:
  - Given an initial estimate of the parameter c^0,
  - An improved estimate of the minimum is obtained by

$$c^{i+1} = c^i - \lambda \left. \frac{d\|\boldsymbol{\varepsilon}\|^2}{dc} \right|_{c=c^i}$$

  - Where λ controls the rate of convergence
    - We had $\lambda = 0.02$
    - Large λ : estimates may oscillate about minimum
    - Small λ : convergence may be slow
  - i is the iteration number

Gradient Descent

- Algorithm (multiple parameter case):
  - Given an initial estimate of the parameters

$$c_k^0,\ k = 0,1,\ldots,n$$

  - An improved estimate of the minimum is obtained by

$$c_k^{i+1} = c_k^i - \lambda \left. \frac{\partial \|\boldsymbol{\varepsilon}\|^2}{\partial c_k} \right|_{c_k = c_k^i},\ k = 0,1,\ldots,n$$