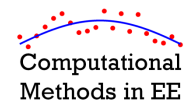




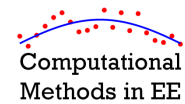
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Topic 5 – Curve Fitting & Interpolation

EE 4386/5301 Computational Methods in EE

Outline

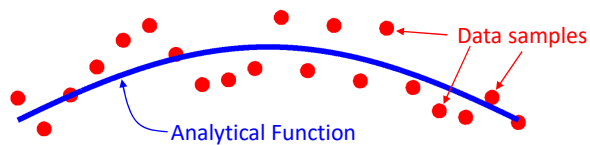


- Introduction
- Statistics of Data Sets
- Best Fit Methods
 - Linear Regression (ugly math)
 - Linear Least Squares (clean math)
 - Nonlinear Regression (moderate math)
- Exact Fit Methods
 - Fitting Polynomials
- Interpolation & Extrapolation

Introduction

What is Curve Fitting?

Curve fitting is simply fitting an analytical equation to a set of measured data.

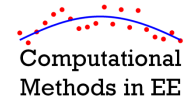


$$f(x) = A + Be^{-\left(\frac{x-C}{D}\right)^2}$$



“Curve fitting” determines the values of A , B , C , and D so that $f(x)$ best represents the given data.

Why Fit Data to a Curve?

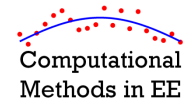


- We may want to estimate data between the discrete values (interpolation)
- We may want to fit measured data to an analytical equation to extract meaningful parameters.
- We may want to reduce noise
- We may want to observe and quantify a general trend

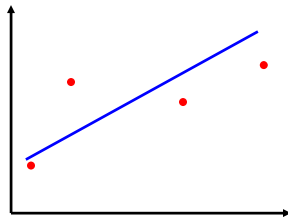
Curve Fitting

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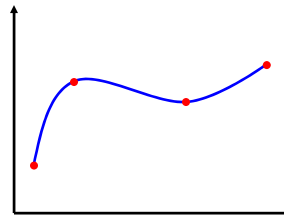
Two Categories of Curve Fitting



Best Fit – Measured data has noise so the curve does not attempt to intercept every point.



Exact Fit – Data samples are assumed to be exact and the curve is forced to pass through each one.



Curve Fitting

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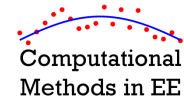
Statistics of Data Sets

Arithmetic Mean

If we had to come up with a single number that represents an entire set of data, the arithmetic mean would probably be it.

$$f_{\text{avg}} = \frac{f_1 + f_2 + \cdots + f_M}{M} = \frac{1}{M} \sum_{m=1}^M f_m$$

Geometric Mean



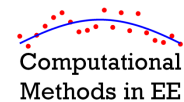
The geometric mean is defined as

$$f_{\text{gm}} = \sqrt[M]{f_1 f_2 \cdots f_M}$$

The arithmetic mean tends to suppress the significance of outlying data samples. With the geometric mean, even a single small value among many large values can dominate the mean.

This is useful in optimizations where multiple parameters must be maximized at the same time and it is not acceptable to have any one of them low.

Variance & Standard Deviation



Standard Deviation σ_f

The standard deviation is a measure of the “spread” of the data about the mean. It is convenient because it shares the same units as the data.

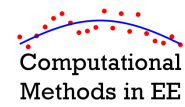
$$\sigma_f = \sqrt{\frac{1}{M} \sum_{m=1}^M (f_m - f_{\text{avg}})^2}$$

Variance v_f

Variance is used more commonly in calculations, but carries the same information as the standard deviation.

$$v_f = \sigma_f^2 = \frac{1}{M} \sum_{m=1}^M (f_m - f_{\text{avg}})^2$$

Coefficient of Variation

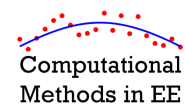


The coefficient of variation (CV) is the standard deviation normalized to the mean.

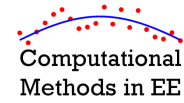
Think of it as “relative standard deviation.”

$$CV = \frac{\sigma_f}{f_{\text{avg}}}$$

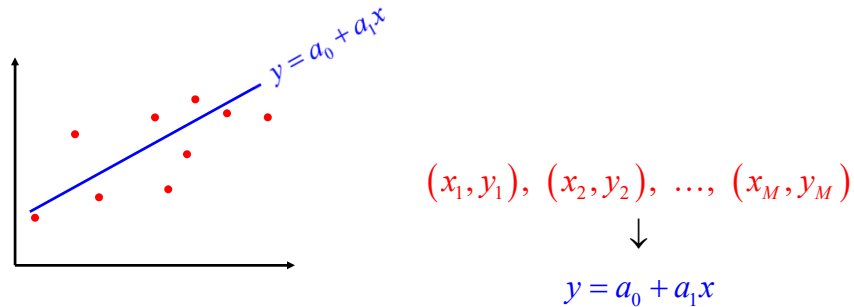
Linear Regression (Best Fit, Ugly Math)



Goal of Linear Regression



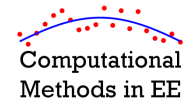
The goal of linear regression is to fit a straight line to a set of measured data that has noise.



Curve Fitting

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Statement of Problem



Given a set of measured data points: $(x_1, y_1), (x_2, y_2), \dots, (x_M, y_M)$, we write our equation of the line for each point.

$$y_1 = a_0 + a_1x_1 + e_1$$

$$y_2 = a_0 + a_1x_2 + e_2$$

$$\vdots$$

$$y_M = a_0 + a_1x_M + e_M$$

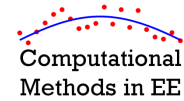
To make these equations correct, we must introduce an error term e called the *residual*.

We wish to determine values of a_0 and a_1 such that the residual terms e_m are as small as possible.

Curve Fitting

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Criteria for “Best Fit”



We must define a single quantity that tells us how “good” the line fits our set of data.

Guess #1 – Sum of Residuals

$$E = \sum_{m=1}^M e_m$$

This does not work because negative and positive residuals can cancel and mislead the overall criteria to think there is no error.

Guess #2 – Sum of Magnitude of Residuals

$$E = \sum_{m=1}^M |e_m|$$

This does not work because it does not lead to a unique best fit.

Guess #3 – Sum of Squares of Residuals

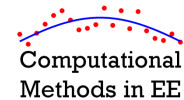
$$E = \sum_{m=1}^M e_m^2$$

This works and leads to a unique solution.

Curve Fitting

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Equation for Criterion



Our line equation for the m th sample is

$$y_m = a_0 + a_1 x_m + e_m$$

Solving this for the residual e_m gives

$$e_m = y_m - (a_0 + a_1 x_m)$$

This is our measured value of y .

This is the value of y of our line at point x_m .

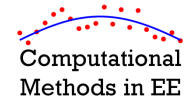
From this, we can write our criterion as

$$E = \sum_{m=1}^M e_m^2 = \sum_{m=1}^M (y_{\text{measured},m} - y_{\text{line},m})^2 = \sum_{m=1}^M (y_m - a_0 - a_1 x_m)^2$$

Curve Fitting

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Least-Squares Fit



We wish to minimize the error criterion E .

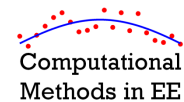
We can identify minimums when the first-order derivative is zero.

$$\frac{\partial E}{\partial a_0} = 0 \quad \text{and} \quad \frac{\partial E}{\partial a_1} = 0$$

We seek the values of a_0 and a_1 that satisfy these equations.

This approach is solving the problem by least-squares (we are minimizing the squares of the residuals).

The Fun Math

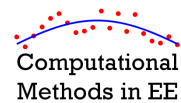


Step 1 – Differential E with respect to each of the unknowns.

$$\begin{aligned} \frac{\partial E}{\partial a_0} &= \frac{\partial}{\partial a_0} \sum_{m=1}^M (y_m - a_0 - a_1 x_m)^2 \\ &= \sum_{m=1}^M \frac{\partial}{\partial a_0} (y_m - a_0 - a_1 x_m)^2 \\ &= \sum_{m=1}^M 2(y_m - a_0 - a_1 x_m)(-1) \\ &= -2 \sum_{m=1}^M (y_m - a_0 - a_1 x_m) \end{aligned}$$

$$\begin{aligned} \frac{\partial E}{\partial a_1} &= \frac{\partial}{\partial a_1} \sum_{m=1}^M (y_m - a_0 - a_1 x_m)^2 \\ &= \sum_{m=1}^M \frac{\partial}{\partial a_1} (y_m - a_0 - a_1 x_m)^2 \\ &= \sum_{m=1}^M 2(y_m - a_0 - a_1 x_m)(-x_m) \\ &= -2 \sum_{m=1}^M (y_m - a_0 - a_1 x_m) x_m \end{aligned}$$

The Fun Math



Step 2 – We set the derivatives to zero to find the minimum of E .

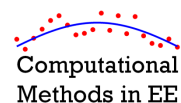
$$\begin{aligned}
 0 &= \frac{\partial E}{\partial a_0} \\
 &= -2 \sum_{m=1}^M (y_m - a_0 - a_1 x_m) \\
 &= \sum_{m=1}^M y_m - \sum_{m=1}^M a_0 - \sum_{m=1}^M a_1 x_m \\
 &= \sum_{m=1}^M y_m - M a_0 - \sum_{m=1}^M a_1 x_m
 \end{aligned}$$

$$\begin{aligned}
 0 &= \frac{\partial E}{\partial a_1} \\
 &= -2 \sum_{m=1}^M (y_m - a_0 - a_1 x_m) x_m \\
 &= \sum_{m=1}^M (y_m - a_0 - a_1 x_m) x_m \\
 &= \sum_{m=1}^M y_m x_m - a_0 \sum_{m=1}^M x_m - \sum_{m=1}^M a_1 x_m^2
 \end{aligned}$$

Curve Fitting

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The Fun Math



Step 3 – We write these as two simultaneous equations. These are called the *normal equations*.

$$\begin{aligned}
 0 &= \frac{\partial E}{\partial a_0} \\
 &= -2 \sum_{m=1}^M (y_m - a_0 - a_1 x_m) \\
 &= \sum_{m=1}^M y_m - \sum_{m=1}^M a_0 - \sum_{m=1}^M a_1 x_m \\
 &= \sum_{m=1}^M y_m - M a_0 - a_1 \sum_{m=1}^M x_m
 \end{aligned}$$

↓

$$M a_0 + a_1 \sum_{m=1}^M x_m = \sum_{m=1}^M y_m$$

$$\begin{aligned}
 0 &= \frac{\partial E}{\partial a_1} \\
 &= -2 \sum_{m=1}^M (y_m - a_0 - a_1 x_m) x_m \\
 &= \sum_{m=1}^M (y_m - a_0 - a_1 x_m) x_m \\
 &= \sum_{m=1}^M y_m x_m - a_0 \sum_{m=1}^M x_m - \sum_{m=1}^M a_1 x_m^2
 \end{aligned}$$

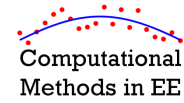
↓

$$a_0 \sum_{m=1}^M x_m + a_1 \sum_{m=1}^M x_m^2 = \sum_{m=1}^M y_m x_m$$

Curve Fitting

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The Fun Math



Step 4 – The normal equations are solved simultaneously and the solution is

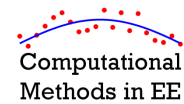
$$a_0 = y_{\text{avg}} - a_1 x_{\text{avg}}$$

$$a_1 = \frac{M \sum_{m=1}^M x_m y_m - \sum_{m=1}^M x_m \sum_{m=1}^M y_m}{M \sum_{m=1}^M x_m^2 - \left(\sum_{m=1}^M x_m \right)^2}$$

$$x_{\text{avg}} = \frac{1}{M} \sum_{m=1}^M x_m$$

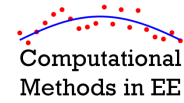
$$y_{\text{avg}} = \frac{1}{M} \sum_{m=1}^M y_m$$

Yikes!
There has to be an easier way!



Linear Least-Squares (Best Fit, Clean Math)

Statement of Problem



We wish to fit a set of M measured data points to a curve containing $N + 1$ terms:

$$f = a_0 z_0 + a_1 z_1 + a_2 z_2 + \cdots + a_N z_N$$

$f \equiv$ measured value

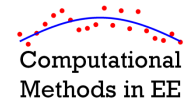
$z_n \equiv$ parameters from which f is evaluated

$a_n \equiv$ coefficients for the curve fit

Curve Fitting

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Formulation of Matrix Equation



We start by writing the function f for each of our M measurements. We also include the residual term.

$$\begin{aligned} f_1 &= a_0 z_{0,1} + a_1 z_{1,1} + \cdots + a_N z_{N,1} + e_1 \\ f_2 &= a_0 z_{0,2} + a_1 z_{1,2} + \cdots + a_N z_{N,2} + e_2 \\ &\vdots \\ f_M &= a_0 z_{0,M} + a_1 z_{1,M} + \cdots + a_N z_{N,M} + e_M \end{aligned}$$

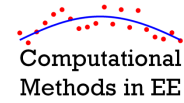
This large set of equations is put into matrix form.

$$\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_{M-1} \\ f_M \end{bmatrix} = \begin{bmatrix} z_{0,1} & z_{1,1} & \cdots & z_{N,1} \\ z_{0,2} & z_{1,2} & \cdots & z_{N,2} \\ z_{0,3} & z_{1,3} & \ddots & z_{N,3} \\ \vdots & \vdots & & \vdots \\ z_{0,M-1} & z_{1,M-1} & \cdots & z_{N,M-1} \\ z_{0,M} & z_{1,M} & \cdots & z_{N,M} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_N \end{bmatrix} + \begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ \vdots \\ e_{M-1} \\ e_M \end{bmatrix} \Rightarrow \begin{aligned} [f] &= [Z][a] + [e] \\ \text{or} \\ \mathbf{f} &= \mathbf{Za} + \mathbf{e} \end{aligned}$$

Curve Fitting

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Formulation of Solution by Least-Squares (1 of 4)



Step 1 – Solve matrix equation for \mathbf{e} .

$$\mathbf{f} = \mathbf{Z}\mathbf{a} + \mathbf{e} \rightarrow \mathbf{e} = \mathbf{f} - \mathbf{Z}\mathbf{a}$$

Step 2 – Calculate the error criterion E from \mathbf{e} .

$$E = \sum_{m=1}^M e_m^2 = [e_1 \ e_2 \ e_3 \ \cdots \ e_{M-1} \ e_M] \begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ \vdots \\ e_{M-1} \\ e_M \end{bmatrix} = \mathbf{e}^T \mathbf{e}$$

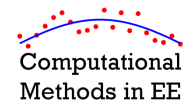
Step 3 – We substitute our equation for \mathbf{e} from Step 1 into our equation for E from Step 2.

$$E = \mathbf{e}^T \mathbf{e} = (\mathbf{f} - \mathbf{Z}\mathbf{a})^T (\mathbf{f} - \mathbf{Z}\mathbf{a})$$

Curve Fitting

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Formulation of Solution by Least-Squares (2 of 4)



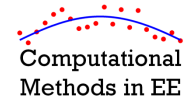
Step 4 – Our new matrix equation is algebraically manipulated as follows in order to make it easier to find its first-order derivative.

$$\begin{aligned} E &= (\mathbf{f} - \mathbf{Z}\mathbf{a})^T (\mathbf{f} - \mathbf{Z}\mathbf{a}) && \text{original equation} \\ &= (\mathbf{f}^T - \mathbf{a}^T \mathbf{Z}^T) (\mathbf{f} - \mathbf{Z}\mathbf{a}) && \text{distribute the transpose} \\ &= \mathbf{f}^T \mathbf{f} - \underbrace{\mathbf{f}^T \mathbf{Z}\mathbf{a} - \mathbf{a}^T \mathbf{Z}^T \mathbf{f}}_{\substack{\text{These are scalars and} \\ \text{transposes of each other} \\ \text{so they are equal.}}} + \mathbf{a}^T \mathbf{Z}^T \mathbf{Z}\mathbf{a} && \text{expand equation} \\ &= \mathbf{f}^T \mathbf{f} - 2\mathbf{a}^T \mathbf{Z}^T \mathbf{f} + \mathbf{a}^T \mathbf{Z}^T \mathbf{Z}\mathbf{a} && \text{combine terms} \end{aligned}$$

Curve Fitting

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Formulation of Solution by Least-Squares (3 of 4)



Step 5 – We differential E with respect to \mathbf{a} .

We wish to determine \mathbf{a} that minimizes E .
We can do this using the first-derivative rule.

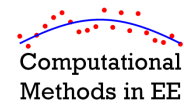
$$E = \mathbf{f}^T \mathbf{f} - 2\mathbf{a}^T \mathbf{Z}^T \mathbf{f} + \mathbf{a}^T \mathbf{Z}^T \mathbf{Z} \mathbf{a}$$

$$\begin{aligned} \frac{\partial E}{\partial \mathbf{a}} &= \frac{\partial}{\partial \mathbf{a}} (\mathbf{f}^T \mathbf{f} - 2\mathbf{a}^T \mathbf{Z}^T \mathbf{f} + \mathbf{a}^T \mathbf{Z}^T \mathbf{Z} \mathbf{a}) && \text{substitute in expression for } E \\ &= \cancel{\frac{\partial}{\partial \mathbf{a}} \mathbf{f}^T \mathbf{f}} - 2 \frac{\partial}{\partial \mathbf{a}} \mathbf{a}^T \mathbf{Z}^T \mathbf{f} + \frac{\partial}{\partial \mathbf{a}} \mathbf{a}^T \mathbf{Z}^T \mathbf{Z} \mathbf{a} && \mathbf{f} \text{ is not a function of } \mathbf{a} \\ &= -2\mathbf{Z}^T \mathbf{f} + 2\mathbf{Z}^T \mathbf{Z} \mathbf{a} && \text{finish differentiation} \end{aligned}$$

Curve Fitting

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Formulation of Solution by Least-Squares (4 of 4)



Step 6 – We find the value of \mathbf{a} that makes the derivative equal to zero.

$$\frac{\partial E}{\partial \mathbf{a}} = -2\mathbf{Z}^T \mathbf{f} + 2\mathbf{Z}^T \mathbf{Z} \mathbf{a} = 0$$

$$-2\mathbf{Z}^T \mathbf{f} + 2\mathbf{Z}^T \mathbf{Z} \mathbf{a} = 0$$

$$2\mathbf{Z}^T \mathbf{Z} \mathbf{a} = 2\mathbf{Z}^T \mathbf{f}$$

$$\mathbf{Z}^T \mathbf{Z} \mathbf{a} = \mathbf{Z}^T \mathbf{f}$$

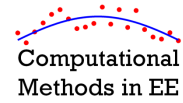
$$\mathbf{a} = (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T \mathbf{f}$$

This is the original equation
premultiplied by \mathbf{Z}^T .

Curve Fitting

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DO NOT SIMPLIFY FURTHER!

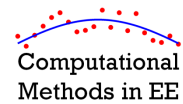


If we were to simplify our least-squares equation, we would get

$$\begin{aligned} \mathbf{a} &= (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T \mathbf{f} \\ &= \mathbf{Z}^{-1} \underbrace{(\mathbf{Z}^T)^{-1} \mathbf{Z}^T}_{\mathbf{I}} \mathbf{f} \\ &= \mathbf{Z}^{-1} \mathbf{f} \end{aligned}$$

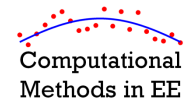
This is just our original equation again ($\mathbf{f} = \mathbf{Z}\mathbf{a}$) without the least-squares approach incorporated.

Visualizing Least-Squares (1 of 3)



We are initially given a matrix equation with more equations than unknowns.

Visualizing Least-Squares (2 of 3)



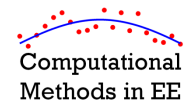
We premultiply by the transpose of \mathbf{A} .

$$\begin{bmatrix} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{bmatrix} \begin{bmatrix} | \\ | \\ | \\ | \end{bmatrix} = \begin{bmatrix} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{bmatrix} \begin{bmatrix} | \\ | \end{bmatrix}$$

Curve Fitting

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Visualizing Least-Squares (3 of 3)



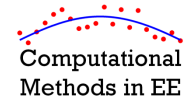
The matrix equations reduces to the same number of equations as unknowns, which is solvable by many standard algorithms.

$$\begin{bmatrix} + & + \\ + & + \end{bmatrix} \begin{bmatrix} | \\ | \end{bmatrix} = \begin{bmatrix} | \\ | \end{bmatrix}$$

Curve Fitting

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Least-Squares Algorithm



Step 1 – Construct matrices. \mathbf{Z} is essentially just a matrix of the coordinates of the data points. \mathbf{f} is a column vector of the measurements.

$$\mathbf{f} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_{M-1} \\ f_M \end{bmatrix} \quad \mathbf{Z} = \begin{bmatrix} z_{0,1} & z_{1,1} & \cdots & z_{N,1} \\ z_{0,2} & z_{1,2} & \cdots & z_{N,2} \\ z_{0,3} & z_{1,3} & \cdots & z_{N,3} \\ \vdots & \vdots & & \vdots \\ z_{0,M-1} & z_{1,M-1} & & z_{N,M-1} \\ z_{0,M} & z_{1,M} & & z_{N,M} \end{bmatrix}$$

Step 2 – Solve for the unknown coefficients \mathbf{a} .

$$\mathbf{a} = (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T \mathbf{f}$$

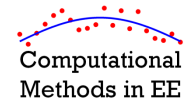
Step 3 – Extract the coefficients from \mathbf{a} .

$$\mathbf{a} = \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_N \end{bmatrix}$$

Curve Fitting

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Least-Squares for Solving $\mathbf{Ax} = \mathbf{b}$



Suppose we wish to solve $\mathbf{Ax} = \mathbf{b}$, but we have more equations than we have unknowns.

We must solve this as a “best fit” because a perfect fit is impossible in the presence of noise.

We apply least-squares by premultiplying by \mathbf{A}^T .

$$\mathbf{Ax} = \mathbf{b} \rightarrow \mathbf{A}'\mathbf{x} = \mathbf{b}'$$

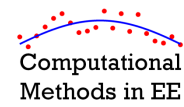
$$\mathbf{A}' = \mathbf{A}^T \mathbf{A}$$

$$\mathbf{b}' = \mathbf{A}^T \mathbf{b}$$

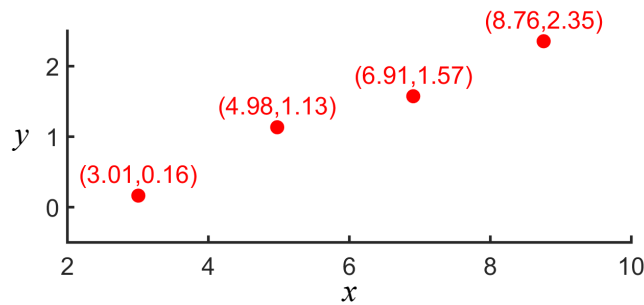
Curve Fitting

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Example 1 (1 of 3)



Let's fit a line to the following set of points.

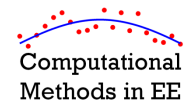


$$y = mx + b$$

Curve Fitting

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Example 1 (2 of 3)



Step 1 – Build matrices

$$\begin{aligned} y_1 &= mx_1 + b \\ y_2 &= mx_2 + b \\ y_3 &= mx_3 + b \\ y_4 &= mx_4 + b \end{aligned} \rightarrow \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ x_3 & 1 \\ x_4 & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} \rightarrow \mathbf{f} = \begin{bmatrix} 0.16 \\ 1.13 \\ 1.57 \\ 2.35 \end{bmatrix} \quad \mathbf{Z} = \begin{bmatrix} 3.01 & 1 \\ 4.98 & 1 \\ 6.91 & 1 \\ 8.76 & 1 \end{bmatrix}$$

With some practice,
you will be able to
write matrices directly
from measured data.

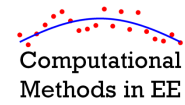
Step 2 – Solve by least squares.

$$\begin{aligned} \mathbf{Z}^T \mathbf{Z} \mathbf{x} &= \mathbf{Z}^T \mathbf{f} \rightarrow \begin{bmatrix} 3.01 & 4.98 & 6.91 & 8.76 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 3.01 & 1 \\ 4.98 & 1 \\ 6.91 & 1 \\ 8.76 & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} 3.01 & 4.98 & 6.91 & 8.76 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 0.16 \\ 1.13 \\ 1.57 \\ 2.35 \end{bmatrix} \\ &\rightarrow \begin{bmatrix} 158.3462 & 23.6600 \\ 23.6600 & 4.0000 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} 37.5437 \\ 5.2100 \end{bmatrix} \\ &\rightarrow \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} 0.3656 \\ -0.8602 \end{bmatrix} \end{aligned}$$

Curve Fitting

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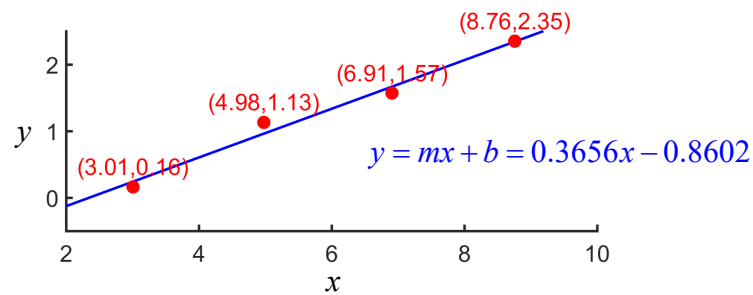
Example 1 (3 of 3)



Step 3 – Extract coefficients

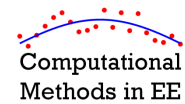
$$\begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} 0.3656 \\ -0.8602 \end{bmatrix} \rightarrow \begin{array}{l} m = 0.3656 \\ b = -0.8602 \end{array}$$

Step 4 – Plot the result



Curve Fitting

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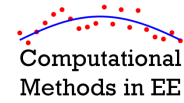


Nonlinear Regression (Best Fit, Moderate Math)

Curve Fitting

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Statement of Problem



We wish to fit a set of M measured data points to a nonlinear function $f(x)$.

$$y = f(x; a_0, a_1, \dots, a_N)$$

$y \equiv$ measured value

$x \equiv$ parameter from which f is evaluated

$a_n \equiv$ coefficients for the function fit

The function can be anything like sine's, logarithms, exponentials...

$$f(x) = A + B \sin(Cx)$$

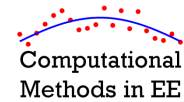
$$f(x) = A + B e^{-Cx^2}$$

$$f(x) = A + B \ln(Cx)$$

Curve Fitting

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Multiple-Parameter Taylor Series



Recall the Taylor series for a single parameter...

$$f(x) = f(\tilde{x}) + \frac{f'(\tilde{x})}{1!}(x - \tilde{x}) + \frac{f''(\tilde{x})}{2!}(x - \tilde{x})^2 + \frac{f'''(\tilde{x})}{3!}(x - \tilde{x})^3 + \dots$$

The two-parameter Taylor series is

$$f(x, y) = f(\tilde{x}, \tilde{y}) + \frac{1}{1!} \left[\frac{\partial f(\tilde{x}, \tilde{y})}{\partial x} (x - \tilde{x}) + \frac{\partial f(\tilde{x}, \tilde{y})}{\partial y} (y - \tilde{y}) \right] \\ + \frac{1}{2!} \left[\frac{\partial^2 f(\tilde{x}, \tilde{y})}{\partial x^2} (x - \tilde{x})^2 + 2 \frac{\partial^2 f(\tilde{x}, \tilde{y})}{\partial x \partial y} (x - \tilde{x})(y - \tilde{y}) + \frac{\partial^2 f(\tilde{x}, \tilde{y})}{\partial y^2} (y - \tilde{y})^2 \right] \\ \vdots$$

We will ignore the higher-order terms.

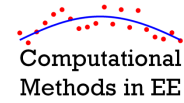
The N -parameter Taylor series using only first-order derivatives is

$$f(x_1, x_2, \dots, x_N) \approx f(\tilde{x}_1, \tilde{x}_2, \dots, \tilde{x}_N) + \sum_{n=1}^N \frac{\partial f}{\partial x_n} \Delta x_n \quad \Delta x_n = x_n - \tilde{x}_n$$

Curve Fitting

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Solution Using Gauss-Newton Method (1 of 5)



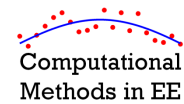
We write our equation for each measured sample.

$$\begin{array}{ccc}
 y_1 = f(x_1; a_0, a_1, \dots, a_N) + e_1 & & y_1 = f(x_1) + e_1 \\
 y_2 = f(x_2; a_0, a_1, \dots, a_N) + e_2 & \rightarrow & y_2 = f(x_2) + e_2 \\
 \vdots & & \vdots \\
 y_M = f(x_M; a_0, a_1, \dots, a_N) + e_M & & y_M = \underbrace{f(x_M)}_{\text{Shorthand notation}} + e_M
 \end{array}$$

Curve Fitting

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Solution Using Gauss-Newton Method (2 of 5)



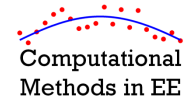
We can convert the nonlinear equations into linear equations by expanding them into multi-parameter Taylor series.

$$\begin{array}{c}
 y_1 = f(x_1) + \frac{\partial f(x_1)}{\partial a_0} \Delta a_0 + \frac{\partial f(x_1)}{\partial a_1} \Delta a_1 + \dots + \frac{\partial f(x_1)}{\partial a_N} \Delta a_N + e_1 \\
 y_2 = f(x_2) + \frac{\partial f(x_2)}{\partial a_0} \Delta a_0 + \frac{\partial f(x_2)}{\partial a_1} \Delta a_1 + \dots + \frac{\partial f(x_2)}{\partial a_N} \Delta a_N + e_2 \\
 \vdots \\
 y_M = f(x_M) + \frac{\partial f(x_M)}{\partial a_0} \Delta a_0 + \frac{\partial f(x_M)}{\partial a_1} \Delta a_1 + \dots + \frac{\partial f(x_M)}{\partial a_N} \Delta a_N + e_M
 \end{array}$$

Curve Fitting

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Solution Using Gauss-Newton Method (3 of 5)



Now that our equations are linear, we can put them in matrix form.

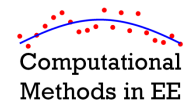
$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{M-1} \\ y_M \end{bmatrix} = \begin{bmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \\ \vdots \\ f(x_{M-1}) \\ f(x_M) \end{bmatrix} + \begin{bmatrix} \frac{\partial f(x_1)}{\partial a_0} & \frac{\partial f(x_1)}{\partial a_1} & \dots & \frac{\partial f(x_1)}{\partial a_N} \\ \frac{\partial f(x_2)}{\partial a_0} & \frac{\partial f(x_2)}{\partial a_1} & \dots & \frac{\partial f(x_2)}{\partial a_N} \\ \frac{\partial f(x_3)}{\partial a_0} & \frac{\partial f(x_3)}{\partial a_1} & \dots & \frac{\partial f(x_3)}{\partial a_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f(x_{M-1})}{\partial a_0} & \frac{\partial f(x_{M-1})}{\partial a_1} & \dots & \frac{\partial f(x_{M-1})}{\partial a_N} \\ \frac{\partial f(x_M)}{\partial a_0} & \frac{\partial f(x_M)}{\partial a_1} & \dots & \frac{\partial f(x_M)}{\partial a_N} \end{bmatrix} \begin{bmatrix} \Delta a_0 \\ \Delta a_1 \\ \vdots \\ \Delta a_N \end{bmatrix} + \begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ \vdots \\ e_{M-1} \\ e_M \end{bmatrix}$$

$$[y] = [f] + [Z][\Delta a] + [e]$$

Curve Fitting

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Solution Using Gauss-Newton Method (4 of 5)



We solve for $[\Delta a]$ using least-squares.

$$[y] = [f] + [Z][\Delta a] + \cancel{[e]}$$

$$[y] - [f] = [Z][\Delta a]$$

$$[d] = [Z][\Delta a]$$

$$[Z]^T [d] = [Z]^T [Z][\Delta a]$$

$$[\Delta a] = \left([Z]^T [Z] \right)^{-1} [Z]^T [d]$$

$$\text{Let } [d] = [y] - [f]$$

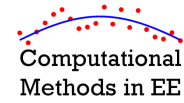
$[d]$ is a new error function.

$[y]$ contains the measured values and $[f]$ contains the calculated values from the curve fit $f(x)$.

Curve Fitting

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Solution Using Gauss-Newton Method (5 of 5)



We now have

$$[\Delta a] = ([Z]^T [Z])^{-1} [Z]^T [d]$$

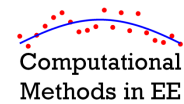
This will only tell us how to change the coefficients $[a]$ given an initial guess $[a]_0$.

We will have to iterate to find the actual coefficients of $[a]$.

Curve Fitting

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Algorithm for Nonlinear Regression (1 of 2)



Step 0 – Derive analytical expressions for partial derivatives of $f(x)$.

Step 1 – Make an initial guess at your coefficients.

$$[a]_0 = [a_{0,0} \quad a_{1,0} \quad \cdots \quad a_{N,0}]^T \quad \text{Make an intelligent guess!}$$

Step 2 – Calculate the function $[f]_i$ at all measured points given the current value of the coefficients $[a]_i$.

$$[f]_i = [f_i(x_1) \quad f_i(x_2) \quad f_i(x_3) \quad \cdots \quad f_i(x_{M-1}) \quad f_i(x_M)]^T$$

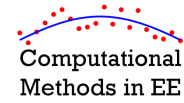
Step 3 – Calculate the error $[d]_i$ in the estimate of $[f]_i$.

$$[d]_i = [y] - [f]_i \quad \begin{array}{l} \% \text{ CALCULATE } d \\ d = \text{fm}(:) - f; \end{array}$$

Curve Fitting

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Algorithm for Nonlinear Regression (2 of 2)



Step 4 – Construct the $[Z]_i$ matrix given the current coefficients $[a]_i$.

$$[Z]_i = \begin{bmatrix} \frac{\partial f_i(x_1)}{\partial a_0} & \frac{\partial f_i(x_1)}{\partial a_1} & \dots & \frac{\partial f_i(x_1)}{\partial a_N} \\ \frac{\partial f_i(x_2)}{\partial a_0} & \frac{\partial f_i(x_2)}{\partial a_1} & \dots & \frac{\partial f_i(x_2)}{\partial a_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_i(x_M)}{\partial a_0} & \frac{\partial f_i(x_M)}{\partial a_1} & \dots & \frac{\partial f_i(x_M)}{\partial a_N} \end{bmatrix}$$

We will need to derive $N+1$ derivatives, one for each coefficient a_n .

We will need to evaluate each of these $N+1$ derivatives at all M points.

This is a lot of work!

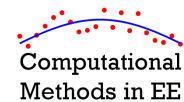
Step 5 – Solve for $[\Delta a]_i$ using least squares.

$$[\Delta a]_i = \left([Z]_i^T [Z]_i \right)^{-1} \left([Z]_i^T [d]_i \right)$$

Curve Fitting

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Algorithm for Nonlinear Regression (3 of 3)



Step 6 – Adjust $[a]_i$ using $[\Delta a]_i$.

$$[a]_{i+1} = [a]_i + [\Delta a]_i$$

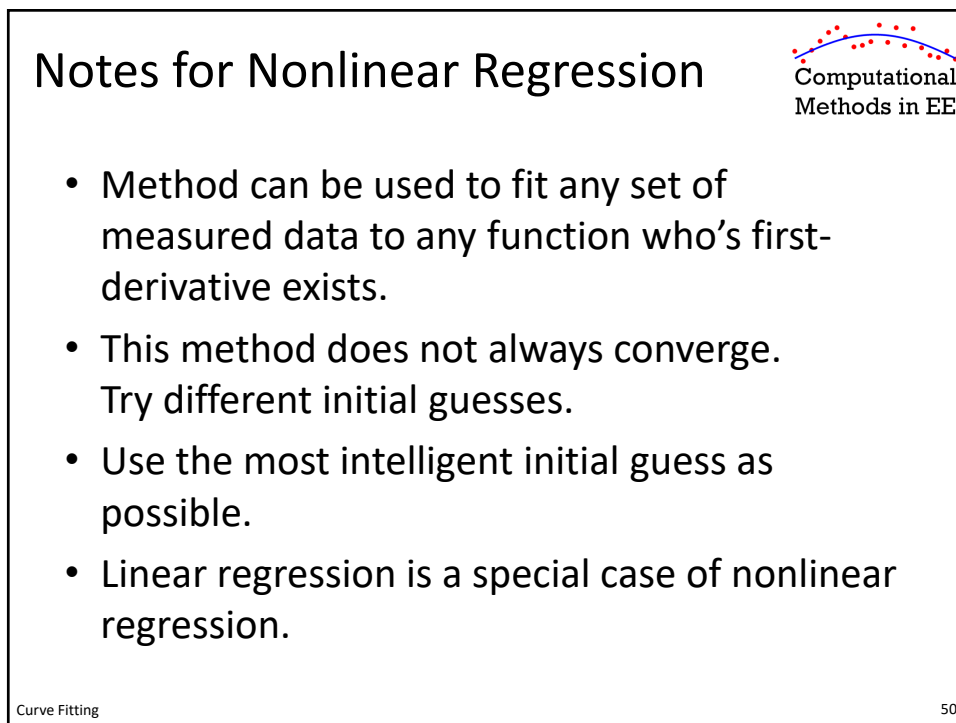
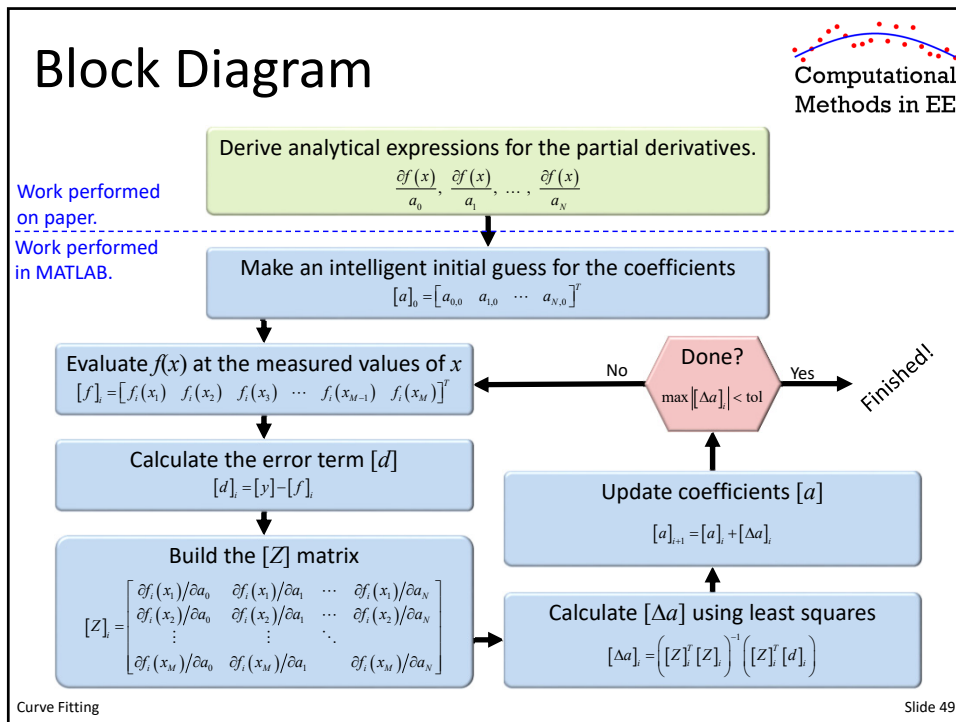
Step 7 – Go back to Step 2 until converged.

Convergence happens when the change in coefficient values $[\Delta a]_i$ falls below some tolerance.

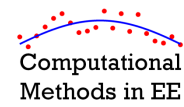
$$\left| \frac{a_{n,i+1} - a_{n,i}}{a_{n,i+1}} \right| \cdot 100\% \leq \text{tol} \quad \text{for all } a_n$$

Curve Fitting

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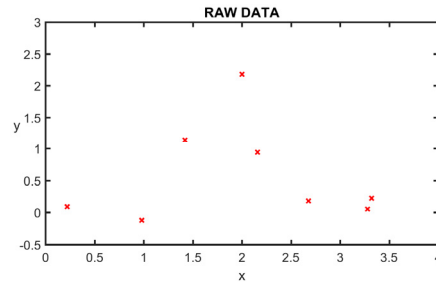


Example 1 – Fit to a Gaussian



We wish to fit a set of measured data to a standard Gaussian function.

$$f(x) = A \exp \left[- \left(\frac{x - x_0}{\sigma} \right)^2 \right]$$



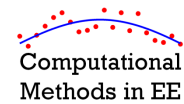
`% MEASURED DATA`

```
xm = [ -0.14 ; 0.22 ; 0.98 ; 1.42 ; 2.00 ; 2.16 ; 2.68 ; 3.28 ; 3.32 ];
fm = [ 0.01 ; 0.09 ; -0.12 ; 1.14 ; 2.18 ; 0.94 ; 0.18 ; 0.05 ; 0.22 ];
```

Curve Fitting

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Example 1 – Fit to a Gaussian



Formulation Step 1 – Identify the unknown parameters.

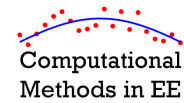
$$[a] = \begin{bmatrix} A \\ x_0 \\ \sigma \end{bmatrix}$$

In this case, we have 3 unknown parameters: A , x_0 , and σ .

Curve Fitting

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Example 1 – Fit to a Gaussian



Formulation Step 2 – Derive terms in $[Z]$ matrix.

$$[Z] = \begin{bmatrix} \frac{\partial f(x_1)}{\partial A} & \frac{\partial f(x_1)}{\partial x_0} & \frac{\partial f(x_1)}{\partial \sigma} \\ \frac{\partial f(x_2)}{\partial A} & \frac{\partial f(x_2)}{\partial x_0} & \frac{\partial f(x_2)}{\partial \sigma} \\ \vdots & \vdots & \vdots \\ \frac{\partial f(x_M)}{\partial A} & \frac{\partial f(x_M)}{\partial x_0} & \frac{\partial f(x_M)}{\partial \sigma} \end{bmatrix}$$

$$\begin{aligned} \frac{\partial f(x)}{\partial A} &= \exp\left[-\left(\frac{x-x_0}{\sigma}\right)^2\right] \\ &= \frac{f(x)}{A} \end{aligned}$$

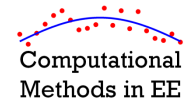
$$\begin{aligned} \frac{\partial f(x)}{\partial x_0} &= A \exp\left[-\left(\frac{x-x_0}{\sigma}\right)^2\right] \cdot \left\{-\frac{2}{\sigma^2}(x-x_0) \cdot (-1)\right\} \\ &= \frac{2(x-x_0)}{\sigma^2} f(x) \end{aligned}$$

$$\begin{aligned} \frac{\partial f(x)}{\partial \sigma} &= A \exp\left[-\left(\frac{x-x_0}{\sigma}\right)^2\right] \cdot \left\{-(x-x_0)^2 \cdot \left(-\frac{2}{\sigma^3}\right)\right\} \\ &= \frac{2(x-x_0)^2}{\sigma^3} f(x) \end{aligned}$$

Curve Fitting

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Example 1 – Fit to a Gaussian



The $[Z]$ matrix is

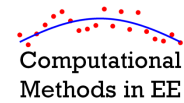
$$[Z] = \begin{bmatrix} \frac{f(x_1)}{A} & \frac{2(x_1-x_0)}{\sigma^2} f(x_1) & \frac{2(x_1-x_0)^2}{\sigma^3} f(x_1) \\ \frac{f(x_2)}{A} & \frac{2(x_2-x_0)}{\sigma^2} f(x_2) & \frac{2(x_2-x_0)^2}{\sigma^3} f(x_2) \\ \vdots & \vdots & \vdots \\ \frac{f(x_M)}{A} & \frac{2(x_M-x_0)}{\sigma^2} f(x_M) & \frac{2(x_M-x_0)^2}{\sigma^3} f(x_M) \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1}{A} f(\mathbf{x}) & \frac{2(\mathbf{x}-x_0)}{\sigma^2} f(\mathbf{x}) & \frac{2(\mathbf{x}-x_0)^2}{\sigma^3} f(\mathbf{x}) \end{bmatrix} \quad \leftarrow \text{We will calculate } [Z] \text{ this way.}$$

Curve Fitting

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Example 1 – Fit to a Gaussian



An example of a more intelligent initial guess...

$$f(x) = A \exp \left[- \left(\frac{x - x_0}{\sigma} \right)^2 \right]$$

$A_1 \leftarrow \max[f_i]$
 Consider using the maximum value of f_i in your measured points as your initial guess for A .

$x_{0,1} \leftarrow \text{average}[x_i]$
 Consider using the average value of x_i as your initial guess for x_0 .

$\sigma \leftarrow s(\max[x_i] - \min[x_i])$
 The standard deviation will likely be on the same order of magnitude as the range of values of x_i . Maybe choose $s = 0.5$?

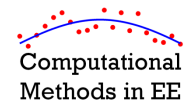
```

% SMART INITIAL GUESS
A = max(fm);
x0 = mean(xm);
s = 0.5*(max(xm) - min(xm));
  
```

Curve Fitting

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Example 1 – Fit to a Gaussian



The main loop...

Step a – Calculate $[f_i]$

$$[f]_i = [f_i(x_1) \quad f_i(x_2) \quad f_i(x_3) \quad \cdots \quad f_i(x_{M-1}) \quad f_i(x_M)]^T$$

```

% COMPUTE COLUMN VECTOR F
f = A*exp(-((xm - x0)/s).^2);
  
```

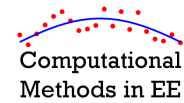
Here is $[f]$ over ten iterations...

0.6452	0.0393	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.9780	0.1218	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1.7707	0.6366	0.0160	0.2244	0.0088	0.0234	0.0131	0.0141	0.0141	0.0141
2.0931	1.0530	0.4043	1.7341	0.7211	1.2323	1.1202	1.1358	1.1357	1.1357
2.1414	1.2289	1.5594	1.3029	2.3184	2.0714	2.1838	2.1829	2.1833	2.1833
2.0714	1.1582	1.2653	0.6630	1.2660	0.9323	0.9277	0.9363	0.9361	0.9362
1.6520	0.7047	0.1130	0.0124	0.0111	0.0042	0.0026	0.0028	0.0028	0.0028
1.0165	0.2228	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.9757	0.2018	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Curve Fitting

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Example 1 – Fit to a Gaussian



The main loop...

Step *b* – Calculate $[d_i]$

$$[d]_i = [y] - [f]_i$$

```
% CALCULATE d
d = fm(:) - f;
```

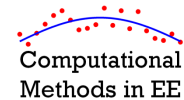
Here is $[d]$ over ten iterations...

```
-0.6352 -0.0293 0.0100 0.0100 0.0100 0.0100 0.0100 0.0100 0.0100 0.0100
-0.8880 -0.0318 0.0900 0.0899 0.0900 0.0900 0.0900 0.0900 0.0900 0.0900
-1.8907 -0.7566 -0.1360 -0.3444 -0.1288 -0.1434 -0.1331 -0.1341 -0.1341 -0.1341
-0.9531 0.0870 0.7357 -0.5941 0.4189 -0.0923 0.0198 0.0042 0.0043 0.0043
0.0386 0.9511 0.6206 0.8771 -0.1384 0.1086 -0.0038 -0.0029 -0.0033 -0.0033
-1.1314 -0.2182 -0.3253 0.2770 -0.3260 0.0077 0.0123 0.0037 0.0039 0.0038
-1.4720 -0.5247 0.0670 0.1676 0.1689 0.1758 0.1774 0.1772 0.1772 0.1772
-0.9665 -0.1728 0.0497 0.0500 0.0500 0.0500 0.0500 0.0500 0.0500 0.0500
-0.7557 0.0182 0.2198 0.2200 0.2200 0.2200 0.2200 0.2200 0.2200 0.2200
```

Curve Fitting

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Example 1 – Fit to a Gaussian



The main loop...

Step *c* – Build $[Z_i]$

$$z_1 = \frac{1}{A} f(\mathbf{x}) \quad z_2 = \frac{2(\mathbf{x} - x_0)}{\sigma^2} f(\mathbf{x})$$

$$z_3 = \frac{2(\mathbf{x} - x_0)^2}{\sigma^3} f(\mathbf{x})$$

$$Z_i = [z_1 \quad z_2 \quad z_3]$$

```
% FORM Z MATRIX
```

```
z1 = f/A;
z2 = 2*f.*(xm - x0)/s^2;
z3 = 2*f.*(xm - x0).^2/s^3;
Z = [ z1 z2 z3 ];
```

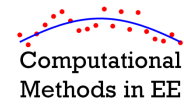
$$Z_1 = \begin{bmatrix} 0.2960 & -0.8230 & 0.9081 \\ 0.4486 & -1.0123 & 0.9063 \\ 0.8123 & -0.9335 & 0.4257 \\ 0.9601 & -0.4880 & 0.0984 \\ 0.9823 & 0.3307 & 0.0442 \\ 0.9502 & 0.5414 & 0.1224 \\ 0.7578 & 1.0058 & 0.5297 \\ 0.4663 & 1.0265 & 0.8966 \\ 0.4476 & 1.0114 & 0.9068 \end{bmatrix}$$

$$Z_{10} = \begin{bmatrix} 0.0000 & -0.0000 & 0.0000 \\ 0.0000 & -0.0000 & 0.0000 \\ 0.0042 & -0.1944 & 0.4552 \\ 0.3352 & -6.9938 & 7.3115 \\ 0.6445 & 8.5245 & 5.6503 \\ 0.2763 & 6.2539 & 7.0924 \\ 0.0008 & 0.0436 & 0.1163 \\ 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 \end{bmatrix}$$

Curve Fitting

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Example 1 – Fit to a Gaussian



The main loop...

Step d – Solve for $[\Delta a]_i$

$$[\Delta a]_i = \left([Z]_i^T [Z]_i \right)^{-1} \left([Z]_i^T [d]_i \right)$$

```
% CALCULATE [Da]
da = (Z'*Z)\(Z'*d);
```

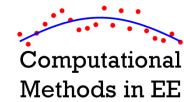
Here is $[\Delta a]$ over ten iterations...

-0.9316	0.3327	0.7433	0.5188	0.3549	0.2022	-0.0135	0.0010	-0.0000	0.0000
0.0958	0.0823	-0.2859	0.1775	-0.0723	0.0092	-0.0006	0.0000	-0.0000	0.0000
-0.6519	-0.6268	-0.0058	-0.0881	-0.0027	-0.0172	0.0022	-0.0001	0.0000	-0.0000

Curve Fitting

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Example 1 – Fit to a Gaussian



The main loop...

Step e – Update coefficients $[a]_i$

$$[a]_{i+1} = [a]_i + [\Delta a]_i$$

```
% UPDATE COEFFICIENTS [a]
A = A + da(1);
x0 = x0 + da(2);
s = s + da(3);
```

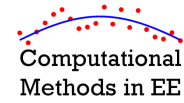
Here is $[a] = [A \ x_0 \ \sigma]^T$ over ten iterations...

1.2484	1.5810	2.3244	2.8432	3.1981	3.4003	3.3868	3.3878	3.3878	3.3878
1.8647	1.9470	1.6611	1.8386	1.7663	1.7755	1.7749	1.7750	1.7750	1.7750
1.0781	0.4513	0.4454	0.3574	0.3546	0.3374	0.3396	0.3395	0.3395	0.3395

Curve Fitting

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Example 1 – Fit to a Gaussian



The main loop...

Step f – Calculate error and check for convergence

$$\varepsilon = \max \left[\left| \frac{a_{n,i+1} - a_{n,i}}{a_{n,i+1}} \right| \right]$$

```
% CALCULATE MAXIMUM ERROR
err = max(abs(da./[A;x0;s]));
```

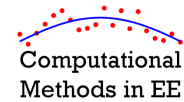
Here is `err` over ten iterations...

```
0.7463  1.3889  0.3198  0.2465  0.1110  0.0595  0.0065  0.0003  0.0000  0.0000
```

Curve Fitting

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Example 1 – Fit to a Gaussian



The final answer is...

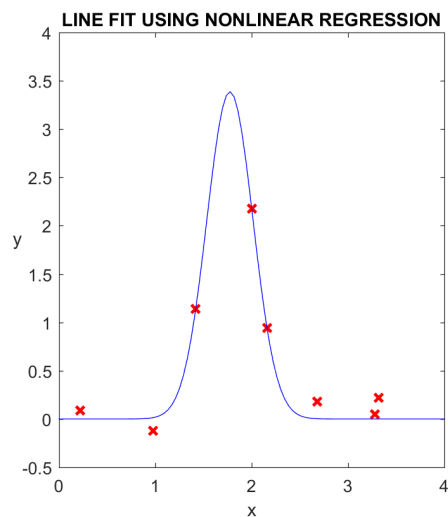
$$A = 3.3878$$

$$x_0 = 1.7750$$

$$\sigma = 0.3395$$

$$f(x) = A \exp \left[- \left(\frac{x - x_0}{\sigma} \right)^2 \right]$$

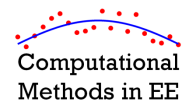
$$= 3.3878 \exp \left[- \left(\frac{x - 1.7750}{0.3395} \right)^2 \right]$$



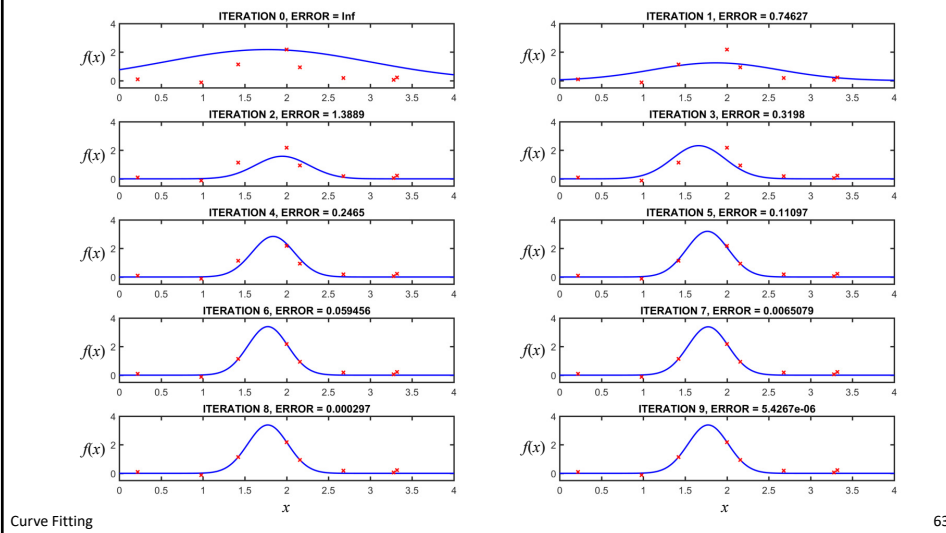
Curve Fitting

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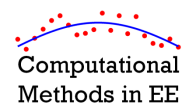
Example 1 – Fit to a Gaussian



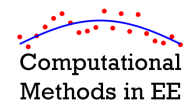
Here are the first 10 iterations of the algorithm visualized...



Fitting Polynomials (Exact Fit, Clean Math)



Statement of the Problem



Suppose we wish to fit the following N th-order polynomial to a set of points.

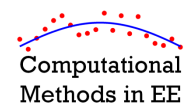
$$f(x) \approx a_0 + a_1x + a_2x^2 + \cdots + a_Nx^N$$

We have $N+1$ unknown coefficients so we need $N+1$ points to calculate the coefficients exactly.

Curve Fitting

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Calculating the Unknown Polynomial Coefficients



First, we write the polynomial at $N+1$ points.

$$f(x_1) = a_0 + a_1x_1 + a_2x_1^2 + \cdots + a_Nx_1^N$$

$$f(x_2) = a_0 + a_1x_2 + a_2x_2^2 + \cdots + a_Nx_2^N$$

$$\vdots$$

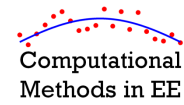
$$f(x_{N+1}) = a_0 + a_1x_{N+1} + a_2x_{N+1}^2 + \cdots + a_Nx_{N+1}^N$$

Since we are doing an exact fit, there are no residual terms.

Curve Fitting

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Calculating the Unknown Polynomial Coefficients



Second, we put the equations into matrix form.

$$\begin{aligned}
 f(x_1) &= a_0 + a_1x_1 + a_2x_1^2 + \dots + a_Nx_1^N \\
 f(x_2) &= a_0 + a_1x_2 + a_2x_2^2 + \dots + a_Nx_2^N \\
 &\vdots \\
 f(x_{N+1}) &= a_0 + a_1x_{N+1} + a_2x_{N+1}^2 + \dots + a_Nx_{N+1}^N
 \end{aligned}
 \quad \Rightarrow \quad
 \begin{bmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \\ \vdots \\ f(x_{N+1}) \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 & \dots & x_1^N \\ 1 & x_2 & x_2^2 & \dots & x_2^N \\ 1 & x_3 & x_3^2 & \dots & x_3^N \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{N+1} & x_{N+1}^2 & \dots & x_{N+1}^N \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_N \end{bmatrix}$$

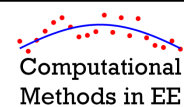
This can be written more compactly as

$$[f] = [X][a]$$

Curve Fitting

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Calculating the Unknown Polynomial Coefficients



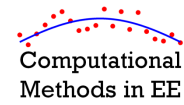
Last, the matrix equation is solved for $[a]$ to find the polynomial coefficients.

$$[a] = [X]^{-1}[f] \qquad [a] = \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_N \end{bmatrix}$$

Curve Fitting

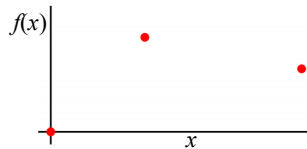
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Example 1 (1 of 2)



Fit the following points to a polynomial..

$$\begin{aligned} f(0) &= 0 \\ f(1.5) &= 1.5 \\ f(4.0) &= 1.0 \end{aligned}$$



Step 1 – Determine order of polynomial

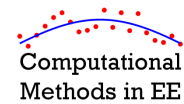
Since we have three points, we can fit a quadratic polynomial.

$$f(x) \approx a_0 + a_1x + a_2x^2$$

Curve Fitting

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Example 1 (2 of 2)



Step 2 – Our matrix equation is

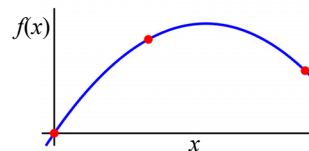
$$\begin{aligned} f_1 &= a_0 + a_1x_1 + a_2x_1^2 \\ f_2 &= a_0 + a_1x_2 + a_2x_2^2 \\ f_3 &= a_0 + a_1x_3 + a_2x_3^2 \end{aligned} \rightarrow \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} \rightarrow \begin{bmatrix} 0 \\ 1.5 \\ 1.0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1.5 & 2.25 \\ 1 & 4 & 16 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix}$$

Step 3 – Calculate unknown polynomial coefficients.

$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1.5 & 2.25 \\ 1 & 4 & 16 \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ 1.5 \\ 1.0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1.45 \\ -0.3 \end{bmatrix}$$

Step 4 – Write the final polynomial.

$$f(x) \approx 1.45x - 0.3x^2$$



Curve Fitting

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Interpolation & Extrapolation

What is Interpolation & Extrapolation?

Sometimes we have some several precisely known values and want to know an intermediate value (interpolation) or a value outside of the range of the known values (extrapolation).

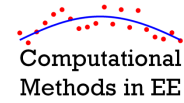
Measuring the new value may be difficult, expensive, or impossible.

Interpolation and extrapolation can be thought of as two steps:

Step 1 – Fit data to a curve.

Step 2 – Use the curve fit to calculate the new value(s).

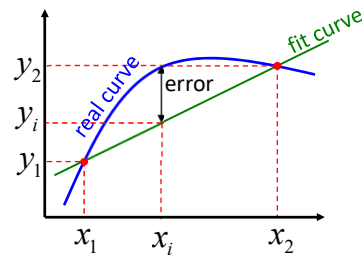
Linear Interpolation



Given two data points, we can fit a line from which we can interpolate or extrapolate anything else.

Given two data points (x_1, y_1) and (x_2, y_2) , the equation for the line is

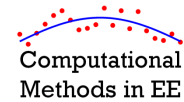
$$y_i = y_1 + \underbrace{\frac{y_2 - y_1}{x_2 - x_1}}_{\text{slope}} (x_i - x_1)$$



Curve Fitting

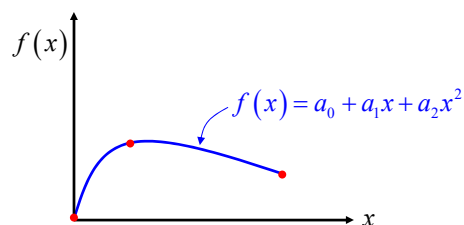
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Polynomial Interpolation (1 of 3)



Interpolation using a quadratic polynomial is likely the most common method of interpolation.

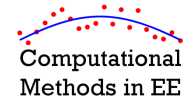
This requires three points.



Curve Fitting

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Polynomial Interpolation (2 of 3)



Write form a matrix equation.

$$\begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix}$$

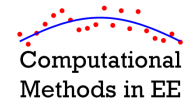
Solve for unknown coefficients.

$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \end{bmatrix}^{-1} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} = \begin{bmatrix} \frac{x_2 x_3}{(x_1 - x_2)(x_1 - x_3)} & -\frac{x_1 x_3}{(x_1 - x_2)(x_2 - x_3)} & \frac{x_1 x_2}{(x_1 - x_3)(x_2 - x_3)} \\ -\frac{x_2 + x_3}{(x_1 - x_2)(x_1 - x_3)} & \frac{x_1 + x_3}{(x_1 - x_2)(x_2 - x_3)} & -\frac{x_1 + x_2}{(x_1 - x_3)(x_2 - x_3)} \\ \frac{1}{(x_1 - x_2)(x_1 - x_3)} & -\frac{1}{(x_1 - x_2)(x_2 - x_3)} & \frac{1}{(x_1 - x_3)(x_2 - x_3)} \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix}$$

Curve Fitting

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Polynomial Interpolation (3 of 3)



The final equations are

$$a_0 = \frac{x_2 x_3}{(x_1 - x_2)(x_1 - x_3)} f_1 - \frac{x_1 x_3}{(x_1 - x_2)(x_2 - x_3)} f_2 + \frac{x_1 x_2}{(x_1 - x_3)(x_2 - x_3)} f_3$$

$$a_1 = -\frac{x_2 + x_3}{(x_1 - x_2)(x_1 - x_3)} f_1 + \frac{x_1 + x_3}{(x_1 - x_2)(x_2 - x_3)} f_2 - \frac{x_1 + x_2}{(x_1 - x_3)(x_2 - x_3)} f_3$$

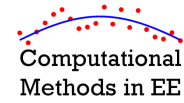
$$a_2 = \frac{1}{(x_1 - x_2)(x_1 - x_3)} f_1 - \frac{1}{(x_1 - x_2)(x_2 - x_3)} f_2 + \frac{1}{(x_1 - x_3)(x_2 - x_3)} f_3$$

Typically, these are not calculated using these equations. Instead, the matrix inversion is performed numerically.

Curve Fitting

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Example 1 – Quadratic Interpolation



Given the following points, interpolate the value at $x = 3$.

$$f(0) = 0$$

$$f(1.5) = 1.5$$

$$f(4.0) = 1.0$$

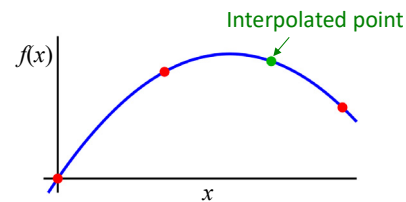
Solution

Step 1 – We already fit these points to a quadratic polynomial. The answer was

$$f(x) = 1.45x - 0.3x^2$$

Step 2 – We evaluate this at $x = 3$.

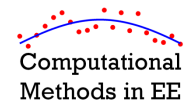
$$f(3) = 1.45(3) - 0.3(3)^2 = \boxed{1.65}$$



Curve Fitting

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Example 2 – Quadratic Extrapolation



Given the following points, extrapolate the value at $x = -0.5$.

$$f(0) = 0$$

$$f(1.5) = 1.5$$

$$f(4.0) = 1.0$$

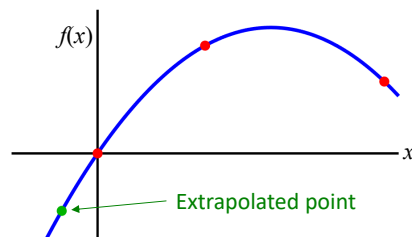
Solution

Step 1 – We already fit these points to a quadratic polynomial. The answer was

$$f(x) = 1.45x - 0.3x^2$$

Step 2 – We evaluate this at $x = -0.5$.

$$f(-0.5) = 1.45(-0.5) - 0.3(-0.5)^2 = \boxed{-0.8}$$



Curve Fitting

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