Exam 2 Review

CH EN 2450
Numerical Methods
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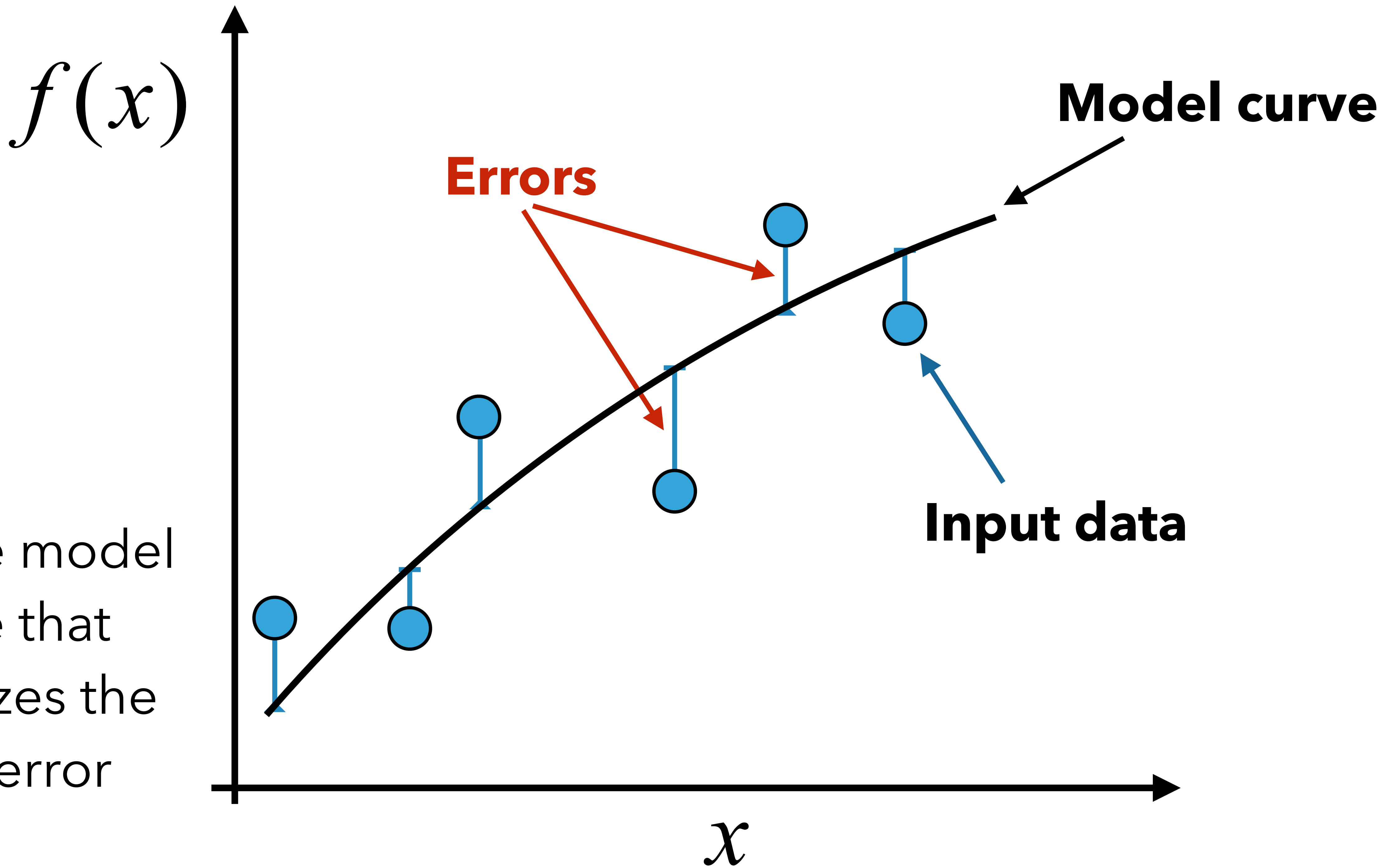
Basic Idea of Regression



Find the model curve that minimizes the total error

regression to high-order polynomials

$$\text{model} : f(x) = a_m x^m + \ldots + a_2 x^2 + a_1 x + a_0$$

$$\begin{bmatrix} N & \sum x_i & \sum x_i^2 & \cdots & \sum x_i^m \\ \sum x_i & \sum x_i^2 & \sum x_i^3 & \cdots & \sum x_i^{m+1} \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 & \cdots & \sum x_i^{m+2} \\ \vdots & & & & \\ \sum x_i^m & \sum x_i^{m+1} & \sum x_i^{m+2} & & \sum x_i^{m+m} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ \vdots \\ a_m \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum x_i y_i \\ \sum x_i^2 y_i \\ \vdots \\ \sum x_i^m y_i \end{bmatrix}$$

$m+1$ Equations, $m+1$ Unknowns

Generalized Linear Regression

$$y_{\text{model}} : f(x) = \alpha_1 \phi_1(x) + \alpha_2 \phi_2(x) + \ldots + \alpha_M \phi_M(x)$$

$$\mathbf{A} = \begin{array}{cc}
\begin{array}{cccc} \text{First basis function} & \text{Second basis function} & & \text{mth basis function} \end{array} & \\
\left[\begin{array}{cccc}
\phi_1(x_1) & \phi_2(x_1) & \ldots & \phi_m(x_1) \\
\phi_1(x_2) & \phi_2(x_2) & \ldots & \phi_m(x_2) \\
\vdots & \vdots & \ldots & \vdots \\
\phi_1(x_N) & \phi_2(x_N) & \ldots & \phi_m(x_N)
\end{array}\right] &
\begin{array}{l} \text{First observation} \\ \text{Second observation} \\ \\ \text{Nth observation} \end{array}
\end{array}$$

$$\mathbf{A}^T\mathbf{A}\boldsymbol{\alpha} = \mathbf{A}^T\mathbf{y}$$

All you need to know is the matrix A!

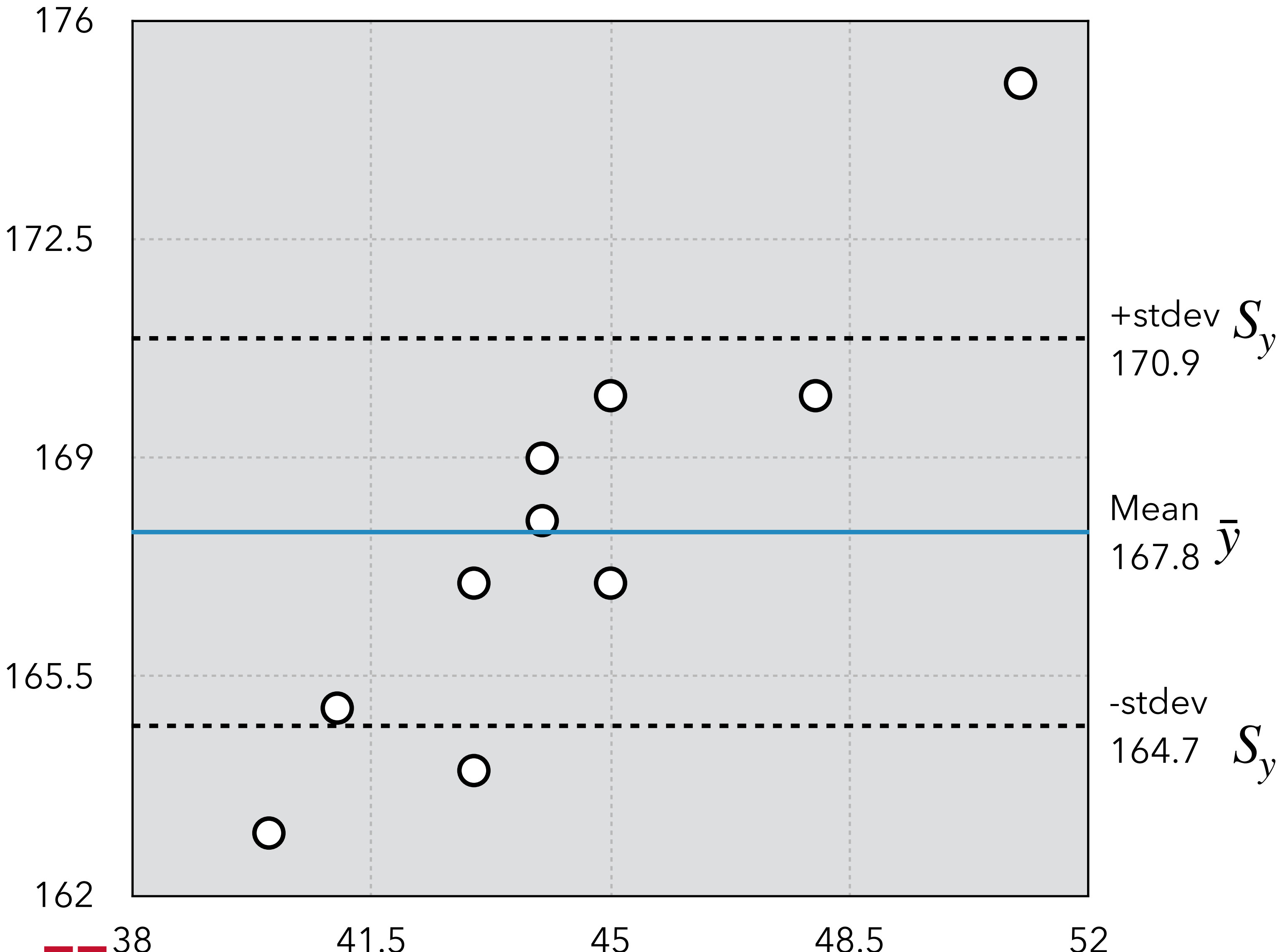
These are called the Normal Equations

Usage

- Given N data pairs in the form $(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)$ and a linear regression model of the form
  $y_{\text{model}} : f(x) = \alpha_1\phi_1(x) + \alpha_2\phi_2(x) + \ldots + \alpha_M\phi_M(x)$
- Build the regression matrix $\mathbf{A}$
  - Column number corresponds to which basis function goes there (first column, first basis function etc…)
  - Row number corresponds to which observation the basis function is applied to (first row corresponds to first observation x_1)
- Build the $\mathbf{y}$ vector which contains the values of the observed dependent variable
- Solve the system: $\mathbf{A}^T\mathbf{A}\boldsymbol{\alpha} = \mathbf{A}^T\mathbf{y}$ - the solution vector, $\boldsymbol{\alpha}$, contains the coefficients of the regression model

Standard Deviation

Standard Deviation: Measures spread of data around the mean value



Mean Value: $\bar{y} = \dfrac{\sum y_i}{n}$

$$S_y = \sqrt{\frac{\sum (y_i - \bar{y})^2}{n-1}}$$

For a normal distribution,

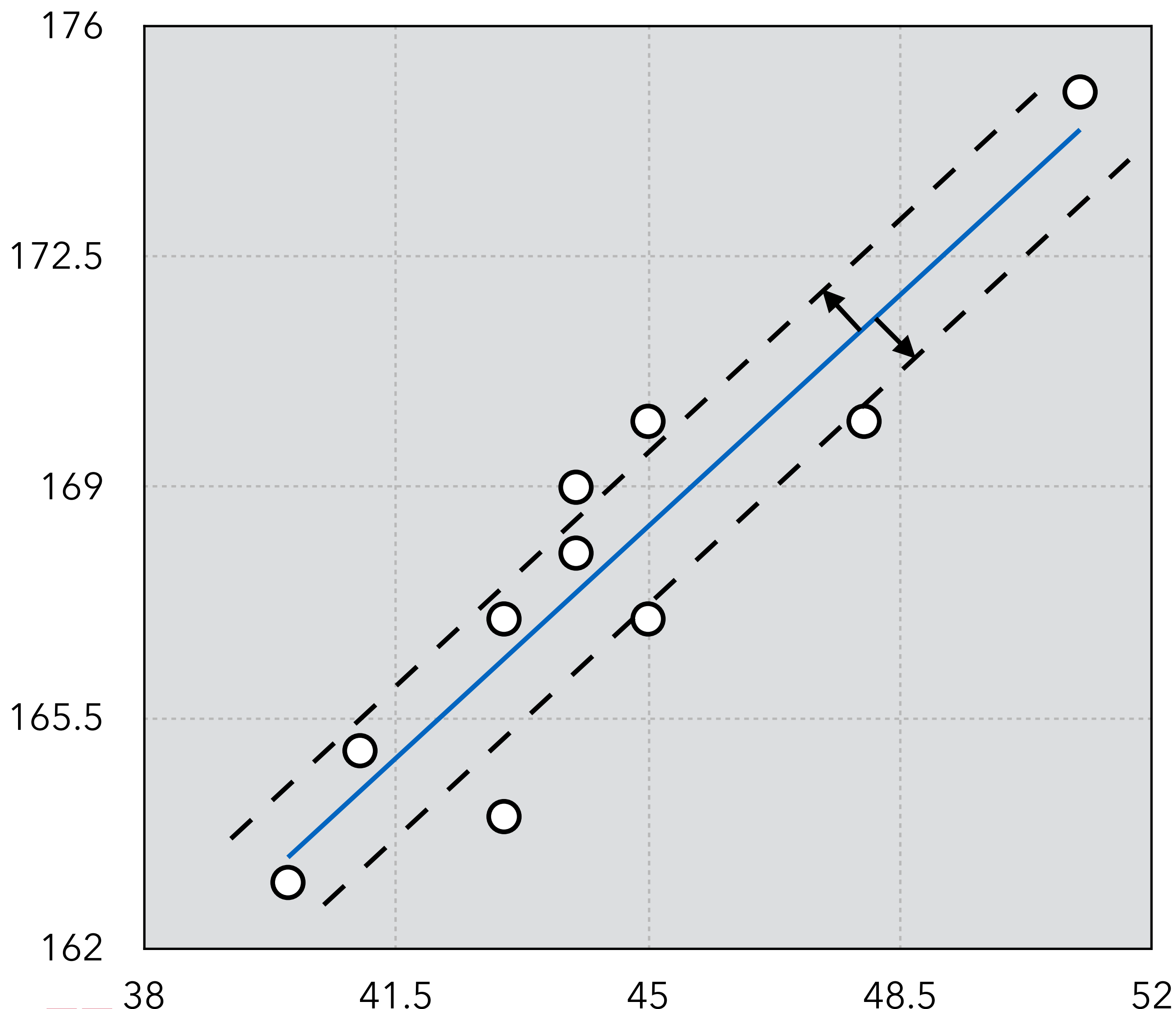
- 68% of the data fall within a standard deviation of the mean
- 95% of the data fall within two standard deviations of the mean

Note that in some cases you will see n used in the denominator for the standard deviation. This has to do with sample vs population stats and is beyond the scope of this course. The standard deviation is a property of a population while it is a statistic for a sample.

Standard Error

Standard Error: Measures spread of data around the regression line

$$S_{y/x} = \sqrt{\frac{\sum (y_i - f_i)^2}{n-2}}$$



For a normal distribution,

- 68% of the data fall within a standard error of the model fit
- 95% of the data fall within two standard errors of the model fit

Standard Error represents the average distance that the observed values fall from the **regression** line. It tells you how wrong the **regression** model is on average using the units of the response variable.

You can think of the standard error as the standard deviation with respect to the regression line

$S_t = \sum (y_i - \bar{y})^2$ Magnitude of error **prior** to regression, with respect to the **mean**

$S_r = \sum (y_i - f_i)^2$ Magnitude of error **after** to regression, with respect to the **regression line**

This is called the R-Squared value
of Coefficient of Determination

$$R^2 = \frac{S_t - S_r}{S_t} = 1 - \frac{S_r}{S_t}$$

- $R^2 \to 0$: Bad fit. No improvement over using a mean value to describe the data
- $R^2 \to 1$: Perfect fit! Significant improvement over just using a mean value to describe the data

What Makes a Regression Model Linear?

- A regression model is linear if
  - The parameters show up linearly OR
  - the least-squares equations can be written as a system of linear equations
- There are two ways to show the latter:
  - Write the least-squares equations (a lot of algebra)
  - Write down part the normal equations (much easier)

y_{model}	**Linear**	**Nonlinear**
$y_{\text{model}} = ax + b$	X	
$y_{\text{model}} = ax + \frac{b}{x}$	X	
$y_{\text{model}} = \sin(a)x + b$	X	
$y_{\text{model}} = \sin(ax) + b$		X
$y_{\text{model}} = (ax)^2 + b$	X	
$y_{\text{model}} = x^a + b$		X
$y_{\text{model}} = a^x + b$		X
$y_{\text{model}} = e^{\alpha}x + \beta x^2$	X	
$y_{\text{model}} = \beta e^{\alpha x}$		X

Nonlinear Least-Squares Regression

Assume that your model, $f(x)$, has n parameters a_k that we want to determine via regression.

$$S = \sum (y_i - f_i)^2$$

$$\frac{\partial S}{\partial a_k} = 0, \quad \forall k$$

$$y_{\text{model}} : f(x) = \cos(a_0 x) + e^{-a_1 x^2} + \sin(a_2 x^2)$$

Same approach as before, but now the parameters of $f(x)$ may enter *nonlinearly*!

Example

$$S = \sum (y_i - f_i)^2 \qquad \frac{\partial S}{\partial a_k} = 0$$

$$f(x) = \alpha e^{\beta x}$$

$$S = \sum (y_i - \alpha e^{\beta x_i})^2$$

$$\frac{\partial S}{\partial \alpha} = 0 \qquad -2\sum e^{\beta x_i}\left(y_i - \alpha e^{\beta x_i}\right) = 0$$

$$\frac{\partial S}{\partial \beta} = 0 \qquad -2\sum \alpha x_i e^{\beta x_i}\left(y_i - \alpha e^{\beta x_i}\right) = 0$$

We will learn how to solve this soon!

Two NONLINEAR equations with two unknowns

$$\sum y_i e^{\beta x_i} - \alpha \sum y_i e^{\beta x_i} = 0$$

$$\alpha \sum x_i y_i e^{\beta x_i} - \alpha^2 \sum x_i y_i e^{\beta x_i} = 0$$

Linear Regression of a Nonlinear Models

Sometimes, it is possible to linearize nonlinear models via appropriate transformations

$$y_{\text{model}} = \alpha e^{\beta f(x)} \quad \text{e.g.} \quad k(T) = A e^{-E\frac{1}{RT}}$$

$$\ln(y_{\text{model}}) = \ln(\alpha) + \beta f(x)$$

$$\underbrace{\ln(y_{\text{model}})}_{Y_{\text{model}}} = \underbrace{\ln(\alpha)}_{A_0} + \underbrace{\beta}_{A_1} \underbrace{f(x)}_{X}$$

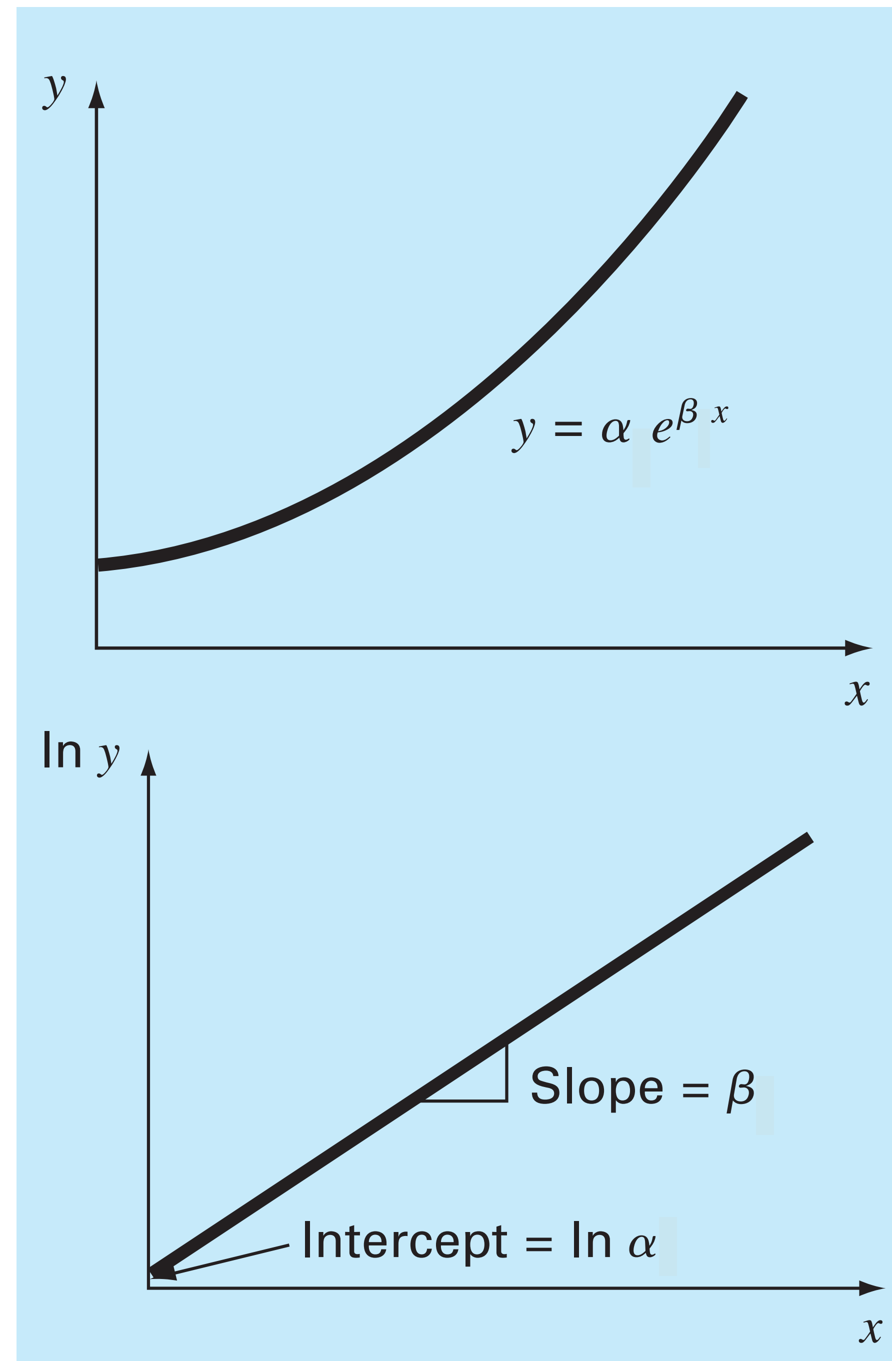
$$Y_{\text{model}} = A_0 + A_1 X$$

$$Y_{\text{model}} = \ln(y_{\text{model}})$$

$$A_0 = \ln(\alpha)$$

$$A_1 = \beta$$

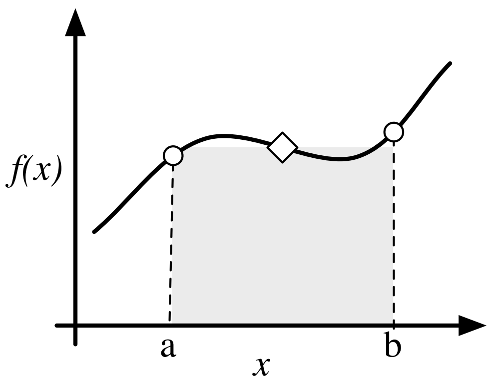
$$X = f(x)$$



Midpoint Rule

<u>Concept</u>: Approximate $f(x)$ as a *constant* on the interval $[a,b]$.

$$\int_a^b f(x)\mathrm{d}x \approx (b-a)\, f\left(\frac{b+a}{2}\right)$$

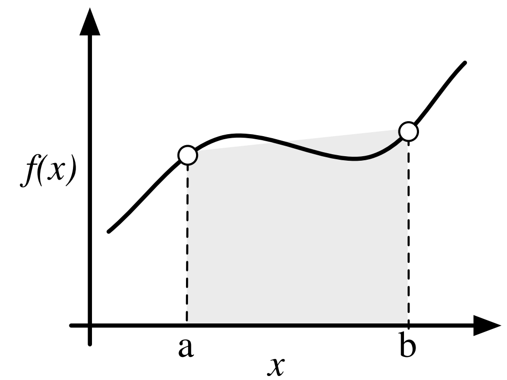


- Requires function value at the midpoint (can be a problem for tabular/discrete data).

Trapezoid Rule

<u>Concept</u>: Approximate $f(x)$ as a *linear* function on the interval $[a,b]$.

$$\int_a^b f(x)\mathrm{d}x \approx \frac{(b-a)}{2}\left[f(a)+f(b)\right]$$

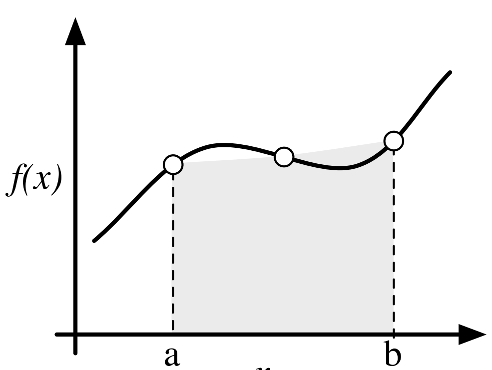


- Convenient form for tabular (discrete) data.
- Doesn't require equally spaced data.
- $\Delta x = b-a$

Simpson's 1/3 Rule

<u>Concept</u>: Approximate $f(x)$ as a *quadratic* on the interval $[a,b]$.

$$\int_a^b f(x)\mathrm{d}x \approx \frac{\Delta x}{3}\left[f(a) + 4f\left(\tfrac{a+b}{2}\right) + f(b)\right]$$

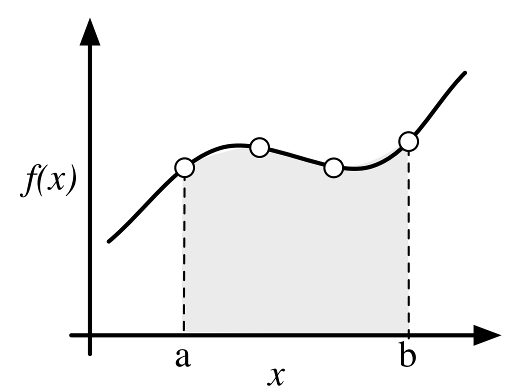


- Requires three equally spaced points on interval $[a,b]$.
- $\Delta x = (b-a)/2$

Simpson's 3/8 Rule

<u>Concept</u>: Approximate $f(x)$ as a *cubic* on the interval $[a,b]$.

$$\int_a^b f(x)\mathrm{d}x \approx \frac{3\Delta x}{8}\left(f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right)$$



- Requires four equally spaced points on interval $[a,b]$.
- $\Delta x = (b-a)/3$
- $x_i = a + i\Delta x$

Error Bounds

$$\int_a^b f(x)\mathrm{d}x \quad |f''(x)| \le K \quad |f''''(x)| \le M$$ on [a,b]

Midpoint

$$E_M \le K\frac{(b-a)^3}{24n^2}$$

Trapezoid

$$E_T \le K\frac{(b-a)^3}{12n^2}$$

Simpson's 1/3

$$E_S \le M\frac{(b-a)^5}{18n^4}$$

n = Number of segments

Note, these are only UPPER bounds. The actual error may be much smaller depending on the function.

First Derivatives

formula	order		Constant Δx ?
$\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right\|_i \approx \frac{f_{i+1}-f_i}{\Delta x}$	Δx	Forward difference	no
$\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right\|_i \approx \frac{f_i-f_{i-1}}{\Delta x}$	Δx	backward difference	no
$\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right\|_i \approx \frac{f_{i+1}-f_{i-1}}{2\Delta x}$	Δx^2	central difference	yes
$\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right\|_i \approx \frac{-3f_i+4f_{i+1}-f_{i+2}}{2\Delta x}$	Δx^2	Forward difference	yes
$\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right\|_i \approx \frac{3f_i-4f_{i-1}+f_{i-2}}{2\Delta x}$	Δx^2	backward difference	yes

Some Approximations for Second Derivatives

All assume constant Δx.

$\frac{\partial^2 f}{\partial x^2}$	Order	Comments
$\left.\frac{\partial^2 f}{\partial x^2}\right\|_i \approx \frac{f_i - 2f_{i+1} + f_{i+2}}{\Delta x^2}$	Δx	Forward difference
$\left.\frac{\partial^2 f}{\partial x^2}\right\|_i \approx \frac{f_i - 2f_{i-1} + f_{i-2}}{\Delta x^2}$	Δx	Backward difference
$\left.\frac{\partial^2 f}{\partial x^2}\right\|_i \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}$	Δx^2	Central difference
$\left.\frac{\partial^2 f}{\partial x^2}\right\|_i \approx \frac{2f_i - 5f_{i+1} + 4f_{i+2} - f_{i+3}}{\Delta x^2}$	Δx^2	Forward difference
$\left.\frac{\partial^2 f}{\partial x^2}\right\|_i \approx \frac{-f_{i-3} + 4f_{i-2} - 5f_{i-1} + 2f_i}{\Delta x^2}$	Δx^2	Backward difference