Numerical Techniques

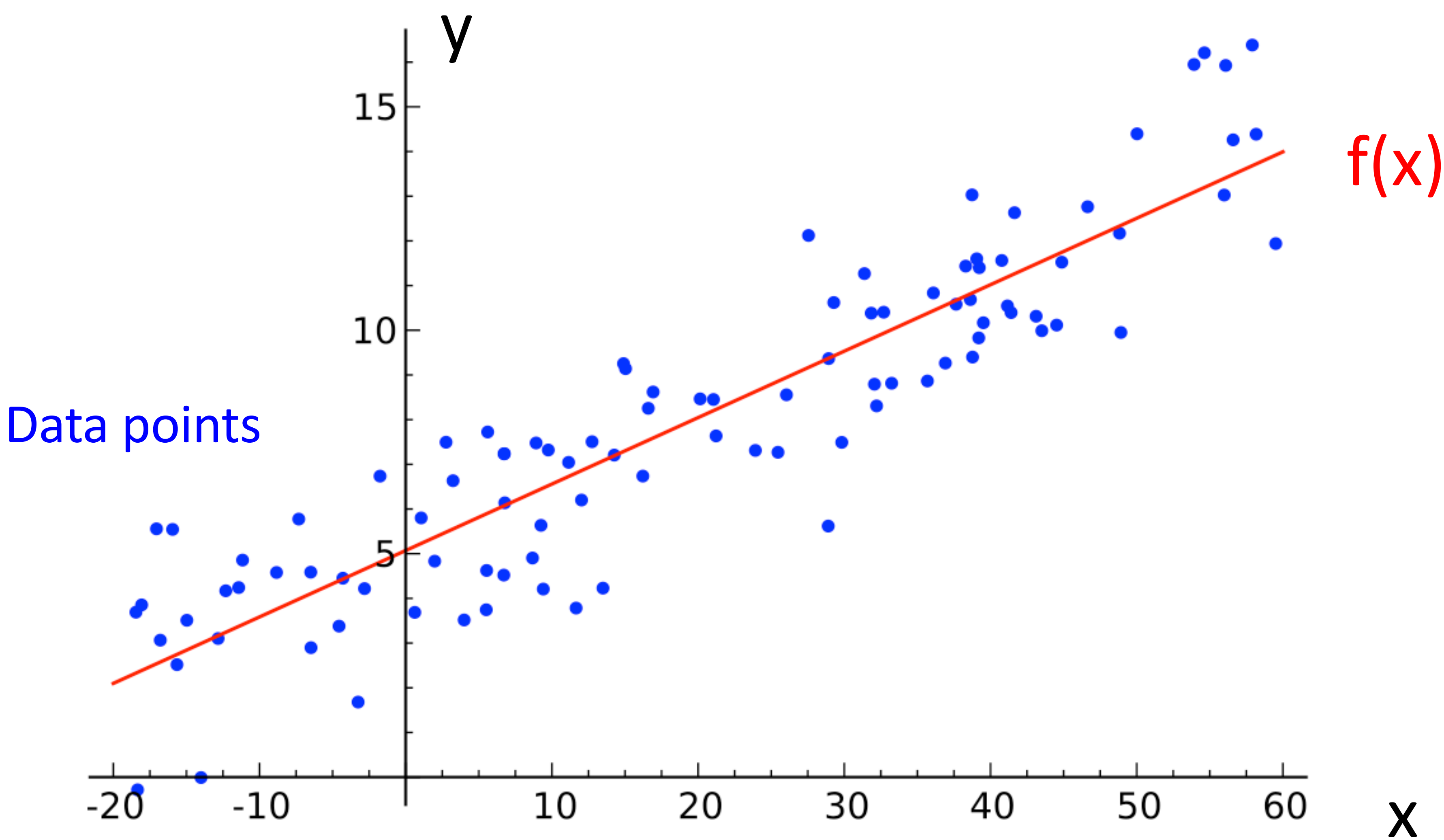
- Numerical Differentiation
- Ordinary Differential Equations
- Numerical Integration
- Root Finding
- **Least Squares Data Fitting**

Chapter 4 in class textbook

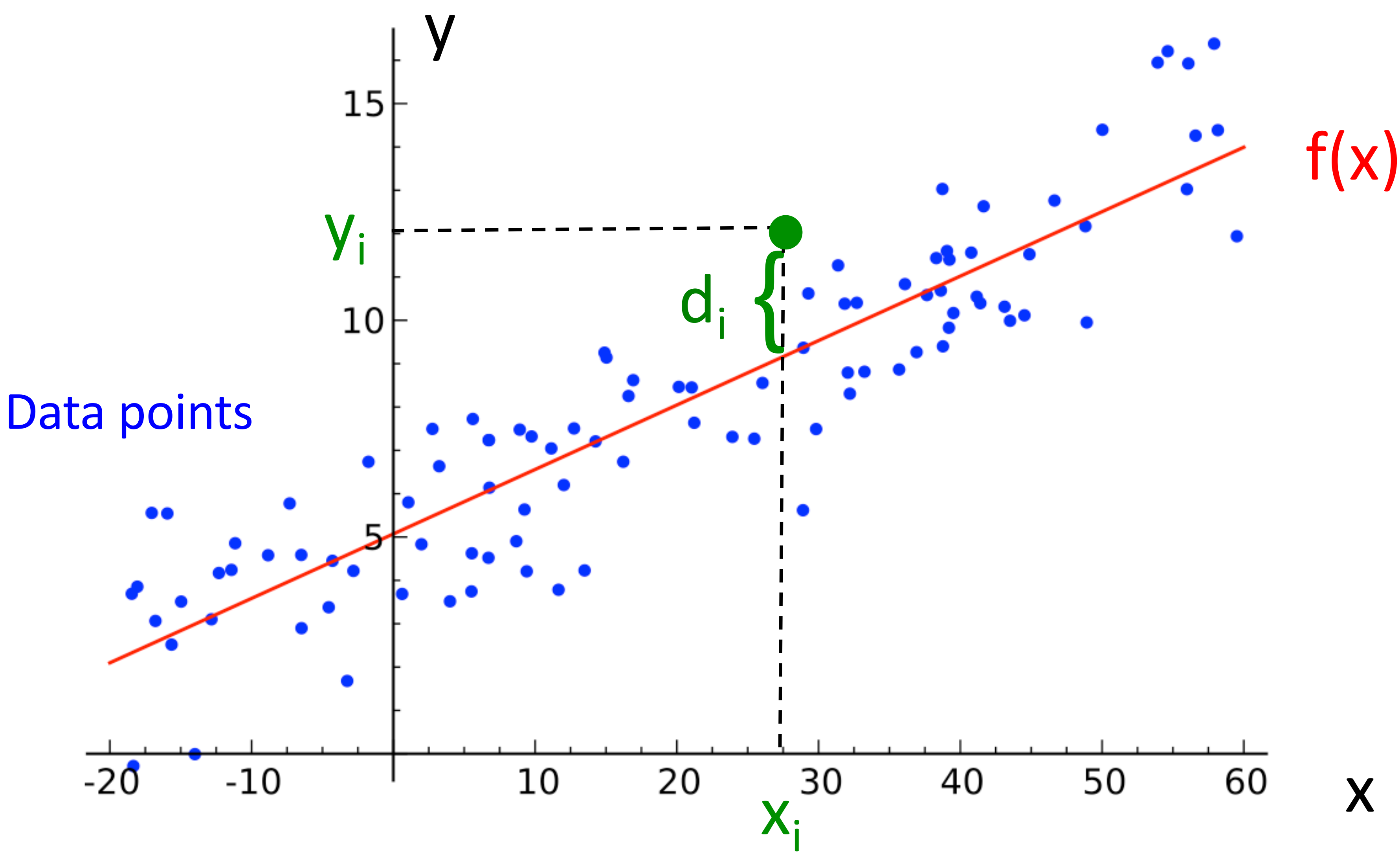
The NIMBUS-7 Satellite Data

Data point i	Altitude (km) x_i	Ozone mixing ratio (ppmv) y_i
1	20.	3.1
2	22.	4.01
3	22.4	4.1
4	23.	4.3
5	24.	4.4
6	26.	5.3
7	28.	6.1
8	29.7	7.2
9	31.	8.3
10	33.	7.5
11	34.	9.3
12	35.	7.7
13	35.	7.8
14	36.	7.7
15	37.	8.1
16	38.	8.4
17	39.4	9.0
18	40.	8.9
19	41.	9.6
20	41.5	10.7

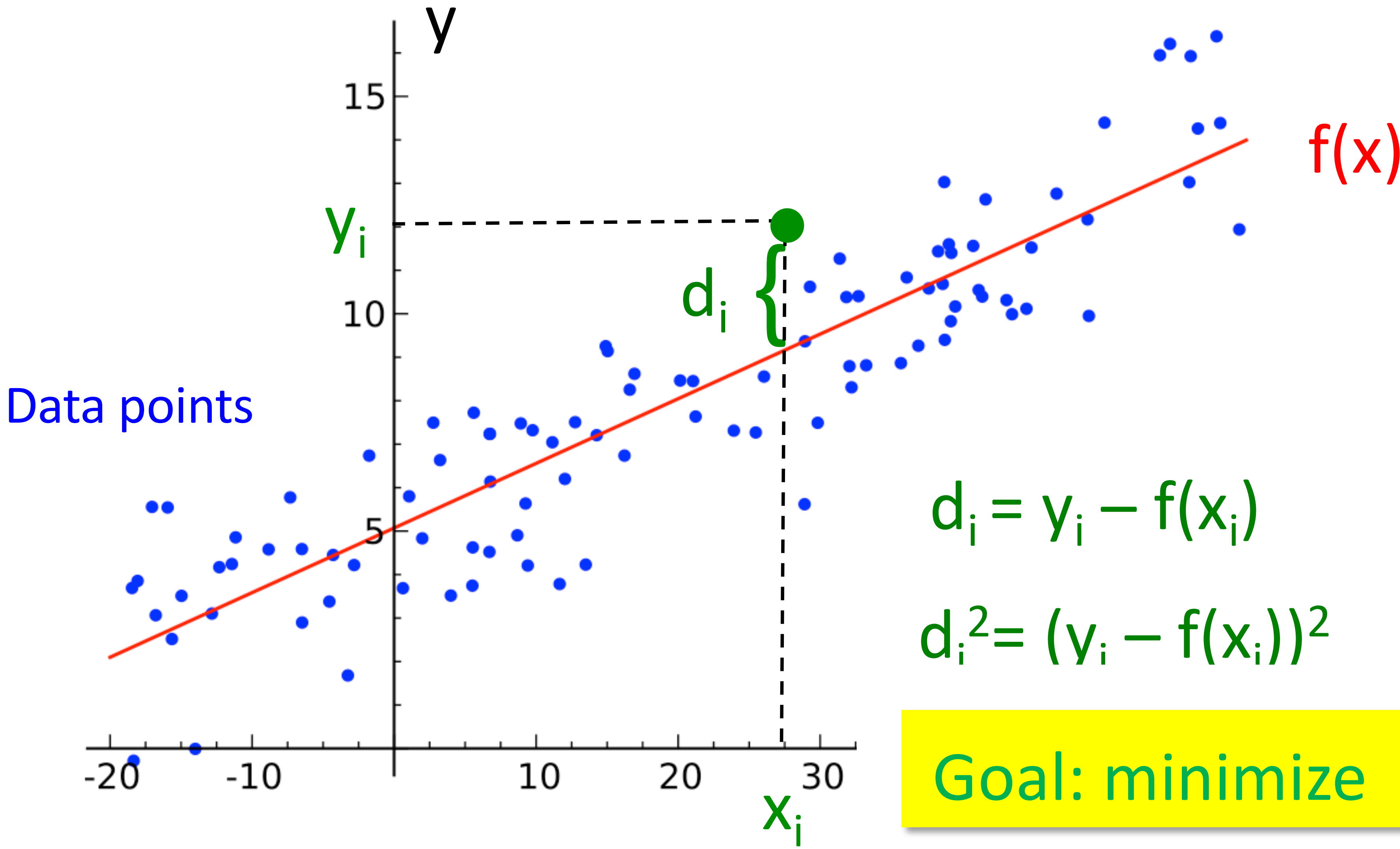
Least-Squares Curve Fitting



Least-Squares Curve Fitting



Least-Squares Curve Fitting



$d_i = y_i - f(x_i)$

$d_i^2 = (y_i - f(x_i))^2$

Goal: minimize d_i^2

The Least-Squares Technique — **Linear Model**

$$\Pi \equiv \sum_{i=1}^{n} \left(y_i - f(x_i)\right)^2 = \sum_{i=1}^{n} \left(y_i - (a + bx_i)\right)^2 = \min.$$

Let's find the minimum possible value of $\Pi(a,b)$:

$$\Rightarrow \quad \left.\begin{aligned} \frac{\partial \Pi(a,b)}{\partial a} &= 0 \\ \frac{\partial \Pi(a,b)}{\partial b} &= 0 \end{aligned}\right\}$$

Two equations for 2 unknowns (*a* and *b*)

The Least-Squares Technique — **Linear Model**

$$\Pi \equiv \sum_{i=1}^{n} \left(y_i - f(x_i)\right)^2 = \sum_{i=1}^{n} \left(y_i - (a + bx_i)\right)^2 = \min.$$

One obtains:

$$\frac{\partial \Pi}{\partial a} = -2 \sum_{i=1}^{n} \left(y_i - (a + bx_i)\right) = 0$$

$$\frac{\partial \Pi}{\partial b} = -2 \sum_{i=1}^{n} x_i \left(y_i - (a + bx_i)\right) = 0$$

The Least-Squares Technique — **Linear Model**

$$\Pi \equiv \sum_{i=1}^{n} \left(y_i - f(x_i)\right)^2 = \sum_{i=1}^{n} \left(y_i - (a + bx_i)\right)^2 = \min.$$

One obtains:

$$\frac{\partial \Pi}{\partial a} = -2 \sum_{i=1}^{n} \left(y_i - (a + bx_i)\right) = 0 \quad \Rightarrow \quad \sum_{i=1}^{n} y_i = a \sum_{i=1}^{n} 1 + b \sum_{i=1}^{n} x_i$$

$$\frac{\partial \Pi}{\partial b} = -2 \sum_{i=1}^{n} x_i \left(y_i - (a + bx_i)\right) = 0 \quad \Rightarrow \quad \sum_{i=1}^{n} x_i\, y_i = a \sum_{i=1}^{n} x_i + b \sum_{i=1}^{n} x_i^2$$

The Least-Squares Technique — **Linear Model**

$$\sum_{i=1}^{n} y_i \quad = \quad a\sum_{i=1}^{n} 1 + b\sum_{i=1}^{n} x_i \qquad \text{(I)}$$

$$\sum_{i=1}^{n} x_i\, y_i \quad = \quad a\sum_{i=1}^{n} x_i + b\sum_{i=1}^{n} x_i^2 \qquad \text{(II)}$$

$$\Leftrightarrow \quad \begin{pmatrix} n & \sum_i x_i \\ \sum_i x_i & \sum_i x_i^2 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \sum_i & y_i \\ \sum_i x_i y_i \end{pmatrix}$$

Matrix inversion $\Rightarrow$

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} n & \sum_i x_i \\ \sum_i x_i & \sum_i x_i^2 \end{pmatrix}^{-1} \begin{pmatrix} \sum_i & y_i \\ \sum_i x_i y_i \end{pmatrix}$$

The equations of the **Linear Model** can be written as

From (I):

$$\sum_{i=1}^{n} y_i = a \cdot n + b \sum_{i=1}^{n} x_i$$

$$\Rightarrow a = \frac{1}{n}\left(\sum_{i=1}^{n} y_i - b \sum_{i=1}^{n} x_i\right)$$

This leads to:

$$a = \frac{\left(\sum_{i=1}^{n} y_i\right)\left(\sum_{i=1}^{n} x_i^2\right) - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} x_i\ y_i\right)}{n\left(\sum_{i=1}^{n} x_i^2\right) - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$$b = \frac{\left(n \sum_{i=1}^{n} x_i\ y_i\right) - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)}{n\left(\sum_{i=1}^{n} x_i^2\right) - \left(\sum_{i=1}^{n} x_i\right)^2}$$

Summary — Linear Model: $f(x)=a+b\,x$

$$a = \frac{\left(\sum_{i=1}^{n} y_i\right)\left(\sum_{i=1}^{n} x_i^2\right) - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} x_i\ y_i\right)}{n\left(\sum_{i=1}^{n} x_i^2\right) - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$$b = \frac{\left(n\sum_{i=1}^{n} x_i\ y_i\right) - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)}{n\left(\sum_{i=1}^{n} x_i^2\right) - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$$\text{Error :} \quad \chi^2 \equiv \frac{1}{n}\sum_{i=1}^{n}\left(y_i - f(x_i)\right)^2$$

The Least-Squares Technique — 2nd order **polynomial** data fitting

$$\Pi \equiv \sum_{i=1}^{n} (y_i - f(x_i))^2 = \sum_{i=1}^{n} \left(y_i - (a + bx_i + cx_i^2)\right)^2 = \text{min.}$$

Least squares error

3 unknowns

$$\frac{\partial \Pi}{\partial a} = -2 \sum_{i=1}^{n} \left(y_i - (a + bx_i + cx_i^2)\right) = 0$$

$$\frac{\partial \Pi}{\partial b} = -2 \sum_{i=1}^{n} x_i \left(y_i - (a + bx_i + cx_i^2)\right) = 0$$

$$\frac{\partial \Pi}{\partial c} = -2 \sum_{i=1}^{n} x_i^2 \left(y_i - (a + bx_i + cx_i^2)\right) = 0$$

Minimize error

The Least-Squares Technique — 2nd order **polynomial** data fitting

$$\sum_{i=1}^{n} \left(y_i - (a + bx_i + cx_i^2)\right) = 0$$

$$\sum_{i=1}^{n} x_i \left(y_i - (a + bx_i + cx_i^2)\right) = 0$$

$$\sum_{i=1}^{n} x_i^2 \left(y_i - (a + bx_i + cx_i^2)\right) = 0$$

$$\begin{aligned}
\sum_{i=1}^{n} y_i &= a\sum_{i=1}^{n} 1 + b\sum_{i=1}^{n} x_i + c\sum_{i=1}^{n} x_i^2 \\
\sum_{i=1}^{n} x_i\, y_i &= a\sum_{i=1}^{n} x_i + b\sum_{i=1}^{n} x_i^2 + c\sum_{i=1}^{n} x_i^3 \\
\sum_{i=1}^{n} x_i^2\, y_i &= a\sum_{i=1}^{n} x_i^2 + b\sum_{i=1}^{n} x_i^3 + c\sum_{i=1}^{n} x_i^4
\end{aligned}$$

The Least-Squares Technique — 2nd order **polynomial** data fitting

$$\sum_{i=1}^{n} y_i = a\sum_{i=1}^{n} 1 + b\sum_{i=1}^{n} x_i + c\sum_{i=1}^{n} x_i^2$$

$$\sum_{i=1}^{n} x_i\, y_i = a\sum_{i=1}^{n} x_i + b\sum_{i=1}^{n} x_i^2 + c\sum_{i=1}^{n} x_i^3$$

$$\sum_{i=1}^{n} x_i^2\, y_i = a\sum_{i=1}^{n} x_i^2 + b\sum_{i=1}^{n} x_i^3 + c\sum_{i=1}^{n} x_i^4$$

$$\begin{pmatrix} n & \sum_i x_i & \sum_i x_i^2 \\ \sum_i x_i & \sum_i x_i^2 & \sum_i x_i^3 \\ \sum_i x_i^2 & \sum_i x_i^3 & \sum_i x_i^4 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} \sum_i y_i \\ \sum_i x_i y_i \\ \sum_i x_i^2 y_i \end{pmatrix}$$

The Least-Squares Technique — 2nd order **polynomial** data fitting

$$\begin{pmatrix} n & \sum_i x_i & \sum_i x_i^2 \\ \sum_i x_i & \sum_i x_i^2 & \sum_i x_i^3 \\ \sum_i x_i^2 & \sum_i x_i^3 & \sum_i x_i^4 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} \sum_i y_i \\ \sum_i x_i y_i \\ \sum_i x_i^2 y_i \end{pmatrix}$$

$$\Leftrightarrow \quad M_{ij}\, u_j = s_j \qquad \text{(i, j = 1,2,3)}$$

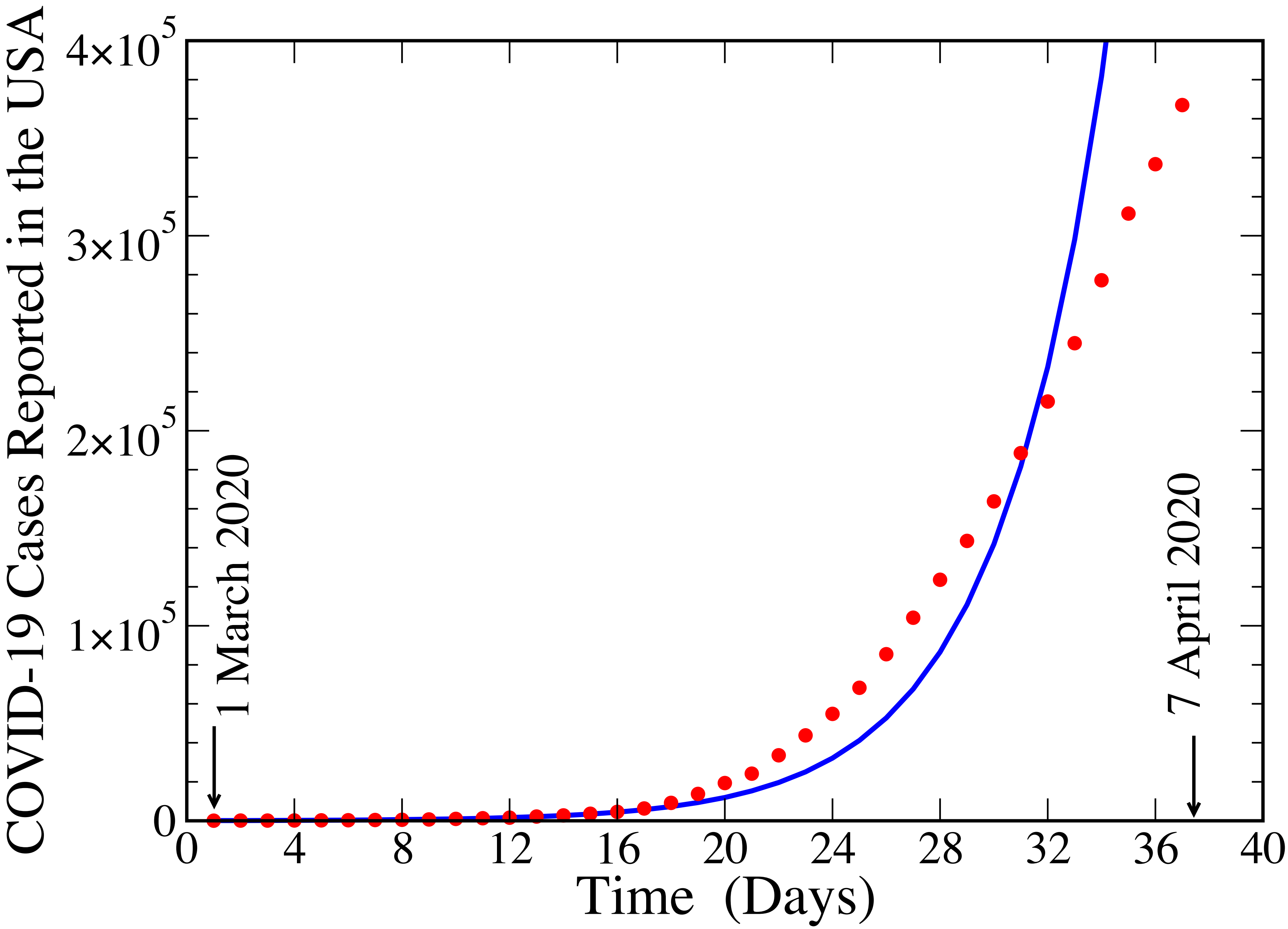
$$\Rightarrow \quad u_i = {M_{ij}}^{-1}\, s_j$$

Tips & Tricks: Fitting Exponential Data

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

$$\Rightarrow \quad \underbrace{\ln f(x)}_{\text{y}} = \ln\left(\alpha\, e^{\beta x}\right) = \underbrace{\ln \alpha}_{\text{a}} + \underbrace{\beta}_{\text{b}}\, x$$

$$\Rightarrow \quad y(x) = a + b\, x$$



COVID-19 Cases Reported in the USA
Time (Days)
4×10^5
3×10^5
2×10^5
1×10^5
0
0
4
8
12
16
20
24
28
32
36
40
1 March 2020
7 April 2020