Computer-Assisted Problem-Solving / Numerical Methods

Curve Fitting

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Legend: Method, Theory, Example, Advanced, Appendix

Theory

Curve Through Data Points

Given: experimental data (x_i, f_i), $i = 1..M$, with M (very) large

Possibility:
construction $M-1$-th order polynomial (exact) through these points (Lagrange Interpolation)

Disadvantages:
(1) problems with higher-order polynomials
(2) experimental data have statistical errors
$\Longrightarrow$ polynomial copies these errors (and amplifies them)

Alternative:
fit smooth curve $y(x)$ through the data points
So: $(x_i, f_i) \longrightarrow (x_i, y(x_i))$, $i = 1..M$

Pay attention to:
(1) choose beforehand the shape of the curve (straight line, parabola, exponential, etc.)
(2) 'overall' error as small as possible: consider errors $\epsilon_i = y(x_i) - f_i$ in all M points

Method

Least Squares Method

Fit the approximating curve such that

$$\sum_{i=1}^{M} \epsilon_i^2 = \sum_{i=1}^{M} \{y(x_i) - f_i\}^2$$

as small as possible.

Fitting Straight Line

Straight line $y(x) = a + bx$ **through** $(x_i, f_i),\ i = 1..M$

How to determine a **and** b**?**

Consider the errors in x_i**,** $i = 1..M$

$$\epsilon_i = y(x_i) - f_i = a + bx_i - f_i$$

Then minimize

$$\psi(a, b) = \epsilon_1^2 + ... + \epsilon_M^2$$

Necessary conditions for minimum: $\frac{\partial \psi}{\partial a} = \frac{\partial \psi}{\partial b} = 0$

Use chain rule

$$\frac{\partial \psi}{\partial a} = \frac{\partial \psi}{\partial \epsilon_1}\frac{\partial \epsilon_1}{\partial a} + ... + \frac{\partial \psi}{\partial \epsilon_M}\frac{\partial \epsilon_M}{\partial a} = 2\epsilon_1 \times \quad 1 + ... + 2\epsilon_M \times \quad 1 = 0$$

$$\frac{\partial \psi}{\partial b} = \frac{\partial \psi}{\partial \epsilon_1}\frac{\partial \epsilon_1}{\partial b} + ... + \frac{\partial \psi}{\partial \epsilon_M}\frac{\partial \epsilon_M}{\partial b} = 2\epsilon_1 \times x_1 + ... + 2\epsilon_M \times x_M = 0$$

So we get $\sum_{i=1}^{M} \epsilon_i = 0$ **and** $\sum_{i=1}^{M} \epsilon_i x_i = 0$

Substitute $\epsilon_i = y(x_i) - f_i = a + bx_i - f_i \Longrightarrow$

$\sum_{i=1}^{M} \{a + bx_i - f_i\} = 0$ **and** $\sum_{i=1}^{M} \{(a + bx_i - f_i)x_i\} = 0$

Elaborate $\Longrightarrow$

$$\begin{aligned} aM + b\sum_{i=1}^{M} x_i &= \sum_{i=1}^{M} f_i \\ a\sum_{i=1}^{M} x_i + b\sum_{i=1}^{M} x_i^2 &= \sum_{i=1}^{M} f_i x_i \end{aligned}$$

Define

$$M_0 = M, \quad M_1 = \sum_{i=1}^{M} x_i \ \textbf{ and } \ M_2 = \sum_{i=1}^{M} x_i^2$$

$$F_0 = \sum_{i=1}^{M} f_i \ \textbf{ and } \ F_1 = \sum_{i=1}^{M} f_i\, x_i$$

Result (Normal Equations of Gauß):

$$\begin{aligned} M_0 a + M_1 b &= F_0 \\ M_1 a + M_2 b &= F_1 \end{aligned}$$

Solving yields a **and** $b \Longrightarrow$ **line** $y(x) = a + bx$

Theorem:
Normal Equations linear and solvable $\Longrightarrow$
$\frac{\partial \psi}{\partial a} = \frac{\partial \psi}{\partial b} = 0$ **necessary and sufficient for minimum**

In other words: smallest 'overall' error

Example

Example Fitting Straight Line

Experimental data

x_i	2	4	6	8	10	12
f_i	2.81	4.30	5.93	7.43	8.85	10.61

Straight line through these data points?

First calculate the summation terms ($M = 6$):

$$\sum_{i=1}^{M} x_i = 42 \qquad \Sigma_{i=1}^{M} x_i^2 = 364$$

$$\sum_{i=1}^{M} f_i = 39.93 \qquad \Sigma_{i=1}^{M} f_i x_i = 333.66$$

So the normal equations are:

$$\begin{aligned} 6\,a + 42\,b &= 39.93 \\ 42\,a + 364\,b &= 333.66 \end{aligned}$$

Solution $a = 1.24$ **and** $b = 0.7736$

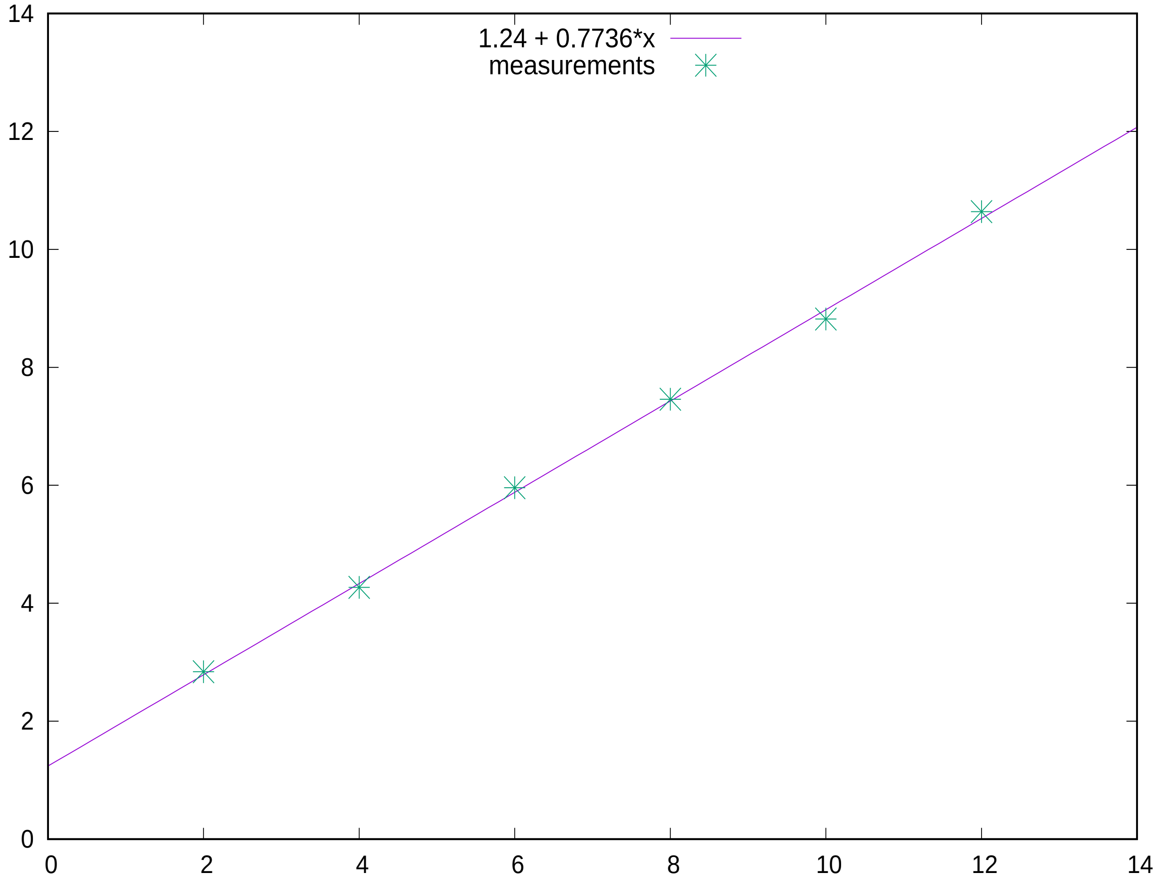
Hence, the best-fitting straight line is

$$y(x) = 1.24 + 0.7736\,x$$

Experimental data

x_i	2	4	6	8	10	12
f_i	2.81	4.30	5.93	7.43	8.85	10.61

Linear fit: $y(x) = 1.24 + 0.7736\,x$



Method

Fitting a Polynomial

Polynomial $y(x) = a_0 + a_1 x + a_2 x^2 + ... + a_N x^N$
through points $(x_i, f_i),\ i = 1..M$ **(with** $N < M - 1$**)**

How to determine $a_j,\ j = 0..N$**?**

Consider the errors in x_i**,** $i = 1..M$

$$\epsilon_i = y(x_i) - f_i = a_0 + a_1 x_i + ... + a_N x_i^N - f_i$$

Then minimize

$$\psi(a_0, a_1, ..., a_N) = \epsilon_1^2 + ... + \epsilon_M^2$$

Necessary conditions: $\frac{\partial \psi}{\partial a_j} = 0,\ j = 0...N$

Apply chain rule:

$$\begin{aligned}
\frac{\partial \psi}{\partial a_0} &= \frac{\partial \psi}{\partial \epsilon_1}\frac{\partial \epsilon_1}{\partial a_0} + ... + \frac{\partial \psi}{\partial \epsilon_M}\frac{\partial \epsilon_M}{\partial a_0} = 2\epsilon_1 \times \ 1 + ... + 2\epsilon_M \times \ 1 = 0 \\
\frac{\partial \psi}{\partial a_1} &= \frac{\partial \psi}{\partial \epsilon_1}\frac{\partial \epsilon_1}{\partial a_1} + ... + \frac{\partial \psi}{\partial \epsilon_M}\frac{\partial \epsilon_M}{\partial a_1} = 2\epsilon_1 \times x_1 + ... + 2\epsilon_M \times x_M = 0 \\
\frac{\partial \psi}{\partial a_2} &= \frac{\partial \psi}{\partial \epsilon_1}\frac{\partial \epsilon_1}{\partial a_2} + ... + \frac{\partial \psi}{\partial \epsilon_M}\frac{\partial \epsilon_M}{\partial a_2} = 2\epsilon_1 \times x_1^2 + ... + 2\epsilon_M \times x_M^2 = 0 \\
\vdots \quad & \quad \vdots \qquad\qquad\qquad \vdots \qquad\qquad\qquad \vdots \qquad\qquad\qquad \vdots \\
\frac{\partial \psi}{\partial a_N} &= \frac{\partial \psi}{\partial \epsilon_1}\frac{\partial \epsilon_1}{\partial a_N} + ... + \frac{\partial \psi}{\partial \epsilon_M}\frac{\partial \epsilon_M}{\partial a_N} = 2\epsilon_1 \times x_1^N + ... + 2\epsilon_M \times x_M^N = 0
\end{aligned}$$

So we have $N+1$ conditions

$$\sum_{i=1}^{M} \epsilon_i = \sum_{i=1}^{M} \epsilon_i x_i = \sum_{i=1}^{M} \epsilon_i x_i^2 = ... = \sum_{i=1}^{M} \epsilon_i x_i^N = 0$$

Substitute $\epsilon_i = a_0 + a_1 x_i + ... + a_N x_i^N - f_i$

and introduce the abbreviations

$$M_0 = M, \quad M_1 = \sum_{i=1}^{M} x_i \quad ... \quad M_N = \sum_{i=1}^{M} x_i^N$$

$$F_0 = \sum_{i=1}^{M} f_i, \quad F_1 = \sum_{i=1}^{M} f_i x_i \quad ... \quad F_N = \sum_{i=1}^{M} f_i x_i^N$$

This gives (after further elaboration)

$$\begin{array}{ccccccccc}
M_0\, a_0 & + & M_1\, a_1 & + & M_2\, a_2 & + ... + & M_{N+0}\, a_N & = & F_0 \\
M_1\, a_0 & + & M_2\, a_1 & + & M_3\, a_2 & + ... + & M_{N+1}\, a_N & = & F_1 \\
M_2\, a_0 & + & M_3\, a_1 & + & M_4\, a_2 & + ... + & M_{N+2}\, a_N & = & F_2 \\
\vdots & & \vdots & & \vdots & & \vdots & & \vdots \\
M_N\, a_0 & + & M_{N+1}\, a_1 & + & M_{N+2}\, a_2 & + ... + & M_{2N}\, a_N & = & F_N
\end{array}$$

These are $N{+}1$ eqns with unknowns $a_j,\ j{=}0..N$

Solution gives the polynomial

$$y(x) = a_0 + a_1 x + a_2 x^2 + ... + a_N x^N$$

Example

Example Fitting Parabola

Experimental data

x_i	2	4	6	8	10
f_i	0.69	8.38	24.35	48.73	80.13

Parabola $y(x) = a + b\,x + c\,x^2$ **through data points?**

Differences in M**-terms are large:**

$M_0 = 5,\ M_4 \approx 10^4 \implies$ **problems with accuracy**

Remedy: transformation $\hat{x} = (x-6)/2$

Transformed data points

$\hat{x}_i$	-2	-1	0	1	2
f_i	0.69	8.38	24.35	48.73	80.13

Calculate the corresponding M **and** F**-terms:**

$M_0 = 5,\ M_1 = 0,\ M_2 = 10,\ M_3 = 0,\ M_4 = 34$

$F_0 = 162.28,\ F_1 = 199.23,\ F_2 = 380.39$

The normal equations then become

$$\begin{array}{rcrcrcl} 5a & + & 0b & + & 10c & = & 162.28 \\ 0a & + & 10b & + & 0c & = & 199.23 \\ 10a & + & 0b & + & 34c & = & 380.39 \end{array}$$

Solution for transformed data:

$a = 24.4803,\ b = 19.9230$ **en** $c = 3.9879$

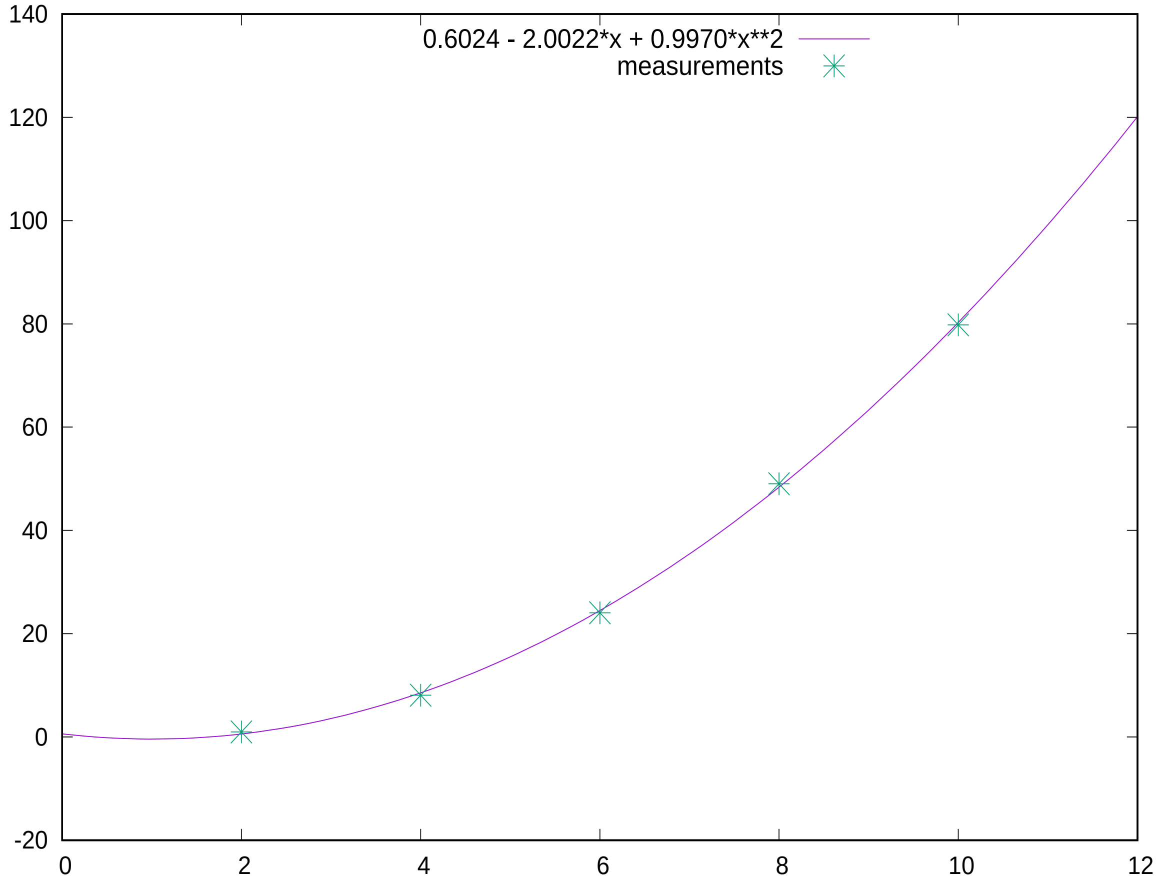
Parabola for transformed data

$$y(\hat{x}) = 24.4803 + 19.9230\,\hat{x} + 3.9879\,\hat{x}^2$$

The transformation was $\hat{x} = (x-6)/2 \Longrightarrow$

Wanted parabola (original data)

$$\begin{aligned} y &= 24.4803 + 19.9230\,\hat{x} + 3.9879\,\hat{x}^2 \\ &= 24.4803 + 19.9230\,\frac{(x-6)}{2} + 3.9879\,\frac{(x-6)^2}{2^2} \\ y(x) &= 0.6024 - 2.0022\,x + 0.9970\,x^2 \end{aligned}$$



Theory

Exponential & Power Functions

Fitting of exponential function $y(x) = a\, e^{bx}$**:**

Apply $ln(\ )$ **to the measured data** f_i
and then determine a linear fit

Because $ln(y) = ln(a) + ln(e^{bx}) = ln(a) + b\, x$
This is of the form $\hat{y} = \hat{a} + \hat{b}\, x$**, and thus linear**

Determine linear fit $(\hat{a}, \hat{b})$**,**
through points $(x_i, ln(f_i))$
Then transform back: $a = e^{\hat{a}}$**,** $b = \hat{b}$

Fitting of $y(x) = a\, x^b$**:**

Using $ln(y) = ln(a) + b\, ln(x)$ **gives** $\hat{y} = \hat{a} + \hat{b}\, ln(x)$
Now apply $ln(\ )$ **to** f_i **and** x_i **values**

Determine linear fit $(\hat{a}, \hat{b})$**,**
through points $(ln(x_i), ln(f_i))$
Then transform back: $a = e^{\hat{a}}$**,** $b = \hat{b}$

This procedure is known as
'data linearization'.

Example

Example Exponential Fit

Experimental data

x_i	2	3	4	5	6	7
f_i	12	16	22	30	40	56

Fit with exponential function $y(x) = a\,e^{bx}$

Transformed data points

x_i	2	3	4	5	6	7
$ln(f_i)$	2.4849	2.7726	3.0910	3.4012	3.6889	4.0254

Calculate M and F-values:

$M_0 = 6, \quad M_1 = 27, \quad M_2 = 139,$
$F_0 = 19.4640, \quad F_1 = 92.9685$

Equations for transformed data:

$$\begin{aligned} 6\hat{a} &+ 27\hat{b} &= 19.4640 \\ 27\hat{a} &+ 139\hat{b} &= 92.9685 \end{aligned}$$

Solution for transformed data:

$\hat{a} = 1.8604,\ \hat{b} = 0.3075$

Transform back: $a = e^{\hat{a}} = 6.4263,\ b = \hat{b} = 0.3075$

Exponential fit for original data:

$$y(x) = 6.4263\,e^{0.3075\,x}$$

Experimental data

x_i	2	3	4	5	6	7
f_i	12	16	22	30	40	56

Exponential fit

$$y(x) = 6.4263\, e^{0.3075\, x}$$