Least Squares - Solutions

1. We have the discrete points

i	0	1	2	3	4	5	6	7
x_i	1	2	3	4	5	6	7	8
y_i	3	3	4	5	5	6	6	7

We wish to fit a straight line

$$y(x) = ax + b$$

to this data using the least-squares method. We have

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

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

Using the given data we find

$$n = 7 \Rightarrow n + 1 = 8$$

$$\left(\sum_{i=0}^{n} x_i\right) = 36 \qquad \left(\sum_{i=0}^{n} x_i^2\right) = 204 \qquad \left(\sum_{i=0}^{n} x_i\right)^2 = 1296$$

$$\left(\sum_{i=0}^{n} y_i\right) = 39 \qquad \left(\sum_{i=0}^{n} x_i y_i\right) = 200$$

and so we have

$$a = \frac{(8)(200) - (36)(39)}{(8)(204) - (1296)} = \frac{1600 - 1404}{1632 - 1296} = \frac{196}{336} = 0.5833$$

$$b = \frac{(204)(39) - (200)(36)}{(8)(204) - (1296)} = \frac{7956 - 7200}{1632 - 1296} = \frac{756}{336} = 2.250.$$

The so-called r^2-coefficient gives an indication of the quality of the fit. If the r^2-coefficient is close to 1, the fit is good; if it is close to 0 the fit is bad. Evaluating the r^2-coefficient for this problem gives

$$\begin{aligned}
r^2 &= \frac{\left[(n+1)\left(\sum_{i=0}^{n} x_i y_i\right) - \left(\sum_{i=0}^{n} x_i\right)\left(\sum_{i=0}^{n} y_i\right)\right]^2}{\left[(n+1)\left(\sum_{i=0}^{n} x_i^2\right) - \left(\sum_{i=0}^{n} x_i\right)^2\right]\left[(n+1)\left(\sum_{i=0}^{n} y_i^2\right) - \left(\sum_{i=0}^{n} y_i\right)^2\right]} \\
&= \frac{[(8)(200) - (36)(39)]^2}{[(8)(204) - (1296)][(8)(205) - (1521)]} = \frac{[1600 - 1404]^2}{[1632 - 1296][1640 - 1521]} \\
&= \frac{[196]^2}{[336][119]} = 0.96
\end{aligned}$$

The fit is thus a pretty good one. Calculating the r^2 coefficient in this problem was optional; we did so simply to indicate how it is done.

2. The discrete data points are

i	0	1	2	3	4
x_i	0	1	2	3	4
y_i	10	12	18	28	42

There are 5 points, and so $n = 4$.

We must fit the function

$$y(x) = a_0 + a_2 x^2$$

to the data, using the least-squares method, which means we need to determine values for a_0 and a_2. To do this we must minimize

$$S \equiv \sum_{i=0}^{n} \Delta_i^2 = \sum_{i=0}^{n} \left(a_0 + a_2 x_i^2 - y_i\right)^2$$

with respect to a_0 and a_2.

First we differentiate S with respect to a_0, and put the result equal to 0 :

$$\begin{aligned}
\frac{\partial S}{\partial a_0} &= 2\sum_{i=0}^{n} \left(a_0 + a_2 x_i^2 - y_i\right)(1) = 0 \\
&\Rightarrow \; a_0\left(\sum_{i=0}^{n} 1\right) + a_2\left(\sum_{i=0}^{n} x_i^2\right) = \left(\sum_{i=0}^{n} y_i\right)
\end{aligned}$$

Differentiating with respect to a_2, and putting the result equal to 0 :

$$\begin{aligned}\frac{\partial S}{\partial a_2} &= 2\sum_{i=0}^{n}\left(a_0 + a_2 x_i^2 - y_i\right)\left(x_i^2\right) = 0 \\ \Rightarrow\ a_0\left(\sum_{i=0}^{n} x_i^2\right) + a_2\left(\sum_{i=0}^{n} x_i^4\right) &= \left(\sum_{i=0}^{n} x_i^2 y_i\right)\end{aligned}$$

Now $n = 4$ and so we have, using the discrete data,

$$\sum_{i=0}^{4} 1 = 5 \qquad \sum_{i=0}^{4} x_i^2 = 30 \qquad \sum_{i=0}^{4} y_i = 110$$

$$\sum_{i=0}^{4} x_i^4 = 354 \qquad \sum_{i=0}^{4} x_i^2 y_i = 1008$$

This gives us the linear system

$$\begin{aligned} 5a_0 + 30a_2 &= 110 \\ 30a_0 + 354a_2 &= 1008 \end{aligned}$$

which is easily solved to yield

$$a_0 = 10 \quad \text{and} \quad a_2 = 2$$

The fitting function $y(x)$ thus has the form

$$y(x) = 10 + 2x^2.$$

We may analyze the quality of the fit using the variance

$$\sigma^2 = \frac{\sum_{i=0}^{n} \Delta_i^2}{n - m}$$

where $m = 2$ (the order of the polynomial that we have fitted). We obtain

$$\sigma^2 = \frac{0 + 0 + 0 + 0 + 0}{4 - 2} = 0$$

In other words, the fit is perfect.

3. From the decay law follows that

$$\ln N = \ln N_0 - \lambda t.$$

Let

$$y \equiv \ln N; \quad x \equiv t; \quad a_0 \equiv \ln N_0; \quad a_1 \equiv -\lambda.$$

Then we have the linear relationship

$$y = a_0 + a_1 x$$

which needs to fit the data

x	1	2	3	4	5	6
$y\,(= \ln N)$	8.4943	8.2314	8.2746	7.9164	7.8842	7.6014

.

For this case $(m = 1; n = 5)$, the we obtain the following:

$$\begin{aligned} 6a_0 + a_1 \sum_i x_1 &= \sum_i y_i \\ a_0 \sum_i x_i + a_1 \sum_i x_i^2 &= \sum_i x_i y_i. \end{aligned}$$

For the data in the table, we then have

$$\begin{aligned} 6a_0 + 21a_1 &= 48.4023 \\ 21a_0 + 91a_1 &= 166.4759 \end{aligned}$$

which is easily solved. The value of a_0 is, in fact, not relevant to the problem, and so we therefore need only find

$$a_1 = -0.1676.$$

(for completeness' sake, $a_0 = 8.6535$). From definition the decay constant is given by

$$\lambda = -a_1 = 0.1676 \text{ min}^{-1}$$

Furthermore, We have

$$N_0 e^{-\lambda(t+t_{half})} = \frac{1}{2} N_0 e^{-\lambda t}$$

so that

$$e^{-\lambda t_{half}} = \frac{1}{2}$$

which gives

$$t_{half} = \frac{\ln 2}{\lambda}.$$

The half-life therefore is $t_{half} \approx 4.14$ min.

4. We have the discrete points

i	0	1	2	3
x_i	0	1	2	3
y_i	-7	-5	-3	θ

We wish to fit a straight line

$$y(x) = ax + b$$

to this data using the least-squares method. We have

$$\begin{aligned} a &= \frac{(n+1)\left(\sum_{i=0}^{n} x_i y_i\right) - \left(\sum_{i=0}^{n} x_i\right)\left(\sum_{i=0}^{n} y_i\right)}{(n+1)\left(\sum_{i=0}^{n} x_i^2\right) - \left(\sum_{i=0}^{n} x_i\right)^2} \\ b &= \frac{\left(\sum_{i=0}^{n} x_i^2\right)\left(\sum_{i=0}^{n} y_i\right) - \left(\sum_{i=0}^{n} x_i y_i\right)\left(\sum_{i=0}^{n} x_i\right)}{(n+1)\left(\sum_{i=0}^{n} x_i^2\right) - \left(\sum_{i=0}^{n} x_i\right)^2} \end{aligned}$$

Using the given data we find

$$n = 3 \Rightarrow n + 1 = 4$$

$$\begin{aligned} \left(\sum_{i=0}^{n} x_i\right) &= 6 \qquad \left(\sum_{i=0}^{n} x_i^2\right) = 14 \qquad \left(\sum_{i=0}^{n} x_i\right)^2 = 36 \\ \left(\sum_{i=0}^{n} y_i\right) &= \theta - 15 \qquad \left(\sum_{i=0}^{n} x_i y_i\right) = 3\theta - 11 \end{aligned}$$

and so

$$\begin{aligned} a &= \frac{23}{10} + \frac{3\theta}{10} \\ b &= -\frac{36}{5} - \frac{\theta}{5} \end{aligned}$$

which gives the fit

$$y(x) = \left(\frac{23}{10} + \frac{3\theta}{10}\right) x + \left(-\frac{36}{5} - \frac{\theta}{5}\right).$$

The variance is given by

$$\sigma^2 = \frac{\sum_{i=0}^{n} \Delta_i^2}{n - m}$$

with $m = 1$. For Δ_1, for example, we have

$$\begin{aligned} \Delta_1^2 &= (y(x_1) - y_1)^2 \\ &= \left(\left(\frac{23}{10} + \frac{3\theta}{10}\right)(1) + \left(-\frac{36}{5} - \frac{\theta}{5}\right) - (-5)\right)^2 \\ &= \frac{\theta^2 + 2\theta + 1}{100} \end{aligned}$$

and similarly for the other Δ's:

$$\begin{aligned} \Delta_0^2 &= \frac{4\left(\theta^2 + 2\theta + 1\right)}{100} \\ \Delta_2^2 &= \frac{16\left(\theta^2 + 2\theta + 1\right)}{100} \\ \Delta_3^2 &= \frac{9\left(\theta^2 + 2\theta + 1\right)}{100} \end{aligned}$$

Hence, we find

$$\sigma^2 = \frac{3\left(\theta^2 + 2\theta + 1\right)}{20}.$$

For $\sigma^2 = 0$ we find

$$\theta = -1$$

which gives

$$\begin{aligned} a &= 2 \\ b &= -7 \end{aligned}$$

and

$$y(x) = 2x - 7$$

which is clearly consistent with the given data.

5. We have

$$S \doteqdot \sum_{i=0}^{3} \left(ax_i^2 + b - y_i\right)^2$$

and so

$$\begin{aligned} \frac{\partial S}{\partial b} = 0 \quad &\Rightarrow \quad 2\sum_{i=0}^{3} \left(ax_i^2 + b - y_i\right) = 0 \\ &\Rightarrow \quad \sum_{i=0}^{3} \left(ax_i^2 + b - y_i\right) = 0 \end{aligned}$$

$$\begin{aligned} \frac{\partial S}{\partial a} = 0 \quad &\Rightarrow \quad 2\sum_{i=0}^{3} \left(ax_i^2 + b - y_i\right) x_i^2 = 0 \\ &\Rightarrow \quad \sum_{i=0}^{3} \left(ax_i^4 + bx_i^2 - x_i^2 y_i\right) = 0 \end{aligned}$$

Hence, the appropriate equations are

$$\begin{aligned} b(n+1) + a\sum_i x_i^2 &= \sum_i y_i \\ b\sum_i x_i^2 + a\sum_i x_i^4 &= \sum_i x_i^2 y_i. \end{aligned}$$

With

$$\begin{array}{ccc} n = 3 & \sum_i x_i^2 = 17 & \sum_i x_i^4 = 113 \\ \sum_i y_i = 27 & \sum_i x_i^2 y_i = 236 & \end{array}$$

we have

$$\begin{aligned} &\begin{bmatrix} 4 & 17 \\ 17 & 113 \end{bmatrix} \begin{bmatrix} b \\ a \end{bmatrix} = \begin{bmatrix} 27 \\ 236 \end{bmatrix} \\ \Rightarrow \; &\begin{bmatrix} b \\ a \end{bmatrix} = \begin{bmatrix} -5.8957 \\ 2.9755 \end{bmatrix}. \end{aligned}$$

Hence,

$$\begin{aligned} f(x) &= ax^2 + b \\ &= 2.9755x^2 - 5.8957 \end{aligned}$$

For the variance σ^2 we have

$$\sigma^2 = \sum_i \frac{\Delta_i^2}{n-m} = \sum_i \frac{\Delta_i^2}{3-2} = \sum_i \Delta_i^2$$

and

$$\begin{aligned} \Delta_0 &= f(-2) - 6 = 0.0061 \\ \Delta_1 &= f(0) - (-7) = 1.1043 \\ \Delta_2 &= f(2) - 8 = -1.9939 \\ \Delta_3 &= f(3) - 20 = 0.8834 \end{aligned}$$

which gives

$$\sigma^2 = \sum_i \Delta_i^2 = 5.9746.$$

6.

$$S = \sum_{i=1}^{4} \left(ax_i^4 + b - y_i\right)^2$$

$$\begin{aligned} \frac{\partial S}{\partial a} = 0 \quad &\Rightarrow \quad 2\sum_{i=1}^{4} \left(ax_i^4 + b - y_i\right) x_i^4 = 0 \\ &\Rightarrow \quad a\sum_{i=1}^{4} x_i^8 + b\sum_{i=1}^{4} x_i^4 = \sum_{i=1}^{4} x_i^4 y_i \end{aligned}$$

$$\begin{aligned} \frac{\partial S}{\partial b} = 0 \quad &\Rightarrow \quad 2\sum_{i=1}^{4} \left(ax_i^4 + b - y_i\right) = 0 \\ &\Rightarrow \quad a\sum_{i=1}^{4} x_i^4 + b\sum_{i=1}^{4} 1 = \sum_{i=1}^{4} y_i \end{aligned}$$

Hence,

$$\begin{aligned} 13378a + 178b &= 12957 \\ 178a + 4b &= 171 \end{aligned}$$

and so

$$f(x) = 0.9799x^4 - 0.8571.$$

7. We have

$$S \equiv \sum_{i=0}^{3} \left(ax_i^3 + bx_i - y_i\right)^2$$

and so

$$\begin{aligned} \frac{\partial S}{\partial b} = 0 \quad &\Rightarrow \quad 2\sum_{i=0}^{3} \left(ax_i^3 + bx_i - y_i\right) x_i = 0 \\ &\Rightarrow \quad \sum_{i=0}^{3} \left(ax_i^4 + bx_i^2 - x_i y_i\right) = 0 \end{aligned}$$

$$\begin{aligned} \frac{\partial S}{\partial a} = 0 \quad &\Rightarrow \quad 2\sum_{i=0}^{3} \left(ax_i^3 + bx_i - y_i\right) x_i^3 = 0 \\ &\Rightarrow \quad \sum_{i=0}^{3} \left(ax_i^6 + bx_i^4 - x_i^3 y_i\right) = 0 \end{aligned}$$

Hence, the appropriate equations are

$$\begin{aligned} b\sum_i x_i^2 + a\sum_i x_i^4 &= \sum_i x_i y_i \\ b\sum_i x_i^4 + a\sum_i x_i^6 &= \sum_i x_i^3 y_i. \end{aligned}$$

With

$$\begin{array}{ccc} n = 3 & \sum_i x_i^2 = 11 & \sum_i x_i^4 = 83 \\ \sum_i x_i^6 = 731 & \sum_i x_i y_i = 4 & \sum_i x_i^3 y_i = -68 \end{array}$$

we have

$$\left[\begin{array}{cc} 11 & 83 \\ 83 & 731 \end{array}\right]\left[\begin{array}{c} b \\ a \end{array}\right] = \left[\begin{array}{c} 4 \\ -68 \end{array}\right]$$

$$\Rightarrow \left[\begin{array}{c} b \\ a \end{array}\right] = \left[\begin{array}{c} 7.4375 \\ -0.9375 \end{array}\right].$$

Hence,

$$\begin{aligned} f(x) &= ax^3 + bx \\ &= -0.9375x^3 + 7.4375x. \end{aligned}$$

8.