[Harold Cohen. Numerical approximation methods, p. 25.]

Given n experimental data points $[x_k, y_k]$ and a *fitting equation*, *aka* model equation, $f[x_k]$ with unknown coefficients $\{\alpha_k\}$ with $1 \leq k \leq n$, the method of least squares consists on minimizing the *square of the root mean square, rms, error*

$$e = \sum_k {\epsilon_k}^2 = \sum_k (f_k - y_k)^2$$

with respect to the coefficients $\{\alpha_k\}$.

For instance, consider that a theory predicts the data in table 1 decreasing with increasing x as a quadratic in $1/x$.

Begin by defining the model to fit the data:

$$f[x] = \alpha_1 + \alpha_2 \frac{1}{x} + \alpha_3 \frac{1}{x^2}\,.$$

Then, find the square of the rms error of the model and the data:

$$e = \sum_k \left(\alpha_1 + \alpha_2 \frac{1}{x} + \alpha_3 \frac{1}{x^2} - y_k \right)^2 .$$

Minimize e with respect to the coefficients $\{\alpha_k\}$:

$$\begin{aligned}
\partial_1 e &= 2 \sum_k \left(\alpha_1 + \alpha_2 \frac{1}{x_k} + \alpha_3 \frac{1}{x_k^2} - y_k \right) = 0\,,\\
\partial_2 e &= 2 \frac{1}{x_k} \sum_k \left(\alpha_1 + \alpha_2 \frac{1}{x_k} + \alpha_3 \frac{1}{x_k^2} - y_k \right) = 0\,,\\
\partial_3 e &= 2 \frac{1}{x_k^2} \sum_k \left(\alpha_1 + \alpha_2 \frac{1}{x_k} + \alpha_3 \frac{1}{x_k^2} - y_k \right) = 0\,.
\end{aligned}$$

x_k	y_k
1.3	5.42
2.2	4.28
3.7	3.81
4.9	3.62

Table 1 Data with inverse power of x decrease

Distribute the sums in every term, perform algebra and replace the values of table 1 to have

$$\begin{aligned}
4.000\alpha_1 + 1.698\alpha_2 + 0.913\alpha_3 &= 17.130\,, \\
1.698\alpha_1 + 0.913\alpha_2 + 0.577\alpha_3 &= 7.883\,, \\
0.913\alpha_1 + 0.577\alpha_2 + 0.400\alpha_3 &= 4.52\,.
\end{aligned}$$

Solve the system of equations to find $\{\alpha_1 = 3.261, \alpha_2 = 1.480, \alpha_3 = 1.722\}$. The model thus becomes

$$f[x] = 3.261 + 1.480\frac{1}{x} + 1.722\frac{1}{x^2}\,,$$

with a fitting error

$$e = \sum_{k=1}^{4}\left(3.261 + 1.480\frac{1}{x} + 1.722\frac{1}{x^2} - y_k\right)^2 = 0.001\,. \qquad \square$$