CHAPTER 7 LEAST SQUARES REGRESSION

SOLVED EXAMPLE PROBLEMS

for

NUMERICAL METHODS FOR SCIENTISTS AND ENGINEERS With Pseudocodes

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EXAMPLE 7.1: Linear Regression

The end product of a filtration process of a slurry, known as *cake*, is to be dried. To determine the optimal drying conditions, the cake was subjected to air flow at various flow rates (Q), and its moisture content (M) was measured. The results are presented in the table below. The theoretical relationship between flow rate and moisture content is given by $M = A + B/Q$. Apply least squares regression to determine the best-fit parameters. What can you say about suitability and the goodness of fit?

Q, m^3/min	0.0044	0.0058	0.0073	0.0145	0.0183	0.0311	0.0377	0.0536
M, w%	31	29.5	28.2	26.5	26.3	25.1	25.2	24.9

SOLUTION:

The given data set consists of eight data pairs ($X = 8$), and the regression model is not exactly linear. However, it can be cast as a linear model by setting $X = 1/Q$. Thus, the model becomes $M = A + BX$. Upon employing the linear regression to determine the model parameters A and B, we obtain the following system of linear equations.

$$\begin{bmatrix} n & \sum_i X_i \\ \sum_i X_i & \sum_i X_i^2 \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} \sum_i M_i \\ \sum_i X_i M_i \end{bmatrix}$$

We construct **Table 7.1** to calculate the coefficients of the linear system.

Table 7.1

i	Q_i	M_i	$X_i = 1/Q_i$	X_i^2	$X_i M_i$	$(M_i - \overline{M})^2$	$(M_i - M(Q_i))^2$
1	0.0044	31	227.27	51652.9	7045.45	15.3077	0.000171
2	0.0058	29.5	172.41	29726.5	5086.21	5.8202	0.006578
3	0.0073	28.2	136.99	18765.2	3863.01	1.2377	0.035862
4	0.0145	26.5	68.97	4756.2	1827.59	0.3452	0.007623
5	0.0183	26.3	54.64	2986.1	1437.16	0.6202	0.092095
6	0.0311	25.1	32.15	1033.9	807.07	3.9502	0.059027
7	0.0377	25.2	26.53	703.6	668.44	3.5627	0.000426
8	0.0536	24.9	18.66	348.1	464.55	4.7852	0.002572
Σ		**216.7**	**737.6194**	**109972.514**	**21199.48**	**35.62875**	**0.204354**

Substituting the numerical sums into the system of equations, we find

$$\begin{bmatrix} 8 & 738.6194 \\ 738.6194 & 109972.514 \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 216.7 \\ 21199.48 \end{bmatrix}$$

which leads to $A = 24.40855$ and $B = 0.029055$ or

$$M(X) = 24.40855 + 0.029055X \quad \text{or} \quad M(Q) = 24.40855 + \frac{0.029055}{Q}$$

This relationship is valid for $0.0044 \leqslant Q \leqslant 0.0536$ m^3/min.

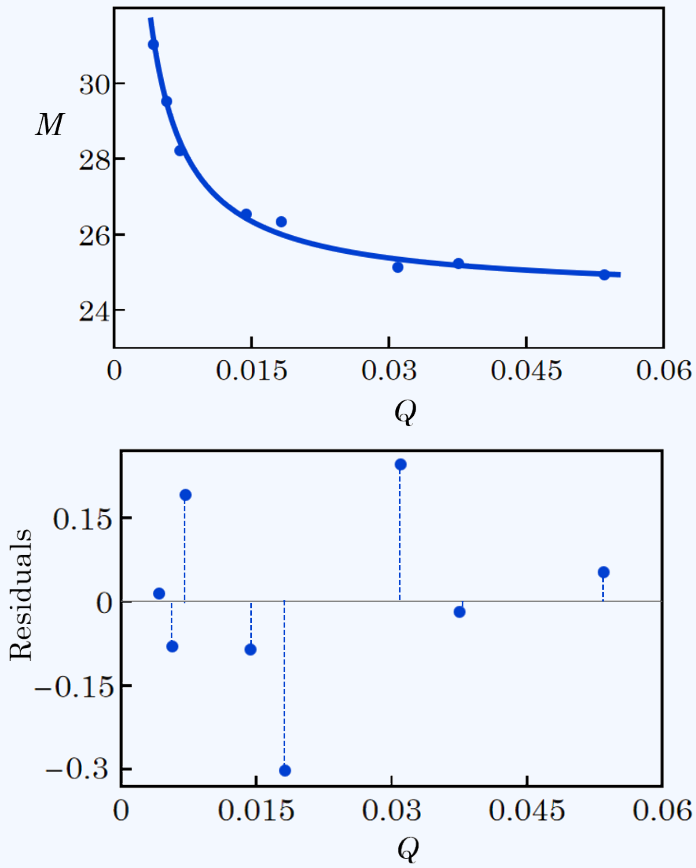
In order to determine the goodness of the fit, we first evaluate r-squared. The following quantities (SSR and SSMD) are needed, and the last two columns of **Table 7.1** are in this regard prepared for this purpose. Finally, we obtain

$$E = \sum_{i=1}^{8} (M(X_i) - M_i)^2 = 0.0253$$

$$\overline{M} = 27.0875, \qquad S = \sum_{i=1}^{8} (M_i - \overline{M})^2 = 8.1841$$

$$r^2 = 1 - \frac{E}{S} = 1 - \frac{0.204354}{35.62875} = 0.99426$$

The r-squared value indicates that 99.43% of the variance in the dependent variable is explained by the independent variable.



(a) (b)

Figure 7.1: Distribution of (a) the data set as well as the best-fit model, (b) the residuals.

Discussion: In **Figure 7.1a**, the best-fit regression represents predicted values (of moisture content) based on the best-fit model, and the original data points represent actual observed values. Note that the original data and the best-fit model are in excellent agreement, meaning that the model fits the data very well, as the high value of the r-squared suggests. The maximum residual corresponds to a relative deviation of about 1.15%. If we had observed wide scatter, the model would not have been a reliable tool.

In **Figure 7.1b**, the residual plot shows no clear trend, meaning the relationship between the flow rate and the inverse of the moisture content is linear, and thus our model is appropriate. If the residuals had shown a systematic curved pattern, this model would not have been the best choice.

EXAMPLE 7.2: Linearizing a Nonlinear Model

Kinetics data for a reaction is presented below:

t, s	200	400	600	800	1000	1200	1400
$A(t)$, M	22	12	8	6	5	4	3.5

It is assumed that the data is best represented by the following nonlinear equation:

$$A(t) = \frac{A_0}{1 + 2kA_0 t}$$

where t denotes reaction time (in seconds), A_0 is the initial concentration (in M), and k is the reaction rate (in $M^{-1}s^{-1}$). Linearize the given model to find the model parameters A_0 and k. Determine the goodness of fit parameters.

SOLUTION:

The given data set consists of $n = 7$ pairs. Inverting the equation results in

$$\frac{1}{A(t)} = \frac{1}{A_0} + 2k\,t$$

Defining $Y(t) = 1/A(t)$, $a = 1/A_0$, and $b = 2k$, we transform the above equation to $Y(t) = a + b\,t$. Then employing the least-squares regression leads to the following system of linear equations:

$$\begin{bmatrix} n & \sum_i t_i \\ \sum_i t_i & \sum_i t_i^2 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \sum_i Y_i \\ \sum_i t_i Y_i \end{bmatrix}$$

Table 7.2

i	t_i	A_i	$Y_i = 1/A_i$	t_i^2	t_iY_i
1	200	22	$0.045\overline{45}$	40000	9.0909
2	400	12	$0.0833\overline{3}$	160000	$33.\overline{3}$
3	600	8	0.1250	360000	75
4	800	6	$0.166\overline{6}$	640000	$133.\overline{3}$
5	1000	5	0.2000	1000000	200
6	1200	4	0.2500	1440000	300
7	1400	3.5	0.285714	1960000	400
Σ	**5600**	**60.5**	**1.15617**	**5600000**	**1150.7576**

We constructed **Table 7.2** to determine the coefficients of this system. Upon substituting the numerical values, we find

$$\begin{bmatrix} 7 & 5600 \\ 5600 & 5600000 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1.15617 \\ 1150.7576 \end{bmatrix}$$

which gives $a = 0.003865182$ and $b = 0.000201627$. We then find $A_0 = 1/a = 258.72$ and $k = b/2 = 0.000100814$.

Discussion: We will accept the result as it is; it is appropriate to investigate how well the obtained model represents the data. The goodness of fit requires evaluating the sum of the squares of the residuals (SSR or E) and the sum of the squares of the mean deviation (SSMD or S). Noting that the mean value of the reaction time $\overline{A} = 60.5/7 = 8.64286$ s, we construct **Table 7.3** from which we find:

$$E = \sum_{i=1}^{7} \left(A_i - A(t_i)\right)^2 = 0.449723 \quad \text{and} \quad S = \sum_{i=1}^{7} \left(A_i - \overline{A}\right)^2 = 258.3571$$

Table 7.3

i	t_i	$(A_i - \overline{A})^2$	$(A_i - A(t_i))^2$
1	200	178.413	0.395932
2	400	11.270	0.028201
3	600	0.413	0.000103
4	800	6.985	0.002968
5	1000	13.270	0.017860
6	1200	21.556	0.004631
7	1400	26.449	0.000028
Σ		258.3571	0.449723

The r-squared, which measures the proportion of variance explained by the model, is found as follows:

$$r^2 = 1 - \frac{E}{S} = 1 - \frac{0.449723}{258.3571} = 0.998259$$

This result implies that 99.83% of the variance in the dependent variable is explained by the independent variable, while the remaining 0.17% is unexplained (due to noise or other unknown factors).

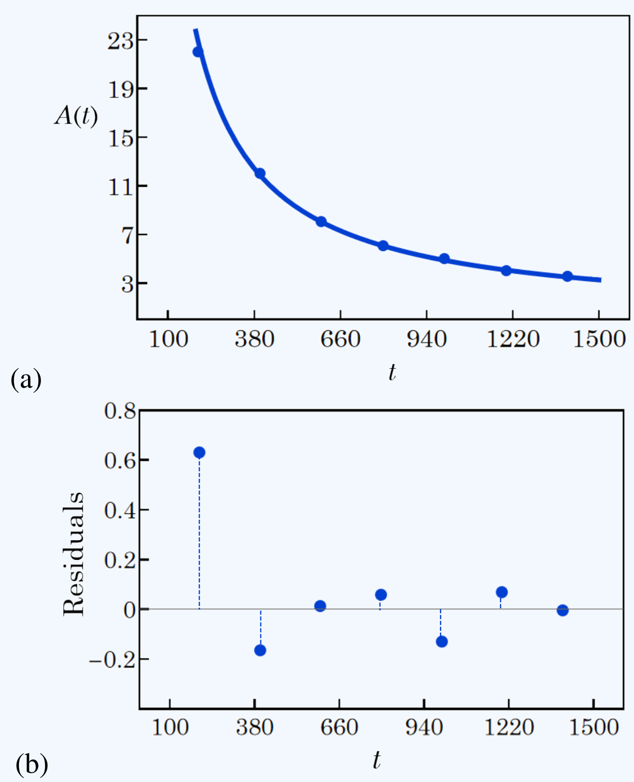


Figure 7.2: Distribution of (a) the data set as well as the best-fit model, (b) the residuals.

In **Figure 7.2**, the agreement of the data with the best-fit model as well as the residuals are depicted. We note that an excellent agreement is obtained. The residuals are very small except for the first data point, which corresponds to a relative error of about 3%. The model is suitable for predictions using the furnished data.

EXAMPLE 7.3: Continuous Least Squares Approximation

In structural engineering, we often need to approximate the deflection $y(x)$ of a beam subjected to a distributed load using a simpler function. Suppose that we have a cantilever beam of length $L = 1$ m that is a fixed beam at both ends, and the deflection follows the differential equation:

$$EI\frac{d^4y}{dx^4} = w(x) = w_0 x, \qquad 0 \leqslant x \leqslant L$$

subject to the following boundary conditions:

$$y(0) = y(L) = 0, \quad y'(0) = y'(L) = 0$$

where $w(x)$ denotes linearly increasing load with $w_0 = 10^3$ kN/m, EI is the flexural rigidity, which is given as 10^3 kN·m^2 for an aluminum beam.

Apply the continuous least squares approximation by approximating the deflection function $y(x)$ of the beam over the interval $x \in [0, L]$ with a polynomial as follows:

$$y(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5$$

where a_2, a_3, a_4 and a_5 are coefficients to be determined.

SOLUTION:

We define the objective function as follows:

$$I = \int_0^L \left(EI\frac{d^4y}{dx^4} - w_0 x \right)^2 dx, \qquad 0 \leqslant x \leqslant L$$

Upon substituting the numerical values, we obtain

$$I(a_4, a_5) = \int_0^1 (24a_4 + 120a_5 x - x)^2\, dx, \qquad 0 \leqslant x \leqslant 1$$

Taking the partial derivatives with respect to a_4 and a_5 results in the following set of linear equations:

$$\frac{\partial I}{\partial a_4} = \int_0^1 2(24)\,(24a_4 + 120a_5 x - x)\, dx = 1152a_4 + 2880a_5 - 24 = 0$$

$$\frac{\partial I}{\partial a_5} = \int_0^1 2(24)\,(24a_4 + 120a_5 x - x)\, dx = 2880a_4 + 9600a_5 - 80 = 0$$

which gives $a_4 = 0$ and $a_5 = 1/120$.

There are still four more coefficients to determine. We will determine these by using the boundary conditions. From $y(0) = y'(0) = 0$, we easily find $a_0 = a_1 = 0$. For $y(1) = y'(1) = 0$, we obtain the following system of equations:

$$y(1) = a_2(1^2) + a_3(1^3) + \frac{1^5}{120} = 0$$

$$y'(1) = 2a_2(1) + 3a_3(1)^2 + \frac{1^4}{24} = 0$$

Solving the system gives $a_2 = 1/60$ and $a_3 = -1/40$. Substituting the coefficients, we arrive at

$$y(x) = \frac{1}{120}\left(x^5 - 3x^3 + 2x^2\right)$$

Discussion: In this example, the solution we have found corresponds to the true solution of the given differential equation. Continuous least squares approximation is used in engineering and applied sciences when you need to approximate a function over a continuous domain. It is particularly useful in the following situations:

When an Exact Analytical Solution is Unavailable: Many engineering problems involve complex differential equations that do not have closed-form solutions. Least squares approximation helps obtain an approximate function. Approximate calculation of the solution of the heat conduction equation in irregular geometries or a source function defined as a discrete function can be given among such problems.

When Experimental or Simulated Data is Noisy: In engineering applications, measured data often contains noise due to sensor limitations or environmental factors. Least squares approximation helps create a smooth function that best represents the underlying trend; e.g., smoothing stress-strain curves in material testing is an example of such a case.

When You Need to Fit a Function Over a Continuous Domain: Unlike discrete least squares (which minimizes errors at specific points), continuous least squares minimizes the error over an entire interval, such as in this example problem.

When Solving Integral Equations or Boundary Value Problems: In structural mechanics, fluid dynamics, and electromagnetics, some problems require approximating a function that satisfies integral constraints. For example, solving the bending of a beam by approximating its deflection function.

When Using Spectral or Orthogonal Methods: Least squares is often used with orthogonal polynomials (Legendre, Chebyshev, Fourier series) to approximate complex functions efficiently. For example, this method is applied to approximate airfoil lift coefficients in aerodynamics.

EXAMPLE 7.4: Solving under-determined systems

Consider a beam with four unknown forces and two strain gauges to measure strain at different points. That is, we have more unknowns than measurements, leading to an under-determined system. Determine the unknown forces if the system of equations based on these measurements is given as follows:

$$\begin{aligned} F_1 + 2F_2 + 4F_3 + F_4 &= 365 \\ 2F_1 + 3F_2 + 2F_3 + 5F_4 &= 395 \end{aligned}$$

SOLUTION:

We can express the under-determined system of linear equations as **Af=b**, where

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 4 & 1 \\ 2 & 3 & 2 & 5 \end{bmatrix}, \qquad \mathbf{b} = \begin{bmatrix} 365 \\ 395 \end{bmatrix}, \quad \text{and} \quad \mathbf{f} = \begin{bmatrix} F_1 \\ F_2 \\ F_3 \\ F_4 \end{bmatrix}.$$

Applying the least squares procedure, the linear system becomes $\mathbf{A}^T\mathbf{A}\mathbf{f}=\mathbf{A}^T\mathbf{b}$, or

$$\begin{bmatrix} 5 & 8 & 8 & 11 \\ 8 & 13 & 14 & 17 \\ 8 & 14 & 20 & 14 \\ 11 & 17 & 14 & 26 \end{bmatrix} \begin{bmatrix} F_1 \\ F_2 \\ F_3 \\ F_4 \end{bmatrix} = \begin{bmatrix} 1155 \\ 1915 \\ 2250 \\ 2340 \end{bmatrix}$$

But $\mathbf{A}^T\mathbf{A}$=0; thus, the system is regularized (*Tikhonov regularization*) as follows:

$$E(\mathbf{f}) = \|\mathbf{A}\mathbf{f} - \mathbf{b}\|_2^2 + \lambda \, \|\mathbf{f}\|_2^2$$

which leads to the following system of equations:

$$(\mathbf{A}^T\mathbf{A} + \lambda\mathbf{I})\mathbf{f} = \mathbf{A}^T\mathbf{b} \quad \Rightarrow \quad \begin{bmatrix} 5+\lambda & 8 & 8 & 11 \\ 8 & 13+\lambda & 14 & 17 \\ 8 & 14 & 20+\lambda & 14 \\ 11 & 17 & 14 & 26+\lambda \end{bmatrix} \begin{bmatrix} F_1 \\ F_2 \\ F_3 \\ F_4 \end{bmatrix} = \begin{bmatrix} 1155 \\ 1915 \\ 2250 \\ 2340 \end{bmatrix}$$

Solving this system for decreasing values of λ result in

$$\begin{array}{lllll} \text{For } \lambda = 1 & F_1 = 18.69, & F_2 = 34.78, & F_3 = 59.20, & F_4 = 26.46\,\text{N} \\ \text{For } \lambda = 0.1 & F_1 = 18.80, & F_2 = 35.42, & F_3 = 62.15, & F_4 = 25.32\,\text{N} \\ \text{For } \lambda = 0.01 & F_1 = 18.81, & F_2 = 35.49, & F_3 = 62.47, & F_4 = 25.20\,\text{N} \\ \text{For } \lambda = 0.001 & F_1 = 18.81, & F_2 = 35.50, & F_3 = 62.50, & F_4 = 25.18\,\text{N} \end{array}$$

Discussion: An under-determined system of linear equations is a system where there are more variables than equations. This means the system has either infinitely many solutions or no solution, depending on the consistency of the equations. Since there are fewer constraints (equations) than unknowns (variables), there is typically at least one free variable that can take on infinitely many values.

To find a unique solution, additional criteria (such as minimizing some function or imposing physical constraints) are necessary. In linear algebra, pseudoinverses (Moore-Penrose inverse) or regularization techniques (Tikhonov regularization) are often used to obtain meaningful solutions. The given program required regularization for fairly small values of λ.