CHAPTER 5

EMPIRICAL LAWS AND CURVE-FITTING

1 Statement of the problem

In mathematics, engineering, and the applied sciences, experimental data often arises from measurements, observations, or simulations rather than from theoretical models. In such cases, an exact functional relationship between variables may not be known, but it is still useful- and often necessary- to approximate this relationship using a suitable mathematical expression.

This chapter addresses the problem of fitting curves to empirical data, a process known as curve fitting. The goal is to determine a function $y = f(x)$ that best describes the observed relationship between a dependent variable y and an independent variable x. This function may be linear, polynomial, exponential, logarithmic, or of a more complex form depending on the data behavior.

Curve fitting techniques are essential in fields such as physics, biology, economics, and engineering, where data-driven models are used for prediction, interpolation, or simplification of complex systems. Key methods to be discussed include:

- Graphical Method (visual estimation)
- Method of Least Squares (error minimization)
- Method of Group Averages
- Fitting curves with two or more constants

Each method has its own applications and limitations, depending on the desired accuracy, complexity of the data, and available computational resources. This chapter presents these techniques in detail, deriving their underlying principles, providing step-by-step procedures, and illustrating their use through worked numerical examples.

2 Linear least squares methods

2.1 Fitting a straight line

Linear models are fundamental tools in data analysis, offering simplicity, interpretability, and computational efficiency. They are particularly effective when the data exhibits a linear relationship or an approximate proportionality. The general form of a linear model is:

$$\hat{y} = ax + b$$

where

- $\hat{y}$ is the predicted value of y from the linear model,
- a is the slope, indicating the rate of change in y for a unit increase in x,
- b is the intercept, representing the expected value of y when $x = 0$.

The parameters a and b are estimated using the least squares method, which minimizes the sum of the squared differences between the observed values y_i and the predicted values $\hat{y}_i$ from the fitted line. This approach ensures that the fitted line best represents the data by minimizing the error between the actual and predicted values.

The residual for a given data point (x_i, y_i) is defined as the difference between the observed value y_i and the predicted value $\hat{y}_i$ based on the fitted model. Mathematically, the residual ε_i is expressed as

$$\varepsilon_i = y_i - \hat{y}_i$$

Residuals provide a measure of the deviation of the observed data points from the fitted line. Minimizing the sum of squared residuals

$$SSE = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

ensures that the fitted line is as close as possible to all the data points, thereby improving the model's accuracy. To visualize the concept of residuals and the fitting process, consider the plot below. This plot illustrates the following

- The red stars represent the observed data points (x_i, y_i).
- The blue line represents the fitted line determined by the least squares method.
- The dotted lines represent the residuals, i.e., the vertical differences between the observed data points and the predicted values from the fitted line.
- The black lines represent the orthogonal distances, which are the minimum distances between the data points and the fitted line, highlighting the accuracy of the fit.

This plot serves to demonstrate the process of fitting a line using the least squares method. The residuals (dotted lines) quantify the error between the observed data and the predicted values from the fitted line. By minimizing the sum of squared residuals, the least squares method ensures the best possible linear approximation of the data. The orthogonal distances (black lines) are essential in evaluating the overall fit of the model, as they represent the true perpendicular distances between each data point and the fitted line.

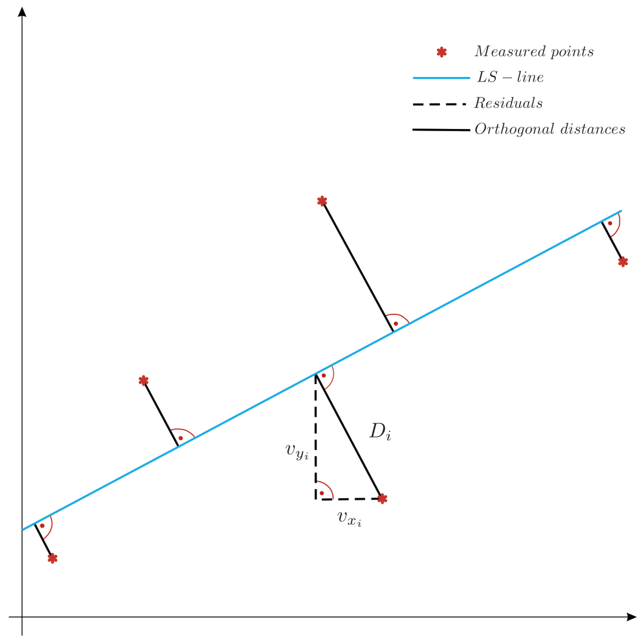

Figure 5.1: Visual representation of least squares fitting and residuals in 2D, where orthogonal distance is $D_i^2 = v_{x_i}^2 + v_{y_i}^2$

Algorithm 15 Fitting a straight line via least squares

Require: Set of data points $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$
Ensure: Slope a and intercept b such that the best-fit line is $y = ax + b$

Compute the means:
$\bar{x} \leftarrow \frac{1}{n}\sum_{i=1}^{n} x_i$
$\bar{y} \leftarrow \frac{1}{n}\sum_{i=1}^{n} y_i$
Compute the slope:
$a \leftarrow \frac{\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y})}{\sum_{i=1}^{n}(x_i-\bar{x})^2}$
Compute the intercept:
$b \leftarrow \bar{y} - a\bar{x}$
Form the regression line:
The fitted line is $y = ax + b$
(Optional) Compute residuals and error:
for $i \leftarrow 1\ n$ **do**
    $\varepsilon_i \leftarrow y_i - (ax_i + b)$ ▷ Residual
end for
$SSE \leftarrow \sum_{i=1}^{n} \varepsilon_i^2$ ▷ Sum of squared errors
return Slope a, intercept b, and optionally residuals and SSE

Example: Fitting a straight line using the least squares method
Given the following dataset:

x_i	1	2	3	4	5
y_i	1.2	1.9	3.2	3.9	5.1

we aim to find the best-fit straight line in the form:

$$y = a + bx$$

using the least squares method, which minimizes the total squared error between the observed data points (x_i, y_i) and the predicted values $\hat{y}_i = a + bx_i$.

Step 1: Compute the necessary summations

$$\begin{aligned}
n &= 5 \\
\sum x_i &= 1 + 2 + 3 + 4 + 5 = 15 \\
\sum y_i &= 1.2 + 1.9 + 3.2 + 3.9 + 5.1 = 15.3 \\
\sum x_i^2 &= 1^2 + 2^2 + 3^2 + 4^2 + 5^2 = 55 \\
\sum x_i y_i &= 1.2 + 3.8 + 9.6 + 15.6 + 25.5 = 55.5
\end{aligned}$$

x_i	y_i	x_i^2	$x_i y_i$
1	1.2	1	1.2
2	1.9	4	3.8
3	3.2	9	9.6
4	3.9	16	15.6
5	5.1	25	25.5
$\sum$	15.3	55	55.5

Step 2: Derive the normal equations
The least squares method leads to the system

$$\begin{aligned}
na + b\sum x_i &= \sum y_i \\
a\sum x_i + b\sum x_i^2 &= \sum x_i y_i
\end{aligned}$$

Substituting known values

$$\begin{aligned}
5a + 15b &= 15.3 \quad \text{(Equation 1)} \\
15a + 55b &= 55.5 \quad \text{(Equation 2)}
\end{aligned}$$

Step 3: Solve for the coefficients

Multiply Equation (1) by 3

$$15a + 45b = 45.9 \quad \text{(Equation 3)}$$

Subtract Equation (3) from Equation (2)

$$(15a + 55b) - (15a + 45b) = 55.5 - 45.9 \Rightarrow 10b = 9.6 \Rightarrow \boxed{b = 0.96}$$

Substitute into Equation (1)

$$5a + 15(0.96) = 15.3 \Rightarrow 5a + 14.4 = 15.3 \Rightarrow a = \frac{0.9}{5} = \boxed{a = 0.18}$$

Step 4: Final fitted equation

$$\boxed{y = 0.18 + 0.96x}$$

This line minimizes the squared error and best approximates the trend in the data.

Step 5: Analyze the residuals and goodness of fit
The residual for each data point is

$$\varepsilon_i = y_i - \hat{y}_i, \quad \text{where } \hat{y}_i = a + bx_i$$

x_i	y_i	$\varepsilon_i = y_i - (0.18 + 0.96x_i)$
1	1.2	$1.2 - (1.14) = 0.06$
2	1.9	$1.9 - (2.10) = -0.20$
3	3.2	$3.2 - (3.06) = -0.06$
4	3.9	$3.9 - (4.02) = -0.12$
5	5.1	$5.1 - (4.98) = 0.12$

Sum of squared residuals (SSE)

$$SSE = \sum_{i=1}^{5} \varepsilon_i^2 = 0.06^2 + (-0.20)^2 + (-0.06)^2 + (-0.12)^2 + 0.12^2 = \boxed{0.0728}$$

Step 6: Compute coefficient of determination R^2
To evaluate how well the model explains the data

$$R^2 = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y})^2}, \quad \bar{y} = \frac{\sum y_i}{n} = 3.06$$

$$\sum (y_i - \bar{y})^2 = (1.2 - 3.06)^2 + (1.9 - 3.06)^2 + \cdots + (5.1 - 3.06)^2 = 10.148$$

$$R^2 = 1 - \frac{0.0728}{10.148} \approx \boxed{0.9928}$$

An R^2 value near 1 indicates an excellent fit: over 99% of the variance in the data is explained by the model.

Conclusion

The least squares method has produced a high-quality linear model:

$$y = 0.18 + 0.96x$$

with minimal residuals and a strong coefficient of determination. This confirms the model is a good representation of the dataset.

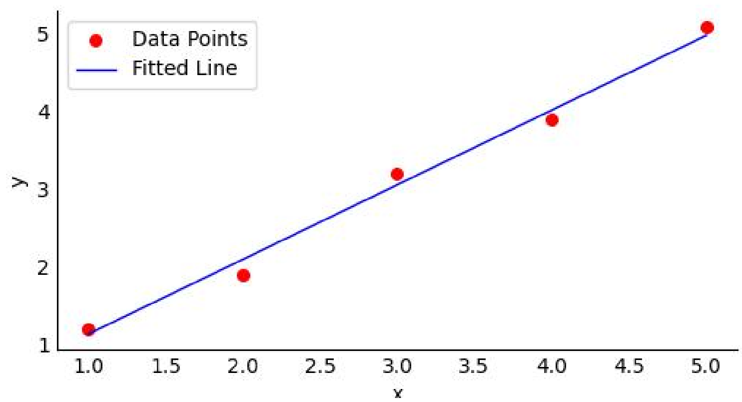

Figure 5.2: Linear Fit Using Least Squares Method

Convergence rate and accuracy

In linear least squares fitting, the solution is obtained analytically by solving a system of two normal equations. Since no iteration is required, the convergence is immediate and exact.

The accuracy of the fit can be evaluated by examining the **residuals**, which have been defined earlier as the differences between observed values y_i and predicted values $\hat{y}_i$. A good fit is indicated by residuals that are randomly scattered around zero, while any patterns (such as curves) suggest that the linear model may be inadequate.

To quantify the total error, the **sum of squared residuals (SSE)** is calculated:

$$SSE = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

A smaller value of SSE indicates a better fit between the model and the data.

The **coefficient of determination** R^2 is another important measure, indicating how much of the variance in the data is explained by the model:

$$R^2 = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y})^2}$$

Values of R^2 close to 1 suggest a strong linear relationship, while values closer to 0 indicate a poor fit. Outliers can reduce the value of R^2 and distort the fitted line. Therefore, it is important to inspect the residuals and ensure that the model appropriately fits the data.

Advantages

- Simple to compute and interpret.
- Provides a good approximation when the data shows a linear trend.
- Requires only two parameters (slope and intercept).
- Efficient in terms of computational cost.
- Applicable in a wide range of practical problems.

Disadvantages

- Inaccurate when the data is nonlinear or curved.
- Sensitive to outliers, which can distort the fitted line.
- May oversimplify complex data patterns.

3 Polynomial least squares methods

3.1 Fitting a second-degree curve

When the relationship between variables displays a curved rather than linear trend, a second-degree polynomial (quadratic) of the form

$$y = ax^2 + bx + c$$

often provides a more accurate approximation. The method of least squares can be extended to estimate the coefficients a, b, and c that define the best-fitting quadratic curve for a given dataset. This model is widely used in physics (projectile motion), economics (marginal cost curves), biology (growth models), and other areas where non-linear relationships arise.

Algorithm 16 Fitting a second-D degree C curve via least squares

Require: Set of data points $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$
Ensure: Coefficients a, b, and c such that the best-fit curve is $y = ax^2 + bx + c$

Compute the necessary sums:
$S_x \leftarrow \sum_{i=1}^{n} x_i$
$S_{x^2} \leftarrow \sum_{i=1}^{n} x_i^2$
$S_{x^3} \leftarrow \sum_{i=1}^{n} x_i^3$
$S_{x^4} \leftarrow \sum_{i=1}^{n} x_i^4$
$S_y \leftarrow \sum_{i=1}^{n} y_i$
$S_{xy} \leftarrow \sum_{i=1}^{n} x_i y_i$
$S_{x^2 y} \leftarrow \sum_{i=1}^{n} x_i^2 y_i$
Construct the normal equations:
Form the system:

$$\begin{bmatrix} S_{x^4} & S_{x^3} & S_{x^2} \\ S_{x^3} & S_{x^2} & S_x \\ S_{x^2} & S_x & n \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} S_{x^2 y} \\ S_{xy} \\ S_y \end{bmatrix}$$

Solve the system for a, b, and c using Gaussian elimination or matrix inversion.
Construct the fitted quadratic curve:
$y = ax^2 + bx + c$
(Optional) Evaluate fit quality:
for $i \leftarrow 1$ n **do**
  $\varepsilon_i \leftarrow y_i - (ax_i^2 + bx_i + c)$ ▷ Compute residual
end for
$SSE \leftarrow \sum_{i=1}^{n} \varepsilon_i^2$ ▷ Sum of squared errors
return Coefficients a, b, c, and optionally the residuals and SSE

Example: Fit a second-degree curve using the least squares method
We are given the dataset:

x_i	1	2	3	4	5
y_i	6	11	18	27	38

Our goal is to fit a quadratic model of the form:

$$y = ax^2 + bx + c$$

using the least squares method, which minimizes the sum of squared deviations between the observed values y_i and the predicted values $\hat{y}_i = ax_i^2 + bx_i + c$.

Step 1: Construct the Extended Table of Summations

x_i	y_i	x_i^2	x_i^3	x_i^4	x_iy_i	$x_i^2y_i$
1	6	1	1	1	6	6
2	11	4	8	16	22	44
3	18	9	27	81	54	162
4	27	16	64	256	108	432
5	38	25	125	625	190	950
$\sum$	15	100	225	979	380	1594

Step 2: Formulate the Normal Equations

The least squares approach leads to a system of three linear equations in three unknowns a, b, c, derived by minimizing the residual sum of squares:

$$\sum y = a\sum x^2 + b\sum x + cn$$
$$\sum xy = a\sum x^3 + b\sum x^2 + c\sum x$$
$$\sum x^2y = a\sum x^4 + b\sum x^3 + c\sum x^2$$

Substitute the computed sums:

$$100 = a(55) + b(15) + 5c$$
$$380 = a(225) + b(55) + 15c$$
$$1594 = a(979) + b(225) + 55c$$

Step 3: Solve the System of Equations

Solving this linear system (by Gaussian elimination, matrix inversion, or symbolic computation), we find:

$$\boxed{a = 1}, \quad \boxed{b = 2}, \quad \boxed{c = 3}$$

Step 4: Final Fitted Equation

Substitute the coefficients into the model:

$$\boxed{y = x^2 + 2x + 3}$$

This equation represents the quadratic curve that best fits the data under the least squares criterion.

Step 5: Residual Analysis and Accuracy Evaluation

To assess the quality of the fit, we compute predicted values $\hat{y}_i = ax_i^2 + bx_i + c$ and residuals $\varepsilon_i = y_i - \hat{y}_i$ for each data point:

x_i	y_i	$\hat{y}_i = x_i^2 + 2x_i + 3$	$\varepsilon_i = y_i - \hat{y}_i$
1	6	6	0
2	11	11	0
3	18	18	0
4	27	27	0
5	38	38	0

Since all residuals are exactly zero, the fit is **perfect** for this dataset. The sum of squared residuals (error) is:

$$SSE = \sum_{i=1}^{5} \varepsilon_i^2 = 0$$

Step 6: Coefficient of Determination R^2

The coefficient of determination quantifies the proportion of variance in y explained by the model:

$$R^2 = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y})^2} = 1 - \frac{0}{\mathrm{Var}(y)} = \boxed{1}$$

This confirms that the fitted model captures 100

Step 7: Interpretation

The model $y = x^2 + 2x + 3$ fits all five data points exactly, suggesting that the original data is either generated from or extremely well-approximated by a second-degree polynomial. In real-world cases, such exact fits are rare, and residuals or R^2 near—but not equal to—1 are more typical.

Step 8: Visualization (Suggested)

To visually confirm the fit, plot the data points and the curve: - Red stars ($*$): Observed data points - Blue curve: Fitted function $y = x^2 + 2x + 3$

This helps interpret both accuracy and trend representation.

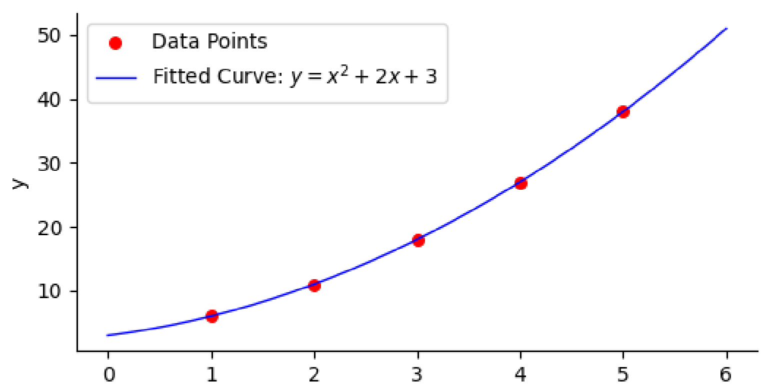

Figure 5.3: Quadratic Fit of the Data Using Least Squares Method

Convergence rate and accuracy

In second-degree least squares fitting, the parameters a, b, and c are obtained by solving a system of three normal equations. These equations form a linear system that can be solved directly without iteration. As a result, the convergence is exact and immediate.

The accuracy of the quadratic model is assessed by computing the residuals:

$$\varepsilon_i = y_i - \hat{y}_i,$$

where $\hat{y}_i = ax_i^2 + bx_i + c$ is the predicted value for each x_i. Ideally, the residuals should be small and randomly distributed around zero, indicating a good fit.

The total residual error is measured by the sum of squared residuals:

$$S = \sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} (y_i - ax_i^2 - bx_i - c)^2$$

This value indicates how closely the curve fits the observed data. A smaller S suggests a better fit.

The coefficient of determination, R^2, quantifies how much of the variation in y is explained by the model:

$$R^2 = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y})^2}$$

A value of R^2 close to 1 implies that the model accurately captures the trend in the data. If residuals show a clear pattern (e.g., increasing or decreasing trend), the model may be insufficient, and a higher-degree polynomial might be more appropriate.

Convergence Rate and Accuracy

Fitting an exponential curve involves transforming the nonlinear model into a linear form by taking logarithms. Once linearized, the parameters are determined using standard least squares, which involves solving a system of two linear equations. This ensures direct computation without iteration, meaning the convergence is exact and immediate.

Accuracy is assessed on the original (non-logarithmic) scale by calculating the residuals $\varepsilon_i = y_i - \hat{y}_i$, where $\hat{y}_i = ae^{bx_i}$. These residuals indicate how well the fitted model predicts the observed data. A good fit is characterized by small residuals that are randomly distributed around zero.

The total error is quantified by the sum of squared residuals, and model quality is further evaluated using the coefficient of determination R^2. A value of R^2 close to 1 indicates that the exponential model effectively captures the trend in the data. However, noticeable patterns in residuals or a low R^2 suggest that a different model may be more appropriate.

Advantages

- Captures curvature in data that cannot be fitted with a straight line.
- Useful when the rate of change itself is changing (acceleration or deceleration).
- Provides better approximation for data with turning points.

Disadvantages

- More complex to compute (requires solving a 3x3 system).
- Risk of overfitting if the actual relationship is linear.
- Interpretation of coefficients is less intuitive than in linear fitting.
- Not suitable for data showing exponential or logarithmic growth.

4 Nonlinear least squares methods

4.1 Fitting an exponential curve

Exponential models arise frequently in natural and social sciences, where growth or decay processes are involved. The general form of an exponential relationship is:

$$y = ae^{bx},$$

where a and b are constants to be determined. Since this model is nonlinear in its parameters, it cannot be fitted directly using standard linear least squares. However, by applying a logarithmic transformation, the model can be reduced to a linear form.

Taking the natural logarithm on both sides

$$\ln y = \ln a + bx$$

Letting $Y = \ln y$ and $A = \ln a$, the equation becomes:

$$Y = A + bx,$$

which is a linear model in x and Y, and can be solved using the method of least squares.

Example: Fit an exponential curve using the least squares method
We are given the following dataset

x_i	1	2	3	4
y_i	2.7	7.4	20.1	54.6

We aim to fit an exponential model of the form

$$y = ae^{bx}$$

using the least squares method. To apply this, we linearize the model by taking logarithms

$$\ln y = \ln a + bx \quad (\text{let } Y = \ln y,\ A = \ln a)$$

This transforms the problem into a linear regression of $Y_i = A + bx_i$.

Step 1: Construct the transformed data table

x_i	y_i	$Y_i = \ln y_i$	x_i^2	x_iY_i
1	2.7	0.9933	1	0.9933
2	7.4	2.0015	4	4.0030
3	20.1	3.0007	9	9.0021
4	54.6	4.0000	16	16.0000
$\sum$	10	10.0000	30	30.0004

Step 2: Derive the normal equations for linear regression
Let the linear model be

$$Y = A + bx$$

From the least squares method, the normal equations are

$$\sum Y = nA + b\sum x, \quad \sum xY = A\sum x + b\sum x^2$$

Substituting values

$$10.0000 = 4A + 10b \quad (1) 30.0004 = 10A + 30b \quad (2)$$

Step 3: Solve the system of equations
From equation (1)

$$A = \frac{10.0000 - 10b}{4}$$

Substitute into (2)

$$30.0004 = 10 \cdot \left(\frac{10.0000 - 10b}{4}\right) + 30b = 25.0000 - 25b + 30b = 25.0000 + 5b \Rightarrow b = 1.0001$$

Then

$$A = \frac{10.0000 - 10(1.0001)}{4} \approx 0 \Rightarrow a = e^A = e^0 = 1$$

Final Result

$$\boxed{y = e^x}$$

This model represents the best exponential fit to the data using the least squares criterion.

Step 4: Compute residuals and evaluate accuracy
We compute the predicted values $\hat{y}_i = ae^{bx_i} = e^{x_i}$, residuals $\varepsilon_i = y_i - \hat{y}_i$, and squared residuals ε_i^2

x_i	y_i	$\hat{y}_i = e^{x_i}$	ε_i	ε_i^2
1	2.7	2.7183	−0.0183	0.0003
2	7.4	7.3891	0.0109	0.0001
3	20.1	20.0855	0.0145	0.0002
4	54.6	54.5982	0.0018	0.0000

$$\text{Total squared error } SSE = \sum \varepsilon_i^2 \approx \boxed{0.00067}$$

The residuals are very small and alternate in sign, indicating no systematic bias. The fit is therefore highly accurate.

Step 5: Visual interpretation (optional)
Plot the data points (x_i, y_i) and the fitted curve $y = e^x$ for comparison. The red stars represent observed data; the blue line shows the exponential model. The close alignment confirms the excellent fit.

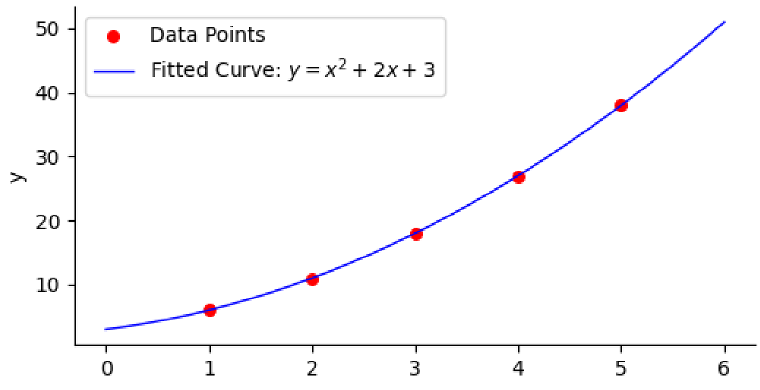

Figure 5.4: Exponential Fit of the Data Using Least Squares Method

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Algorithm 17 Fitting an exponential curve via linearization

Require: A set of data points $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ with $y_i > 0$
Ensure: Parameters a and b for the exponential model $y = ae^{bx}$

Step 1: Transform the data (linearization).
for $i \leftarrow 1$ n **do**
  $Y_i \leftarrow \ln(y_i)$ ▷ Take the natural log of each y_i
end for
Step 2: Compute means of transformed data.
$\bar{x} \leftarrow \frac{1}{n} \sum_{i=1}^{n} x_i$
$\bar{Y} \leftarrow \frac{1}{n} \sum_{i=1}^{n} Y_i$
Step 3: Compute slope and intercept for the linearized model.
$b \leftarrow \frac{\sum_{i=1}^{n}(x_i - \bar{x})(Y_i - \bar{Y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$
$A \leftarrow \bar{Y} - b\bar{x}$ ▷ Intercept of the line
Step 4: Back-transform to obtain exponential model parameters.
$a \leftarrow e^A$ ▷ Since $Y = \ln y = \ln a + bx$, so $a = e^A$
Step 5: Form the exponential regression equation.
Output: $y = ae^{bx}$
Step 6 (Optional): Evaluate residuals and error.
for $i \leftarrow 1$ n **do**
  $\hat{y}_i \leftarrow ae^{bx_i}$ ▷ Predicted value
  $\varepsilon_i \leftarrow y_i - \hat{y}_i$ ▷ Residual
end for
$SSE \leftarrow \sum_{i=1}^{n} \varepsilon_i^2$ ▷ Sum of squared residuals
return Parameters a, b and optionally the residuals and SSE

Convergence rate and accuracy

In exponential least squares fitting, the nonlinear model is first transformed into a linear form using a logarithmic transformation. This results in a system of two normal equations, which can be solved directly without iteration. Therefore, the convergence is immediate and exact.

The accuracy of the exponential model is evaluated by calculating the residuals between the observed and predicted values on the original scale. Ideally, the residuals should be small and randomly distributed, indicating a good fit.

The total error is measured by the sum of squared residuals, which reflects how closely the model approximates the actual data. A smaller value of this sum indicates a more accurate fit.

The coefficient of determination, R^2, expresses the proportion of variation in the observed data that is explained by the model. A value of R^2 close to 1 suggests that the exponential function provides a strong representation of the data trend. If residuals exhibit a clear pattern or if R^2 is low, the exponential model may be inadequate, and an alternative model should be considered.

Advantages

- Suitable for modeling rapid growth or decay processes (e.g., population growth, radioactive decay).
- Provides an excellent fit when the rate of change of y is proportional to y itself.
- Can be linearized through logarithmic transformation, enabling the use of least squares.
- Requires only two parameters, making it computationally efficient.

Disadvantages

- Not appropriate when the data does not follow an exponential trend.
- Logarithmic transformation requires all y-values to be positive.
- Sensitive to data scaling and outliers, which can distort the fit.
- The fitted model is less interpretable when a or b are near zero.

4.2 Fitting a logarithmic curve

A logarithmic model is appropriate when the variable y increases at a decreasing rate as x increases. This behavior is observed in physical, biological, and economic systems where initial rapid growth is followed by a gradual leveling off.

The general form

$$y = a + b \ln x$$

is already linear in parameters a and b, so the method of least squares can be applied directly without transformation of y. However, x must be strictly positive for the logarithm to be defined. The objective is to determine constants a and b such that the curve best represents the observed data points.

Algorithm 18 Fitting a Logarithmic Curve via Linear Regression

Require: A set of data points $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ with $x_i > 0$
Ensure: Coefficients a, b such that the best-fit model is $y = a + b \ln x$

Step 1: Transform the independent variable.
for $i \leftarrow 1\ n$ **do**
  $X_i \leftarrow \ln(x_i)$ ▷ Take natural log of each x_i
end for
Step 2: Compute sample means.
$\bar{X} \leftarrow \frac{1}{n}\sum_{i=1}^{n} X_i$ ▷ Mean of transformed values
$\bar{y} \leftarrow \frac{1}{n}\sum_{i=1}^{n} y_i$ ▷ Mean of original y values
Step 3: Perform linear regression on (X_i, y_i)**.**
Compute slope:

$$b \leftarrow \frac{\sum_{i=1}^{n}(X_i - \bar{X})(y_i - \bar{y})}{\sum_{i=1}^{n}(X_i - \bar{X})^2}$$

Compute intercept:

$$a \leftarrow \bar{y} - b\bar{X}$$

Step 4: Construct the logarithmic regression model.
Output: $y = a + b \ln x$
Step 5 (Optional): Evaluate residuals and model accuracy.
for $i \leftarrow 1\ n$ **do**
  $\hat{y}_i \leftarrow a + b\ln(x_i)$
  $\varepsilon_i \leftarrow y_i - \hat{y}_i$
end for
$SSE \leftarrow \sum_{i=1}^{n} \varepsilon_i^2$ ▷ Sum of squared residuals
return Coefficients a, b, and optionally residuals and SSE

Example: Fit a logarithmic curve using the least squares method
We are given the dataset:

x_i	1	2	3	4
y_i	1.5	2.1	2.8	3.2

Our goal is to fit a logarithmic model of the form:

$$y = a + b \ln x$$

using the least squares method. This approach transforms the independent variable and performs linear regression on the transformed data.

Step 1: Compute the transformed values and construct the table

x_i	y_i	$\ln x_i$	$(\ln x_i)^2$	$y_i \ln x_i$
1	1.5	0.0000	0.0000	0.0000
2	2.1	0.6931	0.4804	1.4555
3	2.8	1.0986	1.2069	3.0759
4	3.2	1.3863	1.9218	4.4362
Totals	10.6	3.1780	3.6091	8.9676

Step 2: Form the normal equations

Let $X_i = \ln x_i$, and use the normal equations for linear regression on the transformed variables (X_i, y_i):

$$\sum y_i = na + b\sum X_i, \quad \sum X_i y_i = a\sum X_i + b\sum X_i^2$$

Substituting the values:

$$10.6 = 4a + 3.1780b \quad (1)$$

$$8.9676 = 3.1780a + 3.6091b \quad (2)$$

Step 3: Solve the system of equations

Solving equations (1) and (2) simultaneously (e.g., by substitution or matrix methods), we obtain:

$$\boxed{a \approx 1.514}, \quad \boxed{b \approx 1.235}$$

Step 4: Final fitted model

The resulting logarithmic model is:

$$\boxed{y = 1.514 + 1.235 \ln x}$$

This equation represents the best-fit curve under the least squares criterion.

Step 5: Compute residuals and assess accuracy

We compute predicted values $\hat{y}_i = a + b\ln x_i$, residuals $\varepsilon_i = y_i - \hat{y}_i$, and squared residuals:

x_i	y_i	$\ln x_i$	$\hat{y}_i$	ε_i	ε_i^2
1	1.5	0.0000	1.514	−0.014	0.0002
2	2.1	0.6931	2.369	−0.269	0.0725
3	2.8	1.0986	2.867	−0.067	0.0045
4	3.2	1.3863	3.227	−0.027	0.0007

Sum of squared residuals:

$$SSE = \sum_{i=1}^{4} \varepsilon_i^2 \approx \boxed{0.0788}$$

The residuals are small and fluctuate around zero, indicating a good fit of the logarithmic model to the observed data.

Step 6: Visual Interpretation (Optional)

To visually assess the model, one may plot the original data points (x_i, y_i) along with the fitted curve:

$$y = 1.514 + 1.235 \ln x$$

- Red dots represent the observed data. - The blue curve shows the fitted model.

Such a plot helps confirm the goodness-of-fit and the appropriateness of using a logarithmic relationship for the given dataset.

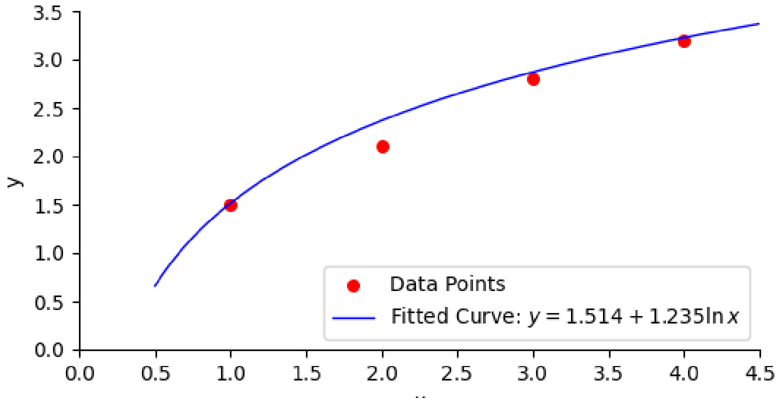

Figure 5.5: Logarithmic fit of the data using least squares method

Convergence rate and accuracy

The logarithmic fitting process involves a linear model in terms of y and $\ln x$, allowing the use of least squares without transforming the dependent variable. Since the resulting normal equations are linear in parameters, the solution is obtained directly and requires no iteration. Thus, convergence is immediate and exact.

Model accuracy is evaluated by comparing observed values y_i to predicted values $\hat{y}_i$, obtained from the fitted equation. Residuals $\varepsilon_i = y_i - \hat{y}_i$ are computed for each point. Ideally, these residuals are small and randomly distributed around zero, suggesting that the model appropriately reflects the data's behavior.

The sum of squared residuals measures the total error, with smaller values indicating a better fit. Additionally, the coefficient of determination R^2 helps quantify the model's explanatory power. A high R^2, along with residuals lacking any pattern, confirms that the logarithmic model is suitable. Otherwise, it may be necessary to consider a different curve type.

Advantages

- Useful for modeling slow-growth behavior or diminishing returns.
- Naturally linear in parameters - no transformation of y is required.
- Efficient for interpolation over a range where growth slows with increasing x.
- Computationally simple and requires only two parameters.

Disadvantages

- Only valid for $x > 0$, since $\ln x$ is undefined for non-positive values.
- Poor fit when data follows exponential or polynomial trends.
- Sensitive to large fluctuations in early values of x.
- Interpretation becomes difficult if the data has large variability.

4.3 Fitting a power curve

Power models are commonly used when both variables follow a multiplicative or proportional relationship. The general form of a power function is

$$y = ax^b,$$

where a and b are constants to be determined. Since this form is nonlinear in its parameters, it is linearized by taking logarithms on both sides

$$\ln y = \ln a + b \ln x$$

Letting $Y = \ln y$, $X = \ln x$, and $A = \ln a$, the model becomes:

$$Y = A + bX,$$

which is a linear equation that can be solved using the method of least squares. After solving for A, we recover $a = e^A$.

Example: Fit a power curve using the least squares method
We are given the dataset

x_i	1	2	3	4
y_i	2.0	4.1	8.9	15.7

We aim to fit the model

$$y = ax^b$$

using the method of least squares. To do so, we linearize the model by taking logarithms on both sides

$$\ln y = \ln a + b \ln x \quad (\text{let } Y_i = \ln y_i,\ X_i = \ln x_i,\ A = \ln a)$$

The linearized model becomes

$$Y = A + bX$$

We now apply linear regression to the transformed data (X_i, Y_i).

Step 1: Compute Transformed Values and Construct the Table

x_i	y_i	$\ln x_i$	$\ln y_i$	$(\ln x_i)^2$	$\ln x_i \cdot \ln y_i$
1	2.0	0.0000	0.6931	0.0000	0.0000
2	4.1	0.6931	1.4100	0.4804	0.9778
3	8.9	1.0986	2.1860	1.2069	2.4044
4	15.7	1.3863	2.7520	1.9218	3.8148
Totals		3.1780	7.0411	3.6091	7.1969

Step 2: Form the Normal Equations
From the least squares method, the normal equations for linear regression are

$$\sum Y = nA + b\sum X, \quad \sum XY = A\sum X + b\sum X^2$$

Substitute the totals into the system

$$7.0411 = 4A + 3.1780b \quad (1) 7.1969 = 3.1780A + 3.6091b \quad (2)$$

Step 3: Solve the System
Solving equations (1) and (2), we obtain

$$A \approx 0.6931 \quad \Rightarrow \quad a = e^A \approx \boxed{2.0}$$

$$b \approx \boxed{1.99}$$

Final Fitted Model

$$\boxed{y = 2.0 \cdot x^{1.99}}$$

This model closely approximates the power law behavior of the data.

Step 4: Compute Predicted Values and Residuals
We calculate the predicted values $\hat{y}_i = 2.0 \cdot x_i^{1.99}$, the residuals $\varepsilon_i = y_i - \hat{y}_i$, and squared residuals

x_i	y_i	$\hat{y}_i = 2.0 \cdot x_i^{1.99}$	ε_i	ε_i^2
1	2.0	2.0000	0.0000	0.0000
2	4.1	3.9760	0.1240	0.0154
3	8.9	8.9045	−0.0045	0.0000
4	15.7	15.6749	0.0251	0.0006

Total sum of squared residuals

$$SSE = \sum_{i=1}^{4} \varepsilon_i^2 \approx \boxed{0.0160}$$

Conclusion
The fitted power curve $y = 2.0 \cdot x^{1.99}$ closely matches the data. The residuals are small and centered near zero, with very low squared error. This confirms that a power-law model is appropriate and provides an excellent fit to the given data. ■

Algorithm 19 Fitting a power curve via linearization

Require: A set of data points $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ with $x_i > 0$ and $y_i > 0$
Ensure: Coefficients a and b such that the best-fit model is $y = ax^b$

Step 1: Transform the data (log-log linearization).
for $i \leftarrow 1$ n **do**
  $X_i \leftarrow \ln(x_i)$
  $Y_i \leftarrow \ln(y_i)$
end for
Step 2: Compute the means of the transformed variables.
$\bar{X} \leftarrow \frac{1}{n} \sum_{i=1}^{n} X_i$
$\bar{Y} \leftarrow \frac{1}{n} \sum_{i=1}^{n} Y_i$
Step 3: Perform linear regression on transformed data.
Compute slope:

$$b \leftarrow \frac{\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})}{\sum_{i=1}^{n}(X_i - \bar{X})^2}$$

Compute intercept:

$$A \leftarrow \bar{Y} - b\bar{X}$$

Recover original parameter:

$$a \leftarrow e^A$$

Step 4: Construct the fitted power model.
Output: $y = ax^b$
Step 5 (Optional): Evaluate residuals and model accuracy.
for $i \leftarrow 1$ n **do**
  $\hat{y}_i \leftarrow a x_i^b$
  $\varepsilon_i \leftarrow y_i - \hat{y}_i$
end for
$SSE \leftarrow \sum_{i=1}^{n} \varepsilon_i^2$
return Parameters a, b, and optionally residuals and SSE

Advantages

– Suitable for data showing multiplicative or scale-invariant patterns.

– Can model wide ranges of behavior with only two parameters.

– Linearized through logarithmic transformation for easy computation.

– Provides excellent fit for polynomial-like growth in many natural systems.

Disadvantages

– Only applicable when $x > 0$ and $y > 0$.

– Sensitive to small errors in logarithmic values, especially near zero.

– May not be appropriate for data that transitions between different regimes.

Summary of Least Squares Curve Fitting Models

Model Type	Equation	Linearized Form	Transformation Required
Linear	$y = ax + b$	$y = ax + b$	None
Quadratic	$y = ax^2 + bx + c$	$y = ax^2 + bx + c$	None
Exponential	$y = ae^{bx}$	$\ln y = \ln a + bx$	Log on y
Logarithmic	$y = a + b \ln x$	$y = a + b \ln x$	Log on x
Power	$y = ax^b$	$\ln y = \ln a + b \ln x$	Log on both x and y

5 Simple statistical methods

5.1 Method of Group averages

The Method of Group averages is a classical empirical technique used to fit a straight-line relationship between two variables, particularly when the data is provided in grouped form or when simplification is preferred over statistical optimization.

It is based on dividing the data into equal-sized groups, calculating the average values within each group, and determining the equation of the line that passes through these average points. Unlike the method of least squares, which minimizes the total squared error, this method approximates the trend using representative group means.

Example: Fit a straight line using the method of group averages
We are given the dataset:

x_i	1	2	3	4	5	6
y_i	2.0	2.8	4.2	5.1	6.3	7.5

Our goal is to fit a linear model of the form

$$y = ax + b$$

using the method of group averages, which simplifies trend estimation by computing average values over data segments.

Step 1: Divide the Data into Two Equal Groups

- Group 1: $x = 1, 2, 3$ with $y = 2.0, 2.8, 4.2$
- Group 2: $x = 4, 5, 6$ with $y = 5.1, 6.3, 7.5$

Step 2: Compute Group Means
For Group 1:

$$\bar{x}_1 = \frac{1+2+3}{3} = 2, \quad \bar{y}_1 = \frac{2.0+2.8+4.2}{3} = 3.0$$

For Group 2:

$$\bar{x}_2 = \frac{4+5+6}{3} = 5, \quad \bar{y}_2 = \frac{5.1+6.3+7.5}{3} = 6.3$$

Step 3: Estimate Slope and Intercept
Compute the slope a as

$$a = \frac{\bar{y}_2 - \bar{y}_1}{\bar{x}_2 - \bar{x}_1} = \frac{6.3 - 3.0}{5 - 2} = \frac{3.3}{3} = 1.1$$

Then compute the intercept b using Group 1

$$b = \bar{y}_1 - a \cdot \bar{x}_1 = 3.0 - 1.1 \cdot 2 = 3.0 - 2.2 = 0.8$$

Final Fitted Model

$$\boxed{y = 1.1x + 0.8}$$

This line approximates the overall trend in the dataset using just two representative points.

Step 4: Evaluate Model Fit (Residuals and Error)
We compute predicted values $\hat{y}_i = 1.1x_i + 0.8$, residuals $\varepsilon_i = y_i - \hat{y}_i$, and squared residuals

x_i	y_i	$\hat{y}_i = 1.1x_i + 0.8$	$\varepsilon_i = y_i - \hat{y}_i$	ε_i^2
1	2.0	1.9	0.1	0.01
2	2.8	3.0	−0.2	0.04
3	4.2	4.1	0.1	0.01
4	5.1	5.2	−0.1	0.01
5	6.3	6.3	0.0	0.00
6	7.5	7.4	0.1	0.01

Total sum of squared residuals

$$SSE = 0.01 + 0.04 + 0.01 + 0.01 + 0.00 + 0.01 = \boxed{0.08}$$

The low total squared error indicates a strong agreement between the fitted model and the observed data.

Step 5: Interpretation
The method of group averages provides a simple yet effective technique for trend estimation, especially useful in exploratory data analysis when a full least squares regression is not necessary.

Algorithm 20 Method of group averages for trend estimation

Require: A dataset of n points $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, and number of groups k
Ensure: Group averages $(\bar{x}_i, \bar{y}_i)$ and optionally the fitted curve

Step 1: Sort the dataset
Arrange the data in ascending order by x-values: $x_1 \leq x_2 \leq \cdots \leq x_n$
Step 2: Divide data into k groups.
Partition the sorted data into k groups $G_1, G_2, \ldots, G_k$ of approximately equal size, with $|G_i| \approx \frac{n}{k}$
Step 3: Compute group averages
for each group G_i **do**
    Compute group mean of x

$$\bar{x}_i = \frac{1}{|G_i|} \sum_{(x_j, y_j) \in G_i} x_j$$

    Compute group mean of y

$$\bar{y}_i = \frac{1}{|G_i|} \sum_{(x_j, y_j) \in G_i} y_j$$

end for
Step 4: Output the group averages
Return k averaged points: $(\bar{x}_1, \bar{y}_1), \ldots, (\bar{x}_k, \bar{y}_k)$
Step 5 (Optional): Fit a regression curve to group averages
Compute the means

$$\bar{x} = \frac{1}{k} \sum_{i=1}^{k} \bar{x}_i, \quad \bar{y} = \frac{1}{k} \sum_{i=1}^{k} \bar{y}_i$$

Fit a linear regression to the averages

$$b = \frac{\sum_{i=1}^{k} (\bar{x}_i - \bar{x})(\bar{y}_i - \bar{y})}{\sum_{i=1}^{k} (\bar{x}_i - \bar{x})^2}, \quad a = \bar{y} - b\bar{x}$$

The resulting trend line is $y = a + bx$
Step 6 (Optional): Compute residuals and error
for $i \leftarrow 1$ k **do**
    $\varepsilon_i \leftarrow \bar{y}_i - (a + b\bar{x}_i)$
end for
Compute total squared error

$$SSE = \sum_{i=1}^{k} \varepsilon_i^2$$

return Grouped points and (optionally) regression coefficients a, b, and SSE

Accuracy and convergence rate

The Method of Group Averages provides a quick estimation of a linear relationship between two variables but does not guarantee an optimal fit. Its accuracy is dependent on how well the selected group means represent the overall distribution of the data.

Since the method does not minimize the total squared error, the resulting line may deviate more from actual observations compared to least squares fitting. The residual sum of squares:

$$S = \sum (y_i - \hat{y}_i)^2$$

can still be calculated to assess the closeness of the fitted model to the data. A smaller value of S indicates a better fit.

This method is not iterative, and therefore it does not have a convergence rate in the numerical analysis sense. The output is computed directly from grouped averages and does not refine over successive steps.

However, its simplicity makes it a useful preliminary method for identifying linear trends before applying more accurate techniques such as the method of least squares.

Advantages

- Simple to apply using basic arithmetic only.
- Effective for grouped or interval-classified data.
- Useful for initial trend estimation.
- No advanced computations or matrix methods required.

Disadvantages

- Does not minimize squared error like least squares.
- Results depend on grouping - different groups yield different lines.
- Ignores individual data point variability within each group.
- Assumes the underlying relationship is linear.

5.2 Graphical method

The **graphical method** is one of the earliest techniques used in curve fitting, relying on the visual interpretation of data to estimate the form and parameters of a functional relationship. It involves plotting observed data points on a coordinate plane and manually drawing a curve or line that best represents the overall trend.

Although limited in precision, the graphical method remains useful for *preliminary analysis*, *model selection*, and *illustrative purposes*, especially when computational tools are unavailable or when an approximate solution is sufficient.

This method is most effective when the underlying relationship is simple (e.g., linear or quadratic) and the dataset is small to moderate in size. It provides insight into whether a linear, exponential, logarithmic, or other form may be appropriate before applying more rigorous numerical methods.

Algorithm 21 Graphical Method for Curve Fitting

Require: A dataset of points $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, and a chosen model type (e.g., linear, exponential, logarithmic)

Ensure: A visually fitted curve and estimated model parameters

Step 1: Plot the raw data.

Plot the dataset (x_i, y_i) on a Cartesian coordinate plane:

- Place the independent variable x on the horizontal axis.
- Place the dependent variable y on the vertical axis.

Step 2: Select the form of the model to fit.

Based on the observed pattern in the plotted data, select a suitable curve type:

- Linear: $y = ax + b$
- Exponential: $y = ae^{bx}$
- Logarithmic: $y = a + b \ln x$
- Power: $y = ax^b$
- Polynomial (e.g., quadratic): $y = ax^2 + bx + c$

Step 3: Visually estimate model parameters.

Manually draw or digitally overlay a curve that best follows the data trend.

- Adjust the curve to visually minimize deviation from the data points.
- Estimate the parameters (e.g., slope and intercept for a line) by inspecting the graph or using software tools.

Step 4: Superimpose the fitted curve.

Draw the estimated curve over the original plot, ensuring it visually aligns with the data.

Step 5 (Optional): Assess fit quality.

Compute predicted values $\hat{y}_i$ from the fitted curve at each x_i

Compute residuals: $\varepsilon_i = y_i - \hat{y}_i$

Calculate sum of squared errors:

$$SSE = \sum_{i=1}^{n} \varepsilon_i^2$$

return Graph of data and fitted curve; optionally estimated parameters and residual analysis

Example: Fitting a straight line graphically
Consider the dataset

x	1	2	3	4	5
y	2.3	3.1	4.5	6.0	6.8

Step 1: Plot the five data points on graph paper or using software. This gives us the visual distribution of the data.

Step 2: Observe that the data roughly follows a linear pattern, indicating a potential linear relationship.

Step 3: Draw a straight line that best balances the distribution of points. The goal is to have an equal spread of points above and below the line, representing the best visual approximation.

Step 4: Select two points on the drawn line. For example, take points $(1, 2.3)$ and $(5, 6.8)$. Then, calculate the slope m using the formula for the slope of a line:

$$m = \frac{y_2 - y_1}{x_2 - x_1} = \frac{6.8 - 2.3}{5 - 1} = \frac{4.5}{4} = 1.125$$

Here, the slope m represents the rate of change in y per unit change in x.

Step 5: Use the slope m and one of the points to calculate the intercept b using the equation $y = mx + b$. Substituting $m = 1.125$ and using the point $(1, 2.3)$, we solve for b:

$$2.3 = 1.125(1) + b \quad \Rightarrow \quad b = 2.3 - 1.125 = 1.175$$

So, the equation of the best-fitting line is:

$$\boxed{y = 1.125x + 1.175}$$

This equation represents the visually best-fitting line obtained using the graphical method.

Advantages

- Provides a quick, intuitive overview of the relationship between variables.
- Helps identify the general form of the curve (linear, nonlinear, etc.).
- Useful for educational, illustrative, or exploratory purposes.
- Requires minimal tools and no numerical computation.

Disadvantages

- Lacks objectivity and reproducibility; results depend on visual judgment.
- Provides only approximate parameter values.
- Not suitable for large or noisy datasets.
- Cannot quantify error or statistical goodness of fit.

Convergence rate and Accuracy

The graphical method does not involve formal computation of errors or residuals. Accuracy is judged visually and subjectively, making it unsuitable for rigorous quantitative analysis. Nonetheless, it plays a valuable role in:

- Detecting outliers or inconsistencies,
- Guiding the selection of appropriate models,
- Comparing general trends across datasets.

In modern applications, graphical fitting is often used in conjunction with numerical techniques to support intuitive understanding of the data.

6 Algebraic curve fitting: Three-constant laws

Many real-world phenomena exhibit nonlinear relationships that cannot be adequately modeled using linear, exponential, or power functions. In such cases, empirical laws involving three constants are used to describe more complex behaviors.

A general three-constant law takes the form

$$y = f(x; a, b, c)$$

where a, b, and c are unknown parameters determined from observed data. These models often arise in chemistry, biology, physics, and economics. They offer greater flexibility and are particularly effective in capturing saturation, asymptotic behavior, or reciprocal relationships.

Several representative models are commonly employed, depending on the nature of the data and the observed behavior. Among the most widely used are

- Michaelis–Menten (Reciprocal) Model

  $$y = \frac{a}{b + cx}$$

  Widely used in enzyme kinetics, reaction rates, and fluid dynamics, this model captures saturation behavior with a horizontal asymptote at $y = \frac{a}{c}$ as $x \to \infty$.

– Rational Saturation Model

$$y = \frac{a + bx}{1 + cx}$$

Commonly applied in economic demand and ecological growth, this model represents rational growth or decay, with asymptotic behavior determined by the parameters a and b.

– Shifted Logarithmic Model

$$y = a + b\ln(x + c)$$

Commonly used in stress-strain analysis, elasticity, and deformation studies, this model exhibits sublinear growth and is undefined for $x + c \leq 0$.

– Modified Exponential Model

$$y = ae^{bx+c}$$

This model is commonly used in population growth, radioactive decay, and fatigue curve analysis, where it captures exponential behavior-rising when $b > 0$ and decaying when $b < 0$.

Example: Fitting a reciprocal model

Fit the model $y = \frac{a}{b+cx}$ to the following data

x	1	2	3	4	5
y	1.80	1.20	0.90	0.72	0.60

Step 1: Take the reciprocal of y

We start by taking the reciprocal of both sides of the equation $y = \frac{a}{b+cx}$. This leads to

$$\frac{1}{y} = \frac{b + cx}{a} = A + Bx$$

where $A = \frac{b}{a}$ and $B = \frac{c}{a}$.

Step 2: Define $z = \frac{1}{y}$ and construct a new table

We now construct a new table with $z = \frac{1}{y}$ as follows

x	y	$z = \frac{1}{y}$
1	1.80	0.5556
2	1.20	0.8333
3	0.90	1.1111
4	0.72	1.3889
5	0.60	1.6667

Step 3: Fit the equation $z = A + Bx$ using least squares
Now, we fit the equation $z = A + Bx$ using the method of least squares. Solving the normal equations, we obtain

$$A \approx 0.278, \quad B \approx 0.278$$

Step 4: Recover the original parameters
Using the values of A and B, we recover the original parameters a, b, and c as follows:

$$a = \frac{1}{B} \approx 3.60, \quad b = \frac{A}{B} \approx 1.00, \quad c = 1.00$$

Thus, the fitted model is

$$\boxed{y = \frac{3.60}{1 + x}}$$

Step 5: Compute the total squared error
To assess the fit of the model, we compute the total squared error, S, by calculating the difference between the observed values and the predicted values. The total squared error is

$$S = \sum (y_i - \hat{y}_i)^2 \approx 0.0062$$

This value represents the total error in the fit. A smaller value suggests that the model is a good approximation of the data. ■

Algorithm 22 Algebraic curve fitting: Three-Constant laws

Require: A dataset $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, and a chosen model form among three-constant nonlinear laws

Ensure: Estimated parameters a, b, and c for the fitted model

Step 1: Select an appropriate three-constant model form.

Choose a model based on the empirical behavior of the data:

- **Michaelis–Menten (Reciprocal) Model:** $y = \frac{a}{b+cx}$
- **Rational Saturation Model:** $y = \frac{a+bx}{1+cx}$
- **Shifted Logarithmic Model:** $y = a + b\ln(x + c)$
- **Modified Exponential Model:** $y = ae^{bx+c}$

Step 2: Apply mathematical transformation to linearize the model.

Examples of transformation:

- For Michaelis–Menten:

$$y = \frac{a}{b + cx} \Rightarrow \frac{1}{y} = \frac{b + cx}{a} = A + Bx$$

  where $A = \frac{b}{a}$, $B = \frac{c}{a}$
- For logarithmic: $y = a + b\ln(x + c) \Rightarrow \text{linear in } \ln(x + c)$
- For exponential: $\ln y = \ln a + bx + c$

Step 3: Prepare transformed dataset.

Compute the transformed variables (e.g., $1/y$, $\ln y$, etc.) for all $i = 1, \ldots, n$

Construct a table with columns for original and transformed values to support regression

Step 4: Perform linear regression on transformed data.

Use the least squares method to estimate parameters in the linearized form

Solve the resulting normal equations to obtain the transformed parameters (e.g., A, B, etc.)

Step 5: Back-substitute to recover original parameters.

Use relationships from the transformation to compute original model constants:

$$a = \frac{1}{A}, \quad b = a \cdot A, \quad c = a \cdot B \quad \text{(example for Michaelis–Menten)}$$

Step 6 (Optional): Evaluate fit.

for $i = 1$ n **do**

  Compute predicted value $\hat{y}_i$ from the original nonlinear model

  Compute residual $\varepsilon_i = y_i - \hat{y}_i$

end for

Compute total squared error:

$$SSE = \sum_{i=1}^{n} \varepsilon_i^2$$

return Estimated parameters a, b, c; optionally predicted values and error statistics

Advantages

– Models complex nonlinear behavior more accurately than basic functions.

– Flexible and applicable to a wide range of scientific domains.

– Some forms can be transformed into linear models.

– Allows parameterized control of curvature and asymptotes.

Disadvantages

– Often requires nonlinear transformation and resubstitution.

– Interpretation of parameters may be non-intuitive.

– Not always solvable by closed-form; may need iterative refinement.

– Susceptible to overfitting with limited data.

Accuracy and convergence rate

Three-constant models are typically nonlinear and require transformation before fitting. The accuracy of the fit depends heavily on the appropriateness of the model form and the quality of transformation.

The total squared error

$$S = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

serves as a measure of fit accuracy. A lower value of S indicates better conformity to the observed data.

Since most of these models are not solved through iterative refinement (unless using numerical nonlinear regression), the concept of convergence rate applies only when nonlinear solvers (e.g., Newton's method) are used. In such cases, the convergence is typically quadratic, depending on initial guesses and function properties.

For linearized forms solved via least squares, convergence is immediate and exact within the transformed system.

Table 5.1: Comparison of Curve Fitting Models

Model Type	Equation	Linearized Form	Transformation
Linear	$y = ax + b$	$y = ax + b$	None
Quadratic	$y = ax^2 + bx + c$	$y = ax^2 + bx + c$	None
Cubic	$y = ax^3 + bx^2 + cx + d$	$y = ax^3 + bx^2 + cx + d$	None
Exponential	$y = ae^{bx}$	$\ln y = \ln a + bx$	Log on y
Power	$y = ax^b$	$\ln y = \ln a + b \ln x$	Log on both x and y
Logarithmic	$y = a + b \ln x$	$y = a + b \ln x$	Log on x
Shifted Log	$y = a + b \ln(x + c)$	Same form	Log on $x + c$
Michaelis–Menten	$y = \frac{a}{b+cx}$	$\frac{1}{y} = A + Bx$	Reciprocal of y
Rational Saturation	$y = \frac{a+bx}{1+cx}$	Nonlinear	Numeric Fitting
Modified Exponential	$y = ae^{bx+c}$	$\ln y = \ln a + bx + c$	Log on y

7 Tasks

1. Fit a straight line $y = ax + b$ to

x	1	2	3	4
y	2.4	3.5	5.1	6.0

2. Fit a quadratic curve $y = ax^2 + bx + c$ to

x	1	2	3	4
y	3.0	4.8	9.0	15.5

3. Fit an exponential curve $y = ae^{bx}$ to

x	1	2	3	4
y	2.0	5.5	14.8	40.2

4. Fit a logarithmic curve $y = a + b \ln x$ to

x	1	2	3	4
y	2.1	3.0	3.6	4.2

5. Fit a power curve $y = ax^b$ to

x	1	2	3	4
y	1.9	3.8	8.1	16.3

6. Determine which model (linear or exponential) fits better for the data

x	1	2	3	4
y	2.5	6.9	18.3	50.1

7. Fit a straight line to this noisy data and discuss the impact of outliers

x	1	2	3	4	5
y	2.0	2.1	2.2	4.5	5.0

8. Fit a second-degree polynomial to

x	1	2	3	4	5
y	1.0	3.9	9.2	16.8	26.1

9. Fit a logarithmic curve to

x	1	2	3	4	5
y	0.8	2.1	2.7	3.2	3.5

10. Compute and compare the residual sum of squares S for two models (exponential and power) fitted to

x	1	2	3	4
y	3.0	7.5	18.9	45.3

11. Fit a linear model $y = mx + c$ to

x	1	2	3	4	5
y	2	3.5	5	7	9

12. Fit a quadratic model $y = ax^2 + bx + c$ to

x	1	2	3	4	5
y	1	4	9	16	25

13. Fit an exponential model $y = ae^{bx}$ to

x	1	2	3	4	5
y	2	4	8	16	32

14. Fit a power model $y = ax^b$ to

x	1	2	3	4	5
y	2	8	18	32	50

15. Fit a logarithmic model $y = a\ln(bx) + c$ to

x	1	2	3	4	5
y	0.5	1.1	1.6	2.1	2.5

16. Using the method of moments, fit a quadratic polynomial $y = ax^2 + bx + c$ to

x	1	2	3	4
y	2.5	4.1	6.3	8.8

17. Perform multiple linear regression to fit $y = a_1x_1 + a_2x_2 + c$ to

x_1	1	2	3	4	5
x_2	2	4	6	8	10
y	5	10	15	20	25

18. Fit a cubic model $y = ax^3 + bx^2 + cx + d$ to

x	1	2	3	4	5
y	3	8	18	32	50

Part II

Second part