Fitting Mathematical Models to Experimental Data with Excel

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By

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Cambridge
Scholars
Publishing

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This book first published 2026

Cambridge Scholars Publishing

Lady Stephenson Library, Newcastle upon Tyne, NE6 2PA, UK

British Library Cataloguing in Publication Data
A catalogue record for this book is available from the British Library

ISBN: 978-1-0364-6678-7
ISBN (Ebook): 978-1-0364-6679-4

I dedicate this book to my wife Esra and to my kids Su and Ateş.

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PREFACE

I started to write a book in Turkish two years ago which was published in March 2024 and the name of it (exact translation from Turkish) was "Describing experimental data by mathematical models in life sciences and engineering applications". After its publication the popularity of the book both surprised and amazed me and I decided to write a similar but more comprehensive book in English to reach out more readers. This is how this book was written. Although there are similarities between this book and its Turkish counterpart, more Excel functions are introduced (e.g. LINEST and TREND functions) and more topics are covered in this book (e.g. "correlation" and "multiple linear regression" are added). Moreover, two user-friendly Excel tool (R-BioXL and ÖK-BUZ GRoFiT) are introduced.

In many disciplines, different mathematical models are fitted to data and mostly these are done with regression analysis. This book is written to help those who want to learn about models and regression with the use of Microsoft Excel.

The first question comes to the mind is "Why Excel?" Readers are right to ask this question as there are several programs to perform regression analysis and some of them are even freely available. The most important reason for using Excel in this book is the popularity of Excel. We (students, instructors, researchers, etc.) are already familiar with Excel and it is installed in our computers because most of the time it is available at the university or in the company in which we work. Moreover, Excel is always a good starting point to learn regression analysis and then more sophisticated statistical software programs can be used such as R (open-source software used for programming, data analysis and data visualization), SigmaPlot, Minitab or SPSS.

I believe this book would be beneficial for those who are engaged in regression analysis for the first time and for those who want to deepen their existing knowledge on the subject. Not only students and researchers but also instructors could be benefitted from this book as it is also designed as one semester course book. There are 14 chapters in the book and there are 48 examples (solved mostly by Excel) in those chapters. Besides, some chapters have their own appendices in which extra solutions of the same examples with different Excel functions exist. A total of 45 end-of-chapter exercises including their solutions (43 solutions as Excel files through a link and also in the appendix at the end of the book) are available.

All comments, criticism and corrections from the readers are truly welcomed and appreciated (Please email me). Without a doubt, I am fully responsible for all errors and mistakes throughout the book. I thank particularly Hasan Basri Öksüz for his extraordinary help for two Excel tools given in Chapters 9 (R-BioXL) and 13 (ÖK-BUZ GRoFiT). Finally, I would like to thank my wife Esra, my daughter Su and my son Ateş for their patience and understanding to whom I dedicated this book.

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July 2025

CHAPTER 1

INTRODUCTION AND SOME BASICS

1.1. Objective of the book

In many basic disciplines such as chemistry and biology as well as engineering fields such as agricultural engineering, food engineering and biomedical engineering, researchers rely on experimental results. These results are afterwards analyzed by using some statistical techniques, and sometimes it may be necessary to describe the experimental data with a suitable mathematical model and further make predictions. In fact, modern data analysis typically involves fitting mathematical models to data. The aim of this book is simple: to show researchers how to describe their experimental data by using Excel. Of course, achieving this simple aim is not that simple! We will start with the basics and step by step we will learn to model more complex situations.

In this chapter, we discuss some important points about modeling and models. Most of the time, models are fitted and parameters of the model are estimated by regression analysis. Therefore, we focus on regression models in the next section.

1.2. Models and modeling

When we say "a model" we refer to a function which has a physical or biological interpretation i.e., parameter(s) of the model has/have physical or biological meaning. A notable example is the famous *D*-value (decimal reduction time) used in food microbiology which is an interpretable parameter of the first-order kinetics that has been used for many years to describe (linear) inactivation curves. However, almost all functions is often referred to as models in regression analysis. What is a model then? Unfortunately, we do not have a straightforward answer but, simply we can say that models are simplifications of the real world that intend to define a process or a system. In other words, a mathematical model is an equation that approximately describe a biological, chemical or physical process.

Models helps us to define our experimental data by simple mathematical expressions. Consider the experimental data given on x-y graph in Fig.1.1A.

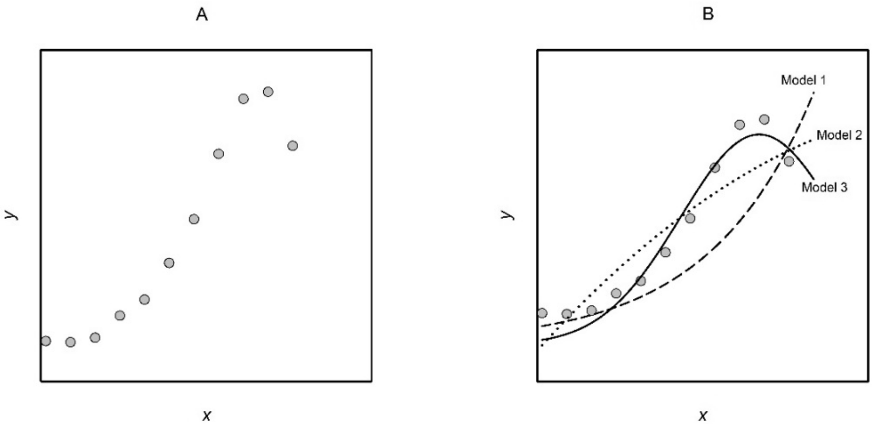

Figure 1.1. Experimental data (gray circles) on the left panel (A) and three models used to describe the data on the right panel (B).

The data are described by three models shown in Fig.1.1B. Without a deep analysis and just by visual examination, it can be said that the best model is Model 3 (continuous line) because it passes closer to the data than Model 1 (dashed line) and Model 2 (dotted line). In fact, one can find even better model than Model 1 but our aim in modeling is not to find a model that passes from all the data points (perfect model) since the models are just approximations. A perfect model may include too many parameters and variables to be useful. Modeling is a word used for many activities and uses; however, in this book, we use the term “modeling” for the development and use of mathematical equations to describe experimental data.

1.3. Independent and dependent variables

Suppose that we design an experiment to monitor the growth of a spoilage bacterium in milk. The organism is inoculated at a level of 10^2 colony forming unit (CFU) per mL and we take samples from the milk every two hours at a constant temperature, say, 25 °C. After taking samples, we try to measure the number of cells with appropriate techniques. It is possible for us to take samples every three or four hours; however, our experimental design requires taking sample at every two hours.

Independent variable is the one that is controlled by the experimenter (in a laboratory experiment it is easy to control a variable) and dependent variable is the one measured by the experimenter. So, for the example above, time is the independent variable (also called explanatory variable) whereas number of spoilage organism is the dependent variable (also called response variable). Let us clarify what do we mean by control. As said above, we could take samples to measure every three hours or every four hours because we control the time and our choice is to take samples every two hours. In general, time is independent variable (especially in kinetic modeling); however, pH, concentration and temperature can be the independent variables as well.

In our example, number of spoilage bacteria at 25 °C depends on time (That's why it is called dependent variable) i.e., it is a function of time. In mathematics, we express it as $y = f(x)$ where x and y are the independent and dependent variables, respectively. The mathematical relation between x and y will be determined by regression analysis in the following chapters.

1.4. Linearity of the models

Consider a simple model in the form of:

$$y = ax + b \tag{1.1}$$

where y is the dependent variable, x is the independent variable, a and b are the model parameters. If the partial derivative with respect to parameters is calculated, we would get:

$$\frac{\partial y}{\partial a} = x, \frac{\partial y}{\partial b} = 1 \tag{1.2}$$

Since the model parameters do not appear in the partial derivatives, the model is considered as a linear model and that is why linear regression is used to obtain the (linear) parameters. Moreover, this model is also linear in independent variable x and hence, a straight line will be observed on an x-y graph.

Now let us consider another model:

$$y = \frac{x}{A} + b \tag{1.3}$$

Partial derivative with respect to parameters will be:

$$\frac{\partial y}{\partial A} = -\frac{1}{A^2}, \frac{\partial y}{\partial b} = 1 \tag{1.4}$$

The model is nonlinear because one of the parameters exists in the partial derivatives and nonlinear regression is required to obtain the parameters. Nevertheless, the model is linear in x and again a straight line would be observed. Models given in Eq.(1.1) and Eq.(1.3) are sketched and shown in Fig.1.2 with all parameter values are set to 1.

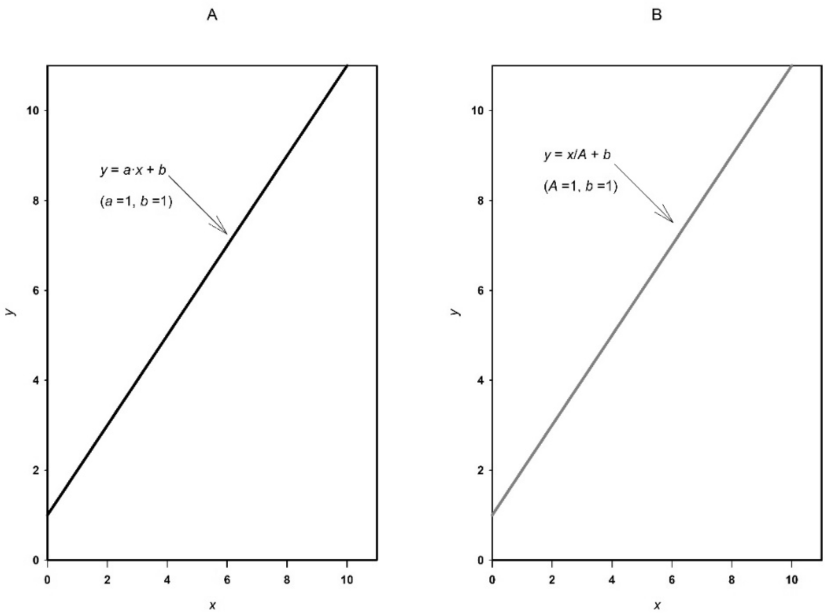

Figure 1.2. The model $y = ax + b$ with $a = 1$ and $b = 1$ which is linear with respect to its parameters and independent variable x (A). The model $y = x/A + b$ with $A = 1$ and $b = 1$ which is nonlinear with respect to its parameter A but linear in x (B).

Although both models appear as straight lines (because they are both linear in x), linear regression should be used to obtain the parameter values for the one on the left panel (black straight line) and nonlinear regression should be used to obtain the parameter values for the one on the right panel (gray straight line). So, when we say linear models we mean linearity of parameters not the linearity of the independent variable.

Consider the following model:

$$y = ax^2 + bx + c \tag{1.5}$$

This model is a linear model because the parameters are linear; however, a curve will appear when it is sketched due to the nonlinearity in x (due to x^2 term in the equation). Now consider:

$$y = Ax + \frac{B}{x} + C \tag{1.6}$$

This model, too, is a linear model and it also appears as a curve due to $1/x$ term. For both models, linear regression (curvilinear regression) can be safely used to obtain parameter values. These models are illustrated in Fig.1.3.

As can be seen, both models appear as curves when fitted but, parameters of both models can be obtained by linear regression. Such regression is called curvilinear regression. From this definition, we can say that all polynomial functions can be fitted by using curvilinear regression.

Next two examples are for nonlinear regression. First one is the exponential (decaying) model:

$$y = ae^{-bx} \tag{1.7}$$

The second one is the hyperbolic model:

$$y = \frac{ax}{b + x} \tag{1.8}$$

Both models are nonlinear in parameters and they are shown in Fig.1.4. To obtain the parameter values of these models, nonlinear regression is required. A timely question here can be “What is the difference between linear and nonlinear regression?” We will see both linear regression and nonlinear regression in the following chapters but suffice to say that linear regression is simple and there is an analytical solution. Moreover, standard errors and confidence intervals of the parameters are symmetric around the best-fit parameter (parameter estimate). On the other hand, nonlinear regression requires iterative solution and initial parameter estimates are needed to start the iteration. Moreover, confidence intervals are not symmetric unlike linear regression.

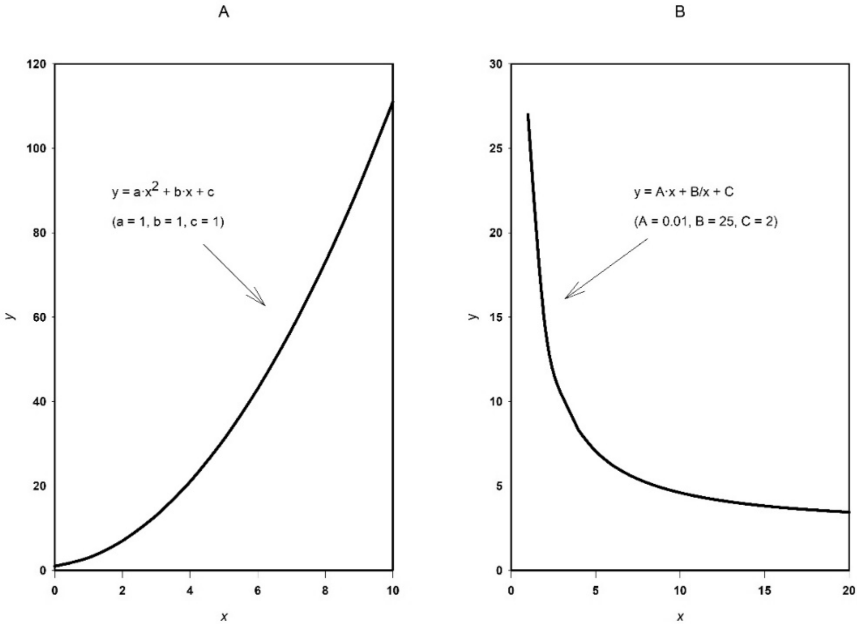

Figure 1.3. Two different linear models. Note that models are nonlinear in x and therefore, they appear as curves not as straight lines. Nevertheless, linear regression (curvilinear regression) can be applied for these linear models: $y = ax^2 + bx + c$ (A), $y = Ax + B/x + C$ (B).

In the past, nonlinear models were generally linearized by transforming whether the data or the parameters. For example, instead of using Eq.(1.3) which is a nonlinear model, the model is converted to $y = A'x + b$ and then after the (simple) linear regression analysis, parameters A' and b can be found. Since in the original model [Eq.(1.3)] we have A not A', A is calculated by using $A'(A = 1/A')$. This method, as we shall see, is no longer valid and application of nonlinear regression is not a big deal in today's world since there are many software programs to be able to perform the analysis.

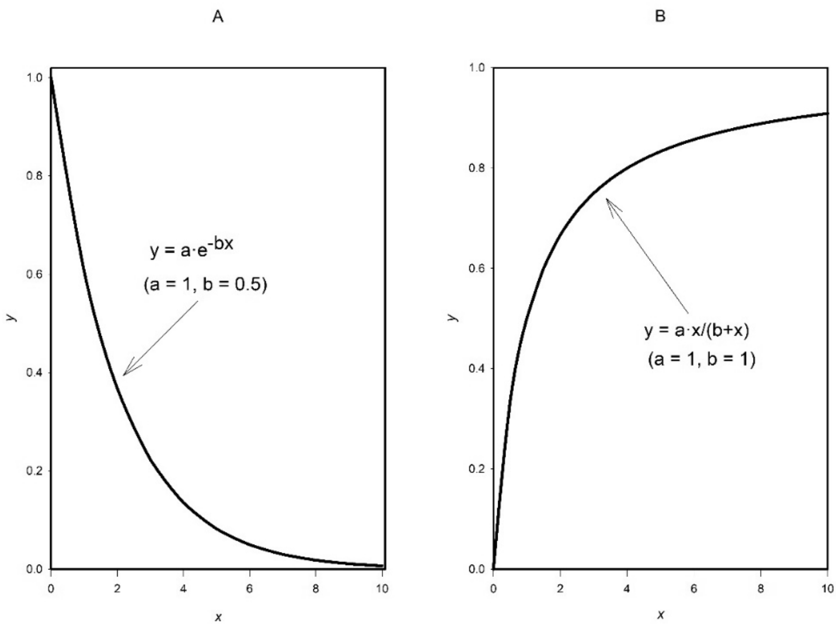

Figure 1.4. Two different nonlinear models. Nonlinear regression should be applied for these nonlinear models: $y = ae^{-bx}$ (A), $y = ax/(b+x)$ (B).

In a similar way, a linear model can be transformed into a nonlinear model by reparametrization. For example, $y = ax + b$ [Eq.(1.1)] can be rearranged into $y = a(x + c)$ with $c = b/a$. Although the mathematical interpretation does not change, regression model is significantly different: Eq.(1.1) is linear in parameters whereas the reparametrized model is a nonlinear model since the partial derivatives with respect to the parameters include parameters indicating that parameters should be estimated iteratively.

1.5. Some key points to remember

- Models represent simplified perspectives of reality.
- Experimenter can control and measure the variables during an (laboratory) experiment.

- The controlled one is the independent variable (e.g., time) while the measured one is the dependent variable (e.g., vitamin concentration).
- "Linear" term in linear regression refers to parameters [not the independent variable (x) in the model].
- Even if there is "x^2" or "$1/x$" term in a model, the model can still be linear.

Exercises

1.1. a) What is a model?
b) What is (are) the independent variable(s)?
c) What is (are) the dependent variable(s)?

1.2. For the models shown below, x is the independent and y is the dependent variable, the rest are the parameters of the models. For which models can linear regression be applied?

a) $y = a \sin x + b$

b) $y = \frac{a}{x} + \frac{b}{x^2} + c$

c) $y = \frac{x}{a} + \frac{x^2}{b} + \frac{1}{c}$

d) $y = ae^{-x} + b \ln x$

e) $y = \frac{bx + c}{a}$

f) $y = a(x - c)$

g) $y = a + bx + cx^2$

h) $y = a\sqrt{x} + \frac{b}{x} + c \log_{10} x + d$

i) $y = ax + \frac{x^2}{b} + \frac{c}{\sqrt{x}} + \log_{10}(dx)$

j) $y = a(x - c)^2$

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CHAPTER 2

CORRELATION & SIMPLE LINEAR REGRESSION

2.1. Correlation coefficient

Correlation coefficient is dimensionless (unitless) number and it is a measure of strength of linear relationship between two variables, namely independent (x) and dependent (y) variables. There are different correlation coefficients but we will use "*Pearson's correlation coefficient*" in this book and we shortly call it correlation coefficient (r). A correlation is a number between –1 and +1 which means it can be either positive or negative. Positive correlation means as x increases y also increases while negative correlation means as x increases y decreases.

If correlation is close to –1 then we say the relationship (between x and y) is negative and strong. If correlation is close to +1 then we say the relationship is positive and strong. There can be (positive or negative) moderate correlation between the variables ($r \approx +0.5$ or $r \approx -0.5$) or there can be zero correlation indicating that there is no relationship between x and y.

The formula for r is given below:

$$r = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2 \sum_{i=1}^{n}(y_i - \bar{y})^2}} \tag{2.1}$$

where n is the sample size (number of data or observations) $\bar{x}$ and $\bar{y}$ are the mean values of independent and dependent variables, respectively. Although the formula seems complicated, there is no reason to memorize it because Excel will do the calculation for us. In Excel, "=CORREL(array1; array2)" calculates Pearson's correlation coefficient where array1 is x and array2 is y (One can enter y into array1 and x into array2, it will not affect the outcome in correlation calculation). Alternatively, "PEARSON" function can be used instead of CORREL in Excel.

Example 2.1. For *x*-*y* data given below, calculate correlation coefficient (i) by using Eq.(2.1), (ii) by using Excel function.

x	1	2	3	4	5
y	1.5	3	5	7.5	9

Solution 2.1. Before the calculation, it is always good to sketch the data (scatter plot) because it will give us an idea about the correlation and direction (whether positive or negative) of it. In Fig.2.1, *x*-*y* graph is shown and as we can see from this sketch there is positive and strong correlation between *x* and *y*. So, without any calculation we can say that *r* is close to +1!

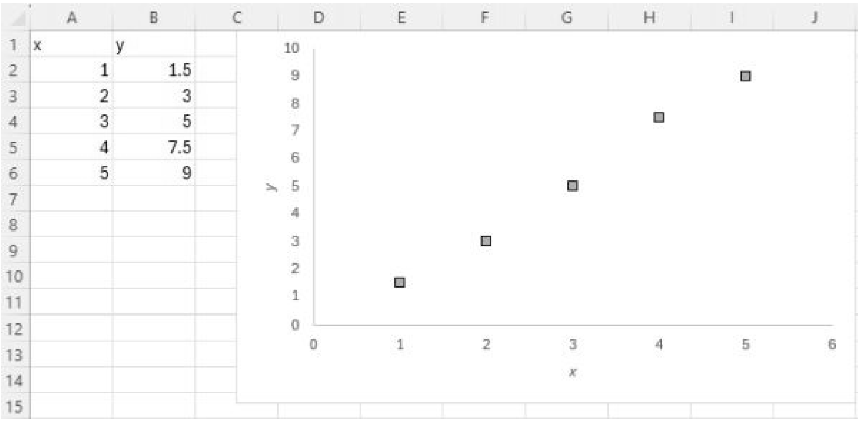

Figure 2.1. Plot of the data given in Example 2.1

Now, let's calculate *r* by using Eq.(1) in Excel. The results of those calculations are shown in Fig.2.2.

The formulas of the calculations are given in Fig.2.3.

	A	B	C	D	E	F	G	H	I
1	x	y	(x-x̄)	(y-ȳ)	(x-x̄)·(y-ȳ)	(x-x̄)^2	(y-ȳ)^2		
2	1	1.5	-2	-3.7	7.4	4	13.69		
3	2	3	-1	-2.2	2.2	1	4.84		
4	3	5	0	-0.2	0	0	0.04		
5	4	7.5	1	2.3	2.3	1	5.29		
6	5	9	2	3.8	7.6	4	14.44		
7						10	38.3	19.5704	sqrt[Σ(x-x̄)^2·Σ(y-ȳ)^2]
8									
9				Σ(x-x̄)·(y-ȳ)	19.5				
10							r	0.9964	
11	x̄	ȳ					r	0.9964	
12	3	5.2							

Figure 2.2. Calculations for correlation coefficient (*r*)

	A	B	C	D	E	F	G	H	I
1	x	y	$(x-\bar{x})$	$(y-\bar{y})$	$(x-\bar{x})\cdot(y-\bar{y})$	$(x-\bar{x})^2$	$(y-\bar{y})^2$		
2	1	1.5	=A2-A12	=B2-B12	=C2*D2	=C2^2	=D2^2		
3	2	3	=A3-A12	=B3-B12	=C3*D3	=C3^2	=D3^2		
4	3	5	=A4-A12	=B4-B12	=C4*D4	=C4^2	=D4^2		
5	4	7.5	=A5-A12	=B5-B12	=C5*D5	=C5^2	=D5^2		
6	5	9	=A6-A12	=B6-B12	=C6*D6	=C6^2	=D6^2		
7						=SUM(F2:F6)	=SUM(G2:G6)	=SQRT(F7*G7)	sqrt[$\Sigma(x-x)^2\cdot\Sigma(y-y)^2$]
8									
9				$\Sigma(x-\bar{x})\cdot(y-\bar{y})$	=SUM(E2:E6)				
10							r	=E9/H7	
11	$\bar{x}$	$\bar{y}$					r	=CORREL(A2:A6;B2:B6)	
12	=AVERAGE(A2:A6)	=AVERAGE(B2:B6)							

Figure 2.3. Formulas for the calculations shown in Fig.2.2.

Note that, r value is obtained as 0.9964 by using whether Eq.(2.1) or Excel function “CORREL”. We stated that r should be positive and close to +1 before starting the calculation and our calculation proves this statement. Also note that, we used the sign “$” to fix the cells (Fig.2.3) otherwise, cells will be shifted as we glide the calculation. Alternatively, users can write the average (mean) values by hand instead of using $ sign.

This example also shows that we do not need to memorize the formula of correlation coefficient as said above because Excel has a function to do that. However, it is always good to know and understand the logic of such numbers. Another remark which was also mentioned above, is that while using the CORREL function of Excel, you may first enter array for x and then for y or vice versa. You will end up with the same result.

Before closing this section, we will give some examples where there is both positive and negative strong, moderate and weak correlations between x and y. In Fig.2.4, six different data sets (x-y pairs) are shown. Positive strong (r = +1, i.e., perfect positive correlation is not likely possible to observe in many disciplines such as biology and biotechnology; however, r can be as high as, say 0.9987), positive moderate (r = +0.6) and positive weak (r = +0.1) correlations as well as negative strong (r = –1, again not likely possible to see in many disciplines), negative moderate (r = –0.6) and negative weak (r = –0.1) correlations are given together with the scatter plots (Fig.2.4).

2.2. Simple (ordinary) linear regression

The word “simple” in the title indicates that there is only one independent variable (x) in our equation. We saw this equation in Chapter 1 but let’s recall it here once more:

$$y = mx + c \tag{2.2}$$

where y is the dependent variable, x is the independent variable, m and c are the model parameters. Since the model is linear in parameters we can use linear regression and furthermore model is also linear in x so, it is not surprising to observe a straight line not a curved line on a graph. In other words, variables x and y are linearly related. In the previous section, we have seen that correlation coefficient tells us about the linear relationship between x and y; however, it does not say anything about the mathematical relationship between the variables. We will use simple linear regression for this purpose. In most statistical books, linear regression is used instead of simple linear regression; however, we will continue to use the term simple linear regression throughout this book.

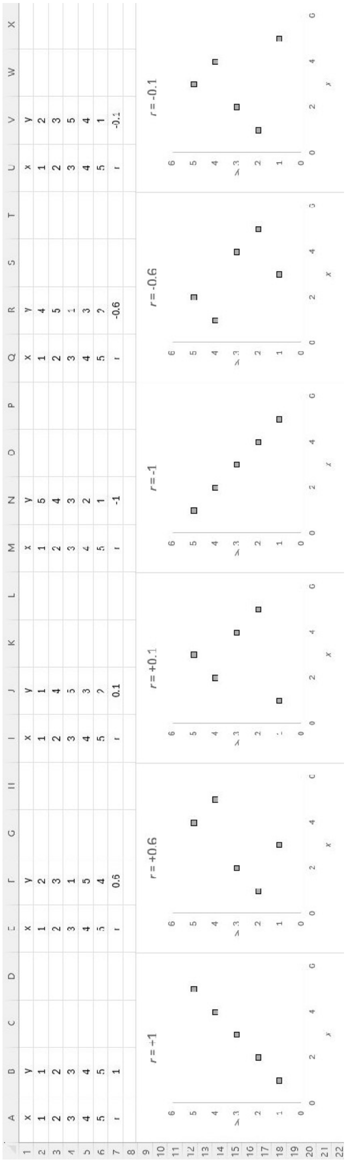

Figure 2.4. Examples of positive strong, positive moderate and positive weak correlations, and negative strong, negative moderate and negative weak correlations

Let us try to understand our model better. If $x = 0$ then $y = c$ and parameter c is known as intercept. In some books it is called y intercept to specify that it is the y value of the line when $x = 0$. (Similarly, x intercept is the value when $y = 0$, but throughout the book when we say intercept it is y intercept.) The intercept has the same unit as y. If $x \to \infty$ then $y \to \infty$ (if $m > 0$) or $y \to -\infty$ (if $m < 0$). Parameter m is known as slope. Simple linear regression fits "best line" through a sketch of data points (straight line that comes closest to the data points) to obtain the intercept and the slope. The objective may be to learn how y depends on x or to predict y from x. In Fig.2.5, two straight lines, one with a positive slope and the other with a negative slope are shown.

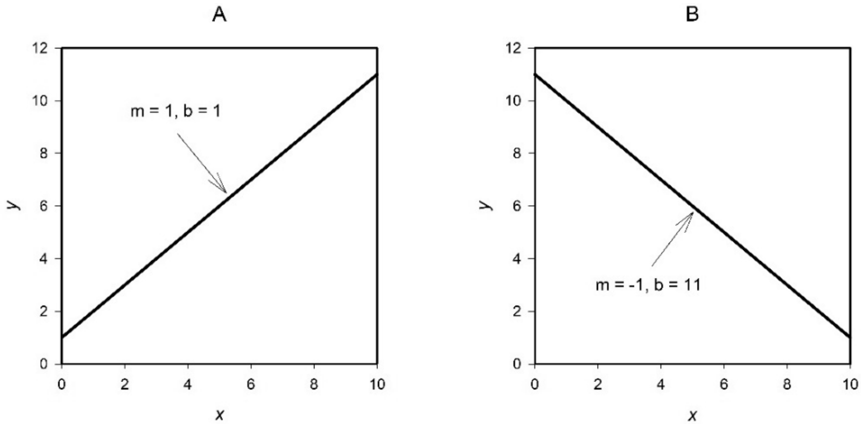

Figure 2.5. Examples of straight lines with a positive slope (A) and a negative slope (B)

The slope is the steepness of the line and it is equal to change in y for each unit change in x i.e., $\Delta y/\Delta x$. It is positive if y increases as x increases (Fig.2.5A) and negative if y decreases as x increases (Fig.2.5B). The unit of the slope is the unit of y divided by the unit of x. Best way to learn simple linear regression is to apply it! Here is an example.

Example 2.2. Heights of soybean plants (cm) versus time (week) is given below. Apply simple linear regression, obtain parameter values and their uncertainties as well as goodness-of-fit statistics.

time (week)	1	2	3	4	5	6	7
height (cm)	5	13	16	23	33	38	40

Solution 2.2. Dependent variable (y) is the height and independent variable (x) is the time. Let us label these and plot x-y graph (Fig.2.6)

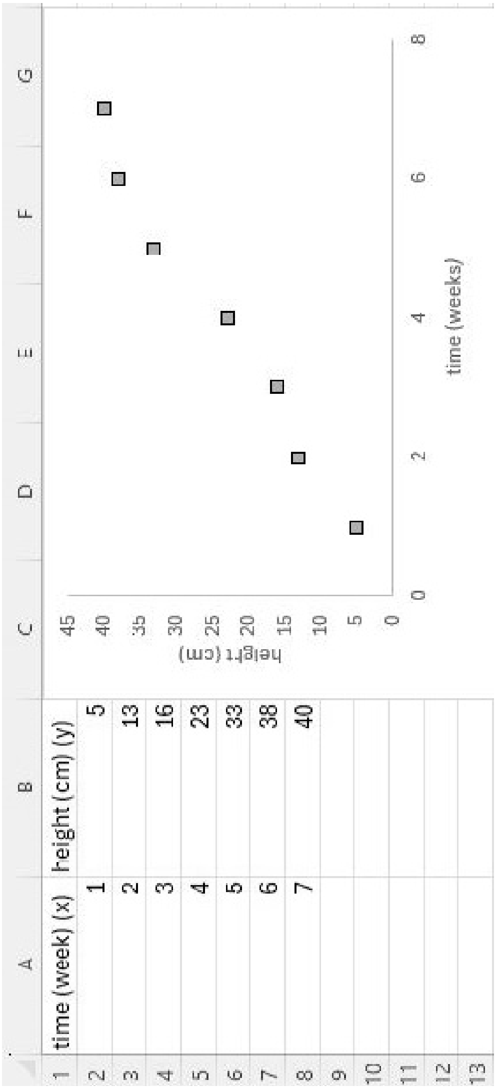

Figure 2.6. Labeling the titles as x and y, and sketching the graph

Labeling the titles as x and y is important because, as we shall see, unlike correlation in regression, it is important to enter x as the independent variable and y as the dependent variable. Remember that in CORREL function it is unimportant whether the user enter x as array 1 or array 2. In either case, the same r will be found.

After plotting the graph, right-click on any of the data points (gray squares) and select "Add Trendline". This is shown in Fig.2.7.

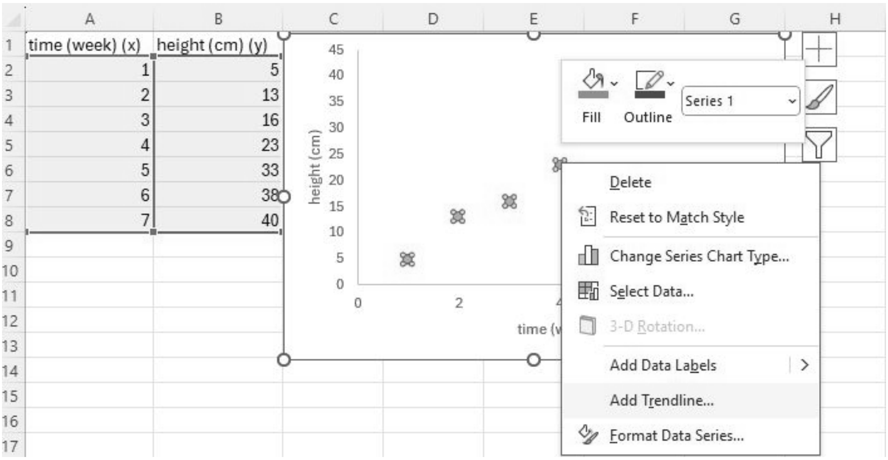

Figure 2.7. Menu appeared after right-clicking the data

When "Add Trendline" (Trendline option) is selected, a menu on the right-hand side of Excel screen will be appeared. Linear model [Eq.(2.2)] is selected by default and user may select "Display Equation on chart" and "Display R-squared value on chart" on the bottom of the menu (Fig.2.8).

Most Excel users will be satisfied by these results because we find $y = 6.1429x - 0.5714$ and $R^2 = 0.9783$. (R^2 is known as coefficient of determination.) Unfortunately, these results are not enough and the question asks about not only the parameter values but their uncertainties (standard error or confidence intervals of the parameters) as well. Uncertainties are as important as the parameters themselves. Parameters should be precise and uncertainties are the ways to express the precision of parameter estimates. Many researchers rely on R^2 for the goodness-of-fit of a model (if it is close to 1 then the model fit is good); however, this may not be always true. Other indices should also be calculated.

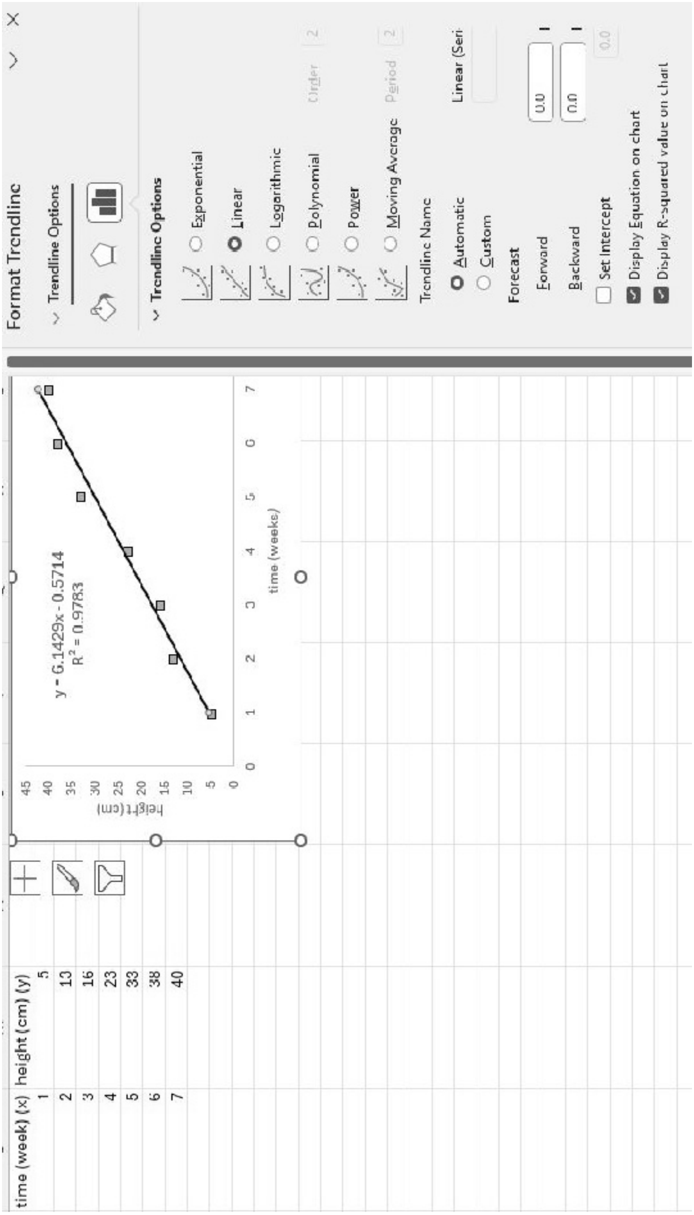

Figure 2.8. Fitting a straight line to the data

Let us summarize our results up to now (Fig.2.8): $m = 6.1429$ (slope) and $c = -0.5714$ (intercept), and visually our model (black straight line) is close to the data (gray squares). We may predict height of the soybean plants when $x = 3.5$ weeks or 5.2 weeks for example just by placing these values into the equation (in place of x) we obtained. They are 20.9 cm and 31.4 cm, respectively. This is interpolation since 3.5 weeks or 5.2 weeks are within our x values. However, it is also possible to predict the height at week 8, which is out of our x range and that is 48.6 cm. This is called extrapolation, and extrapolation should be used with caution and sometimes it should be avoided. In extrapolation, we assume that line goes beyond x values where we developed our model and this may not be true or there is no reason for us to think that linear relationship continues beyond the range of data. Interpolation or extrapolation can also be calculated by "FORECAST.LINEAR" function (Appendix 2.1) or "TREND" function (Appendix 2.2) of Excel.

We may also want to predict the time (x) when height (y) is 30 cm then 30 cm should be placed in our equation (in place of y) and time should be calculated. According to our data (see data in Example 2.2) 30 cm is in between weeks 4 and 5, and our model predicts it as 4.98 weeks.

It is also possible to calculate the slope, the intercept and R^2 by using Excel functions "SLOPE", "INTERCEPT" and "RSQ", respectively. For each function, user should enter "(known ys; known xs)" that is; y should be entered first and x should be entered afterwards for those functions otherwise wrong results will be found. That is one of the reasons for labeling the titles as x and y. These calculations are shown in Fig.2.9. "LINEST" function of Excel can also be used to calculate the slope (m) and intercept (c) together in one step – see Appendix 2.3.

In order to find uncertainties of the slope (m) and intercept (c) we can use "Regression" application (macro) in "Data Analysis" tool (Analysis Toolpak) known as Regression routine. Users may follow the path Data > Data Analysis > Regression and then a menu will appear (Fig.2.10).

The tool asks for y (dependent variable) and x (independent variable). We can enter those from our data which has already been labelled so that we will not make any mistake such as selecting x instead of y or vice versa (Fig.2.11)