UMAP

Modules in Undergraduate Mathematics and its Applications

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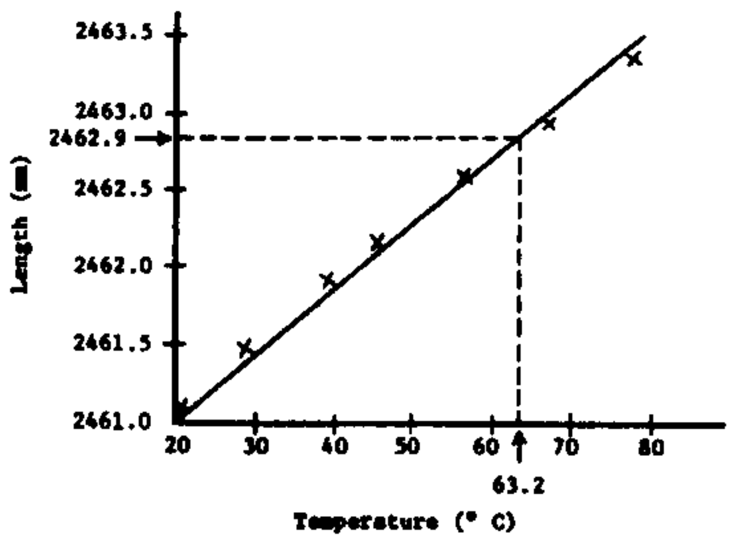
Module 321

Curve Fitting via the Criterion of Least Squares

John W. Alexander, Jr.



Applications of Algebra and Elementary Calculus to Curve Fitting

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Intermodular Description Sheet: *UMAP Unit 321*

Title: CURVE FITTING VIA THE CRITERION OF LEAST SQUARES

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Review Stage/Date: III 9/3/79

Classification: APPL ALG & ELEM CALC/CURVE FITTING

Suggested Support Materials: A computer terminal on line to a system with BASIC compiler (to be used for the appendix).

Prerequisite Skills:

1. Be able to do partial differentiation.
2. Be able to maximize functions.
3. Know how to solve simultaneous equations by elimination or substitution for 2 x 2 cases.
4. Know how to graph elementary, exponential, and logarithmic functions.

Output Skills:

1. Be able to construct scatter diagrams.
2. Be able to choose an appropriate function to fit specific data.
3. To understand the underlying theory of the method of least squares.
4. To be able to use a computer program to do desired curve-fitting.
5. Be able to use augmented matrix approach to solve simultaneous equations.

CURVE FITTING VIA THE CRITERION OF LEAST SQUARES

by

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Modules and Monographs in Undergraduate Mathematics and Its Applications (UMAP) Project

The goal of UMAP was to develop, through a community of users and developers, a system of instructional modules in undergraduate mathematics and its applications to be used to supplement existing courses and from which complete courses may eventually be built.

The Project was guided by a National Advisory Board of mathematicians, scientists, and educators. UMAP was funded by a grant from the National Science Foundation and is now supported by the Consortium for Mathematics and Its Applications (COMAP), Inc., a non-profit corporation engaged in research and development in mathematics education.

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CURVE FITTING VIA THE CRITERION OF LEAST SQUARES

1. INTRODUCTION

In many instances, we wish to be able to predict the outcome of certain phenomena. For example, we may want to know which students in a graduating high-school class will do well in their first year of college.

One way to get a measure or at least an indication would be to observe the high-school grades in English of 20 or so students who have gone to college. If we match the students' English grades with their grade point average after one semester, we would be able to see if good grades in English matched with high grade point averages.

If the "correlation" is high, then, we might wish to assert that students who do well in high-school English do well in college. There may be exceptions of course. We may want to look at other indicators (e.g., math grades) but, the point is, we wish to look at two or more statistics on the same individual, and we are interested to know how these statistics relate.

Ideas of the sort alluded to above are the subject of this module.

2. SCATTER DIAGRAMS

Many statistical problems are concerned with more than a single characteristic of an individual. For instance, the weight and height of a number of people could be recorded so that an examination of the relationship between the two measurements could be made. As a further example, consider how the length of a copper rod relates to its temperature.

TABLE 1

Temperature (° C)	Length (mm)
x	y
20.1	2461.16
28.2	2461.49
38.5	2461.88
44.6	2462.10
57.4	2462.62
66.2	2462.93
78.1	2463.38

When we draw a scatter diagram letting the horizontal axis be the scale for the temperature and the vertical axis the scale for the length, we note that the plotted points lie very close to a straight line. It is, therefore, reasonable to make a quick and accurate estimate of the length of the rod for any temperature between 20.1° and

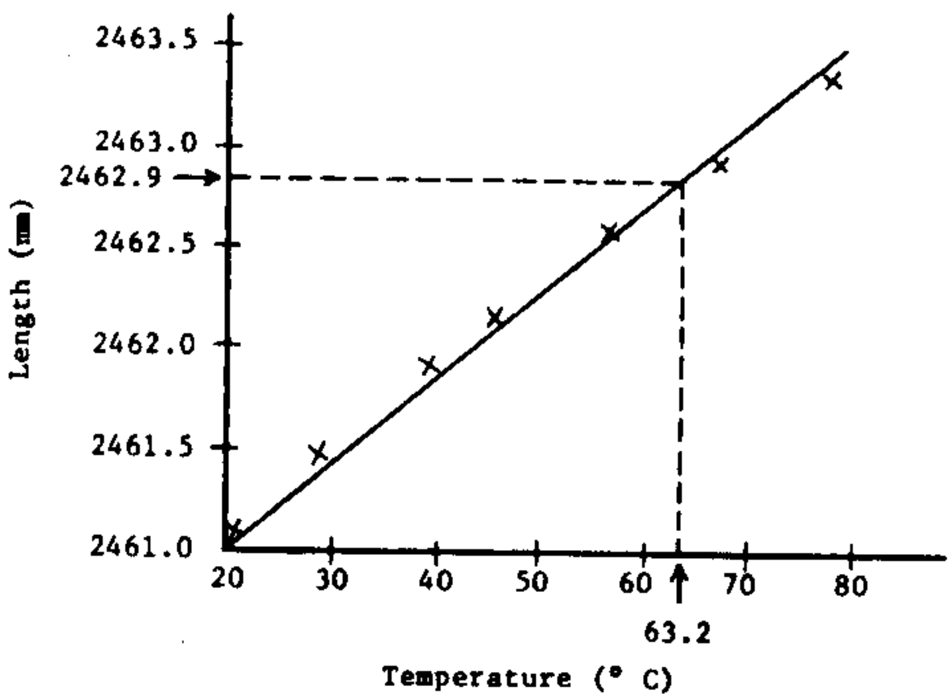

Figure 1.

78.1°.* For example, if the temperature was 63.2° the dotted lines in Figure 1 indicate that the corresponding point on the line gives a length of approximately 2462.9 mm.

Let us explore another example that gives us a scatter diagram where the points are more scattered. Table 2 gives us the weight in grams, x, and the length of the right hind foot in millimeters, y, of a sample of 14 adult field mice.

TABLE 2

Weight (g) x	Length (mm) y
22.3	23.0
16.0	22.6
18.8	23.2
18.2	22.5
16.0	22.2
20.4	23.3
17.9	22.8
19.4	22.4
16.9	21.8
17.6	22.4
16.5	22.4
18.8	21.5
17.2	21.9
20.4	23.3

The point in Figure 2 that is circled indicates where two points of the data coincide. The points here are much more scattered than those of the previous set. It would be extremely difficult to determine which straight line best fits this set of points. In fact, if a number of people were to attempt to fit a line to these points, there is little doubt that each person would come up with a different line. What we need is a mathematical method for determining the line that comes "closest" to all of the points.

*We are not in a position to speculate about values outside of this range.

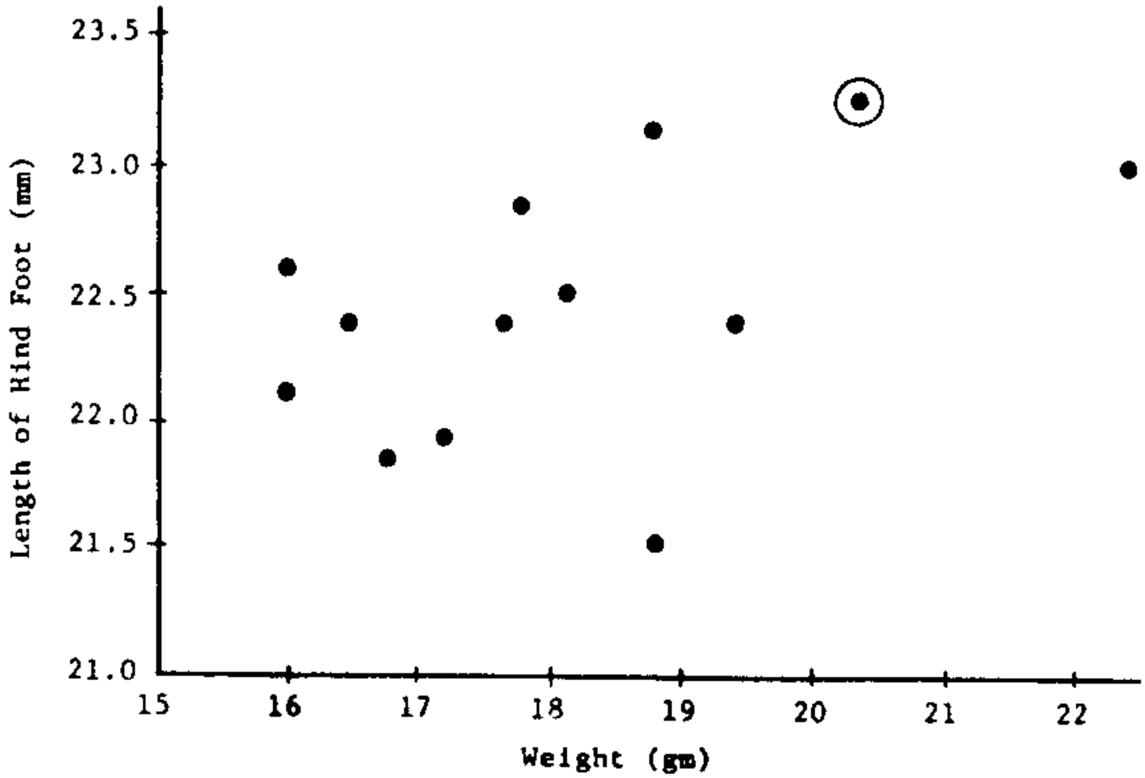

Figure 2.

3. THE LINE OF REGRESSION

The criterion traditionally used to define a "best" fit dates back to the nineteenth century French mathematician Adrien Legendre. It is called the *criterion*, or *method, of least squares*. This criterion requires the line of regression which we fit to our data to minimize *the sum of the squares of the vertical deviations (distances) from the points to the line.* In other words, the method requires the sum of the squares of the distances represented by the solid line segments of Figure 3 to be as small as possible.

From the figure, we see that the actual grade received for a student who studied 11 hours was 79. Reading from the line of regression we predict a grade of about 71.

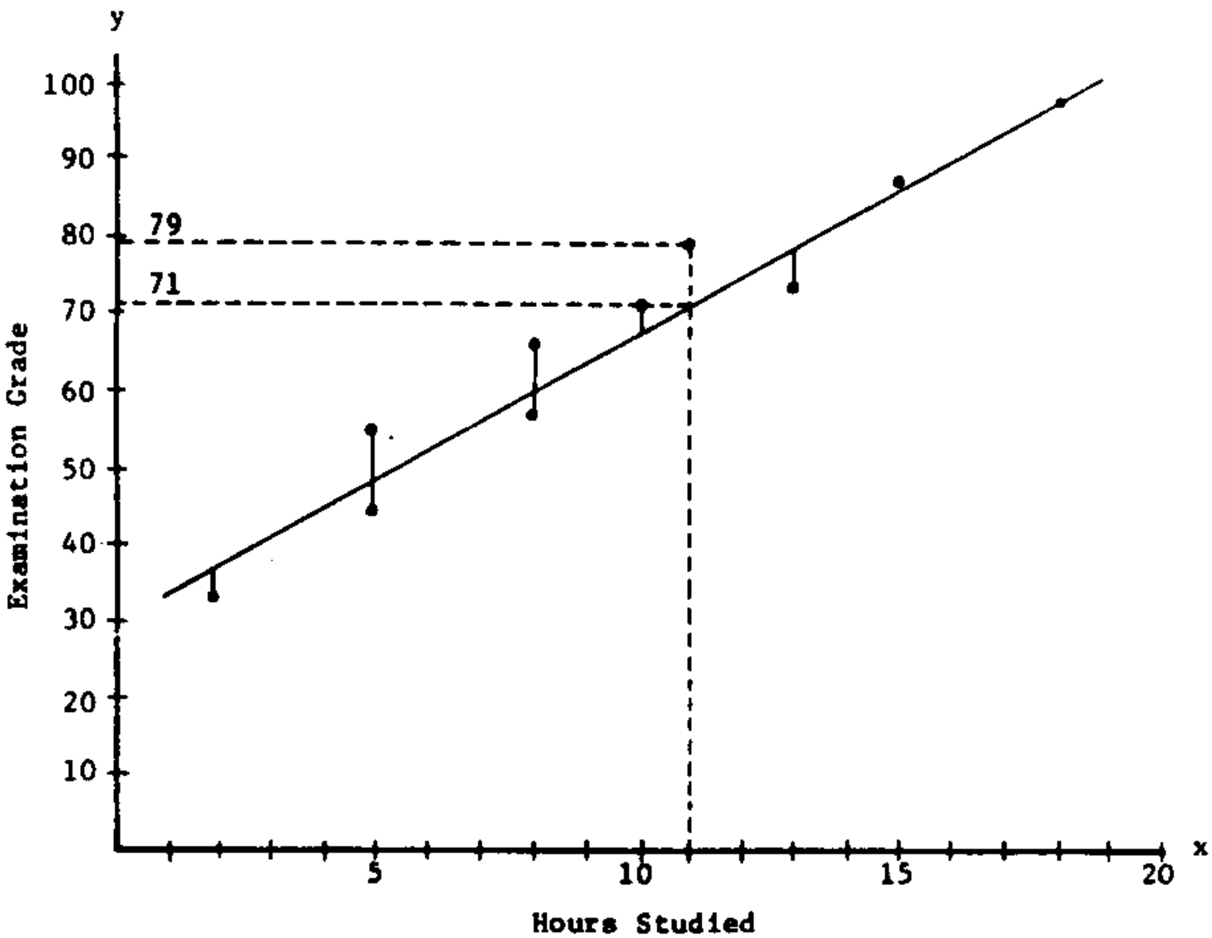

Figure 3. Line of regression fitted to data on hours studied and examination grades.

Observe that any line can be expressed:

(1) $$y = bx + c$$

or

(2) $$x = b'y + c',$$

where the b's represent the slope of the line and the c's are interpreted as the intercept of the axis.

If we consider Equation (1), knowing the values of b and c will allow us to compare the actual values in the y column with $bx + c$. We take the difference in each case and square the result. Consider the values of x and y in Table 3.

TABLE 3

x	y	bx + c	[Difference]^2
25	30	b25 + c	$[30 - (25b + c)]^2$
30	46	b30 + c	$[46 - (30b + c)]^2$
50	51	b50 + c	$[51 - (50b + c)]^2$
20	28	b20 + c	$[28 - (20b + c)]^2$
70	48	b70 + c	$[48 - (70b + c)]^2$
80	88	b80 + c	$[88 - (80b + c)]^2$
91	75	b91 + c	$[75 - (91b + c)]^2$
46	52	b46 + c	$[52 - (46b + c)]^2$
35	35	b35 + c	$[35 - (35b + c)]^2$
25	28	b25 + c	$[28 - (25b + c)]^2$
80	95	b80 + c	$[95 - (80b + c)]^2$

We add up all of these squared differences. It must then be determined what values of b and c must be used in order to have a line such that the sum of the vertical distances from the line to the data points is at a minimum.

<u>The Problem</u>: Find the values of b and c such that the sum indicated below is a minimum.

$$\sum D^2 = (30-25b-c)^2 + (46-30b-c)^2 + (51-50b-c)^2 + (28-20b-c)^2$$
$$+ (48-70b-c)^2 + (88-80b-c)^2 + (75-91b-c)^2 + (52-46b-c)$$
$$+ (35-35b-c)^2 + (28-25b-c)^2 + (95-80b-c)^2.$$

The symbol sigma can be employed on both sides of the equation above (i.e., $\Sigma D^2 = \sum_{i=1}^{n}(y_i - bx_i - c)^2$). Since $\sum D^2$ is a function of b and c we can write

$$\sum D^2 = f(b,c) = \sum_{i=1}^{n}(y_i - bx_i - c).$$

To find our desired minimum we find the partial derivatives with respect to b and c and set the results equal to zero. We obtain two equations in two unknowns which we solve simultaneously. This gives us the desired values of b and c and thus our line of best fit (the line of regression).

Trace through the actual development given below.

$$f(b,c) = \sum_{i=1}^{n}(y_i - bx_i - c)^2$$

$$\frac{\partial f}{\partial b} = \sum_{i=1}^{n} 2(y_i - bx_i - c)(-x_i) = 0$$

$$= \sum_{i=1}^{n}(-2y_i x_i + 2bx_i^2 + 2cx_i) = 0,$$

finally,

$$\sum_{i=1}^{n} bx_i^2 + \sum_{i=1}^{n} cx_i = \sum_{i=1}^{n} x_i y_i .$$

To continue with the other derivatives:

$$\frac{\partial f}{\partial c} = \sum_{i=1}^{n} 2(y_i - bx_i - c)(-1) = 0$$

$$= 2\sum_{i=1}^{n}(-y_i + bx_i + c) = 0$$

and

$$\sum_{i=1}^{n} bx_i + \sum_{i=1}^{n} c = \sum_{i=1}^{n} y_i .$$

Thus our two equations which are traditionally called *normal equations* are:

(3) $$b\sum_{i=1}^{n} x_i^2 + c\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} x_i y_i .$$

(4) $$b\sum_{i=1}^{n} x_i + nc = \sum_{i=1}^{n} y_i .$$

In order to solve these equations, we must calculate the indicated sums as is done in Table 4. We have also included the table of y_i^2's because we can use the sum $\sum_{i=1}^{n} y_i^2$ to find the line of regression $x = b'y + c'$.

The normal equations for this line are obtained merely by interchanging x and y in the original two equations (3) and (4).

TABLE 4

x	y	x^2	y^2	xy
25	30	625	900	750
30	46	900	2116	1380
50	51	2500	2601	2550
20	28	400	784	560
70	48	4900	2304	3360
80	88	6400	7744	7040
91	75	8281	5625	6825
46	52	2116	2704	2392
35	35	1225	1225	1225
25	28	625	784	700
80	95	6400	9025	7600
552	576	34372	35812	34382

As an example, for x = b'y + c' we have:

(3') $$b'\sum_{i=1}^{n} y_i^2 + c'\sum_{i=1}^{n} y_i = \sum_{i=1}^{n} y_i x_i.$$

(4') $$b'\sum_{i=1}^{n} y_i + nc' = \sum_{i=1}^{n} x_i.$$

From Table 4, our equations become:

(3) $$34372b + 552c = 34382.$$

and

(4) $$552b + 11c = 576.$$

Thus,

$$11c = 576 - 552b$$

$$c = \frac{576 - 552b}{11}.$$

Substituting the value of c into (3) we get

$$34372b + 552\left(\frac{576 - 552b}{11}\right) = 34382$$

$$378092b + 317952 - 304704b = 378202$$

$$73388b = 60250$$

$$\therefore \quad b = 0.8209789$$

$$\text{and} \quad c = 11.165422.$$

Hence, $y = 0.8209789x + 11.165422$. Similarly,

$$(3') \qquad 35812b' + 576c' = 34382$$

$$(4') \qquad 576b' + 11c' = 552$$

$$\therefore \quad 11c' = 552 - 576b'$$

$$c' = \frac{552 - 576b'}{11}.$$

Substituting in (3') we get

$$35812b' + 576\left(\frac{552 - 576b'}{11}\right) = 34382$$

$$393932b' + 317952 - 331776b' = 378202$$

$$62156b' = 60250$$

$$\therefore \quad b' = 0.9693352$$

and

$$c' = -0.5760972$$

$$\therefore \quad x = 0.9693352y - 0.5760972.$$

So, we now have the lines of best fit with respect to y and with respect to x. (See Figures 4a and 4b.) We can use either one, depending on our needs. Further than that, having the two lines allows us to calculate what is called the coefficient of correlation.

4. COEFFICIENT OF CORRELATION

In order to get a numerical indicator of how well the two sets of scores compare, we take the geometric mean of the slopes of the two lines of regression (i.e., $r = \pm\sqrt{bb'}$).

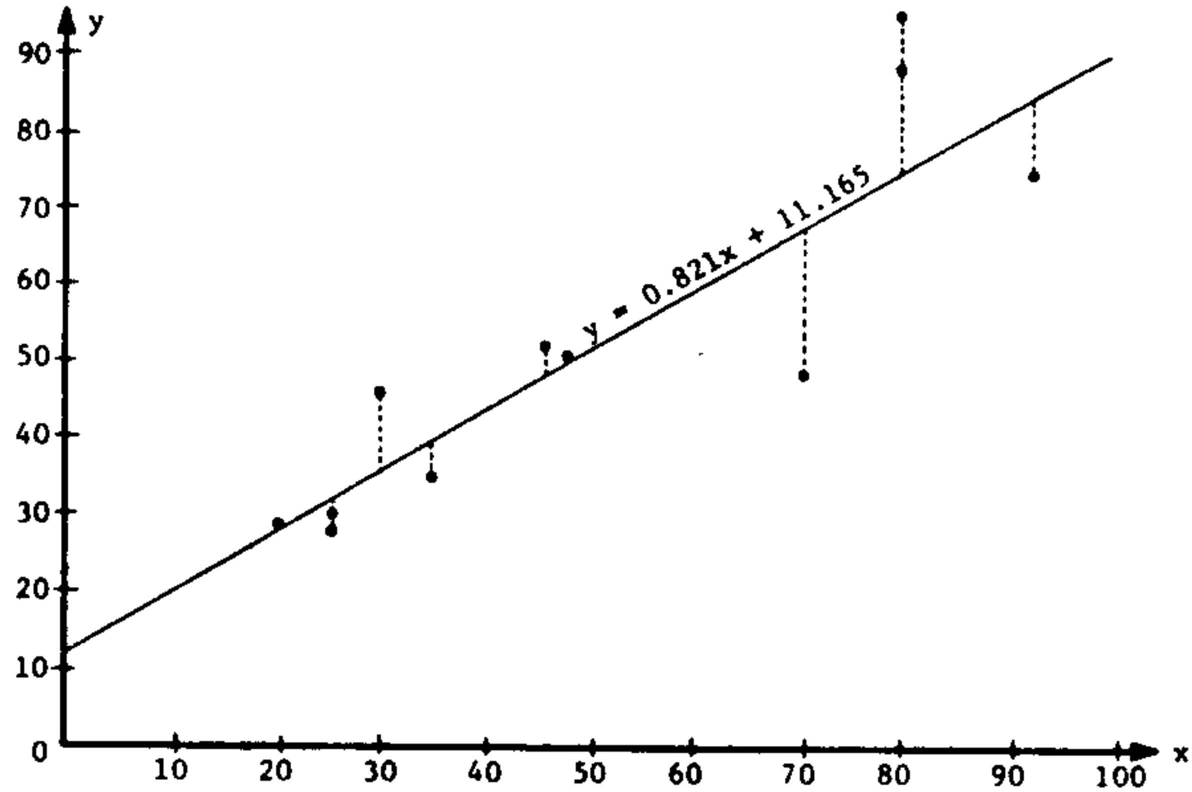

Figure 4a. Regression of y on x.

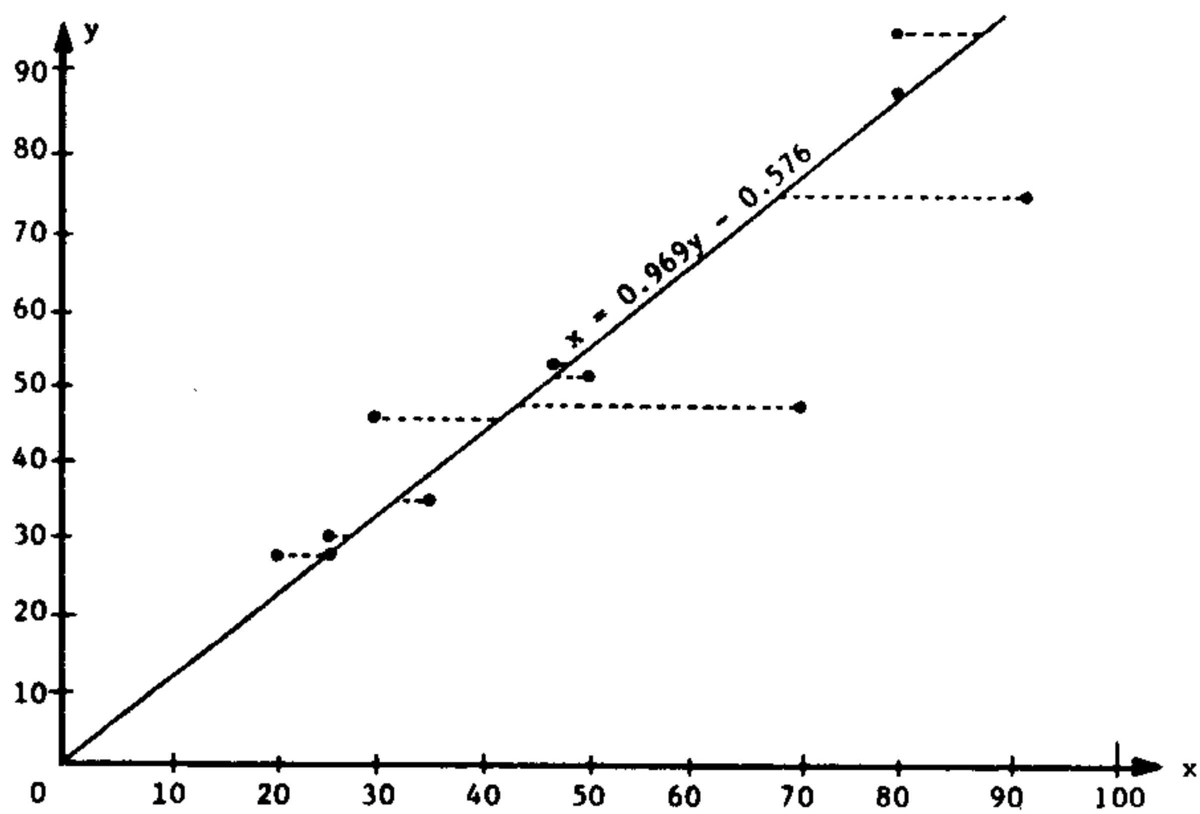

Figure 4b. Regression of x on y.

The sign is chosen to be negative if both slopes are negative, and positive if both slopes are positive. This value, which ranges from -1 to 1 is called the coefficient of correlation. If we have good correlation the value r is close to 1. Poor correlation is indicated by a value near 0. If high values of one characteristic are associated with low values of the other, the correlation is considered negative. Observe the distribution of points in the graphs of Figure 5.

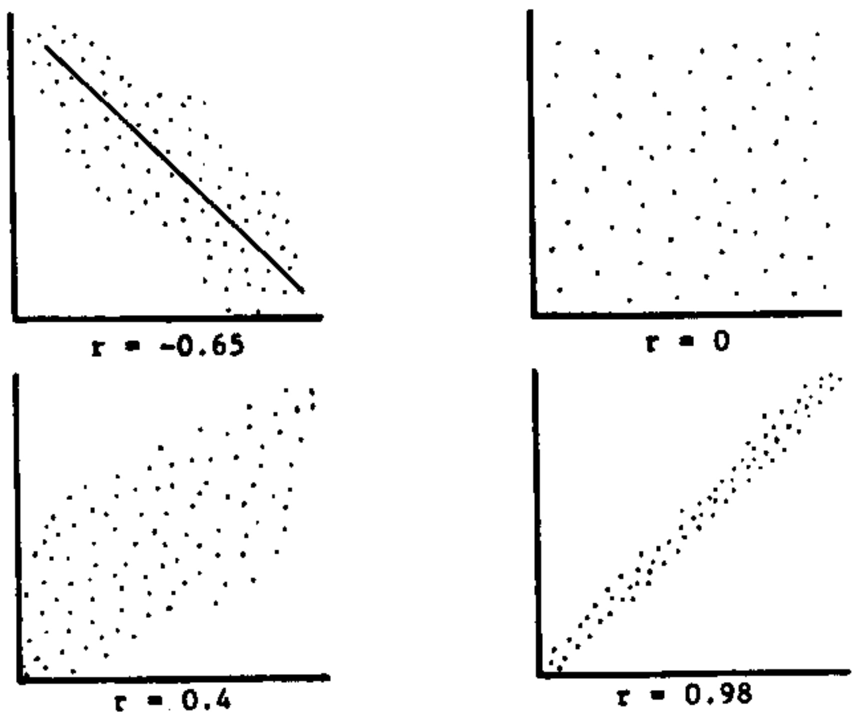

Figure 5.

Using the data from the example in the previous section we have:

$$r = \sqrt{bb'} = \sqrt{(0.8209789)(0.9693352)}$$

$$= \sqrt{0.7958037}$$

$$= 0.8921.$$

The value of r indicates a reasonably good correlation.

We can determine b and b' directly from the two normal equations. This allows us to calculate r without the trouble of finding the lines of regression. With a little algebra we can write:

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

and

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

Exercise 1.

Given the normal equations (3), (4), (3'), and (4'), use algebra to obtain b and b' above.

Since $r = \sqrt{bb'}$ we can write:

$$r = \sqrt{\frac{\left[n\sum_{i=1}^{n} x_i y_i - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)\right]^2}{\left[n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2\right]\left[n\sum_{i=1}^{n} y_i^2 - \left(\sum_{i=1}^{n} y_i\right)^2\right]}}.$$

More simply:

$$r = \frac{n\sum_{i=1}^{n} x_i y_i - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)}{\sqrt{\left[n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2\right]\left[n\sum_{i=1}^{n} y_i^2 - \left(\sum_{i=1}^{n} y_i\right)^2\right]}}.$$

As a check we substitute the indicated sums in this new formula:

$$r = \frac{11(34382) - 552(576)}{\sqrt{(11(34372) - (552)^2)(11(35812) - (576)^2)}}$$

$$= \frac{378202 - 317952}{\sqrt{(73388)(62156)}} = \frac{60250}{67540}$$

$$\therefore \qquad r \doteq 0.8920639 \doteq 0.8921.$$

This agrees with the results obtained by employing the explicit slopes, b and b' of the two lines of regression.

5. REGRESSION FOR LOGARITHMIC SCATTERS

Consider the graph in Figure 6 of a man's growth measured every three years after birth. Notice that there is a great deal of growth between birth and 15 years. After that time, growth tapers off. Table 5 gives the data used in plotting the graph.

TABLE 5

Age in Yrs.	Birth	3	6	9	12	15	18	21	24	27	...
Height in Ft.	1.5	3	3.75	4.5	5	5.8	6.1	6.15	6.17	6.18	...

Using the techniques developed in Section 3, we can easily fit a line to the data. See the calculations below in Table 6.

Figure 6.

TABLE 6

x	x^2	y	xy
0	0	1.60	0
3	9	2.90	8.70
6	36	3.75	22.50
9	81	4.50	40.50
12	144	5.00	60.00
15	225	5.80	87.00
18	324	6.10	109.80
21	441	6.15	129.15
24	576	6.17	148.08
27	729	6.18	166.86
135	2565	46.55	772.59

Using $b\Sigma x^2 + c\Sigma x = \Sigma xy$

$b\Sigma x + cn = \Sigma y$.

Therefore we can write:

$$2565b + 135c = 772.59$$

$$135b + 10c = 46.55$$

$$c = \frac{46.55 - 135b}{10}$$

and we can further write

$$2565b + 135\left(\frac{46.55 - 135b}{10}\right) = 772.59$$

$$25650b + 135(46.55) - (135)^2 b = 7725.9$$

$$25650b + 6284.25 - 18225b = 7725.9$$

$$7425b = 1441.65$$

$$b = 1441.65/7425$$

$$b = 0.1942$$

$$\therefore \quad c = 2.0333$$

and we have our line of regression:

$$y = 0.1942x + 2.0333.$$

In order to draw the line we need only locate two points.

For $x = 0$, $y = 2.0333$,

for $x = 3$, $y = 0.1942(3) + 2.0333 = 2.6159$.

While this is not a bad fit, we can do better. It turns out that the data will fit a logarithmic curve much better than a straight line. In general, logarithmic curves look like the one shown in Figure 8.

We can take the $\log_e$* of each of the x values (age in this example). We then use the same technique of least squares to find a log line of best fit. The calculations are given below. Notice how much closer this curve is to the actual data.

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*Log_e is also written ln. We are using $\log_e$ here to emphasize the general nature of logarithms. We can arbitrarily use any base.

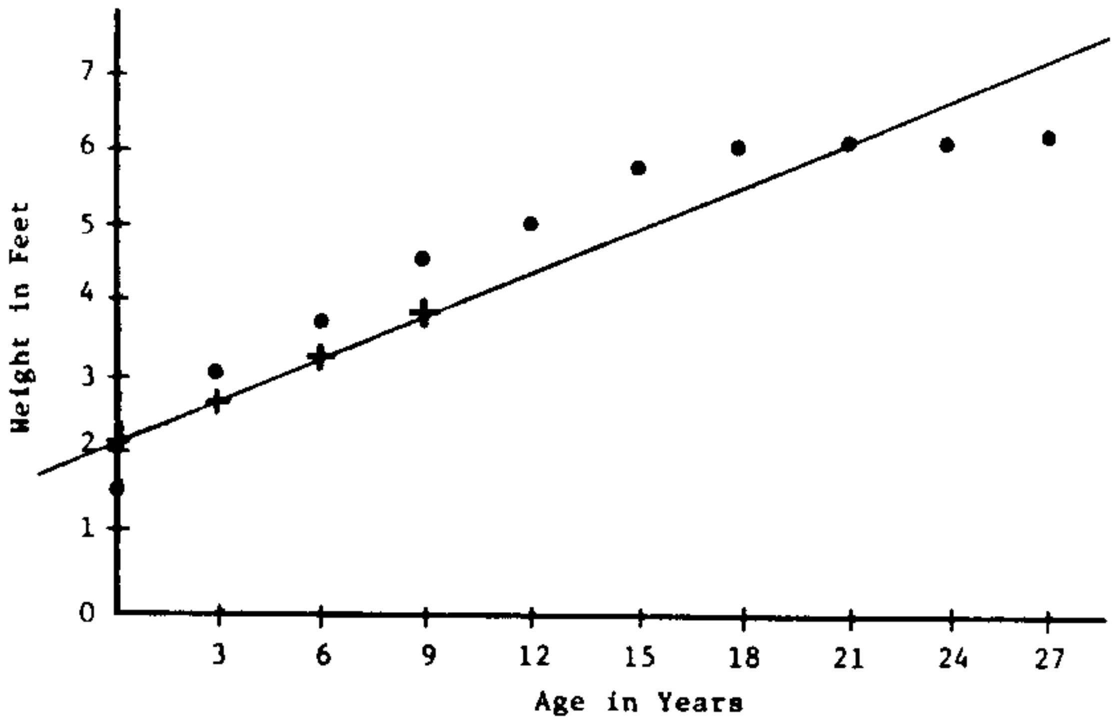

Figure 7.

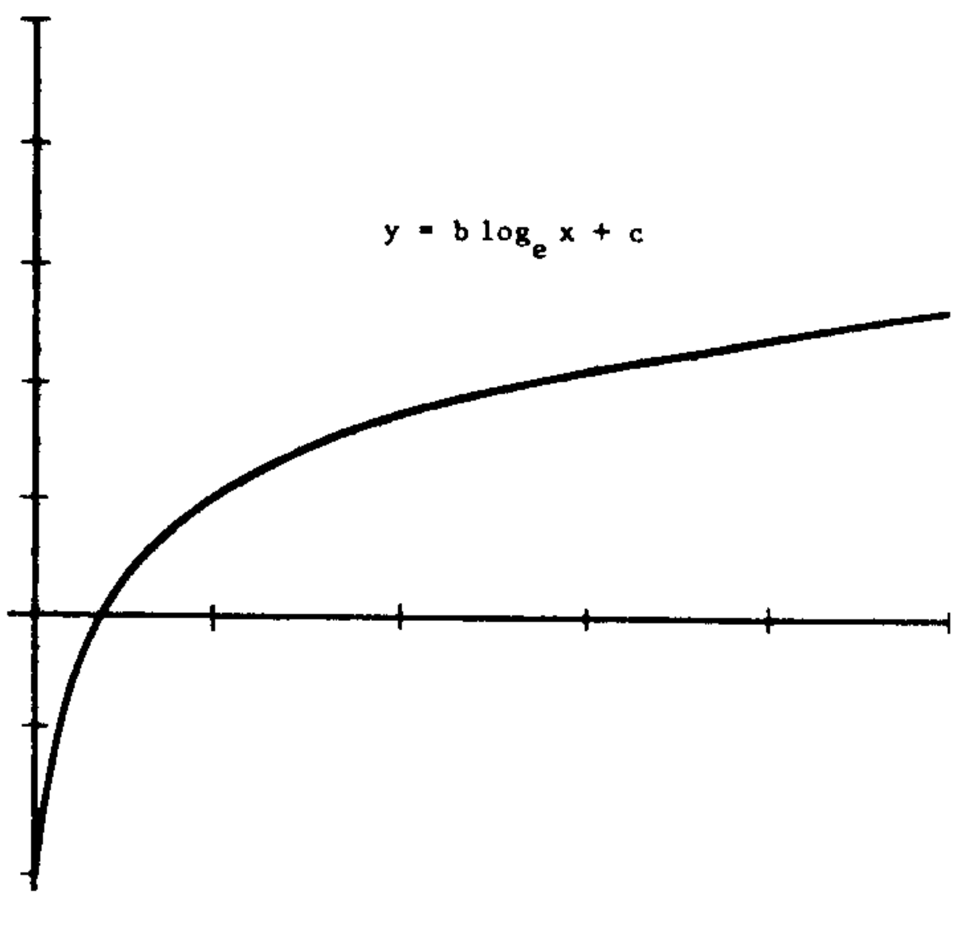

Figure 8.

TABLE 7

x	$\log_e x$	$(\log_e x)^2$	y	$(\log_e x)y$
0	$-\infty$			
3	1.0986	1.2069	2.90	3.1859
6	1.7918	3.2105	3.75	6.7193
9	2.1972	4.8277	4.50	9.8874
12	2.4849	6.1743	5.00	12.4245
15	2.7081	7.3338	5.80	15.5707
18	2.8904	8.3544	6.10	17.6314
21	3.0445	9.2690	6.15	18.7237
24	3.1781	10.1003	6.17	19.6089
27	3.2958	10.8623	6.18	20.3680
	22.6894	61.3392	46.55	124.1198

We use

$$b\Sigma(\log_e x)^2 + c\Sigma\log_e x = \Sigma(\log_e x)y$$

$$b\Sigma\log_e x + cn = \Sigma y.$$

Therefore we can write:

$$61.3392b + 22.6894c = 124.1198$$

$$22.6894b + 9c = 46.55$$

$$c = \frac{46.55 - 22.6894b}{9}$$

therefore

$$61.3392b + 22.6895\left(\frac{46.55-22.6894b}{9}\right) = 124.1198$$

$$9(61.3392b) + 22.6894(46.55) - (22.6984)^2b = 9(124.1198)$$

$$552.0528b + 1056.1915 - 515.2174b = 1117.0782$$

$$36.8354b = 60.8867$$

$$b = 1.6529$$

$$c = \frac{46.55 - 22.6894(1.6529)}{9} = \frac{46.55 - 37.5033}{9}$$

$$= \frac{9.0467}{9} = 1.0052$$

$$y = 1.6529 \log_e x + 1.0052.$$

Let $x = 3$, then $y = 1.6529(1.0986) + 1.0052 = 2.821.$

$x = 6$, then $y = 1.6529(1.7918) + 1.0052 = 3.9669.$

$x = 9$, then $y = 1.6529(2.1972) + 1.0052 = 4.637.$

$x = 12$, then $y = 1.6529(2.4849) + 1.0052 = 5.1125.$

$x = 15$, then $y = 1.6529(2.7081) + 1.0052 = 5.4814.$

$x = 18$, then $y = 1.6529(2.8904) + 1.0052 = 5.7827.$

$x = 21$, then $y = 1.6529(3.0445) + 1.0052 = 6.0375.$

$x = 24$, then $y = 1.6529(3.1781) + 1.0052 = 6.2583.$

$x = 27$, then $y = 1.6529(3.2958) + 1.0052 = 6.4528.$

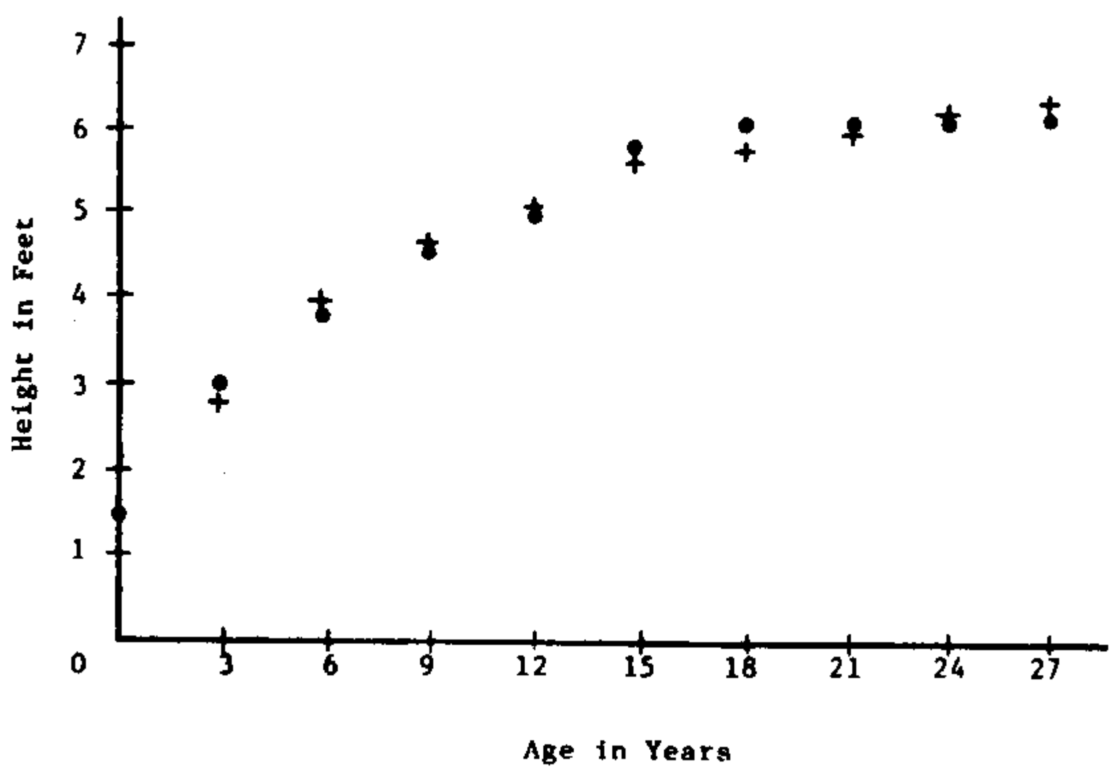

Figure 9.

Exercise 2.

Fit a logarithmic curve to the data given in the table below.

x	1	6	11	16	21	...
y	12	42	53	71	76	...

6. REGRESSION FOR EXPONENTIAL SCATTERS

Consider now, an experiment where a large number of corn seedlings were grown under favorable conditions. Every two weeks a few plants were weighed, and the average of their weights was recorded. (See Table 8.) We also give a graph in Figure 10. It would be difficult to find a straight line that would fit very well. The logarithmic curve does not fit so well either.

TABLE 8

Age in Weeks	2	4	6	8	10	12	14	16	18	20	...
Average Weight in Grams	21	28	58	76	170	422	706	853	924	966	...

This set of data is probably best fit to an exponential curve. The general shape of such curves ($y = e^x$) is given in Figure 11. Algebraically $y = e^x$ can be written $\log_e y = x$. For a general exponential we can write:

$$y = ce^{bx}.$$

With a little algebra, we can get a form that will allow us to use the least squares method. Analyze the development below.

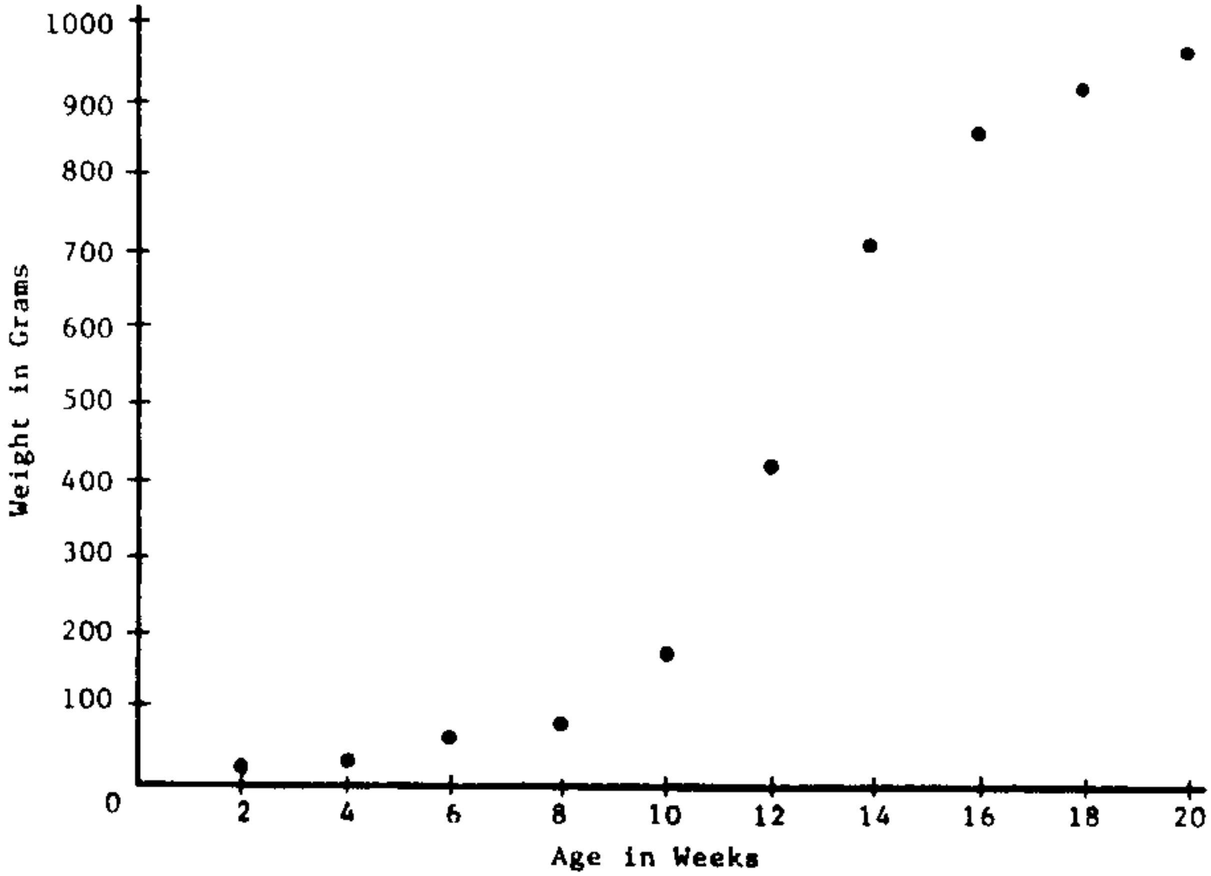

Figure 10.

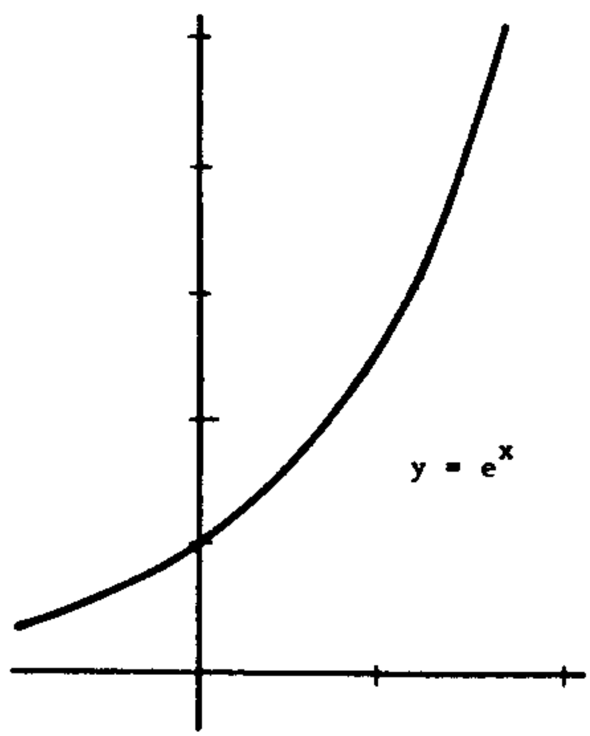

Figure 11.

$$y = ce^{bx} \rightarrow \frac{y}{c} = e^{bx} \rightarrow \log_e \frac{y}{c} = bx.$$

And further we have:

$$\log_e y - \log_e c = bx \quad \text{or} \quad \log_e y = bx + \log_e c.$$

We can find the "line" of best exponential fit by taking the $\log_e$ of the y values and then proceeding with the least squares technique. (See Table 9.)

TABLE 9

x	y	$\log_e y$	x^2	$x(\log_e y)$
2	21	3.0445	4	6.0890
4	28	3.3322	16	13.3288
6	58	4.0604	36	24.3624
8	76	4.3307	64	34.6456
10	170	5.1358	100	51.3580
12	422	6.0450	144	72.5400
14	706	6.5596	196	91.8344
16	853	6.7488	256	107.9808
18	924	6.8287	324	122.9166
20	966	6.8732	400	137.4640
110		52.9597	1540	662.5196

Keeping the equation

$$\log_e y = bx + \log_e c$$

in mind, we calculate

$$1540b + 110 \log_e c = 662.5196$$

$$110b + 10 \log_e c = 52.9597$$

$$b = \frac{52.9597 - 10 \log_e c}{110}$$

$$\log_e c = \frac{52.9597 - 110b}{10}$$

$$1540b + 110\left(\frac{52.9597 - 110b}{10}\right) = 662.5196$$

$$1540b + 5825.567 - 12100b = 6625.196$$

$$3300b = 799.629$$

$$b = 0.2423$$

$$\log_e c = \frac{52.9597 - 26.653}{10} = 2.63067$$

$$\log_e y = 0.2423x + 2.63067.$$

For $x = 2$, $\log_e y = 0.2423(2) + 2.63067$

$$= 3.11527$$

therefore

$$y = e^{3.11527} \doteq 2.71828^{3.11527}$$

$$= 22.5395.$$

For $x = 4$, $\log_e y = 0.2423(4) + 2.6307$

therefore

$$y = 36.5946.$$

For $x = 6$, $y = 59.4122$
for $x = 8$, $y = 96.4573$
for $x = 10$, $y = 156.6008$
for $x = 12$, $y = 254.2454$
for $x = 14$, $y = 412.7739$
for $x = 16$, $y = 670.1489$
for $x = 18$, $y = 1088.0038$
for $x = 20$, $y = 1766.4019$.

We could have solved for c when we obtained $\log_e c = 2.63067$.

If $\log_e c = 2.63067$, then $c \doteq 13.8831$, therefore

$$y = 13.8831e^{0.2423x}.$$

If we substitute 2 for x we get a value which is virtually the same as we got using the other form. That is,

$$y = 13.8831e^{0.2423(2)} = 22.5395.$$

Observe the fitted curve in Figure 12.

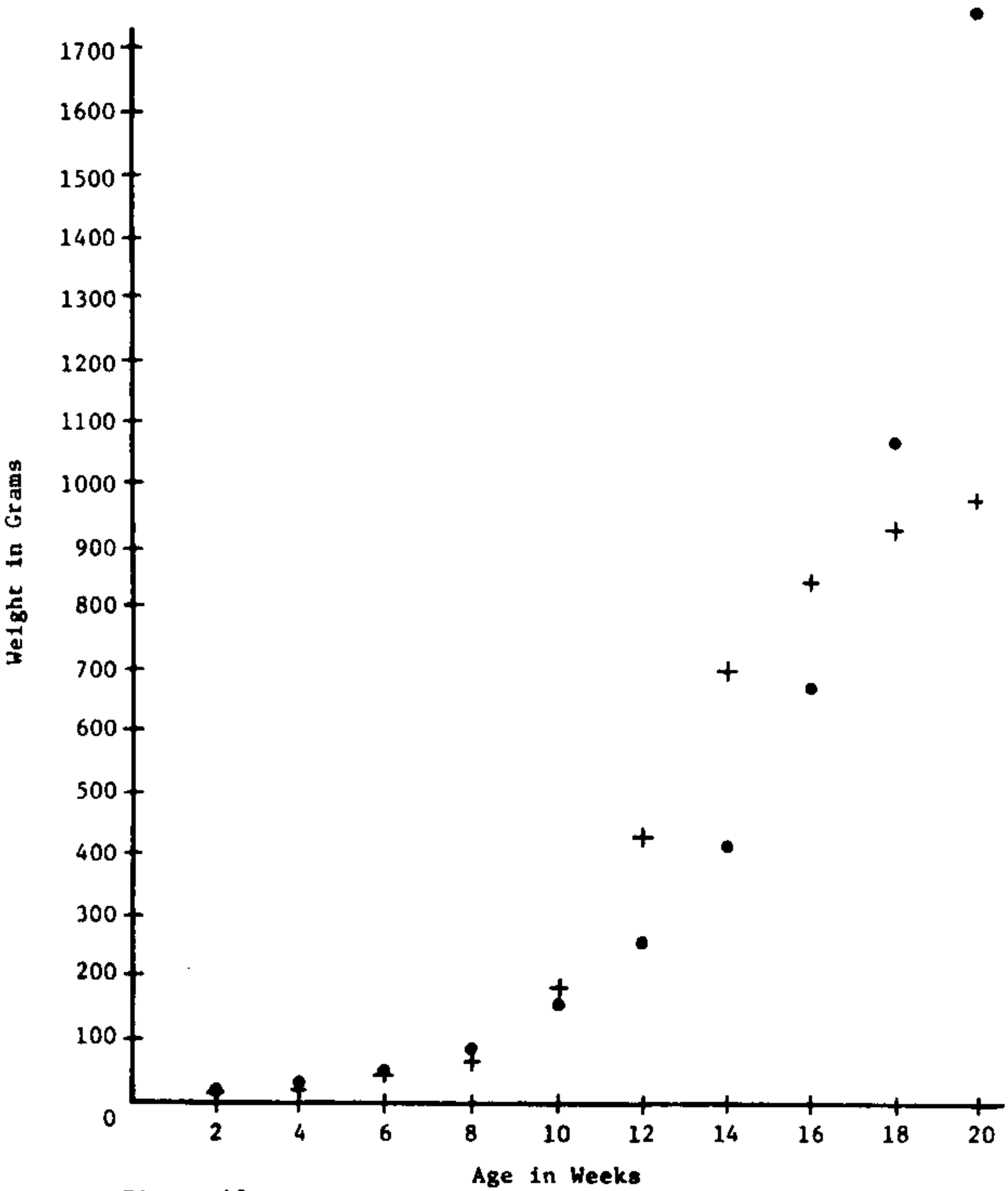

Figure 12.

Exercise 3.

Try to fit the data for the growth of the corn seedlings using 15 as a base instead of 10.

A disc was rolled down an inclined plane and the distance it travelled was measured after 0, 2, 4, ..., seconds. The results are organized in Table 10.

TABLE 10

Time (x)	0	2	4	6	8	10	12	14	16
Distance (y)	0	1	3	5	8	12	17	23	29

We give a graph of the data in Figure 13. Notice that it looks as if it could be fitted to an exponential. However, this data fits closer to a second degree polynomial or a parabola, $y = ax^2 + bx + c$.

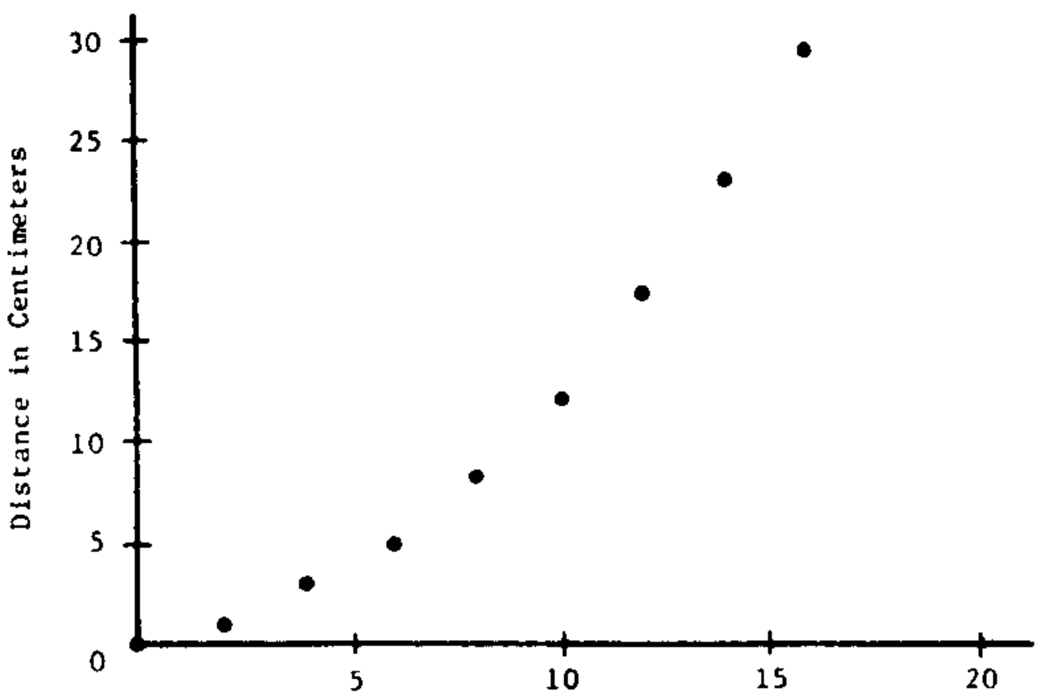

Figure 13.

In order to fit a polynomial we must do a little more mathematics. Notice, that we now have three constants to identify, namely a, b, and c.

We must consider minimizing the sum

$$\sum_{i=1}^{n} [y_i - (ax_i^2 + bx_i + c)]^2.$$