MAP 2220 – FUNDAMENTOS DE ANÁLISE NUMÉRICA

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Prof. Dr. Luis Carlos de Castro Santos

lsantos@ime.usp.br/lccs13@yahoo.com

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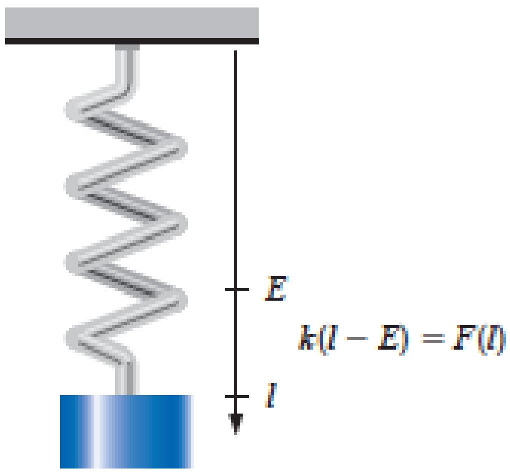
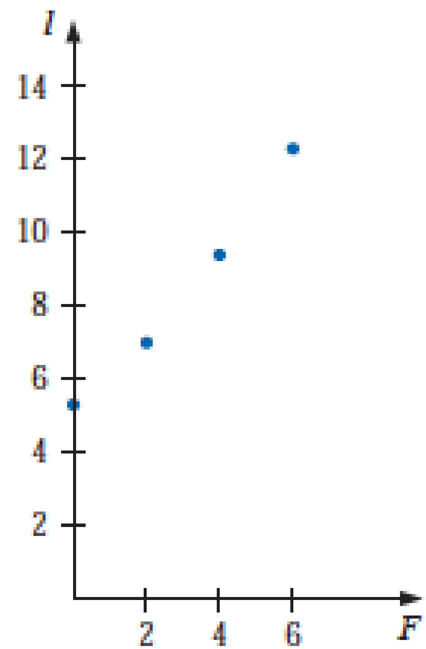
CHAPTER 8

Approximation Theory

Introduction

Hooke's law states that when a force is applied to a spring constructed of uniform material, the length of the spring is a linear function of that force. We can write the linear function as $F(l) = k(l - E)$, where $F(l)$ represents the force required to stretch the spring l units, the constant E represents the length of the spring with no force applied, and the constant k is the spring constant.





Approximation theory involves two general types of problems. One problem arises when a function is given explicitly, but we wish to find a "simpler" type of function, such as a polynomial, to approximate values of the given function. The other problem in approximation theory is concerned with fitting functions to given data and finding the "best" function in a certain class to represent the data.

Both problems have been touched upon in Chapter 3. The nth Taylor polynomial about the number x_0 is an excellent approximation to an $(n+1)$-times differentiable function f in a small neighborhood of x_0. The Lagrange interpolating polynomials, or, more generally, osculatory polynomials, were discussed both as approximating polynomials and as polynomials to fit certain data. Cubic splines were also discussed in that chapter. In this chapter, limitations to these techniques are considered, and other avenues of approach are discussed.

8.1 Discrete Least Squares Approximation

Consider the problem of estimating the values of a function at nontabulated points, given the experimental data in Table 8.1.

Figure 8.1 shows a graph of the values in Table 8.1. From this graph, it appears that the actual relationship between x and y is linear. The likely reason that no line precisely fits the data is because of errors in the data. So it is unreasonable to require that the approximating function agree exactly with the data. In fact, such a function would introduce oscillations that were not originally present. For example, the graph of the ninth-degree interpolating polynomial shown in unconstrained mode for the data in Table 8.1 is obtained in Maple

Table 8.1

x_i	y_i	x_i	y_i
1	1.3	6	8.8
2	3.5	7	10.1
3	4.2	8	12.5
4	5.0	9	13.0
5	7.0	10	15.6

Figure 8.1

x_i	y_i
1	1.3
2	3.5
3	4.2
4	5.0
5	7.0
6	8.8
7	10.1
8	12.5
9	13.0
10	15.6

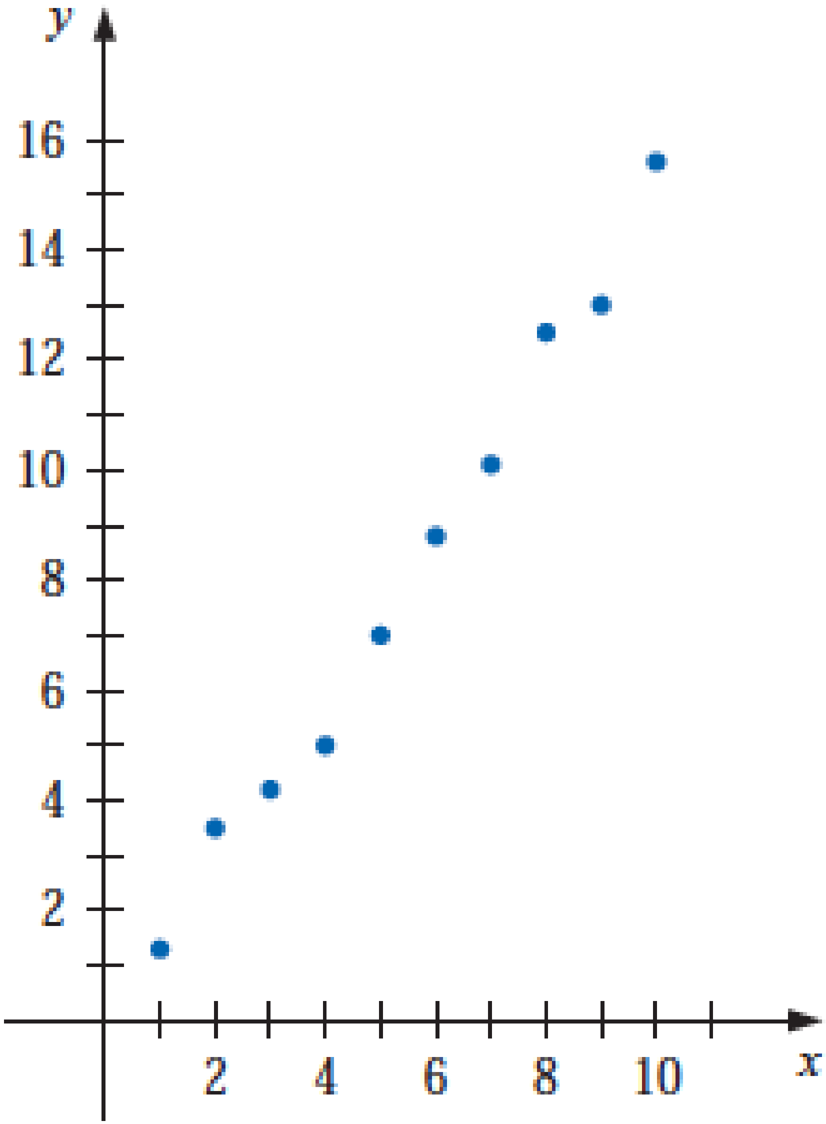
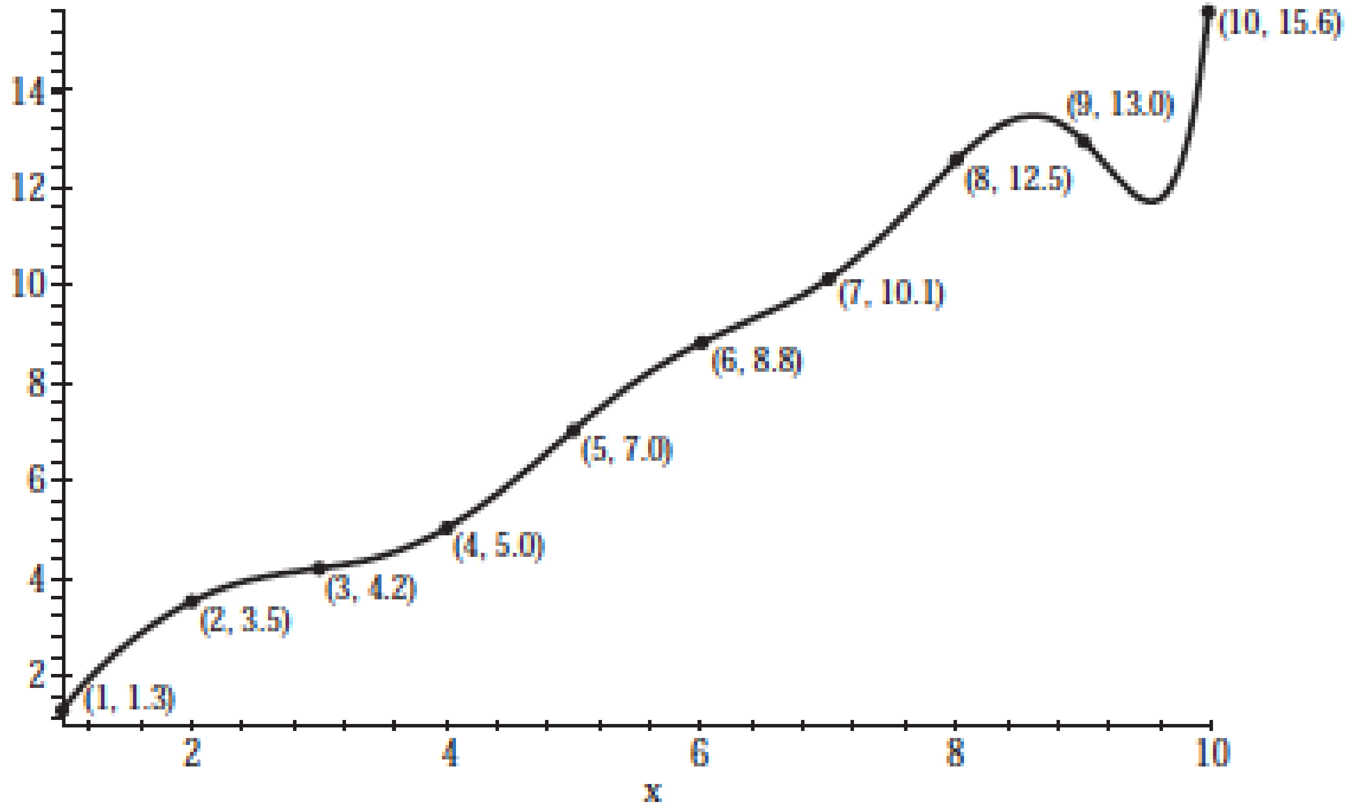


Figure 8.2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(3, 4.2)
(4, 5.0)
(5, 7.0)
(6, 8.8)
(7, 10.1)
(8, 12.5)
(9, 13.0)
(10, 15.6)

Let $a_1x_i + a_0$ denote the ith value on the approximating line and y_i be the ith given y-value. We assume throughout that the independent variables, the x_i, are exact, it is the dependent variables, the y_i, that are suspect. This is a reasonable assumption in most experimental situations.

The problem of finding the equation of the best linear approximation in the absolute sense requires that values of a_0 and a_1 be found to minimize

$$E_\infty(a_0, a_1) = \max_{1 \le i \le 10} \{|y_i - (a_1x_i + a_0)|\}.$$

This is commonly called a **minimax** problem and cannot be handled by elementary techniques.

Another approach to determining the best linear approximation involves finding values of a_0 and a_1 to minimize

$$E_1(a_0, a_1) = \sum_{i=1}^{10} |y_i - (a_1x_i + a_0)|.$$

This quantity is called the **absolute deviation**. To minimize a function of two variables, we need to set its partial derivatives to zero and simultaneously solve the resulting equations. In the case of the absolute deviation, we need to find a_0 and a_1 with

$$0 = \frac{\partial}{\partial a_0} \sum_{i=1}^{10} |y_i - (a_1x_i + a_0)| \quad \text{and} \quad 0 = \frac{\partial}{\partial a_1} \sum_{i=1}^{10} |y_i - (a_1x_i + a_0)|.$$

The problem is that the absolute-value function is not differentiable at zero, and we might not be able to find solutions to this pair of equations.

Linear Least Squares

The **least squares** approach to this problem involves determining the best approximating line when the error involved is the sum of the squares of the differences between the y-values on the approximating line and the given y-values. Hence, constants a_0 and a_1 must be found that minimize the least squares error:

$$E_2(a_0, a_1) = \sum_{i=1}^{10} \left[y_i - (a_1 x_i + a_0)\right]^2 .$$

The least squares method is the most convenient procedure for determining best linear approximations, but there are also important theoretical considerations that favor it. The minimax approach generally assigns too much weight to a bit of data that is badly in error, whereas the absolute deviation method does not give sufficient weight to a point that is considerably out of line with the approximation. The least squares approach puts substantially more weight on a point that is out of line with the rest of the data, but will not permit that point to completely dominate the approximation. An additional reason for considering the least squares approach involves the study of the statistical distribution of error. (See [Lar], pp. 463–481.)

The general problem of fitting the best least squares line to a collection of data $\{(x_i, y_i)\}_{i=1}^{m}$ involves minimizing the total error,

$$E \equiv E_2(a_0, a_1) = \sum_{i=1}^{m} \left[y_i - (a_1 x_i + a_0)\right]^2,$$

with respect to the parameters a_0 and a_1. For a minimum to occur, we need both

$$\frac{\partial E}{\partial a_0} = 0 \quad \text{and} \quad \frac{\partial E}{\partial a_1} = 0,$$

that is,

$$0 = \frac{\partial}{\partial a_0} \sum_{i=1}^{m} \left[(y_i - (a_1 x_i - a_0)\right]^2 = 2 \sum_{i=1}^{m} (y_i - a_1 x_i - a_0)(-1)$$

and

$$0 = \frac{\partial}{\partial a_1} \sum_{i=1}^{m} \left[y_i - (a_1 x_i + a_0)\right]^2 = 2 \sum_{i=1}^{m} (y_i - a_1 x_i - a_0)(-x_i).$$

These equations simplify to the **normal equations**:

$$a_0 \cdot m + a_1 \sum_{i=1}^{m} x_i = \sum_{i=1}^{m} y_i \quad \text{and} \quad a_0 \sum_{i=1}^{m} x_i + a_1 \sum_{i=1}^{m} x_i^2 = \sum_{i=1}^{m} x_i y_i.$$

The solution to this system of equations is

$$a_0 = \frac{\sum_{i=1}^{m} x_i^2 \sum_{i=1}^{m} y_i - \sum_{i=1}^{m} x_i y_i \sum_{i=1}^{m} x_i}{m\left(\sum_{i=1}^{m} x_i^2\right) - \left(\sum_{i=1}^{m} x_i\right)^2} \tag{8.1}$$

and

$$a_1 = \frac{m \sum_{i=1}^{m} x_i y_i - \sum_{i=1}^{m} x_i \sum_{i=1}^{m} y_i}{m\left(\sum_{i=1}^{m} x_i^2\right) - \left(\sum_{i=1}^{m} x_i\right)^2}. \tag{8.2}$$

Example 1 Find the least squares line approximating the data in Table 8.1.

Solution We first extend the table to include x_i^2 and $x_i y_i$ and sum the columns. This is shown in Table 8.2.

Table 8.2

x_i	y_i	x_i^2	$x_i y_i$	$P(x_i) = 1.538x_i - 0.360$
1	1.3	1	1.3	1.18
2	3.5	4	7.0	2.72
3	4.2	9	12.6	4.25
4	5.0	16	20.0	5.79
5	7.0	25	35.0	7.33
6	8.8	36	52.8	8.87
7	10.1	49	70.7	10.41
8	12.5	64	100.0	11.94
9	13.0	81	117.0	13.48
10	15.6	100	156.0	15.02
55	81.0	385	572.4	$E = \sum_{i=1}^{10} (y_i - P(x_i))^2 \approx 2.34$

The normal equations (8.1) and (8.2) imply that

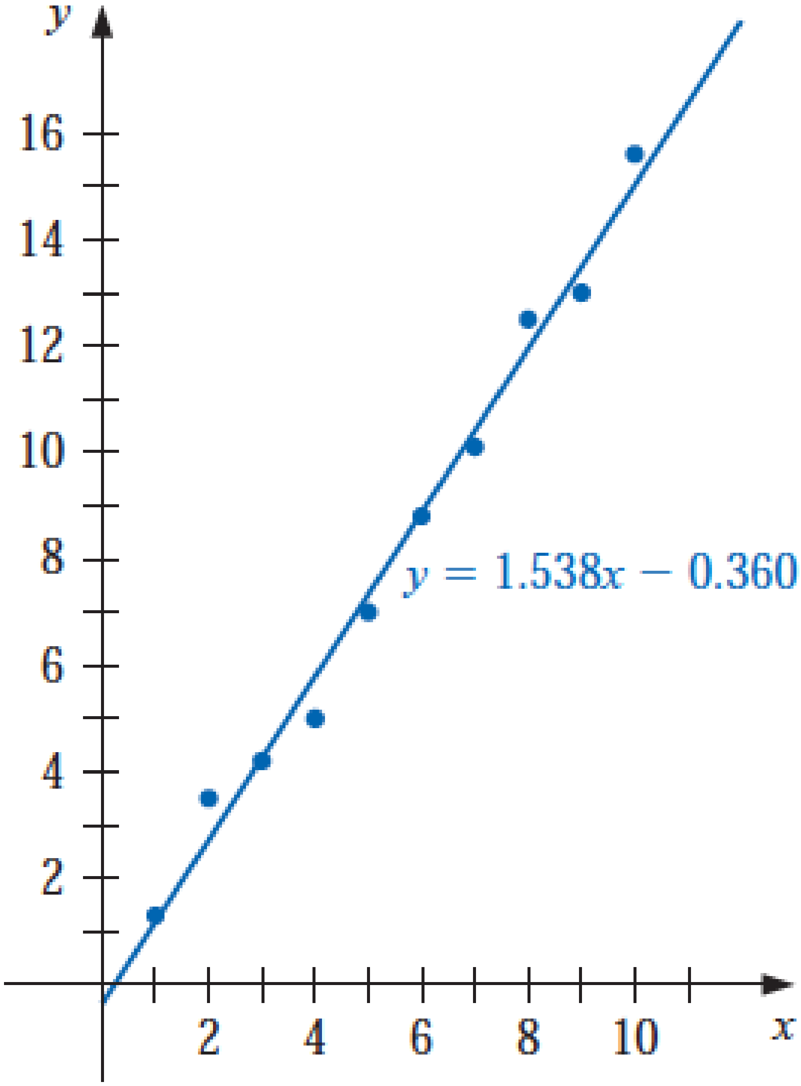
$$a_0 = \frac{385(81) - 55(572.4)}{10(385) - (55)^2} = -0.360$$

and

$$a_1 = \frac{10(572.4) - 55(81)}{10(385) - (55)^2} = 1.538,$$

so $P(x) = 1.538x - 0.360$. The graph of this line and the data points are shown in Figure 8.3. The approximate values given by the least squares technique at the data points are in Table 8.2. ■

Figure 8.3



Polynomial Least Squares

The general problem of approximating a set of data, $\{(x_i, y_i) \mid i = 1, 2, \ldots, m\}$, with an algebraic polynomial

$$P_n(x) = a_n x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0,$$

of degree $n < m - 1$, using the least squares procedure is handled similarly. We choose the constants $a_0, a_1, \ldots, a_n$ to minimize the least squares error $E = E_2(a_0, a_1, \ldots, a_n)$, where

$$\begin{aligned} E &= \sum_{i=1}^{m} (y_i - P_n(x_i))^2 \\ &= \sum_{i=1}^{m} y_i^2 - 2\sum_{i=1}^{m} P_n(x_i) y_i + \sum_{i=1}^{m} (P_n(x_i))^2 \end{aligned}$$

$$= \sum_{i=1}^{m} y_i^2 - 2\sum_{i=1}^{m}\left(\sum_{j=0}^{n} a_j x_i^j\right) y_i + \sum_{i=1}^{m}\left(\sum_{j=0}^{n} a_j x_i^j\right)^2$$

$$= \sum_{i=1}^{m} y_i^2 - 2\sum_{j=0}^{n} a_j\left(\sum_{i=1}^{m} y_i x_i^j\right) + \sum_{j=0}^{n}\sum_{k=0}^{n} a_j a_k\left(\sum_{i=1}^{m} x_i^{j+k}\right).$$

As in the linear case, for E to be minimized it is necessary that $\partial E/\partial a_j = 0$, for each $j = 0, 1, \ldots, n$. Thus, for each j, we must have

$$0 = \frac{\partial E}{\partial a_j} = -2\sum_{i=1}^{m} y_i x_i^j + 2\sum_{k=0}^{n} a_k \sum_{i=1}^{m} x_i^{j+k}.$$

This gives $n + 1$ **normal equations** in the $n + 1$ unknowns a_j. These are

$$\sum_{k=0}^{n} a_k \sum_{i=1}^{m} x_i^{j+k} = \sum_{i=1}^{m} y_i x_i^j, \quad \text{for each } j = 0, 1, \ldots, n. \tag{8.3}$$

It is helpful to write the equations as follows:

$$a_0 \sum_{i=1}^{m} x_i^0 + a_1 \sum_{i=1}^{m} x_i^1 + a_2 \sum_{i=1}^{m} x_i^2 + \cdots + a_n \sum_{i=1}^{m} x_i^n = \sum_{i=1}^{m} y_i x_i^0,$$

$$a_0 \sum_{i=1}^{m} x_i^1 + a_1 \sum_{i=1}^{m} x_i^2 + a_2 \sum_{i=1}^{m} x_i^3 + \cdots + a_n \sum_{i=1}^{m} x_i^{n+1} = \sum_{i=1}^{m} y_i x_i^1,$$

$$\vdots$$

$$a_0 \sum_{i=1}^{m} x_i^n + a_1 \sum_{i=1}^{m} x_i^{n+1} + a_2 \sum_{i=1}^{m} x_i^{n+2} + \cdots + a_n \sum_{i=1}^{m} x_i^{2n} = \sum_{i=1}^{m} y_i x_i^n.$$

These *normal equations* have a unique solution provided that the x_i are distinct (see Exercise 14).

Example 2

Fit the data in Table 8.3 with the discrete least squares polynomial of degree at most 2.

Table 8.3

i	x_i	y_i
1	0	1.0000
2	0.25	1.2840
3	0.50	1.6487
4	0.75	2.1170
5	1.00	2.7183

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Solution For this problem, $n = 2, m = 5$, and the three normal equations are

$$\begin{aligned} 5a_0 + \quad 2.5a_1 + \quad 1.875a_2 &= 8.7680, \\ 2.5a_0 + \quad 1.875a_1 + 1.5625a_2 &= 5.4514, \\ 1.875a_0 + 1.5625a_1 + 1.3828a_2 &= 4.4015. \end{aligned}$$

Thus the least squares polynomial of degree 2 fitting the data in Table 8.3 is

$$P_2(x) = 1.0051 + 0.86468x + 0.84316x^2,$$

whose graph is shown in Figure 8.4. At the given values of x_i we have the approximations shown in Table 8.4.

The total error,

$$E = \sum_{i=1}^{5} (y_i - P(x_i))^2 = 2.74 \times 10^{-4},$$

is the least that can be obtained by using a polynomial of degree at most 2. ■

Figure 8.4

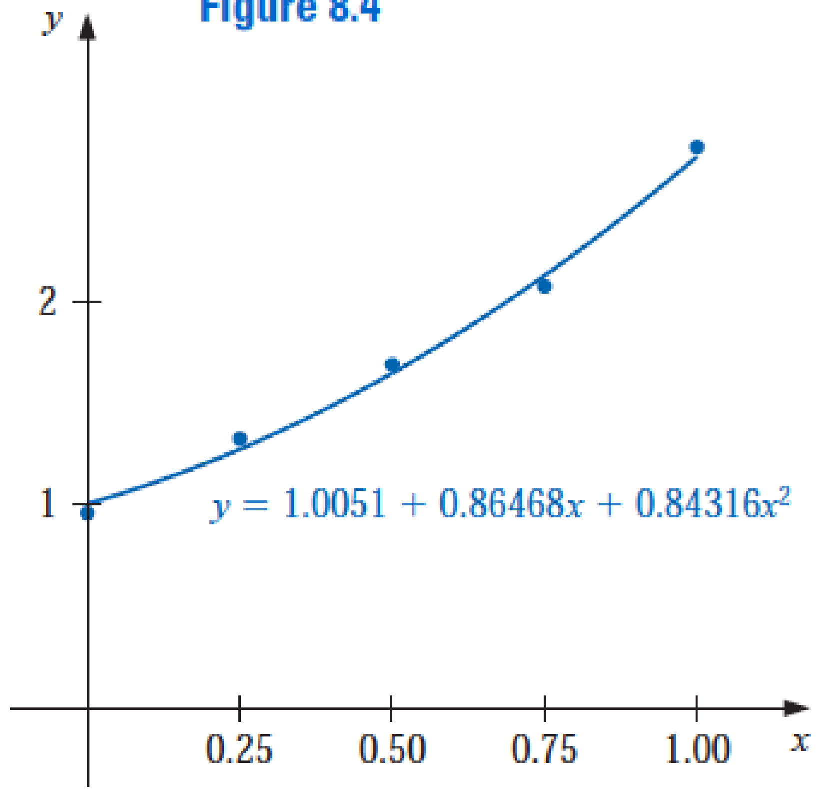


Table 8.4

i	1	2	3	4	5
x_i	0	0.25	0.50	0.75	1.00
y_i	1.0000	1.2840	1.6487	2.1170	2.7183
$P(x_i)$	1.0051	1.2740	1.6482	2.1279	2.7129
$y_i - P(x_i)$	−0.0051	0.0100	0.0004	−0.0109	0.0054

At times it is appropriate to assume that the data are exponentially related. This requires the approximating function to be of the form

$$y = be^{ax} \tag{8.4}$$

or

$$y = bx^{a}, \tag{8.5}$$

for some constants a and b. The difficulty with applying the least squares procedure in a situation of this type comes from attempting to minimize

$$E = \sum_{i=1}^{m}(y_i - be^{ax_i})^2, \quad \text{in the case of Eq. (8.4)},$$

or

$$E = \sum_{i=1}^{m}(y_i - bx_i^{a})^2, \quad \text{in the case of Eq. (8.5)}.$$

The normal equations associated with these procedures are obtained from either

$$0 = \frac{\partial E}{\partial b} = 2\sum_{i=1}^{m}(y_i - be^{ax_i})(-e^{ax_i})$$

and

$$0 = \frac{\partial E}{\partial a} = 2\sum_{i=1}^{m}(y_i - be^{ax_i})(-bx_i e^{ax_i}), \quad \text{in the case of Eq. (8.4);}$$

or

$$0 = \frac{\partial E}{\partial b} = 2\sum_{i=1}^{m}(y_i - bx_i^a)(-x_i^a)$$

and

$$0 = \frac{\partial E}{\partial a} = 2\sum_{i=1}^{m}(y_i - bx_i^a)(-b(\ln x_i)x_i^a), \quad \text{in the case of Eq. (8.5).}$$

No exact solution to either of these systems in a and b can generally be found.

The method that is commonly used when the data are suspected to be exponentially related is to consider the logarithm of the approximating equation:

$$\ln y = \ln b + ax, \quad \text{in the case of Eq. (8.4)},$$

and

$$\ln y = \ln b + a \ln x, \quad \text{in the case of Eq. (8.5)}.$$

In either case, a linear problem now appears, and solutions for $\ln b$ and a can be obtained by appropriately modifying the normal equations (8.1) and (8.2).

However, the approximation obtained in this manner is *not* the least squares approximation for the original problem, and this approximation can in some cases differ significantly from the least squares approximation to the original problem. The application in Exercise 13 describes such a problem. This application will be reconsidered as Exercise 11 in Section 10.3, where the exact solution to the exponential least squares problem is approximated by using methods suitable for solving nonlinear systems of equations.

Illustration Consider the collection of data in the first three columns of Table 8.5.

Table 8.5

i	x_i	y_i	$\ln y_i$	x_i^2	$x_i \ln y_i$
1	1.00	5.10	1.629	1.0000	1.629
2	1.25	5.79	1.756	1.5625	2.195
3	1.50	6.53	1.876	2.2500	2.814
4	1.75	7.45	2.008	3.0625	3.514
5	2.00	8.46	2.135	4.0000	4.270
	7.50		9.404	11.875	14.422

If x_i is graphed with $\ln y_i$, the data appear to have a linear relation, so it is reasonable to assume an approximation of the form

$$y = be^{ax}, \quad \text{which implies that} \quad \ln y = \ln b + ax.$$

Extending the table and summing the appropriate columns gives the remaining data in Table 8.5.

Using the normal equations (8.1) and (8.2),

$$a = \frac{(5)(14.422) - (7.5)(9.404)}{(5)(11.875) - (7.5)^2} = 0.5056$$

and

$$\ln b = \frac{(11.875)(9.404) - (14.422)(7.5)}{(5)(11.875) - (7.5)^2} = 1.122.$$

With $\ln b = 1.122$ we have $b = e^{1.122} = 3.071$, and the approximation assumes the form

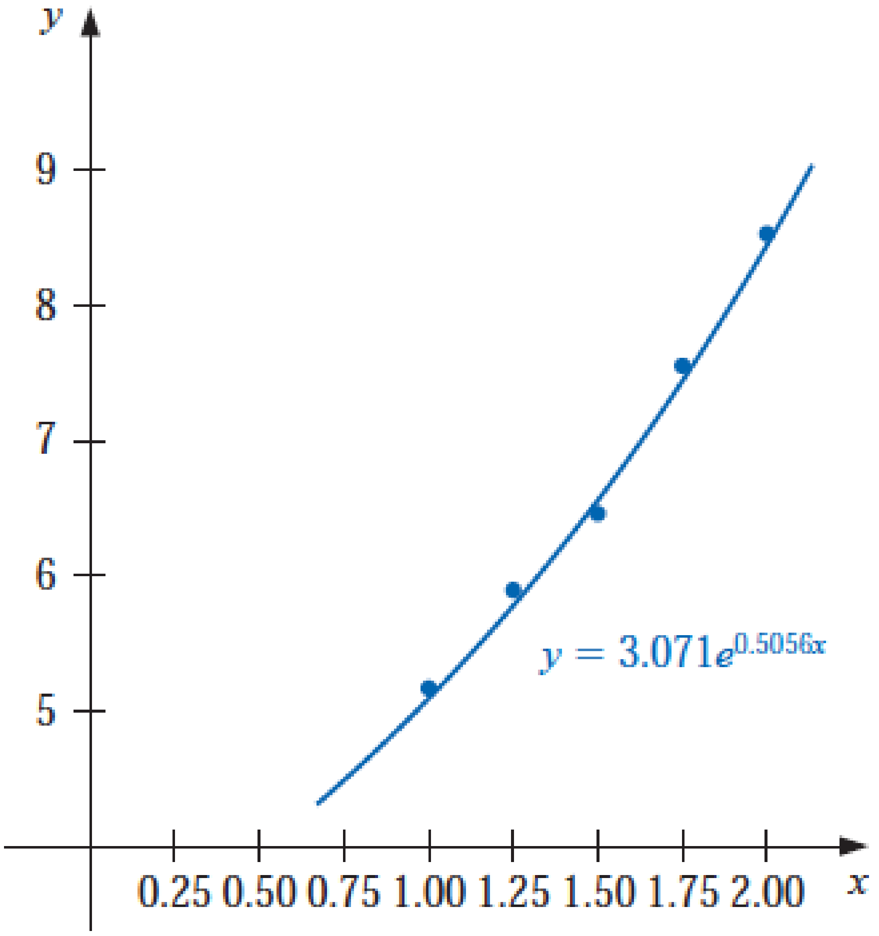
$$y = 3.071e^{0.5056x}.$$

At the data points this gives the values in Table 8.6. (See Figure 8.5.) □

Table 8.6

i	x_i	y_i	$3.071e^{0.5056x_i}$	$\|y_i - 3.071e^{0.5056x_i}\|$
1	1.00	5.10	5.09	0.01
2	1.25	5.79	5.78	0.01
3	1.50	6.53	6.56	0.03
4	1.75	7.45	7.44	0.01
5	2.00	8.46	8.44	0.02

Figure 8.5



5. Given the data:

x_i	4.0	4.2	4.5	4.7	5.1	5.5	5.9	6.3	6.8	7.1
y_i	102.56	113.18	130.11	142.05	167.53	195.14	224.87	256.73	299.50	326.72

a. Construct the least squares polynomial of degree 1, and compute the error.

b. Construct the least squares polynomial of degree 2, and compute the error.

c. Construct the least squares polynomial of degree 3, and compute the error.

d. Construct the least squares approximation of the form be^{ax}, and compute the error.

e. Construct the least squares approximation of the form bx^a, and compute the error.

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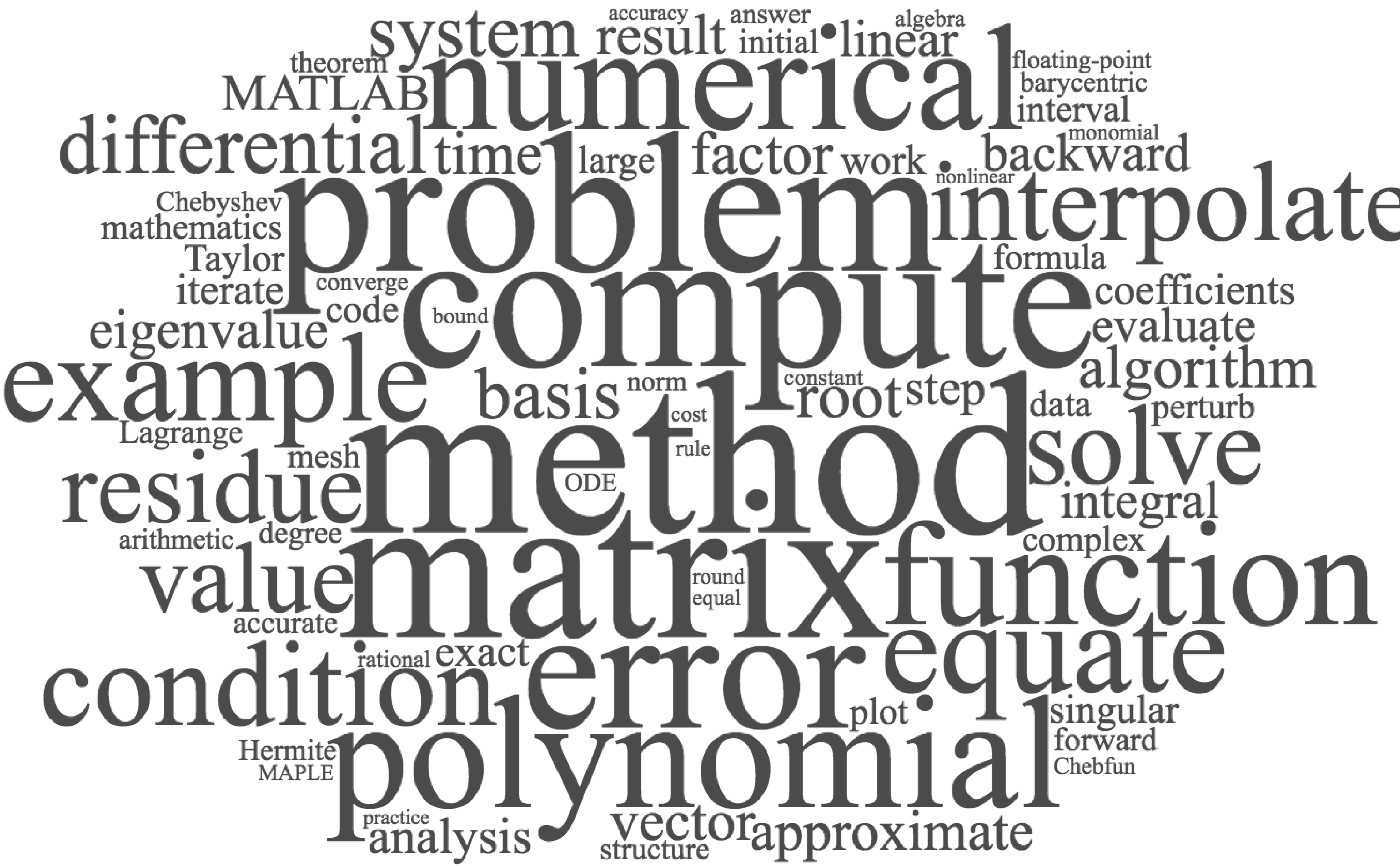
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solve
mesh
rule
residue
ODE
integral
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accurate
exact
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equate
condition
plot
singular
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Hermite
MAPLE
Chebfun
practice
analysis
vector
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