Contents 31

Numerical Methods of Approximation

Learning outcomes

In this Workbook you will learn about some numerical methods widely used in engineering applications.

You will learn how certain data may be modelled, how integrals and derivatives may be approximated and how estimates for the solutions of non-linear equations may be found.

Polynomial Approximations

31.1

Introduction

Polynomials are functions with useful properties. Their relatively simple form makes them an ideal candidate to use as approximations for more complex functions. In this second Workbook on Numerical Methods, we begin by showing some ways in which certain functions of interest may be approximated by polynomials.

Prerequisites

Before starting this Section you should ...

- revise material on maxima and minima of functions of two variables
- be familiar with polynomials and Taylor series

Learning Outcomes

On completion you should be able to ...

- interpolate data with polynomials
- find the least squares best fit straight line to experimental data

1. Polynomials

A polynomial in x is a function of the form

$$p(x) = a_0 + a_1x + a_2x^2 + \dots a_nx^n \qquad (a_n \neq 0, \quad n \text{ a non-negative integer})$$

where $a_0, a_1, a_2, \dots, a_n$ are constants. We say that this polynomial p has **degree** equal to n. (The degree of a polynomial is the highest power to which the argument, here it is x, is raised.) Such functions are relatively simple to deal with, for example they are easy to differentiate and integrate. In this Section we will show ways in which a function of interest can be approximated by a polynomial. First we briefly ensure that we are certain what a polynomial is.

Example 1

Which of these functions are polynomials in x? In the case(s) where f *is* a polynomial, give its degree.

(a) $f(x) = x^2 - 2 - \frac{1}{x}$, (b) $f(x) = x^4 + x - 6$, (c) $f(x) = 1$,

(d) $f(x) = mx + c$, m and c are constants. (e) $f(x) = 1 - x^6 + 3x^3 - 5x^3$

Solution

(a) This is not a polynomial because of the $\frac{1}{x}$ term (no negative powers of the argument are allowed in polynomials).
(b) This is a polynomial in x of degree 4.
(c) This is a polynomial of degree 0.
(d) This straight line function is a polynomial in x of degree 1 if $m \neq 0$ and of degree 0 if $m = 0$.
(e) This is a polynomial in x of degree 6.

Task

Which of these functions are polynomials in x? In the case(s) where f *is* a polynomial, give its degree.

(a) $f(x) = (x-1)(x+3)$ (b) $f(x) = 1 - x^7$ (c) $f(x) = 2 + 3e^x - 4e^{2x}$

(d) $f(x) = \cos(x) + \sin^2(x)$

Your solution

Answer
(a) This function, like all quadratics, is a polynomial of degree 2.
(b) This is a polynomial of degree 7.
(c) and (d) These are not polynomials in x. Their Maclaurin expansions have infinitely many terms.

We have in fact already seen, in HELM 16, one way in which some functions may be approximated by polynomials. We review this next.

2. Taylor series

In HELM 16 we encountered Maclaurin series and their generalisation, Taylor series. Taylor series are a useful way of approximating functions by polynomials. The Taylor series expansion of a function $f(x)$ about $x = a$ may be stated

$$f(x) = f(a) + (x-a)f'(a) + \tfrac{1}{2}(x-a)^2 f''(a) + \tfrac{1}{3!}(x-a)^3 f'''(a) + \dots .$$

(The special case called Maclaurin series arises when $a = 0$.)
The general idea when using this formula in practice is to consider only points x which are near to a. Given this it follows that $(x-a)$ will be small, $(x-a)^2$ will be even smaller, $(x-a)^3$ will be smaller still, and so on. This gives us confidence to simply neglect the terms beyond a certain power, or, to put it another way, to **truncate** the series.

Example 2

Find the Taylor polynomial of degree 2 about the point $x = 1$, for the function $f(x) = \ln(x)$.

Solution

In this case $a = 1$ and we need to evaluate the following terms

$$f(a) = \ln(a) = \ln(1) = 0, \qquad f'(a) = 1/a = 1, \qquad f''(a) = -1/a^2 = -1.$$

Hence

$$\ln(x) \approx 0 + (x-1) - \frac{1}{2}(x-1)^2 = -\frac{3}{2} + 2x - \frac{x^2}{2}$$

which will be reasonably accurate for x close to 1, as you can readily check on a calculator or computer. For example, for all x between 0.9 and 1.1, the polynomial and logarithm agree to at least 3 decimal places.

One drawback with this approach is that we need to find (possibly many) derivatives of f. Also, there can be some doubt over what is the best choice of a. The statement of Taylor series is an extremely useful piece of theory, but it can sometimes have limited appeal as a means of approximating functions by polynomials.

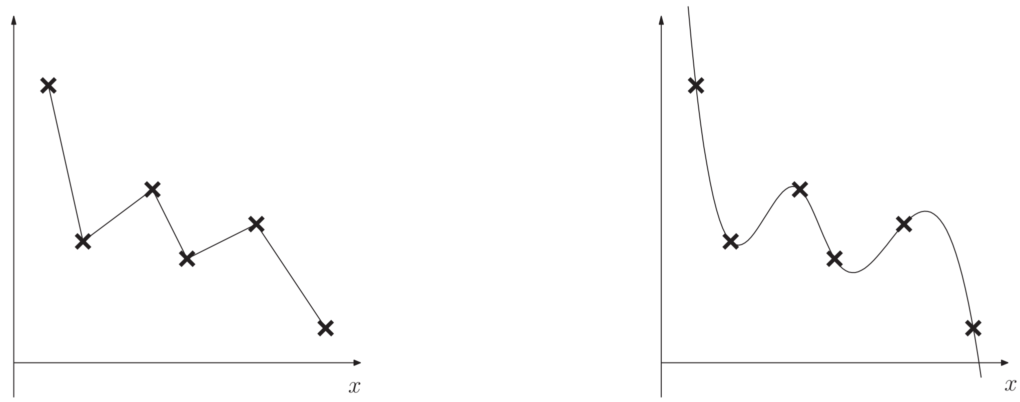
Next we will consider two alternative approaches.

3. Polynomial approximations - exact data

Here and in subsections 4 and 5 we consider cases where, rather than knowing an expression for the function, we have a list of point values. Sometimes it is good enough to find a polynomial that passes *near* these points (like putting a straight line through experimental data). Such a polynomial is an approximating polynomial and this case follows in subsection 4. Here and in subsection 5 we deal with the case where we want a polynomial to pass *exactly* through the given data, that is, an **interpolating polynomial**.

Lagrange interpolation

Suppose that we know (or choose to sample) a function f *exactly* at a few points and that we want to approximate how the function behaves between those points. In its simplest form this is equivalent to a dot-to-dot puzzle (see Figure 1(a)), but it is often more desirable to seek a curve that does not have"corners" in it (see Figure 1(b)).



(a) Linear, or "dot-to-dot", interpolation, with corners at all of the data points.

(b) A smoother interpolation of the data points.

Figure 1

Let us suppose that the data are in the form (x_1, f_1), (x_2, f_2), (x_3, f_3), $\ldots$, these are the points plotted as crosses on the diagrams above. (For technical reasons, and those of common sense, we suppose that the x-values in the data are all distinct.)

Our aim is to find a polynomial which passes exactly through the given data points. We want to find $p(x)$ such that

$$p(x_1) = f_1, \quad p(x_2) = f_2, \quad p(x_3) = f_3, \quad \ldots$$

There is a mathematical trick we can use to achieve this. We define **Lagrange polynomials** L_1, L_2, L_3, $\ldots$ which have the following properties:

$$\begin{array}{rclll} L_1(x) &=& 1, & \text{at } x = x_1, & L_1(x) = 0, \quad \text{at } x = x_2, x_3, x_4 \ldots \\ L_2(x) &=& 1, & \text{at } x = x_2, & L_2(x) = 0, \quad \text{at } x = x_1, x_3, x_4 \ldots \\ L_3(x) &=& 1, & \text{at } x = x_3, & L_3(x) = 0, \quad \text{at } x = x_1, x_2, x_4 \ldots \\ & \vdots & & & \vdots \end{array}$$

Each of these functions acts like a filter which "turns off" if you evaluate it at a data point other than its own. For example if you evaluate L_2 at any data point other than x_2, you will get zero.

Furthermore, if you evaluate any of these Lagrange polynomials at its own data point, the value you get is 1. These two properties are enough to be able to write down what $p(x)$ must be:

$$p(x) = f_1 L_1(x) + f_2 L_2(x) + f_3 L_3(x) + \ldots$$

and this does work, because if we evaluate p at one of the data points, let us take x_2 for example, then

$$p(x_2) = f_1 \underbrace{L_1(x_2)}_{=0} + f_2 \underbrace{L_2(x_2)}_{=1} + f_3 \underbrace{L_3(x_2)}_{=0} + \cdots = f_2$$

as required. The filtering property of the Lagrange polynomials picks out exactly the right f-value for the current x-value. Between the data points, the expression for p above will give a smooth polynomial curve.
This is all very well as long as we can work out what the Lagrange polynomials are. It is not hard to check that the following definitions have the right properties.

Key Point 1

Lagrange Polynomials

$$L_1(x) = \frac{(x-x_2)(x-x_3)(x-x_4)\ldots}{(x_1-x_2)(x_1-x_3)(x_1-x_4)\ldots}$$

$$L_2(x) = \frac{(x-x_1)(x-x_3)(x-x_4)\ldots}{(x_2-x_1)(x_2-x_3)(x_2-x_4)\ldots}$$

$$L_3(x) = \frac{(x-x_1)(x-x_2)(x-x_4)\ldots}{(x_3-x_1)(x_3-x_2)(x_3-x_4)\ldots}$$

and so on.

The numerator of $L_i(x)$ does not contain $(x - x_i)$.

The denominator of $L_i(x)$ does not contain $(x_i - x_i)$.

In each case the numerator ensures that the filtering property is in place, that is that the functions switch off at data points other than their own. The denominators make sure that the value taken at the remaining data point is equal to 1.

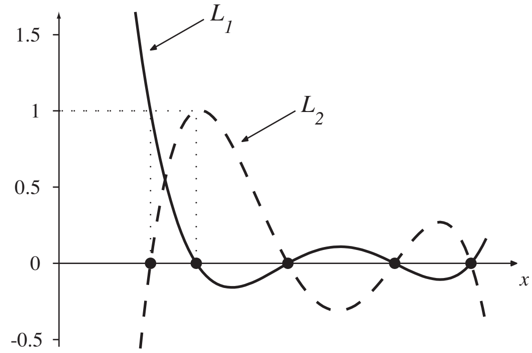


Figure 2

Figure 2 shows L_1 and L_2 in the case where there are five data points (the x positions of these data points are shown as large dots). Notice how both L_1 and L_2 are equal to zero at four of the data points and that $L_1(x_1) = 1$ and $L_2(x_2) = 1$.

In an implementation of this idea, things are simplified by the fact that we do not generally require an expression for $p(x)$. (This is good news, for imagine trying to multiply out all the algebra in the expressions for L_1, L_2, ...) What we *do* generally require is p evaluated at some specific value. The following Example should help show how this can be done.

Example 3

Let $p(x)$ be the polynomial of degree 3 which interpolates the data

x	0.8	1	1.4	1.6
$f(x)$	-1.82	-1.73	-1.40	-1.11

Evaluate $p(1.1)$.

Solution

We are interested in the Lagrange polynomials at the point $x = 1.1$ so we consider

$$L_1(1.1) = \frac{(1.1 - x_2)(1.1 - x_3)(1.1 - x_4)}{(x_1 - x_2)(x_1 - x_3)(x_1 - x_4)} = \frac{(1.1 - 1)(1.1 - 1.4)(1.1 - 1.6)}{(0.8 - 1)(0.8 - 1.4)(0.8 - 1.6)} = -0.15625.$$

Similar calculations for the other Lagrange polynomials give

$$L_2(1.1) = 0.93750, \quad L_3(1.1) = 0.31250, \quad L_4(1.1) = -0.09375,$$

and we find that our interpolated polynomial, evaluated at $x = 1.1$ is

$$\begin{aligned} p(1.1) &= f_1L_1(1.1) + f_2L_2(1.1) + f_3L_3(1.1) + f_4L_4(1.1) \\ &= -1.82 \times -0.15625 + -1.73 \times 0.9375 + -1.4 \times 0.3125 + -1.11 \times -0.09375 \\ &= -1.670938 \\ &= -1.67 \qquad \text{to the number of decimal places to which the data were given.} \end{aligned}$$

Key Point 2

Quote the answer only to the same number of decimal places as the given data (or to less places).

Task

Let $p(x)$ be the polynomial of degree 3 which interpolates the data

x	0.1	0.2	0.3	0.4
$f(x)$	0.91	0.70	0.43	0.52

Evaluate $p(0.15)$.

Your solution

Answer

We are interested in the Lagrange polynomials at the point $x = 0.15$ so we consider

$$L_1(0.15) = \frac{(0.15 - x_2)(0.15 - x_3)(0.15 - x_4)}{(x_1 - x_2)(x_1 - x_3)(x_1 - x_4)} = \frac{(0.15 - 0.2)(0.15 - 0.3)(0.15 - 0.4)}{(0.1 - 0.2)(0.1 - 0.3)(0.1 - 0.4)} = 0.3125.$$

Similar calculations for the other Lagrange polynomials give

$$L_2(0.15) = 0.9375, \quad L_3(0.15) = -0.3125, \quad L_4(0.15) = 0.0625,$$

and we find that our interpolated polynomial, evaluated at $x = 0.15$ is

$$\begin{aligned} p(0.15) &= f_1 L_1(0.15) + f_2 L_2(0.15) + f_3 L_3(0.15) + f_4 L_4(0.15) \\ &= 0.91 \times 0.3125 + 0.7 \times 0.9375 + 0.43 \times -0.3125 + 0.52 \times 0.0625 \\ &= 0.838750 \\ &= 0.84, \quad \text{to 2 decimal places.} \end{aligned}$$

The next Example is very much the same as Example 3 and the Task above. Try not to let the specific application, and the slight change of notation, confuse you.

Example 4

A designer wants a curve on a diagram he is preparing to pass through the points

x	0.25	0.5	0.75	1
y	0.32	0.65	0.43	0.10

He decides to do this by using an interpolating polynomial $p(x)$. What is the y-value corresponding to $x = 0.8$?

Solution

We are interested in the Lagrange polynomials at the point $x = 0.8$ so we consider

$$L_1(0.8) = \frac{(0.8 - x_2)(0.8 - x_3)(0.8 - x_4)}{(x_1 - x_2)(x_1 - x_3)(x_1 - x_4)} = \frac{(0.8 - 0.5)(0.8 - 0.75)(0.8 - 1)}{(0.25 - 0.5)(0.25 - 0.75)(0.25 - 1)} = 0.032.$$

Similar calculations for the other Lagrange polynomials give

$$L_2(0.8) = -0.176, \quad L_3(0.8) = 1.056, \quad L_4(0.8) = 0.088,$$

and we find that our interpolated polynomial, evaluated at $x = 0.8$ is

$$\begin{aligned} p(0.8) &= y_1 L_1(0.8) + y_2 L_2(0.8) + y_3 L_3(0.8) + y_4 L_4(0.8) \\ &= 0.32 \times 0.032 + 0.65 \times -0.176 + 0.43 \times 1.056 + 0.1 \times 0.088 \\ &= 0.358720 \\ &= 0.36 \quad \text{to 2 decimal places.} \end{aligned}$$

In this next Task there are five points to interpolate. It therefore takes a polynomial of degree 4 to interpolate the data and this means we must use five Lagrange polynomials.

Task

The hull drag f of a racing yacht as a function of the hull speed, v, is known to be

v	0.0	0.5	1.0	1.5	2.0
f	0.00	19.32	90.62	175.71	407.11

(Here, the units for f and v are N and m s^{-1}, respectively.)

Use Lagrange interpolation to fit this data and hence approximate the drag corresponding to a hull speed of 2.5 m s^{-1}.

Your solution

Answer

We are interested in the Lagrange polynomials at the point $v = 2.5$ so we consider

$$\begin{aligned} L_1(2.5) &= \frac{(2.5 - v_2)(2.5 - v_3)(2.5 - v_4)(2.5 - v_5)}{(v_1 - v_2)(v_1 - v_3)(v_1 - v_4)(v_1 - v_5)} \\ &= \frac{(2.5 - 0.5)(2.5 - 1.0)(2.5 - 1.5)(2.5 - 2.0)}{(0.0 - 0.5)(0.0 - 1.0)(0.0 - 1.5)(0.0 - 2.0)} = 1.0 \end{aligned}$$

Similar calculations for the other Lagrange polynomials give

$$L_2(2.5) = -5.0, \quad L_3(2.5) = 10.0, \quad L_4(2.5) = -10.0, \quad L_5(2.5) = 5.0$$

and we find that our interpolated polynomial, evaluated at $x = 2.5$ is

$$\begin{aligned} p(2.5) &= f_1 L_1(2.5) + f_2 L_2(2.5) + f_3 L_3(2.5) + f_4 L_4(2.5) + f_5 L_5(2.5) \\ &= 0.00 \times 1.0 + 19.32 \times -5.0 + 90.62 \times 10.0 + 175.71 \times -10.0 + 407.11 \times 5.0 \\ &= 1088.05 \end{aligned}$$

This gives us the approximation that the hull drag on the yacht at 2.5 m s^{-1} is about 1100 N.

The following Example has time t as the independent variable, and two quantities, x and y, as dependent variables to be interpolated. We will see however that exactly the same approach as before works.

Example 5

An animator working on a computer generated cartoon has decided that her main character's right index finger should pass through the following (x, y) positions on the screen at the following times t

t	0	0.2	0.4	0.6
x	1.00	1.20	1.30	1.25
y	2.00	2.10	2.30	2.60

Use Lagrange polynomials to interpolate these data and hence find the (x, y) position at time $t = 0.5$. Give x and y to 2 decimal places.

Solution

In this case t is the independent variable, and there are two dependent variables: x and y. We are interested in the Lagrange polynomials at the time $t = 0.5$ so we consider

$$L_1(0.5) = \frac{(0.5 - t_2)(0.5 - t_3)(0.5 - t_4)}{(t_1 - t_2)(t_1 - t_3)(t_1 - t_4)} = \frac{(0.5 - 0.2)(0.5 - 0.4)(0.5 - 0.6)}{(0 - 0.2)(0 - 0.4)(0 - 0.6)} = 0.0625$$

Similar calculations for the other Lagrange polynomials give

$$L_2(0.5) = -0.3125, \quad L_3(0.5) = 0.9375, \quad L_4(0.5) = 0.3125$$

Solution (contd.)

These values for the Lagrange polynomials can be used for both of the interpolations we need to do. For the x-value we obtain

$$\begin{aligned} x(0.5) &= x_1L_1(0.5) + x_2L_2(0.5) + x_3L_3(0.5) + x_4L_4(0.5) \\ &= 1.00 \times 0.0625 + 1.20 \times -0.3125 + 1.30 \times 0.9375 + 1.25 \times 0.3125 \\ &= 1.30 \quad \text{to 2 decimal places} \end{aligned}$$

and for the y value we get

$$\begin{aligned} y(0.5) &= y_1L_1(0.5) + y_2L_2(0.5) + y_3L_3(0.5) + y_4L_4(0.5) \\ &= 2.00 \times 0.0625 + 2.10 \times -0.3125 + 2.30 \times 0.9375 + 2.60 \times 0.3125 \\ &= 2.44 \quad \text{to 2 decimal places} \end{aligned}$$

Error in Lagrange interpolation

When using Lagrange interpolation through n points $(x_1, f_1), (x_2, f_2), \ldots, (x_n, f_n)$ the error, in the estimate of $f(x)$ is given by

$$E(x) = \frac{(x - x_1)(x - x_2)\ldots(x - x_n)}{n!} f^{(n)}(\eta) \qquad \text{where } \eta \in [x, x_1, x_n]$$

N.B. The value of η is not known precisely, only the interval in which it lies. Normally x will lie in the interval $[x_1, x_n]$ (that's **interpolation**). If x lies outside the interval $[x_1, x_n]$ then that's called **extrapolation** and a larger error is likely.

Of course we will not normally know what f is (indeed no f may exist for experimental data). However, sometimes f can at least be estimated. In the following (somewhat artificial) example we will be told f and use it to check that the above error formula is reasonable.

Example 6

In an experiment to determine the relationship between power gain (G) and power output (P) in an amplifier, the following data were recorded.

P	5	7	8	11
G	0.00	1.46	2.04	3.42

(a) Use Lagrange interpolation to fit an appropriate quadratic, $q(x)$, to estimate the gain when the output is 6.5. Give your answer to an appropriate accuracy.

(b) Given that $G \equiv 10\log_{10}(P/5)$ show that the actual error which occurred in the Lagrange interpolation in (a) lies withing the theoretical error limits.

Solution

For a quadratic, $q(x)$, we need to fit **three** points and those most appropriate (nearest 6.5) are for P at $5, 7, 8$:

$$\begin{aligned} q(6.5) &= \frac{(6.5-7)(6.5-8)}{(5-7)(5-8)} \times 0.00 \\ &+ \frac{(6.5-5)(6.5-8)}{(7-5)(7-8)} \times 1.46 \\ &+ \frac{(6.5-5)(6.5-7)}{(8-5)(8-7)} \times 2.04 \\ &= 0 + 1.6425 - 0.5100 \\ &= 1.1325 \qquad \text{working to } 4 \text{ d.p.} \\ &\approx 1.1 \qquad \text{(rounding to sensible accuracy)} \end{aligned}$$

(b) We use the error formula

$$E(x) = \frac{(x-x_1)\ldots(x-x_n)}{n!} f^{(n)}(\eta), \qquad \eta \in [x, x_1, \ldots, x_n]$$

Here $f(x) \equiv G(x) = \log_{10}(P/5)$ and $n = 3$:

$$\begin{aligned} \frac{d(\log_{10}(P/5))}{dP} &= \frac{d(\log_{10}(P) - \log_{10}(5))}{dP} = \frac{d(\log_{10}(P))}{dP} \\ &= \frac{d}{dP}\left(\frac{\ln P}{\ln 10}\right) = \frac{1}{\ln 10}\frac{1}{P} \end{aligned}$$

So $\dfrac{d^3}{dP^3}(\log_{10}(P/5)) = \dfrac{1}{\ln 10}\dfrac{2}{P^3}$.

Substituting for $f^{(3)}(\eta)$:

$$\begin{aligned} E(6.5) &= \frac{(6.5-6)(6.5-7)(6.5-8)}{6} \times \frac{10}{\ln 10} \times \frac{2}{\eta^3}, \qquad \eta \in [5, 8] \\ &= \frac{1.6286}{\eta^3} \qquad \eta \in [5, 8] \end{aligned}$$

Taking $\eta = 5$: $\quad E_{\mathsf{max}} = 0.0131$

Taking $\eta = 8$: $\quad E_{\mathsf{min}} = 0.0031$

Taking $x = 6.5$: $\quad E_{\mathsf{actual}} = G(6.5) - q(6.5)$

$$\begin{aligned} &= 10\log_{10}(6.5/5) - 1.1325 \\ &= 1.1394 - 1.1325 \\ &= 0.0069 \end{aligned}$$

The theory is satisfied because $E_{\mathsf{min}} < E_{\mathsf{actual}} < E_{\mathsf{max}}$.

Task

(a) Use Lagrange interpolation to estimate $f(8)$ to appropriate accuracy given the table of values below, by means of the appropriate cubic interpolating polynomial

x	2	5	7	9	10
$f(x)$	0.980067	0.8775836	0.764842	0.621610	0.540302

Your solution

Answer

The most appropriate cubic passes through x at $5, 7, 9, 10$

$x = 8 \quad x_1 = 5, \quad x_2 = 7, \quad x_3 = 9, \quad x_4 = 10$

$$\begin{aligned}
p(8) &= \frac{(8-7)(8-9)(8-10)}{(5-7)(5-9)(5-10)} \times 0.877583 \\
&+ \frac{(8-5)(8-9)(8-10)}{(7-5)(7-9)(7-10)} \times 0.764842 \\
&+ \frac{(8-5)(8-7)(8-10)}{(9-5)(9-7)(9-10)} \times 0.621610 \\
&+ \frac{(8-5)(8-7)(8-9)}{(10-5)(10-7)(10-9)} \times 0.540302 \\
&= -\frac{1}{20} \times 0.877583 + \frac{1}{2} \times 0.764842 + \frac{3}{4} \times 0.621610 - \frac{1}{5} \times 0.540302 \\
&= 0.6966689
\end{aligned}$$

Suitable accuracy is 0.6967 (rounded to 4 d.p.).

(b) Given that the table in (a) represents $f(x) \equiv \cos(x/10)$, calculate theoretical bounds for the estimate obtained:

Your solution

Answer

$$E(8) = \frac{(8-5)(8-7)(8-9)(8-10)}{4!} f^{(4)}(\eta), \qquad 5 \leq \eta \leq 10$$

$$f(\eta) = \cos\left(\frac{\eta}{10}\right) \qquad \text{so} \qquad f^{(4)}(\eta) = \frac{1}{10^4}\cos\left(\frac{\eta}{10}\right)$$

$$E(8) = \frac{1}{4\times 10^4}\cos\left(\frac{\eta}{10}\right), \qquad \eta \in [5, 10]$$

$$E_{\text{min}} = \frac{1}{4\times 10^4}\cos(1) \qquad E_{\text{max}} = \frac{1}{4\times 10^4}\cos(0.5)$$

This leads to

$$0.696689 + 0.000014 \leq \text{True Value} \leq 0.696689 + 0.000022$$

$$\Rightarrow \qquad 0.696703 \leq \text{True Value} \leq 0.696711$$

We can conclude that the True Value is 0.69670 or 0.69671 to 5 d.p. or 0.6967 to 4 d.p. (actual value is 0.696707).

4. Polynomial approximations - experimental data

You may well have experience in carrying out an experiment and then trying to get a straight line to pass as near as possible to the data plotted on graph paper. This process of adjusting a clear ruler over the page until it looks "about right" is fine for a rough approximation, but it is not especially scientific. Any software you use which provides a "best fit" straight line must obviously employ a less haphazard approach.

Here we show one way in which best fit straight lines may be found.

Best fit straight lines

Let us consider the situation mentioned above of trying to get a straight line $y = mx + c$ to be as near as possible to experimental data in the form (x_1, f_1), (x_2, f_2), (x_3, f_3), $\ldots$.

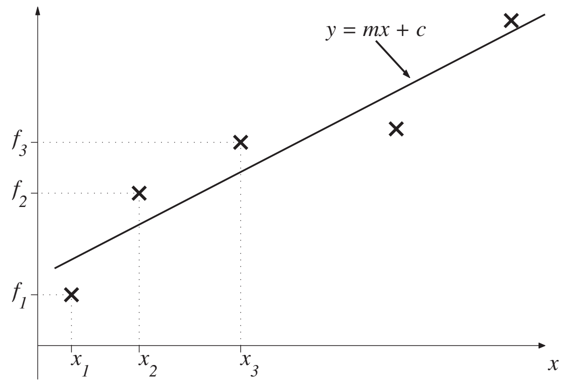


Figure 3

We want to minimise the overall distance between the crosses (the data points) and the straight line. There are a few different approaches, but the one we adopt here involves minimising the quantity

$$R = \underbrace{(mx_1 + c - f_1)}_{\substack{\text{vertical distance}\\ \text{between line and}\\ \text{the point } (x_1, f_1)}}{}^2 + \underbrace{(mx_2 + c - f_2)}_{\substack{\text{second data point}\\ \text{distance}}}{}^2 + \underbrace{(mx_3 + c - f_3)}_{\substack{\text{third data point}\\ \text{distance}}}{}^2 + \ldots$$

$$= \sum \Big(mx_n + c - f_n\Big)^2.$$

Each term in the sum measures the vertical distance between a data point and the straight line. (Squaring the distances ensures that distances above and below the line do not cancel each other out. It is because we are minimising the distances squared that the straight line we will find is called the **least squares** best fit straight line.)

In order to minimise R we can imagine sliding the clear ruler around on the page until the line looks right; that is we can imagine varying the slope m and y-intercept c of the line. We therefore think of R as a function of the two variables m and c and, as we know from our earlier work on maxima and minima of functions, the minimisation is achieved when

$$\frac{\partial R}{\partial c} = 0 \qquad \text{and} \qquad \frac{\partial R}{\partial m} = 0.$$

(We know that this will correspond to a minimum because R has no maximum, for whatever value R takes we can always make it bigger by moving the line further away from the data points.)
Differentiating R with respect to m and c gives

$$\begin{aligned}
\frac{\partial R}{\partial c} &= 2\,(mx_1 + c - f_1) + 2\,(mx_2 + c - f_2) + 2\,(mx_3 + c - f_3) + \ldots \\
&= 2\sum \Big(mx_n + c - f_n\Big) \qquad \text{and} \\
\frac{\partial R}{\partial m} &= 2\,(mx_1 + c - f_1)\,x_1 + 2\,(mx_2 + c - f_2)\,x_2 + 2\,(mx_3 + c - f_3)\,x_3 + \ldots \\
&= 2\sum \Big(mx_n + c - f_n\Big)\,x_n,
\end{aligned}$$

respectively. Setting both of these quantities equal to zero (and cancelling the factor of 2) gives a pair of simultaneous equations for m and c. This pair of equations is given in the Key Point below.

Key Point 3

The least squares best fit straight line to the experimental data

$$(x_1, f_1), \quad (x_2, f_2), \quad (x_3, f_3), \quad \ldots (x_n, f_n)$$

is

$$y = mx + c$$

where m and c are found by solving the pair of equations

$$\begin{aligned}
c\left(\sum_1^n 1\right) + m\left(\sum_1^n x_n\right) &= \sum_1^n f_n, \\
c\left(\sum_1^n x_n\right) + m\left(\sum_1^n x_n^2\right) &= \sum_1^n x_n f_n.
\end{aligned}$$

(The term $\sum_1^n 1$ is simply equal to the number of data points, n.)

Example 7

An experiment is carried out and the following data obtained:

x_n	0.24	0.26	0.28	0.30
f_n	1.25	0.80	0.66	0.20

Obtain the least squares best fit straight line, $y = mx + c$, to these data. Give c and m to 2 decimal places.

Solution

For a hand calculation, tabulating the data makes sense:

x_n	f_n	x_n^2	$x_n f_n$
0.24	1.25	0.0576	0.3000
0.26	0.80	0.0676	0.2080
0.28	0.66	0.0784	0.1848
0.30	0.20	0.0900	0.0600
1.08	2.91	0.2936	0.7528

The quantity $\sum 1$ counts the number of data points and in this case is equal to 4.
It follows that the pair of equations for m and c are:

$$\begin{aligned} 4c + 1.08m &= 2.91 \\ 1.08c + 0.2936m &= 0.7528 \end{aligned}$$

Solving these gives $c = 5.17$ and $m = -16.45$ and we see that the least squares best fit straight line to the given data is

$$y = 5.17 - 16.45x$$

Figure 4 shows how well the straight line fits the experimental data.

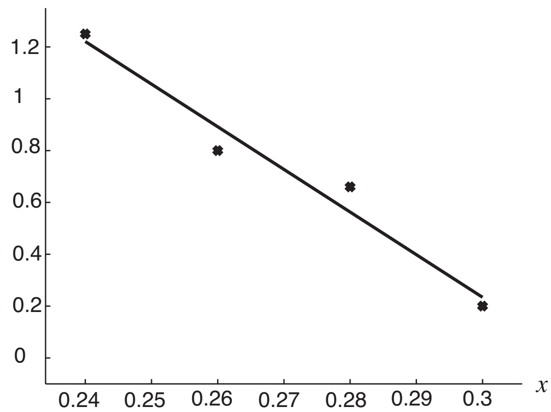


Figure 4

Example 8

Find the best fit straight line to the following experimental data:

x_n	0.00	1.00	2.00	3.00	4.00
f_n	1.00	3.85	6.50	9.35	12.05

Solution

In order to work out all of the quantities appearing in the pair of equations we tabulate our calculations as follows

	x_n	f_n	x_n^2	$x_n f_n$
	0.00	1.00	0.00	0.00
	1.00	3.85	1.00	3.85
	2.00	6.50	4.00	13.00
	3.00	9.35	9.00	28.05
	4.00	12.05	16.00	48.20
$\sum$	10.00	32.75	30.00	93.10

The quantity $\sum 1$ counts the number of data points and is in this case equal to 5.

Hence our pair of equations is

$$5c + 10m = 32.95$$

$$10c + 30m = 93.10$$

Solving these equations gives $c = 1.03$ and $m = 2.76$ and this means that our best fit straight line to the given data is

$$y = 1.03 + 2.76x$$

Task

An experiment is carried out and the data obtained are as follows:

x_n	0.2	0.3	0.5	0.9
f_n	5.54	4.02	3.11	2.16

Obtain the least squares best fit straight line, $y = mx + c$, to these data. Give c and m to 2 decimal places.

Your solution

Answer

Tabulating the data gives

	x_n	f_n	x_n^2	$x_n f_n$
	0.2	5.54	0.04	1.108
	0.3	4.02	0.09	1.206
	0.5	3.11	0.25	1.555
	0.9	2.16	0.81	1.944
$\sum$	1.9	14.83	1.19	5.813

The quantity $\sum 1$ counts the number of data points and in this case is equal to 4.
It follows that the pair of equations for m and c are:

$$\begin{aligned} 4c + 1.9m &= 14.83 \\ 1.9c + 1.19m &= 5.813 \end{aligned}$$

Solving these gives $c = 5.74$ and $m = -4.28$ and we see that the least squares best fit straight line to the given data is

$$y = 5.74 - 4.28x$$

Task

Power output P of a semiconductor laser diode, operating at $35°$C, as a function of the drive current I is measured to be

I	70	72	74	76
P	1.33	2.08	2.88	3.31

(Here I and P are measured in mA and mW respectively.)

It is known that, above a certain threshold current, the laser power increases linearly with drive current. Use the least squares approach to fit a straight line, $P = mI + c$, to these data. Give c and m to 2 decimal places.

Your solution

Answer

Tabulating the data gives

	I	P	I^2	$I \times P$
	70	1.33	4900	93.1
	72	2.08	5184	149.76
	74	2.88	5476	213.12
	76	3.31	5776	251.56
	292	9.6	21336	707.54

The quantity $\sum 1$ counts the number of data points and in this case is equal to 4.
It follows that the pair of equations for m and c are:

$$\begin{aligned} 4c + 292m &= 9.6 \\ 292c + 21336m &= 707.54 \end{aligned}$$

Solving these gives $c = -22.20$ and $m = 0.34$ and we see that the least squares best fit straight line to the given data is

$$P = -22.20 + 0.34I.$$

5. Polynomial approximations - splines

We complete this Section by briefly describing another approach that can be used in the case where the data are exact.

Why are splines needed?

Fitting a polynomial to the data (using Lagrange polynomials, for example) works very well when there are a small number of data points. But if there were 100 data points it would be silly to try to fit a polynomial of degree 99 through all of them. It would be a great deal of work and anyway polynomials of high degree can be very oscillatory giving poor approximations between the data points to the underlying function.

What are splines?

Instead of using a polynomial valid for all x, we use one polynomial for $x_1 < x < x_2$, then a different polynomial for $x_2 < x < x_3$ then a different one again for $x_3 < x < x_4$, and so on.
We have already seen one instance of this approach in this Section. The "dot to dot" interpolation that we abandoned earlier (Figure 1(a)) is an example of a **linear spline**. There is a different straight line between each pair of data points.

The most commonly used splines are **cubic splines**. We use a different polynomial of degree three between each pair of data points. Let $s = s(x)$ denote a cubic spline, then

$$\begin{aligned} s(x) &= a_1(x-x_1)^3 + b_1(x-x_1)^2 + c_1(x-x_1) + d_1 \qquad (x_1 < x < x_2) \\ s(x) &= a_2(x-x_2)^3 + b_2(x-x_2)^2 + c_2(x-x_2) + d_2 \qquad (x_2 < x < x_3) \\ s(x) &= a_3(x-x_3)^3 + b_3(x-x_3)^2 + c_3(x-x_3) + d_3 \qquad (x_3 < x < x_4) \\ &\vdots \end{aligned}$$

And we need to find a_1, b_1, c_1, d_1, a_2, ... to determine the full form for the spline $s(x)$. Given the large number of quantities that have to be assigned (four for every pair of adjacent data points) it is possible to give s some very nice properties:

- $s(x_1) = f_1$, $s(x_2) = f_2$, $s(x_3) = f_3$, ... This is the least we should expect, as it simply states that s interpolates the given data.
- $s'(x)$ is continuous at the data points. This means that there are no "corners" at the data points - the whole curve is smooth.
- $s''(x)$ is continuous. This reduces the occurrence of points of inflection appearing at the data points and leads to a smooth interpolant.

Even with all of these requirements there are still two more properties we can assign to s. A **natural cubic spline** is one for which s'' is zero at the two end points. The natural cubic spline is, in some sense, the smoothest possible spline, for it minimises a measure of the curvature.

How is a spline found?

Now that we have described what a **natural cubic spline** is, we briefly describe how it is found. Suppose that there are N data points. For a natural cubic spline we require $s''(x_1) = s''(x_N) = 0$ and values of s'' taken at the other data points are found from the system of equations in Key Point 4.

Key Point 4

Cubic Spline Equations

$$\begin{bmatrix} k_2 & h_2 & & & \\ h_2 & k_3 & h_3 & & \\ & \ddots & \ddots & \ddots & \\ & & h_{N-3} & k_{N-2} & h_{N-2} \\ & & & h_{N-2} & k_{N-1} \end{bmatrix} \begin{bmatrix} s''(x_2) \\ s''(x_3) \\ \vdots \\ s''(x_{N-2}) \\ s''(x_{N-1}) \end{bmatrix} = \begin{bmatrix} r_2 \\ r_3 \\ \vdots \\ r_{N-2} \\ r_{N-1} \end{bmatrix}$$

in which

$$h_1 = x_2 - x_1, \quad h_2 = x_3 - x_2, \quad h_3 = x_4 - x_3, \quad h_4 = x_5 - x_4, \ldots$$

$$k_2 = 2(h_1 + h_2), \quad k_3 = 2(h_2 + h_3), \quad k_4 = 2(h_3 + h_4), \ldots$$

$$r_2 = 6\left(\frac{f_3 - f_2}{h_2} - \frac{f_2 - f_1}{h_1}\right), \quad r_3 = 6\left(\frac{f_4 - f_3}{h_3} - \frac{f_3 - f_2}{h_2}\right), \ldots$$

Admittedly the system of equations in Key Point 4 looks unappealing, but this is a “nice” system of equations. It was pointed out at the end of HELM 30 that some applications lead to systems of equations involving matrices which are **strictly diagonally dominant**. The matrix above is of that type since the diagonal entry is always twice as big as the sum of off-diagonal entries.

Once the system of equations is solved for the second derivatives s'', the spline s can be found as follows:

$$a_i = \frac{s''(x_{i+1}) - s''(x_i)}{6h_i}, \quad b_i = \frac{s''(x_i)}{2}, \quad c_i = \frac{f_{i+1} - f_i}{h_i} - \left(\frac{s''(x_{i+1}) + 2s''(x_i)}{6}\right) h_i, \quad d_i = f_i$$

We now present an Example illustrating this approach.

Example 9

Find the natural cubic spline which interpolates the data

x_j	1	3	5	8
f_j	0.85	0.72	0.34	0.67

Solution

In the notation now established we have $h_1 = 2$, $h_2 = 2$ and $h_3 = 3$. For a *natural* cubic spline we require s'' to be zero at x_1 and x_4. Values of s'' at the other data points are found from the system of equations given in Key Point 4. In this case the matrix is just 2×2 and the pair of equations are:

$$\begin{aligned} h_1 \underbrace{s''(x_1)}_{=0} + 2(h_1 + h_2)s''(x_2) + h_2 s''(x_3) &= 6\left(\frac{f_3 - f_2}{h_2} - \frac{f_2 - f_1}{h_1}\right) \\ h_2 s''(x_2) + 2(h_2 + h_3)s''(x_3) + h_3 \underbrace{s''(x_4)}_{=0} &= 6\left(\frac{f_4 - f_3}{h_3} - \frac{f_3 - f_2}{h_2}\right) \end{aligned}$$

In this case the equations become

$$\begin{pmatrix} 8 & 2 \\ 2 & 10 \end{pmatrix} \begin{pmatrix} s''(x_2) \\ s''(x_3) \end{pmatrix} = \begin{pmatrix} -0.75 \\ 1.8 \end{pmatrix}$$

Solving the coupled pair of equations leads to

$$s''(x_2) = -0.146053 \qquad s''(x_3) = 0.209211$$

We now find the coefficients a_1, b_1, etc. from the formulae and deduce that the spline is given by

$$\begin{aligned} s(x) &= -0.01217(x-1)^3 - 0.016316(x-1) + 0.85 \qquad (1 < x < 3) \\ s(x) &= 0.029605(x-3)^3 - 0.073026(x-3)^2 - 0.162368(x-3) + 0.72 \qquad (3 < x < 5) \\ s(x) &= -0.01162(x-5)^3 + 0.104605(x-5)^2 - 0.099211(x-5) + 0.34 \qquad (5 < x < 8) \end{aligned}$$

Figure 5 shows how the spline interpolates the data.

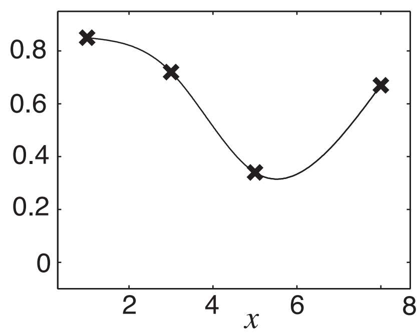


Figure 5

Task

Find the natural cubic spline which interpolates the data

x_j	1	2	3	5
f_j	0.1	0.24	0.67	0.91

Your solution

Answer

In the notation now established we have $h_1 = 1$, $h_2 = 1$ and $h_3 = 2$. For a *natural* cubic spline we require s'' to be zero at x_1 and x_4. Values of s'' at the other data points are found from the system of equations

$$\begin{aligned} h_1 \underbrace{s''(x_1)}_{=0} + 2(h_1 + h_2)s''(x_2) + h_2 s''(x_3) &= 6\left(\frac{f_3 - f_2}{h_2} - \frac{f_2 - f_1}{h_1}\right) \\ h_2 s''(x_2) + 2(h_2 + h_3)s''(x_3) + h_3 \underbrace{s''(x_4)}_{=0} &= 6\left(\frac{f_4 - f_3}{h_3} - \frac{f_3 - f_2}{h_2}\right) \end{aligned}$$

In this case the equations become

$$\begin{pmatrix} 4 & 1 \\ 1 & 6 \end{pmatrix}\begin{pmatrix} s''(x_2) \\ s''(x_3) \end{pmatrix} = \begin{pmatrix} 1.74 \\ -1.86 \end{pmatrix}$$

Solving the coupled pair of equations leads to $\quad s''(x_2) = 0.534783 \qquad s''(x_3) = -0.399130$

We now find the coefficients a_1, b_1, etc. from the formulae and deduce that the spline is

$$\begin{aligned} s(x) &= 0.08913(x-1)^3 + 0.05087(x-1) + 0.1 \qquad (1 < x < 2) \\ s(x) &= -0.15565(x-2)^3 + 0.267391(x-2)^2 + 0.318261(x-2) + 0.24 \qquad (2 < x < 3) \\ s(x) &= 0.033261(x-3)^3 - 0.199565(x-3)^2 + 0.386087(x-3) + 0.67 \qquad (3 < x < 5) \end{aligned}$$

Exercises

1. A political analyst is preparing a dossier involving the following data

x	10	15	20	25
$f(x)$	9.23	8.41	7.12	4.13

   She interpolates the data with a polynomial $p(x)$ of degree 3 in order to find an approximation $p(22)$ to $f(22)$. What value does she find for $p(22)$?

2. Estimate $f(2)$ to an appropriate accuracy from the table of values below by means of an appropriate quadratic interpolating polynomial.

x	1	3	3.5	6
$f(x)$	99.8	295.5	342.9	564.6

3. An experiment is carried out and the data obtained as follows

x_n	2	3	5	7
f_n	2.2	5.4	6.5	13.2

   Obtain the least squares best fit straight line, $y = mx + c$, to these data. (Give c and m to 2 decimal places.)

4. Find the natural cubic spline which interpolates the data

x_j	2	4	5	7
f_j	1.34	1.84	1.12	0.02

Answers

1. We are interested in the Lagrange polynomials at the point $x = 22$ so we consider

$$L_1(22) = \frac{(22-x_2)(22-x_3)(22-x_4)}{(x_1-x_2)(x_1-x_3)(x_1-x_4)} = \frac{(22-15)(22-20)(22-25)}{(10-15)(10-20)(10-25)} = 0.056.$$

Similar calculations for the other Lagrange polynomials give

$$L_2(22) = -0.288, \quad L_3(22) = 1.008, \quad L_4(22) = 0.224,$$

and we find that our interpolated polynomial, evaluated at $x = 22$ is

$$\begin{aligned} p(22) &= f_1L_1(22) + f_2L_2(22) + f_3L_3(22) + f_4L_4(22) \\ &= 9.23 \times 0.056 + 8.41 \times -0.288 + 7.12 \times 1.008 + 4.13 \times 0.224 \\ &= 6.197 \\ &= 6.20, \quad \text{to 2 decimal places,} \end{aligned}$$

which serves as the approximation to $f(22)$.

2.

$$\begin{aligned} f(2) &= \frac{(2-1)(2-3)}{(3.5-1)(3.5-3)} \times 342.9 + \frac{(2-1)(2-3.5)}{(3-1)(3-3.5)} \times 295.5 + \frac{(2-3)(2-3.5)}{(1-3)(1-3.5)} \times 99.8 \\ &= -274.32 + 443.25 + 29.94 \\ &= 198.87 \end{aligned}$$

Estimate is 199 (to 3 sig. fig.)

3. We tabulate the data for convenience:

	x_n	f_n	x_n^2	x_nf_n
	2	2.2	4	4.4
	3	5.4	9	16.2
	5	6.5	25	32.5
	7	13.2	49	92.4
$\sum$	17	27.3	87	145.5

The quantity $\sum 1$ counts the number of data points and in this case is equal to 4.
It follows that the pair of equations for m and c are as follows:

$$\begin{aligned} 4c + 17m &= 27.3 \\ 17c + 87m &= 145.5 \end{aligned}$$

Solving these gives $c = -1.67$ and $m = 2.00$, to 2 decimal places, and we see that the least squares best fit straight line to the given data is

$$y = -1.67 + 2.00x$$

Answers

4. In the notation now established we have $h_1 = 2$, $h_2 = 1$ and $h_3 = 2$. For a *natural* cubic spline we require s'' to be zero at x_1 and x_4. Values of s'' at the other data points are found from the system of equations

$$\begin{aligned} h_1 \underbrace{s''(x_1)}_{=0} + 2(h_1+h_2)s''(x_2) + h_2 s''(x_3) &= 6\left(\frac{f_3-f_2}{h_2} - \frac{f_2-f_1}{h_1}\right) \\ h_2 s''(x_2) + 2(h_2+h_3)s''(x_3) + h_3 \underbrace{s''(x_4)}_{=0} &= 6\left(\frac{f_4-f_3}{h_3} - \frac{f_3-f_2}{h_2}\right) \end{aligned}$$

In this case the equations become

$$\begin{pmatrix} 6 & 1 \\ 1 & 6 \end{pmatrix}\begin{pmatrix} s''(x_2) \\ s''(x_3) \end{pmatrix} = \begin{pmatrix} -5.82 \\ 1.02 \end{pmatrix}$$

Solving the coupled pair of equations leads to

$$s''(x_2) = -1.026857 \qquad s''(x_3) = 0.341143$$

We now find the coefficients a_1, b_1, etc. from the formulae and deduce that the spline is given by

$$\begin{aligned} s(x) &= -0.08557(x-2)^3 + 0.592286(x-2) + 1.34 \qquad (2 < x < 4) \\ s(x) &= 0.228(x-4)^3 - 0.513429(x-4)^2 - 0.434571(x-4) + 1.84 \qquad (4 < x < 5) \\ s(x) &= -0.02843(x-5)^3 + 0.170571(x-5)^2 - 0.777429(x-5) + 1.12 \qquad (5 < x < 7) \end{aligned}$$