Contens numerical methods of approximation

- 1. Polynomial approximations
- 2. Numerical integration
- 3. Numerical differentiation
- 4. Nonlinear equations

Learning outcomes

Time allocation

You are expected to spend approximately thirteen hours of independent study on the material presented in this workbook. However, depending upon your ability to concentrate and on your previous experience with certain mathematical topics this time may vary considerably.

Polynomial approximations





Polynomials are functions with useful properties. Their relatively simple form makes them an ideal candidate to use as approximations.

In this second Workbook on Numerical Methods, we begin by showing some ways in which certain functions of interest may be approximated by polynomials.

Before starting this Section you should	 revise material on maxima and minima of functions of two variables reacquaint yourself with polynomials and Taylor series
Learning Outcomes	✓ interpolate data with polynomials

After completing this Section you should be able to ...

чg to experimental data

1. Polynomials

A polynomial in x is a function of the form

$$p(x) = a_0 + a_1 x + a_2 x^2 + \dots a_n x^n \qquad (a_n \neq 0)$$

where $a_0, a_1, a_2, \ldots, a_n$ are constants. We say that this 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, they are easy to differentiate and integrate, for example. 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 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) A polynomial of degree 0.

- (d) This straight line function is a polynomial of degree 1 if $m \neq 0$ and of degree 0 if m = 0.
- (e) Finally, a polynomial in x of degree 6.



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

- (c) and (d) These are not polynomials in x.
 - .7 sergeb to faimonylog a si sidT (d)
- (a) This function, like all quadratics, is a polynomial of degree 2.

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

2. Taylor series

In Workbook 16 we encountered Maclaurin series and its 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

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

(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 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

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

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

Here 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 a few pages. First we deal with the case where we want a polynomial to pass *exactly* through the given data, that is, an interpolating polynomial.

Exact data

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 boils down to a dot-to-dot puzzle, but it is often more desirable to seek an **interpolation** that does not have "corners" in it.



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

A smoother interpolation of the data points.

Let us suppose that the data we have is in the form (x_1, f_1) , (x_2, f_2) , (x_3, f_3) , ..., 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

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

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

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:

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

HELM (VERSION 1: March 18, 2004): Workbook Level 1 31.1: Numerical Methods of Approximation and this does work, because if we evaluate p at one of the data points, let us take x_2 for example, then

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

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

$$L_{1}(x) = \frac{(x - x_{2})(x - x_{3})(x - x_{4})\dots}{(x_{1} - x_{2})(x_{1} - x_{3})(x_{1} - x_{4})\dots}$$

$$L_{2}(x) = \frac{(x - x_{1})(x - x_{3})(x - x_{4})\dots}{(x_{2} - x_{1})(x_{2} - x_{3})(x_{2} - x_{4})\dots}$$

$$L_{3}(x) = \frac{(x - x_{1})(x - x_{2})(x - x_{4})\dots}{(x_{3} - x_{1})(x_{3} - x_{2})(x_{3} - x_{4})\dots}$$
:



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.



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The diagram above 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, \ldots) What we do generally require is p evaluated at some specific value. The following example should help show how this can be done.

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

Evaluate p(1.1).

Solution

We are only 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

$$p(1.1) = f_1 L_1(1.1) + f_2 L_2(1.1) + f_3 L_3(1.1) + f_4 L_4(1.1)$$

= -1.82 × -0.15625 + -1.73 × 0.9375 + -1.4 × 0.3125 + -1.11 × -0.09375
= -1.670938
= -1.67 to the number of decimal places to which the data was given.



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



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

Evaluate p(0.15).

We are only interested in the Lagrange polynomials at the point x = 0.15 so we consider $L_1(0.15) = \frac{(0.15 - x_3)(0.15 - x_3)(0.15 - x_4)}{(x_1 - x_3)(x_1 - x_4)} = \frac{(0.15 - 0.3)(0.15 - 0.3)(0.1 - 0.4)}{(0.1 - 0.4)} = 0.3125.$ Similar calculations for the other Lagrange polynomials give $L_2(0.15) = J_1L_1(0.15) + J_2L_2(0.15) + J_3L_3(0.15) + J_4L_4(0.15) = 0.0625,$ and we find that our interpolated polynomial, evaluated at x = 0.15 is $p(0.15) = J_1L_1(0.15) + J_2L_2(0.15) + J_3L_3(0.15) + J_4L_4(0.15) = 0.0625,$ $= 0.91 \times 0.3125 + 0.7 \times 0.9375 + 0.43 \times -0.3125 + 0.52 \times 0.0625$ = 0.838750 = 0.84, to 2 decimal places. The next example is very much the same as the exercise and example above. Try not to let the specific application, and the slight change of notation, confuse the main issues.

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

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 only 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

$$p(0.8) = y_1 L_1(0.8) + y_2 L_2(0.8) + y_3 L_3(0.8) + y_4 L_4(0.8)$$

= 0.32 × 0.032 + 0.65 × -0.176 + 0.43 × 1.056 + 0.1 × 0.088
= 0.358720 = 0.36 to 2 decimal places.

In this next exercise 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.



Your solution

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, respectively.) Use Lagrange interpolation to fit this data and hence approximate the drag corresponding to a hull speed of 2.5 m/s.



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 works.

Example 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 this 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 only 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

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

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

$$\begin{aligned} x(0.5) &= x_1 L_1(0.5) + x_2 L_2(0.5) + x_3 L_3(0.5) + x_4 L_4(0.5) \\ &= 1.00 \times 0.0625 + 1.20 \times -0.3125 + 1.30 \times 0.9375 + 1.25 \times 0.3125 \\ &= 1.30 \quad \text{to } 2 \text{ decimal places} \end{aligned}$$

and for the y value we get

$$y(0.5) = y_1 L_1(0.5) + y_2 L_2(0.5) + y_3 L_3(0.5) + y_4 L_4(0.5)$$

= 2.00 × 0.0625 + 2.10 × -0.3125 + 2.30 × 0.9375 + 2.60 × 0.3125
= 2.44 to 2 decimal places

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 on a piece of 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. Also, 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 $(x_1, f_1), (x_2, f_2), (x_3, f_3), \ldots$



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

$$R = \underbrace{(mx_1 + c - f_1)}_{\text{vertical distance}}^2 + \underbrace{(mx_2 + c - f_2)}_{\text{second data point}}^2 + \underbrace{(mx_3 + c - f_3)}_{\text{third data point}}^2 + \dots$$

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

Each term in the sum measures the vertical distance between a data point and the straight line. (The distance is squared so that large distances above and below the line do not cancel each other out. It is because the distances are 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

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

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(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

$$\frac{\partial R}{\partial c} = 2(mx_1 + c - f_1) + 2(mx_2 + c - f_2) + 2(mx_3 + c - f_3) + \dots$$

$$= 2\sum (mx_n + c - f_n) \quad \text{and}$$

$$\frac{\partial R}{\partial m} = 2(mx_1 + c - f_1)x_1 + 2(mx_2 + c - f_2)x_2 + 2(mx_3 + c - f_3)x_3 + \dots$$

$$= 2\sum (mx_n + c - f_n)x_n,$$

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.



The "least squares" best fit straight line to the experimental data

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

is

y = mx + c

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

$$c\left(\sum 1\right) + m\left(\sum x_n\right) = \sum f_n,$$

$$c\left(\sum x_n\right) + m\left(\sum x_n^2\right) = \sum x_n f_n$$

(The term $\sum 1$ is simply equal to the number of data points.)

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

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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
$\boldsymbol{\Sigma}$	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



Your solution

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

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

 $x82.\hbar - 47.\delta = \psi$

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

 $\begin{array}{rcl} 88.41 &=& m0.1 + 54 \\ 818.6 &=& m0.1 + 50.1 \\ \end{array}$

It follows that the pair of equations for m and c are as follows:

The quantity $\sum 1$ counts the number of data points and in this case is equal to 4.

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₽₽6.I	18.0	2.16	6.0	
$\ddot{c}\ddot{c}\ddot{c}.I$	0.25	11.6	d.0	
1.206	60.0	4.02	0.3	
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${}^{u}\!f^{\overline{u}x}$	$\frac{u}{z}x$	$^{u}\!f$	^{u}x	

Tabulating the data as in the example gives

at the least squares best fit straight	dt 998	s əm put	3.4€.0	= 111	bus $02.22 - 222.20$ and Solving these gives $c = -22.20$
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					Tabulating as before

P = -22.20 + 0.34I.

current. Use the least squares approach to fit a straight line, P = mI + c, to this data. Give c and m to 2 decimal places. Your solution

(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



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

ine to the given data is

Exercises

1. A politician is preparing a dossier involving the following data

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

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

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

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

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

$$p(22) = f_1 L_1(22) + f_2 L_2(22) + f_3 L_3(22) + f_4 L_4(22)$$

= 9.23 × 0.056 + 8.41 × -0.288 + 7.12 × 1.008 + 4.13 × 0.224
= 6.197 = 6.20, to 2 decimal places,

which serves as the approximation to f(22).

2. We tabulate the data for convenience:

ð.ð∳1	28	27.3	LΙ	\sum
₽.20	$6 \overline{\nu}$	13.2	L	
32.5	25	$\mathbf{\tilde{d}.0}$	\mathbf{G}	
16.2	6	${\bf h}.{\bf d}$	3	
$\overline{\Lambda}.\overline{\Lambda}$	\overline{V}	5.2	3	
$uf^{u}x$	$\frac{u}{z}x$	^u f	ux	

The quantity $\sum I$ 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:

$$8.72 = m71 + 24$$

 $8.72 = m78 + 271$

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

$$x00.2 + 70.1 - = y$$