

Extra \leftrightarrow Lecture 2

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Chapter 1

Finite difference approximations

Our goal is to approximate solutions to differential equations, *i.e.*, to find a function (or some discrete approximation to this function) which satisfies a given relationship between various of its derivatives on some given region of space and/or time, along with some boundary conditions along the edges of this domain. In general this is a difficult problem and only rarely can an analytic formula be found for the solution. A finite difference method proceeds by replacing the derivatives in the differential equations by finite difference approximations. This gives a large algebraic system of equations to be solved in place of the differential equation, something that is easily solved on a computer.

Before tackling this problem, we first consider the more basic question of how we can approximate the derivatives of a known function by finite difference formulas based only on values of the function itself at discrete points. Besides providing a basis for the later development of finite difference methods for solving differential equations, this allows us to investigate several key concepts such as the *order of accuracy* of an approximation in the simplest possible setting.

Let $u(x)$ represent a function of one variable that, unless otherwise stated, will always be assumed to be smooth, meaning that we can differentiate the function several times and each derivative is a well-defined bounded function over an interval containing a particular point of interest \bar{x} .

Suppose we want to approximate $u'(\bar{x})$ by a finite difference approximation based only on values of u at a finite number of points near \bar{x} . One obvious choice would be to use

$$D_+ u(\bar{x}) \equiv \frac{u(\bar{x} + h) - u(\bar{x})}{h} \quad (1.1)$$

for some small value of h . This is motivated by the standard definition of the derivative as the limiting value of this expression as $h \rightarrow 0$. Note that $D_+ u(\bar{x})$ is the slope of the line interpolating u at the points \bar{x} and $\bar{x} + h$ (see Figure 1.1).

The expression (1.1) is a *one-sided* approximation to u' since u is evaluated only at values of $x \geq \bar{x}$. Another one-sided approximation would be

$$D_- u(\bar{x}) \equiv \frac{u(\bar{x}) - u(\bar{x} - h)}{h}. \quad (1.2)$$

Each of these formulas gives a *first order accurate* approximation to $u'(\bar{x})$, meaning that the size of the error is roughly proportional to h itself.

Another possibility is to use the *centered approximation*

$$D_0 u(\bar{x}) \equiv \frac{u(\bar{x} + h) - u(\bar{x} - h)}{2h} = \frac{1}{2}(D_+ u(\bar{x}) + D_- u(\bar{x})). \quad (1.3)$$

This is the slope of the line interpolating u at $\bar{x} - h$ and $\bar{x} + h$, and is simply the average of the two one-sided approximations defined above. From Figure 1.1 it should be clear that we would expect $D_0 u(\bar{x})$ to give a better approximation than either of the one-sided approximations. In fact this gives a



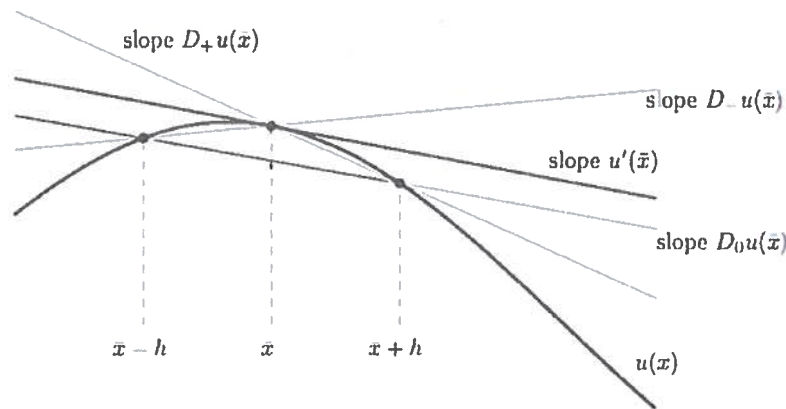


Figure 1.1: Various approximations to $u'(x)$ interpreted as the slope of secant lines.

Table 1.1: Errors in various finite difference approximations to $u'(x)$.

h	D+	D-	D0	D3
1.0000e-01	-4.2939e-02	4.1138e-02	-9.0005e-04	6.8207e-05
5.0000e-02	-2.1257e-02	2.0807e-02	-2.2510e-04	8.6491e-06
1.0000e-02	-4.2163e-03	4.1983e-03	-9.0050e-06	6.9941e-08
5.0000e-03	-2.1059e-03	2.1014e-03	-2.2513e-06	8.7540e-09
1.0000e-03	-4.2083e-04	4.2065e-04	-9.0050e-08	6.9979e-11

second order accurate approximation — the error is proportional to h^2 and hence is much smaller than the error in a first order approximation when h is small.

Other approximations are also possible, for example

$$D_3u(\bar{x}) \equiv \frac{1}{6h} [2u(\bar{x} + h) + 3u(\bar{x}) - 6u(\bar{x} - h) + u(\bar{x} - 2h)]. \quad (1.4)$$

It may not be clear where this came from or why it should approximate u' at all, but in fact it turns out to be a third order accurate approximation — the error is proportional to h^3 when h is small.

Our first goal is to develop systematic ways to derive such formulas and to analyze their accuracy and relative worth. First we will look at a typical example of how the errors in these formulas compare.

Example 1.1. Let $u(x) = \sin(x)$ and $\bar{x} = 1$, so we are trying to approximate $u'(1) = \cos(1) = 0.5403023$. Table 1.1 shows the error $Du(\bar{x}) - u'(\bar{x})$ for various values of h for each of the formulas above.

We see that D_+u and D_-u behave similarly though one exhibits an error that is roughly the negative of the other. This is reasonable from Figure 1.1 and explains why D_0u , the average of the two, has an error that is much smaller than either.

We see that

$$\begin{aligned} D_+u(\bar{x}) - u'(\bar{x}) &\approx -0.42h \\ D_0u(\bar{x}) - u'(\bar{x}) &\approx -0.09h^2 \\ D_3u(\bar{x}) - u'(\bar{x}) &\approx 0.007h^3 \end{aligned}$$

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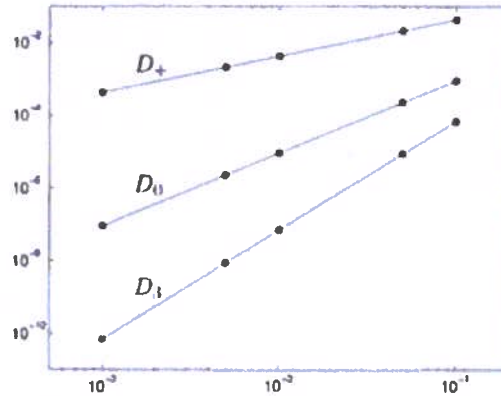


Figure 1.2: The errors in $Du(\bar{x})$ from Table 1.1 plotted against h on a log-log scale.

confirming that these methods are first order, second order, and third order, respectively.

Figure 1.2 shows these errors plotted against h on a log-log scale. This is a good way to plot errors when we expect them to behave like some power of h , since if the error $E(h)$ behaves like

$$E(h) \approx Ch^p$$

then

$$\log |E(h)| \approx \log |C| + p \log h.$$

So on a log-log scale the error behaves linearly with a slope that is equal to p , the order of accuracy.

1.1 Truncation errors

The standard approach to analyzing the error in a finite difference approximation is to expand each of the function values of u in a *Taylor series* about the point \bar{x} , e.g.,

$$u(\bar{x} + h) = u(\bar{x}) + hu'(\bar{x}) + \frac{1}{2}h^2u''(\bar{x}) + \frac{1}{6}h^3u'''(\bar{x}) + O(h^4) \quad (1.5a)$$

$$u(\bar{x} - h) = u(\bar{x}) - hu'(\bar{x}) + \frac{1}{2}h^2u''(\bar{x}) - \frac{1}{6}h^3u'''(\bar{x}) + O(h^4) \quad (1.5b)$$

These expansions are valid provided that u is sufficiently smooth. Readers unfamiliar with the “big-oh” notation $O(h^4)$ are advised to read Section A1.2 of Appendix A1 at this point since this notation will be heavily used and a proper understanding of its use is critical.

Using (1.5a) allows us to compute that

$$D_+u(\bar{x}) = \frac{u(\bar{x} + h) - u(\bar{x})}{h} = u'(\bar{x}) + \frac{1}{2}hu''(\bar{x}) + \frac{1}{6}h^2u'''(\bar{x}) + O(h^3).$$

Recall that \bar{x} is a fixed point so that $u''(\bar{x})$, $u'''(\bar{x})$, etc., are fixed constants independent of h . They depend on u of course, but the function is also fixed as we vary h .

For h sufficiently small, the error will be dominated by the first term $\frac{1}{2}hu''(\bar{x})$ and all the other terms will be negligible compared to this term, so we expect the error to behave roughly like a constant times h , where the constant has the value $\frac{1}{2}u''(\bar{x})$.

Note that in Example 1.1, where $u(x) = \sin x$, we have $\frac{1}{2}u''(1) = -0.4207355$ which agrees with the behavior seen in Table 1.1.

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Similarly, from (1.5b) we can compute that the error in $D_-u(\bar{x})$ is

$$D_-u(\bar{x}) - u'(\bar{x}) = -\frac{1}{2}hu''(\bar{x}) + \frac{1}{6}h^2u'''(\bar{x}) + O(h^3)$$

which also agrees with our expectations.

Combining (1.5a) and (1.5b) shows that

$$u(\bar{x} + h) - u(\bar{x} - h) = 2hu'(\bar{x}) + \frac{1}{3}h^3u'''(\bar{x}) + O(h^5)$$

so that

$$D_0u(\bar{x}) - u'(\bar{x}) = \frac{1}{6}h^2u'''(\bar{x}) + O(h^4). \quad (1.6)$$

This confirms the second order accuracy of this approximation and again agrees with what is seen in Table 1.1, since in the context of Example 1.1 we have

$$\frac{1}{6}u'''(\bar{x}) = -\frac{1}{6}\cos(1) = -0.09005038.$$

Note that all of the odd order terms drop out of the Taylor series expansion (1.6) for $D_0u(\bar{x})$. This is typical with *centered* approximations and typically leads to a higher order approximation.

In order to analyze D_+u we need to also expand $u(\bar{x} - 2h)$ as

$$u(\bar{x} - 2h) = u(\bar{x}) - 2hu'(\bar{x}) + \frac{1}{2}(2h)^2u''(\bar{x}) - \frac{1}{6}(2h)^3u'''(\bar{x}) + O(h^4). \quad (1.7)$$

Combining this with (1.5a) and (1.5b) shows that

$$D_+u(\bar{x}) = u'(\bar{x}) + \frac{1}{12}h^3u'''(\bar{x}) + O(h^4). \quad (1.8)$$

1.2 Deriving finite difference approximations

Suppose we want to derive a finite difference approximation to $u'(\bar{x})$ based on some given set of points. We can use Taylor series to derive an appropriate formula, using the *method of undetermined coefficients*.

Example 1.2. Suppose we want a one-sided approximation to $u'(\bar{x})$ based on $u(\bar{x})$, $u(\bar{x} - h)$ and $u(\bar{x} - 2h)$, of the form

$$D_2u(\bar{x}) = au(\bar{x}) + bu(\bar{x} - h) + cu(\bar{x} - 2h). \quad (1.9)$$

We can determine the coefficients a , b , and c to give the best possible accuracy by expanding in Taylor series and collecting terms. Using (1.5b) and (1.7) in (1.9) gives

$$\begin{aligned} D_2u(\bar{x}) &= (a + b + c)u(\bar{x}) - (b + 2c)hu'(\bar{x}) + \frac{1}{2}(b + 4c)h^2u''(\bar{x}) \\ &\quad - \frac{1}{6}(b + 8c)h^3u'''(\bar{x}) + \dots \end{aligned}$$

If this is going to agree with $u'(\bar{x})$ to high order then we need

$$\begin{aligned} a + b + c &= 0 \\ b + 2c &= -1/h \\ b + 4c &= 0 \end{aligned} \quad (1.10)$$

We might like to require that higher order coefficients be zero as well, but since there are only three unknowns a , b , and c we cannot in general hope to satisfy more than three such conditions. Solving the linear system (1.10) gives

$$a = 3/2h \quad b = -2/h \quad c = 1/2h$$

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so that the formula is

$$D_2 u(\bar{x}) = \frac{1}{2h} [3u(\bar{x}) - 4u(\bar{x} - h) + u(\bar{x} - 2h)]. \quad (1.11)$$

The error in this approximation is clearly

$$\begin{aligned} D_2 u(\bar{x}) - u'(\bar{x}) &= -\frac{1}{6}(b + 8c)h^3 u'''(\bar{x}) + \dots \\ &= \frac{1}{12}h^2 u'''(\bar{x}) + O(h^3). \end{aligned}$$

1.3 Polynomial interpolation

There are other ways to derive the same finite difference approximations. One way is to approximate the function $u(x)$ by some polynomial $p(x)$ and then use $p'(\bar{x})$ as an approximation to $u'(\bar{x})$. If we determine the polynomial by interpolating u at an appropriate set of points, then we obtain the same finite difference methods as above.

Example 1.3. To derive the method of Example 1.2 in this way, let $p(x)$ be the quadratic polynomial that interpolates u at \bar{x} , $\bar{x} - h$ and $\bar{x} - 2h$ and then compute $p'(\bar{x})$. The result is exactly (1.11).

1.4 Second order derivatives

Approximations to the second derivative $u''(x)$ can be obtained in an analogous manner. The standard second order centered approximation is given by

$$\begin{aligned} D^2 u(\bar{x}) &= \frac{1}{h^2} [u(\bar{x} - h) - 2u(\bar{x}) + u(\bar{x} + h)] \\ &= u''(\bar{x}) + \frac{1}{2}h^2 u''''(\bar{x}) + O(h^4). \end{aligned}$$

Again, since this is a symmetric centered approximation all of the odd order terms drop out. This approximation can also be obtained by the method of undetermined coefficients, or alternatively by computing the second derivative of the quadratic polynomial interpolating $u(x)$ at $\bar{x} - h$, \bar{x} and $\bar{x} + h$.

Another way to derive approximations to higher order derivatives is by repeatedly applying first order differences. Just as the second derivative is the derivative of u' , we can view $D^2 u(x)$ as being a difference of first differences. In fact,

$$D^2 u(\bar{x}) = D_+ D_- u(\bar{x})$$

since

$$\begin{aligned} D_+(D_- u(\bar{x})) &= \frac{1}{h} [D_- u(\bar{x} + h) - D_- u(\bar{x})] \\ &= \frac{1}{h} \left[\left(\frac{u(\bar{x} + h) - u(\bar{x})}{h} \right) - \left(\frac{u(\bar{x}) - u(\bar{x} - h)}{h} \right) \right] \\ &= D^2 u(\bar{x}). \end{aligned}$$

Alternatively, $D^2(x) = D_- D_+ u(\bar{x})$ or we can also view it as a centered difference of centered differences, if we use a step size $h/2$ in each centered approximation to the first derivative. If we define

$$\hat{D}_0 u(x) = \frac{1}{h} (u(x + h/2) - u(x - h/2))$$

then we find that

$$\hat{D}_0(\hat{D}_0 u(\bar{x})) = \frac{1}{h} \left(\left(\frac{u(\bar{x} + h) - u(\bar{x})}{h} \right) - \left(\frac{u(\bar{x}) - u(\bar{x} - h)}{h} \right) \right) = D^2 u(\bar{x}).$$

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1.5 Higher order derivatives

Finite difference approximations to higher order derivatives can also be obtained using any of the approaches outlined above. Repeatedly differencing approximations to lower order derivatives is a particularly simple way.

Example 1.4. As an example, here are two different approximations to $u'''(\bar{x})$. The first one is uncentered and first order accurate:

$$\begin{aligned} D_+ D^2 u(\bar{x}) &= \frac{1}{h^3} (u(\bar{x} + 2h) - 3u(\bar{x} + h) + 3u(\bar{x}) - u(\bar{x} - h)) \\ &= u'''(\bar{x}) + \frac{1}{2} h u''''(\bar{x}) + O(h^2). \end{aligned}$$

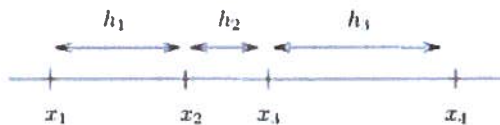
The next approximation is centered and second order accurate:

$$\begin{aligned} D_0 D_+ D_- u(\bar{x}) &= \frac{1}{2h^3} (u(\bar{x} + 2h) - 2u(\bar{x} + h) + 2u(\bar{x} - h) - u(\bar{x} - 2h)) \\ &= u'''(\bar{x}) + \frac{1}{4} h^2 u''''(\bar{x}) + O(h^4). \end{aligned}$$

Finite difference approximations of the sort derived above are the basic building blocks of finite difference methods for solving differential equations.

1.6 Exercises

Exercise 1.1 Consider the nonuniform grid:



1. Use polynomial interpolation to derive a finite difference approximation for $u''(x_2)$ that is as accurate as possible for smooth functions u , based on the four values $U_1 = u(x_1)$, \dots , $U_4 = u(x_4)$. Give an expression for the dominant term in the error.
2. Verify your expression for the error by testing your formula with a specific function and various values of h_1 , h_2 , h_3 .
3. Can you define an "order of accuracy" for your method in terms of $h = \max(h_1, h_2, h_3)$? To get a better feel for how the error behaves as the grid gets finer, do the following. Take a large number (say 500) of different values of H spanning two or three orders of magnitude, choose h_1 , h_2 , and h_3 as random numbers in the interval $[0, H]$ and compute the error in the resulting approximation. Plot these values against H on a log-log plot to get a scatter plot of the behavior as $H \rightarrow 0$. (Note: in `matlab` the command `h = H * rand(1)` will produce a single random number uniformly distributed in the range $[0, H]$.) Of course these errors will not lie exactly on a straight line since the values of h_k may vary quite a lot even for H 's that are nearby, but you might expect the upper limit of the error to behave reasonably.
4. Estimate the "order of accuracy" by doing a least squares fit of the form

$$\log(E(H)) = K + p \log(H)$$

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formula		error term
$f'(x_i) = \frac{f(x_{i-2}) - 4f(x_{i-1}) + 3f(x_i)}{2h}$		$\frac{1}{3} h^2 f'''$
$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1}))}{2h}$	$f' \approx$	$\frac{1}{6} h^2 f'''$
$f'(x_i) = \frac{-3f(x_{i+4}) + 4f(x_{i+1}) - f(x_{i+2}))}{2h}$		$\frac{1}{3} h^2 f'''$
$f'(x_i) = \frac{3f(x_{i-4}) - 16f(x_{i-3}) + 36f(x_{i-2}) - 48f(x_{i-1}) + 25f(x_i)}{12h}$		$\frac{1}{5} h^4 f^{(5)}$
$f'(x_i) = \frac{-f(x_{i-3}) + 6f(x_{i-2}) - 10f(x_{i-1}) + 10f(x_i) + 3f(x_{i+1}))}{12h}$		$\frac{1}{20} h^4 f^{(5)}$
$f'(x_i) = \frac{f(x_{i-2}) - 8f(x_{i-1}) + 8f(x_{i+1}) - f(x_{i+2}))}{12h}$		$\frac{1}{30} h^4 f^{(5)}$
$f'(x_i) = \frac{-3f(x_{i-1}) - 10f(x_i) + 18f(x_{i+1}) - 6f(x_{i+2}) + f(x_{i+3}))}{12h}$		$\frac{1}{20} h^4 f^{(5)}$
$f'(x_i) = \frac{-25f(x_{i+4}) + 48f(x_{i+1}) - 36f(x_{i+2}) + 16f(x_{i+3}) - 3f(x_{i+4}))}{12h}$		$\frac{1}{5} h^4 f^{(5)}$
$f'(x_i) = \frac{10f(x_{i-6}) - 72f(x_{i-5}) + 225f(x_{i-4}) - 400f(x_{i-3}) + 450f(x_{i-2}) - 360f(x_{i-1}) + 147f(x_i)}{60h}$		$\frac{1}{7} h^6 f^{(7)}$
$f'(x_i) = \frac{-2f(x_{i-5}) + 15f(x_{i-4}) - 50f(x_{i-3}) + 100f(x_{i-2}) - 150f(x_{i-1}) + 77f(x_i) + 10f(x_{i+1}))}{60h}$		$\frac{1}{42} h^6 f^{(7)}$
$f'(x_i) = \frac{f(x_{i-4}) - 8f(x_{i-3}) + 30f(x_{i-2}) - 80f(x_{i-1}) + 35f(x_i) + 24f(x_{i+1}) - 2f(x_{i+2}))}{60h}$		$\frac{1}{105} h^6 f^{(7)}$
$f'(x_i) = \frac{-f(x_{i-3}) + 9f(x_{i-2}) - 45f(x_{i-1}) + 45f(x_{i+1}) - 9f(x_{i+2}) + f(x_{i+3}))}{60h}$		$\frac{1}{140} h^6 f^{(7)}$
$f'(x_i) = \frac{2f(x_{i-2}) - 24f(x_{i-1}) - 35f(x_i) + 80f(x_{i+1}) - 30f(x_{i+2}) + 8f(x_{i+3}) - f(x_{i+4}))}{60h}$		$\frac{1}{105} h^6 f^{(7)}$
$f'(x_i) = \frac{-10f(x_{i-1}) - 77f(x_i) + 150f(x_{i+1}) - 100f(x_{i+2}) + 50f(x_{i+3}) - 15f(x_{i+4}) + 3f(x_{i+5}))}{60h}$		$\frac{1}{42} h^6 f^{(7)}$
$f'(x_i) = \frac{-147f(x_{i+3}) + 360f(x_{i+1}) - 450f(x_{i+2}) + 400f(x_{i+3}) - 225f(x_{i+4}) + 72f(x_{i+5}) - 10f(x_{i+6}))}{60h}$		$\frac{1}{7} h^6 f^{(7)}$

Finite difference formulas on uniform grids for the first derivative

formula		error term
$f''(x_i) = \frac{-f(x_{i-3}) + 4f(x_{i-2}) - 5f(x_{i-1}) + 2f(x_i)}{h^2}$		$\frac{11}{12} h^2 f^{(4)}$
$f''(x_i) = \frac{f(x_{i-1}) - 2f(x_i) + f(x_{i+1}))}{h^2}$	$f'' \approx$	$\frac{1}{12} h^2 f^{(4)}$
$f''(x_i) = \frac{2f(x_{i+1}) - 5f(x_{i+2}) + 4f(x_{i+3}) - f(x_{i+4}))}{h^2}$		$\frac{11}{12} h^2 f^{(4)}$
$f''(x_i) = \frac{-10f(x_{i-5}) + 61f(x_{i-4}) - 156f(x_{i-3}) + 214f(x_{i-2}) - 154f(x_{i-1}) + 45f(x_i)}{12h^2}$		$\frac{137}{180} h^4 f^{(6)}$
$f''(x_i) = \frac{f(x_{i-4}) - 6f(x_{i-3}) + 14f(x_{i-2}) - 4f(x_{i-1}) - 15f(x_i) + 10f(x_{i+1}))}{12h^2}$		$\frac{13}{180} h^4 f^{(6)}$
$f''(x_i) = \frac{-f(x_{i-2}) + 16f(x_{i-1}) - 30f(x_i) + 16f(x_{i+1}) - f(x_{i+2}))}{12h^2}$		$\frac{1}{90} h^4 f^{(6)}$
$f''(x_i) = \frac{10f(x_{i-1}) - 15f(x_i) - 4f(x_{i+1}) + 14f(x_{i+2}) - 6f(x_{i+3}) + f(x_{i+4}))}{12h^2}$		$\frac{13}{180} h^4 f^{(6)}$
$f''(x_i) = \frac{45f(x_{i+1}) - 154f(x_{i+2}) + 214f(x_{i+3}) - 156f(x_{i+4}) + 61f(x_{i+5}) - 10f(x_{i+6}))}{12h^2}$		$\frac{137}{180} h^4 f^{(6)}$
$f''(x_i) = \frac{-126f(x_{i-7}) + 1019f(x_{i-6}) - 3618f(x_{i-5}) + 7380f(x_{i-4}) - 9490f(x_{i-3}) + 7911f(x_{i-2}) - 4014f(x_{i-1}) + 938f(x_i)}{180h^2}$		$\frac{363}{560} h^6 f^{(8)}$
$f''(x_i) = \frac{11f(x_{i-6}) - 90f(x_{i-5}) + 324f(x_{i-4}) - 670f(x_{i-3}) + 855f(x_{i-2}) - 486f(x_{i-1}) - 70f(x_i) + 126f(x_{i+1}))}{180h^2}$		$\frac{29}{560} h^6 f^{(8)}$
$f''(x_i) = \frac{-2f(x_{i-5}) + 16f(x_{i-4}) - 54f(x_{i-3}) + 85f(x_{i-2}) + 130f(x_{i-1}) - 378f(x_i) + 214f(x_{i+1}) - 11f(x_{i+2}))}{180h^2}$		$\frac{47}{5040} h^6 f^{(8)}$
$f''(x_i) = \frac{2f(x_{i-3}) - 27f(x_{i-2}) + 270f(x_{i-1}) - 490f(x_i) + 270f(x_{i+1}) - 27f(x_{i+2}) + 2f(x_{i+3}))}{180h^2}$		$\frac{1}{560} h^6 f^{(8)}$
$f''(x_i) = \frac{-11f(x_{i-2}) + 214f(x_{i-1}) - 378f(x_i) + 130f(x_{i+1}) + 85f(x_{i+2}) - 54f(x_{i+3}) + 16f(x_{i+4}) - 2f(x_{i+5}))}{180h^2}$		$\frac{47}{5040} h^6 f^{(8)}$
$f''(x_i) = \frac{126f(x_{i-1}) - 70f(x_i) - 486f(x_{i+1}) + 855f(x_{i+2}) - 670f(x_{i+3}) + 324f(x_{i+4}) - 90f(x_{i+5}) + 11f(x_{i+6}))}{180h^2}$		$\frac{29}{560} h^6 f^{(8)}$
$f''(x_i) = \frac{938f(x_{i+3}) - 4014f(x_{i+1}) + 7911f(x_{i+2}) - 9490f(x_{i+3}) + 7380f(x_{i+4}) - 3618f(x_{i+5}) + 1019f(x_{i+6}) - 126f(x_{i+7}))}{180h^2}$		$\frac{363}{560} h^6 f^{(8)}$

Finite difference formulas on uniform grids for the second derivative

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The eigenvalues of tridiagonal matrices Autumn 2009

Note TMA4205

Tridiagonal matrices are often found in connection with finite differences.

Tridiagonal matrices are easy to deal with since there exists efficient numerical methods both for solving their linear systems of equations and eigenvalue problem. Here we consider the eigenvalue problem for a general tridiagonal matrix of the form

$$A = \begin{bmatrix} a & b & & & \\ c & a & b & & \\ & c & \ddots & \ddots & \\ & & \ddots & a & b \\ & & & c & a \end{bmatrix} \in \mathbf{R}^{m \times m}.$$

We solve the eigenvalue problem

$$Ax = \lambda x,$$

where $\lambda \in \mathbf{R}$ and $x = [x_1, \dots, x_m]^T \neq 0$. We write out the eigenvalue problem for A to obtain the difference equation

$$\begin{aligned} cx_{j-1} + ax_j + bx_{j+1} &= \lambda x_j, & j = 1, \dots, m \\ x_0 = x_{m+1} &= 0 \end{aligned}$$

which is equivalent to

$$\begin{aligned} cx_{j-1} + (a - \lambda)x_j + bx_{j+1} &= 0, & j = 1, \dots, m \\ x_0 = x_{m+1} &= 0 \end{aligned}$$

You may remember from earlier exercises that the solution of such an equation can be expressed in terms of the roots of the characteristic polynomial, which in this case is

$$p(r) = br^2 + (a - \lambda)r + c.$$

So assume that the roots of p are given as r_1 and r_2 . Then the solution of the difference equation is

$$x_j = \alpha r_1^j + \beta r_2^j$$

for $j = 0, \dots, m + 1$. We determine the unknown coefficients by using the initial condition:

$$x_0 = \alpha + \beta = 0 \Leftrightarrow \beta = -\alpha,$$

which gives

$$x_j = \alpha(r_1^j - r_2^j), \quad j = 0, \dots, m + 1.$$

Furthermore we have

$$x_{m+1} = \alpha(r_1^{m+1} - r_2^{m+1}) = 0.$$

Since $x \neq 0$ we need $\alpha \neq 0$, so we find that

$$r_1^{m+1} = r_2^{m+1} \Leftrightarrow \left(\frac{r_1}{r_2}\right)^{m+1} = 1.$$

We can eliminate r_2 from this equation through the identity

$$\begin{aligned} r_1 r_2 &= \left(\frac{-(a-\lambda) + \sqrt{(a-\lambda)^2 - 4bc}}{2b}\right) \left(\frac{-(a-\lambda) - \sqrt{(a-\lambda)^2 - 4bc}}{2b}\right) \\ &= \frac{(a-\lambda)^2 - ((a-\lambda)^2 - 4bc)}{4b^2} \\ &= \frac{c}{b}. \end{aligned}$$

Thus

$$\left(\frac{r_1}{r_2}\right)^{m+1} = \left(\frac{r_1^2}{r_2 r_1}\right)^{m+1} = \left(\frac{r_1^2}{\frac{c}{b}}\right)^{m+1} = 1$$

The roots of a quadratic polynomial are in general complex, so the above equation can be written in the form

$$\frac{r_1^2}{\frac{c}{b}} = e^{2\pi i(\frac{s}{m+1})}, \quad s = 1, \dots, m.$$

We immediately see that the possible roots are

$$\begin{aligned} r_{1,s} &= \sqrt{\frac{c}{b}} e^{\pi i(\frac{s}{m+1})} \\ r_{2,s} &= \sqrt{\frac{c}{b}} e^{-\pi i(\frac{s}{m+1})}, \end{aligned}$$

where $s = 1, \dots, m$. For every $s = 1, \dots, m$ there is thus an eigenvalue λ_s given by the equation

$$\begin{aligned} r_{1,s} + r_{2,s} &= \frac{\lambda_s - a}{b} \\ &\Downarrow \\ \sqrt{\frac{c}{b}}(e^{\pi i(\frac{s}{m+1})} + e^{-\pi i(\frac{s}{m+1})}) &= \frac{\lambda_s - a}{b} \\ &\Downarrow \\ 2\sqrt{\frac{c}{b}} \cos\left(\frac{\pi s}{m+1}\right) &= \frac{\lambda_s - a}{b} \\ &\Downarrow \\ \lambda_s &= a + 2\sqrt{bc} \cos\left(\frac{\pi s}{m+1}\right) \end{aligned}$$

The corresponding eigenvector $x_{s,j}$ is then

$$\begin{aligned} x_{s,j} &= \alpha(r_{1,s}^j + r_{2,s}^j) \\ &= \alpha \left(\frac{c}{b}\right)^{j/2} (e^{\pi i(\frac{js}{m+1})} - e^{-\pi i(\frac{js}{m+1})}) \\ &= 2i\alpha \left(\frac{c}{b}\right)^{j/2} \sin\left(\frac{\pi js}{m+1}\right), \end{aligned}$$

i.e.

$$x_s = \left[\left(\frac{c}{b}\right)^{1/2} \sin\left(\frac{\pi s}{m+1}\right), \dots, \left(\frac{c}{b}\right)^{m/2} \sin\left(\frac{\pi m s}{m+1}\right) \right],$$

for $s = 1, \dots, m$.

EXAMPLE: Consider the eigenvalues of the matrix

$$A = I + rD,$$

where

$$D = \begin{bmatrix} -2 & 1 & & & \\ & 1 & \ddots & & \\ & & \ddots & \ddots & \\ & & & \ddots & 1 \\ & & & & 1 & -2 \end{bmatrix} \in \mathbf{R}^{n \times n}.$$

Set $\lambda_s(A) = 1 + r\lambda_s(D)$ for $s = 1, \dots, n$, from the discussion above we then have

$$\lambda_s(D) = -2 + 2 \cos\left(\frac{\pi s}{n+1}\right) = -4 \sin^2\left(\frac{\pi s}{2(n+1)}\right).$$

Therefore,

$$\lambda_s(A) = 1 - 4r \sin^2\left(\frac{\pi s}{2(n+1)}\right)$$

for $s = 1, \dots, n$.