Taylor Series and Numerical Approximations

Hilary Weller h.weller@reading.ac.uk

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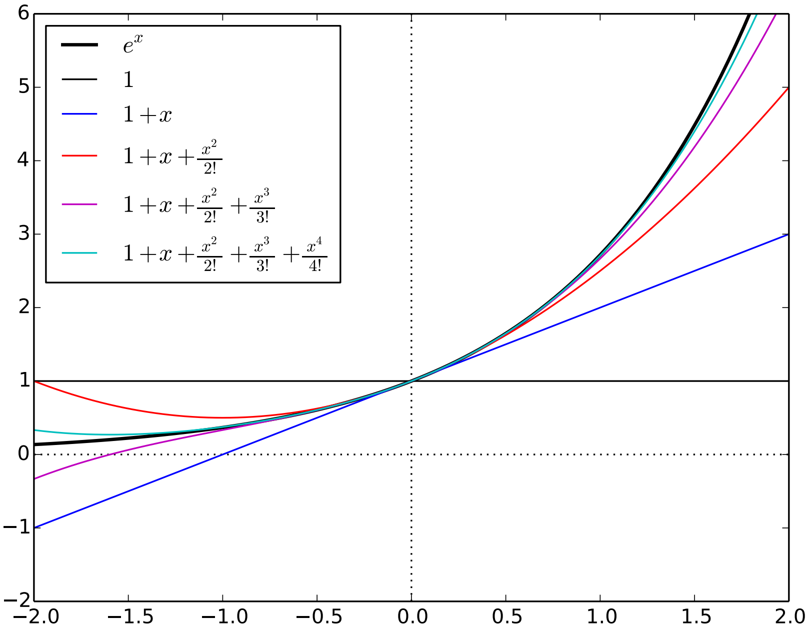
An introduction to the concept of a Taylor series and how these are used in numerical analysis to find numerical approximations and estimate their accuracy.

This is a series of four short videos to accompany the printed notes. You can download the printed notes and fill parts in as we go along. Alternatively, you can work through the notes without the videos.

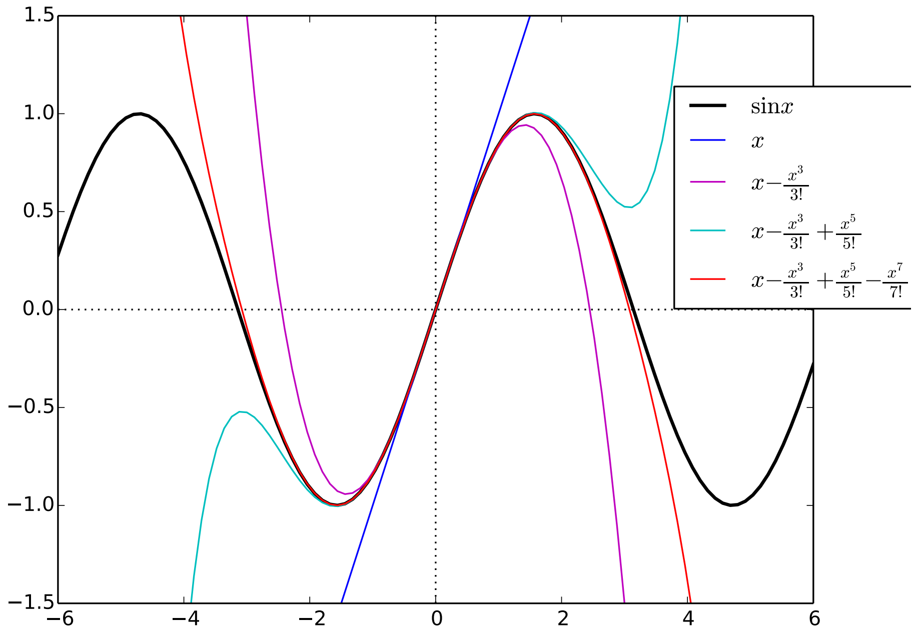
1 Taylor Series

- Many functions can be expressed as Taylor series
- Taylor series are infinite polynomials

For example an exponential:

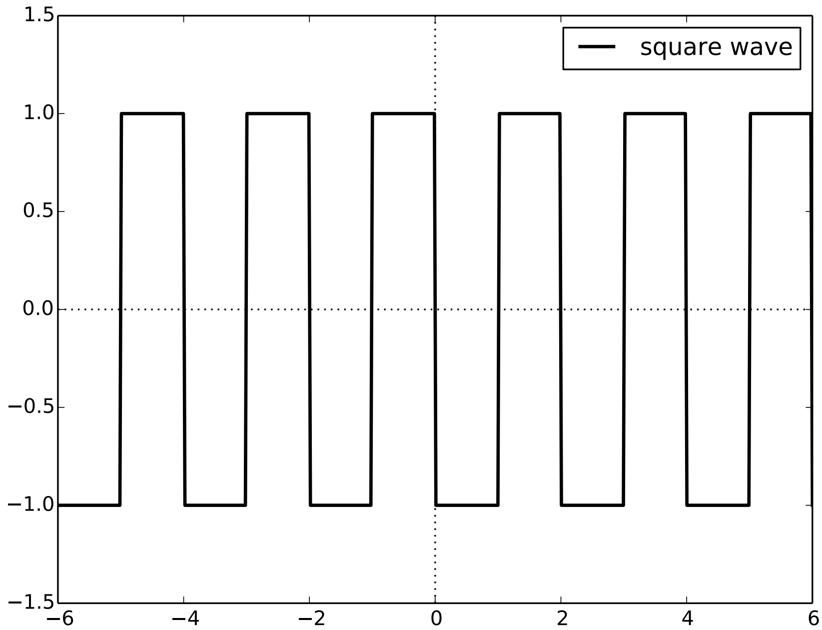


For example a sine wave:



The more terms you include, the more accurate it should get.

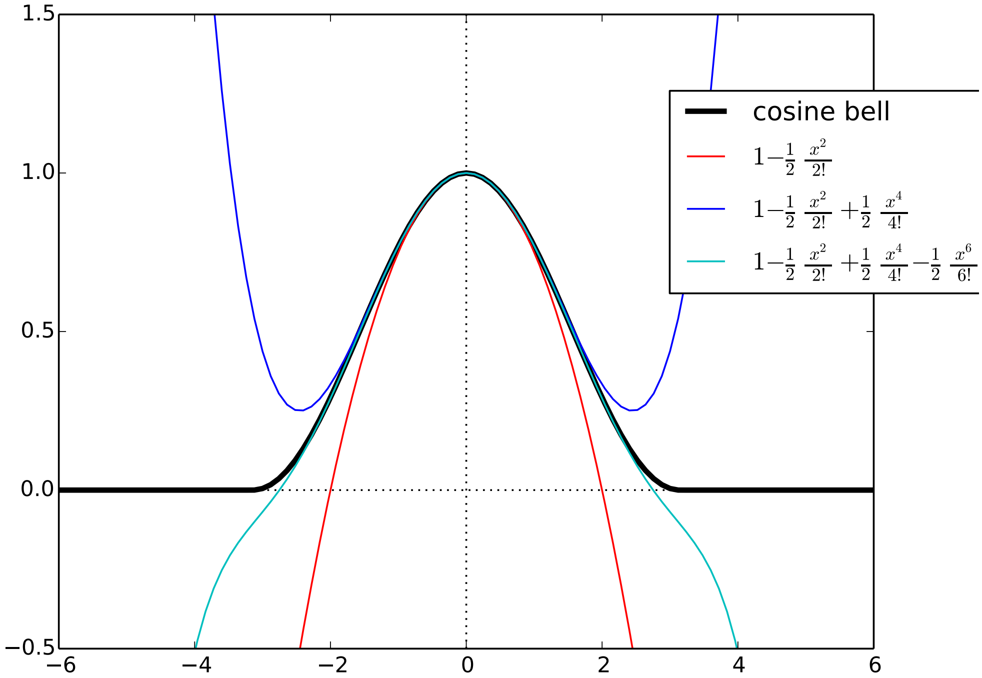
Functions with discontinuities cannot be expressed as Taylor series:



A polynomial cannot jump between 1 and -1

Functions with discontinuities in some of their derivatives cannot be expressed as Taylor series:

Eg. cosine bell, $f(x) = \begin{cases} {}^1\!/_2(1+\cos x) & |x| < \pi \\ 0 & \text{otherwise} \end{cases}$



A polynomial cannot be uniform in one place and non-uniform in another

The Taylor Series:

A function, f, can be represented as a Taylor series about position a if:

- is continuous near a and
- all of its derivatives are continuous near a

Using the notation $\Delta x = x - a$:

$$f(x) = f(a) + \Delta x f'(a) + \frac{\Delta x^2}{2!} f''(a) + \frac{\Delta x^3}{3!} f'''(a) + \cdots + \frac{\Delta x^j}{j!} f^{(j)}(a) + \cdots$$

where $f'(x) = \dfrac{df}{dx}(x)$, $f''(x) = \dfrac{d^2 f}{dx^2}(x)$, ...

- If infinitely many terms are used then this approximation is exact near a.
- If all terms of order n and above are discarded then the error is approximately proportional to Δx^n (assuming that Δx is small). Then the approximation is said to be n^{th} order accurate
- A third order accurate approximation for $f(x)$ has error proportional to Δx^3:

$$f(x) = f(a) + \Delta x f'(a) + \frac{\Delta x^2}{2!} f''(a) + O\left(\Delta x^3\right).$$

  We say that the error is of order Δx^3 or $O\left(\Delta x^3\right)$.
- If Δx is small, then higher order accuracy generally means higher accuracy

1.1 **Exercises** (answers at end)

1. Write down the infinite Taylor series for function f at position $x+\Delta x$ about x

2. Write the third order approximation for $f(x-\Delta x)$ in terms of $f(x)$, $f'(x)$ and $f''(x)$. Write the error term using the $O(\Delta x^n)$ notation.

3. Write the third order approximation for $f(x+\Delta x)$ in terms of $f(x-\Delta x)$, $f'(x-\Delta x)$ and $f''(x-\Delta x)$.

2 Numerical Differentiation

Consider a set of points, $x_0, x_1, \cdots x_j, \cdots x_n$ where $x_j = j\Delta x$ (the points are distance Δx apart). Assume that we know the value of the function $f(x)$ at these points, as shown in figure 1.

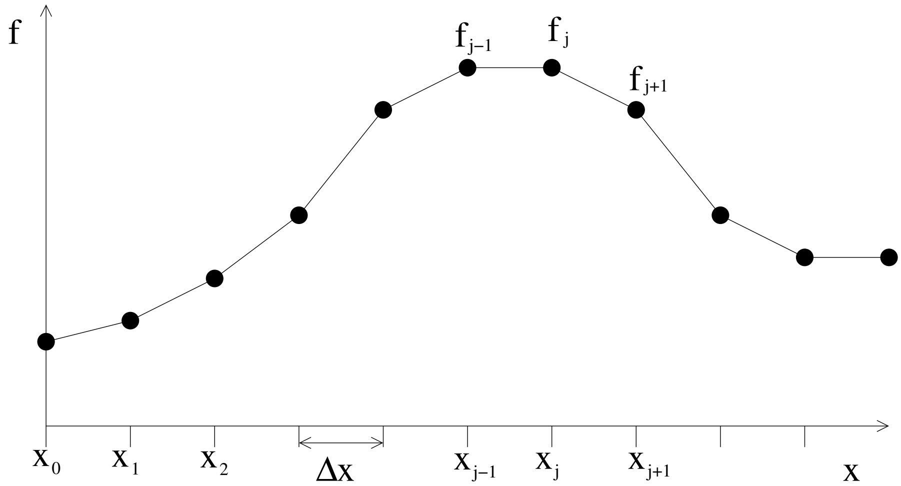


Figure 1: Values of a function f at points $x_0,\ x_1, \cdots, x_j, \cdots$.

Some possible estimate of $f'_j = f'(x_j)$ are:

forward difference	backward difference	centred difference
$f'_j \approx$	$f'_j \approx$	$f'_j \approx$

Taylor series can be used to derive estimates of derivatives and to find their order of accuracy.

3 Taylor Series to find Finite Difference Gradients

In order to use a Taylor series (below) to find an approximation for f'

$$f(x+\Delta x) = f(x) + \Delta x f'(x) + \frac{\Delta x^2}{2!} f''(x) + \frac{\Delta x^3}{3!} f'''(x) + \cdots + \frac{\Delta x^j}{j!} f^{(j)}(x) + \cdots$$

1. write down the knowns
2. consider *where* we want to find f'
3. consider what order of accuracy we want
4. write down Taylor series for some of the knowns
5. eliminate the additional unknowns to find f'

3.1 Example

1. Assume that we know $f_j = f(x_j)$
   $$f_{j-1} = f(x_{j-1}) = f(x - \Delta x)$$
   $$f_{j+1} = f(x_{j+1}) = f(x + \Delta x)$$
2. and we want to find f'_j.
3. For 3 knowns we wonder if we can get second order accuracy
4. We do not want to generate too many unknowns. We don't know f'_{j-1} or f'_{j+1} so no Taylor series about x_{j-1} or x_{j+1}. So let's try Taylor series for f_{j+1} and f_{j-1} about x_j

   $$f_{j+1} = \qquad\qquad\qquad\qquad + O(\Delta x^4)$$

   $$f_{j-1} = \qquad\qquad\qquad\qquad + O(\Delta x^4)$$

5. Eliminate f''_j by taking the difference of the two equations

   $$+ O(\Delta x^4)$$

   Rearrange to get f'_j

   $$f'_j =$$

   We cannot eliminate f'''_j so this is part of the error:

   $$f'_j =$$

   The error, ε, is proportional to Δx^2 ($\varepsilon \propto \Delta x^2$) so this approximation is second order accurate.

This is a worked example on my YouTube page:
`https://www.youtube.com/channel/UCO0YwmerBCvW-BrR8kcjLzw`
called TaylorSeries2

3.2 **Exercises** (answers at the end)

1. Use the Taylor series to find an approximation for f'_j in terms of f_j and f_{j-1}. What order accuracy is it?

2. Derive an uncentred, second order difference formula for f'_j that uses f_j, f_{j+1} and f_{j+2}. (And show that it is second order accurate)

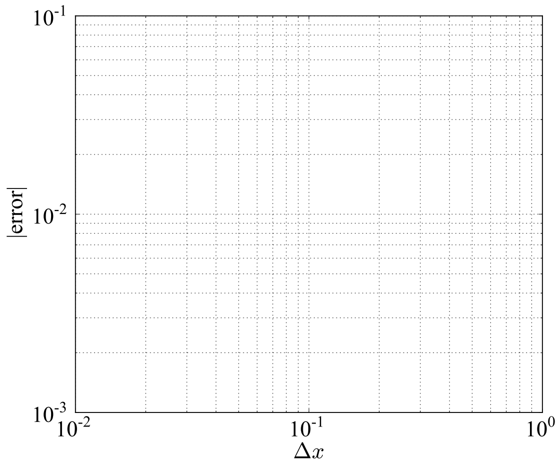
3. Find an uncentred approximation for f''_j using f_j, f_{j+1} and f_{j+2}. What order accurate is it?
4. Derive a second order approximation for f'_b from f_a, f_b and f_c at x locations $a < b < c$ when the grid spacing is not regular. (And show that it is second order accurate)

4 Order of Accuracy of Numerical Solutions

In order to demonstrate the order of accuracy (or order of convergence) of a numerical method, we can calculate the error of solving a problem that has an analytic solution. For example our numerical method calculates the gradient of $\sin x$ and gives these results:

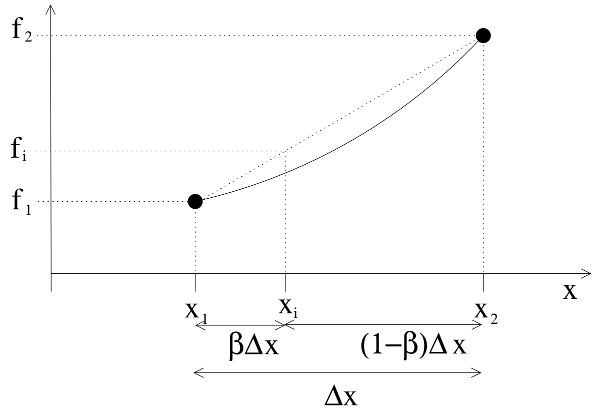
Δx	numerical gradient of $\sin x$ at $x = 0$	Error, ε (Difference from $\cos(0)$)
0.4	0.97355	-0.02645
0.2	0.99335	-0.00666
0.1	0.99833	-0.00167

Assume that $\varepsilon = A\Delta x^n$ where n is the order of accuracy and A is unknown. From the data, eliminate A and find two possible values for n.



Plot $|\varepsilon|$ as a function of Δx on log paper. Then the order of accuracy is the gradient. Does this value agree with the values found from calculating n directly from the data above? (both should give about $n = 2$. See YouTube video for a worked example.

5 Interpolation



An Example:

- Function f is known at points x_1 and x_2 (values f_1 and f_2)
- We want to estimate the value of f at point x_i in between x_1 and x_2

- **Exercise**: Use linear interpolation (ie assume that f_i lies on a straight line between f_1 and f_2): to find f at x_i
  Hint: First write down expressions for Δx, β and the gradient, f' between x_1 and x_2. Then find an expression for f at x_i along the straight line between x_1 and x_2.

$\Delta x =$ $\qquad\qquad$ $\beta =$ $\qquad\qquad$ $f' =$ $\qquad\qquad$ $\Longrightarrow f_i =$

- If f is known at n points then a polynomial of degree $n-1$ can be fit to estimate f

Eg. Cubic Lagrange interpolation for constant grid spacing, Δx:

$$\begin{aligned}\hat{f}(x) = &-\frac{1}{6}\beta(1-\beta)(2-\beta)f_{k-1} + \frac{1}{2}(1+\beta)(1-\beta)(2-\beta)f_k \\ &+\frac{1}{2}(1+\beta)\beta(2-\beta)f_{k+1} - \frac{1}{6}(1+\beta)\beta(1-\beta)f_{k+2}\end{aligned}$$

5.1 Finding Finite Difference Formulae for Interpolation using Taylor Series

An Example:

Assume that we know $f_j = f(x_j)$ and $f_{j+1} = f(x_{j+1})$ and we want to find the interpolated value, $f_{j+1/2}$, mid-way between x_j and x_{j+1}.

- Start by writing down Taylor series for f_j and f_{j+1} about $f_{j+1/2}$

$$f_{j+1} = f_{j+1/2} + \frac{\Delta x}{2} f'_{j+1/2} + \frac{1}{2!}\left(\frac{\Delta x}{2}\right)^2 f''_{j+1/2} + \frac{1}{3!}\left(\frac{\Delta x}{2}\right)^3 f'''_{j+1/2} + O(\Delta x)^4$$

$$f_j = f_{j+1/2} - \frac{\Delta x}{2} f'_{j+1/2} + \frac{1}{2!}\left(\frac{\Delta x}{2}\right)^2 f''_{j+1/2} - \frac{1}{3!}\left(\frac{\Delta x}{2}\right)^3 f'''_{j+1/2} + O(\Delta x)^4$$

- Eliminate the largest unknown, $f'_{j+1/2}$ by adding the two equations

$$f_j + f_{j+1} = 2f_{j+1/2} + \frac{\Delta x^2}{4} f''_{j+1/2} + O(\Delta x)^4$$

- Rearrange to find $f_{j+1/2}$ and express the error based on the largest unknown
  $f_{j+1/2} = (f_j + f_{j+1})/2 + O(\Delta x)^2$
- So this is a second-order accurate approximation

5.2 Exercises (answers at the end)

1. Derive a centred, second order difference interpolation formula for f_j that uses f_{j-1} and f_{j+1}. (And show that it is second order accurate)
2. Derive a centred fourth order difference formula for $f'_{j+1/2}$ that uses f_{j-1}, f_j, f_{j+1} and f_{j+2}. (And show that it is fourth order accurate)
3. Show that the first order forward difference formula for f'_j is exact for linear functions, $f(x) = ax+b$.
4. Show that the centred second order difference formula for f'_j is exact for quadratic functions $f(x) = ax^2+bx+c$.

Solutions

Solutions to Exercises 1.1

1. Write down the infinite Taylor series for function f at position $x+\Delta x$ about x

$$f(x+\Delta x) = f(x) + \Delta x f'(x) + \frac{\Delta x^2}{2!} f''(x) + \frac{\Delta x^3}{3!} f'''(x) + \cdots + \frac{\Delta x^j}{j!} f^{(j)}(x) + \cdots$$

2. Write the third order approximation for $f(x-\Delta x)$ in terms of $f(x)$, $f'(x)$ and $f''(x)$. Write the error term using the $O(\Delta x^n)$ notation.

$$f(x-\Delta x) = f(x) - \Delta x f'(x) + \frac{\Delta x^2}{2!} f''(x) + O\left(\Delta x^3\right)$$

3. Write the third order approximation for $f(x+\Delta x)$ in terms of $f(x-\Delta x)$, $f'(x-\Delta x)$ and $f''(x-\Delta x)$.

$$f(x+\Delta x) = f(x-\Delta x) + 2\Delta x f'(x-\Delta x) + 2\Delta x^2 f''(x-\Delta x) + \frac{4\Delta x^3}{3} f'''(x-\Delta x) + O\left(\Delta x^3\right)$$

Solutions to Exercises 3.2

1. Use the Taylor series to find an approximation for f'_j in terms of f_j and f_{j-1}. What order accuracy is it?
   Write the Taylor series for f_{j-1} in terms of f_j:
   $f_{j-1} = f_j - \Delta x f'_j + O(\Delta x^2)$
   Rearrange to find f'_j:
   $f'_j = (f_j - f_{j-1})/\Delta x + O(\Delta x)$
   Note dividing $O(\Delta x^2)$ by Δx gives $O(\Delta x)$ so the approximation is first order accurate
2. Derive an uncentred, second order difference formula for f'_j that uses f_j, f_{j+1} and f_{j+2}. (And show that it is second order accurate)

Taylor approximations for f_{j+1} and f_{j+2} about f_j:

$$f_{j+1} = f_j + \Delta x f_j' + \frac{\Delta x^2}{2!} f_j'' + \frac{\Delta x^3}{3!} f_j''' + \frac{\Delta x^4}{4!} f_j'''' + O(\Delta x^5)$$

$$f_{j+2} = f_j + 2\Delta x f_j' + 2\Delta x^2 f_j'' + \frac{4\Delta x^3}{3} f_j''' + \frac{2\Delta x^4}{3} f_j'''' + O(\Delta x^5)$$

Eliminate the largest unknown, f_j'' by calculating $f_{j+2} - 4f_{j+1}$:

$$f_{j+2} - 4f_{j+1} = -3f_j - 2\Delta x\, f_j' + O(\Delta x^3)$$

Rearrange to find f_j':

$$f_j' = \left(-f_{j+2} + 4f_{j+1} - 3f_j\right)/(2\Delta x) + O(\Delta x^2)$$

3. Find an uncentred approximation for f_j'' using f_j, f_{j+1} and f_{j+2}. What order accurate is it?
   Taylor approximations for f_{j+1} and f_{j+2} about f_j:

$$f_{j+1} = f_j + \Delta x f_j' + \frac{\Delta x^2}{2!} f_j'' + \frac{\Delta x^3}{3!} f_j''' + \frac{\Delta x^4}{4!} f_j'''' + O(\Delta x^5)$$

$$f_{j+2} = f_j + 2\Delta x f_j' + 2\Delta x^2 f_j'' + \frac{4\Delta x^3}{3} f_j''' + \frac{2\Delta x^4}{3} f_j'''' + O(\Delta x^5)$$

Eliminate the largest unknown, f_j' by calculating $f_{j+2} - 2f_{j+1}$:

$$f_{j+2} - 2f_{j+1} = -f_j - \Delta x^2\, f_j'' + O(\Delta x^3)$$

Rearrange to find f_j'':

$$f_j'' = \left(-f_{j+2} + 2f_{j+1} - f_j\right)/\Delta x^2 + O(\Delta x)$$

4. Derive a second order approximation for f_b' from f_a, f_b and f_c at x locations $a < b < c$ when the grid spacing is not regular. (And show that it is second order accurate)
   Define $\Delta x_1 = b - a$ and $\Delta x_2 = c - b$ and $\Delta x = \max(\Delta x_1, \Delta x_2)$
   Taylor approximations for f_a and f_c about f_b:

$$f_a = f_b - \Delta x_1\, f_b' + \frac{\Delta x_1^2}{2!} f_b'' - \frac{\Delta x_1^3}{3!} f_b''' + \frac{\Delta x_1^4}{4!} f_b'''' + O(\Delta x_1^5)$$

$$f_c = f_b + \Delta x_2\, f_b' + \frac{\Delta x_2^2}{2!} f_b'' + \frac{\Delta x_2^3}{3!} f_b''' + \frac{\Delta x_2^4}{4!} f_b'''' + O(\Delta x_2^5)$$

Eliminate the largest unknown, f_b'':

$$\Delta x_1^2 f_c - \Delta x_2^2 f_a = \Delta x_1^2 \left\{f_b + \Delta x_2 f_b' + O(\Delta x_2^3)\right\} - \Delta x_2^2 \left\{f_b - \Delta x_1 f_b' + O(\Delta x_1^3)\right\}$$

Rearrange to find f_b':

$$\Delta x_1^2 f_c - \Delta x_2^2 f_a = \Delta x_1^2 f_b + \Delta x_1^2 \Delta x_2 f_b' + O(\Delta x_2^3 \Delta x_1^2) - \Delta x_2^2 f_b + \Delta x_1 \Delta x_2^2 f_b' + O(\Delta x_1^3 \Delta x_2^2)$$

$$\implies \Delta x_1^2 f_c - \Delta x_2^2 f_a = \left(\Delta x_1^2 - \Delta x_2^2\right) f_b + \Delta x_1 \Delta x_2 \left(\Delta x_1 + \Delta x_2\right) f_b' + O(\Delta x^5)$$

$$\implies f_b' = \frac{\Delta x_1^2 f_c - \Delta x_2^2 f_a - \left(\Delta x_1^2 - \Delta x_2^2\right) f_b}{\Delta x_1 \Delta x_2 \left(\Delta x_1 + \Delta x_2\right)} + O(\Delta x^2)$$

Solutions to Exercises 5.2

1. Use 2 Taylor series about f_j so that they both contain f_j' so that we can eliminate it:

$$f_{j-1} = f_j - \Delta x f_j' + \frac{1}{2!}\Delta x^2 f_j'' + O(\Delta x^3)$$

$$f_{j+1} = f_j + \Delta x f_j' + \frac{1}{2!}\Delta x^2 f_j'' + O(\Delta x^3)$$

Eliminate f_j' by adding the two equations:

$$f_{j-1} + f_{j+1} = 2f_j + \Delta x^2 f_j'' + O(\Delta x^3)$$

Rearrange for f_j and express the unknowns as the order of accuracy:

$$f_j = (f_{j-1} + f_{j+1})/2 + O(\Delta x^2)$$

2. Taylor series about $f_{j+1/2}$:

$$f_{j-1} = f_{j+1/2} - \frac{3}{2}\Delta x f_{j+1/2}' + \frac{1}{2!}\frac{9}{4}\Delta x^2 f_{j+1/2}'' - \frac{1}{3!}\frac{27}{8}\Delta x^3 f_{j+1/2}''' + \frac{1}{4!}\frac{81}{16}\Delta x^4 f_{j+1/2}'''' + O(\Delta x^5)$$

$$f_j = f_{j+1/2} - \frac{1}{2}\Delta x f_{j+1/2}' + \frac{1}{2!}\frac{1}{4}\Delta x^2 f_{j+1/2}'' - \frac{1}{3!}\frac{1}{8}\Delta x^3 f_{j+1/2}''' + \frac{1}{4!}\frac{1}{16}\Delta x^4 f_{j+1/2}'''' + O(\Delta x^5)$$

$$f_{j+1} = f_{j+1/2} + \frac{1}{2}\Delta x f_{j+1/2}' + \frac{1}{2!}\frac{1}{4}\Delta x^2 f_{j+1/2}'' + \frac{1}{3!}\frac{1}{8}\Delta x^3 f_{j+1/2}''' + \frac{1}{4!}\frac{1}{16}\Delta x^4 f_{j+1/2}'''' + O(\Delta x^5)$$

$f_{j+2} = f_{j+1/2} + \frac{3}{2}\Delta x f'_{j+1/2} + \frac{1}{2!}\frac{9}{4}\Delta x^2 f''_{j+1/2} + \frac{1}{3!}\frac{27}{8}\Delta x^3 f'''_{j+1/2} + \frac{1}{4!}\frac{81}{16}\Delta x^4 f''''_{j+1/2} + O(\Delta x^5)$

First eliminate f''_j, the biggest unknown (we only need to leave two equations):

$f_{j+2} - f_{j-1} = 3\Delta x f'_{j+1/2} + \frac{9}{8}\Delta x^3 f'''_j + O(\Delta x^5)$

$f_{j+1} - f_j = \Delta x f'_{j+1/2} + \frac{1}{3}\frac{1}{8}\Delta x^3 f'''_j + O(\Delta x^5)$

Next eliminate f'''_j leaving one equation for f'_j:

$f_{j+2} - f_{j-1} - 27 f_{j+1} + 27 f_j = -24\Delta x f'_{j+1/2} + O(\Delta x^5)$

$\Longrightarrow f'_{j+1/2} = \dfrac{f_{j-1} - 27 f_j + 27 f_{j+1} - f_{j+2}}{24\Delta x} + O(\Delta x^4)$

3. If $f(x) = ax + b$ and we use the approximation $f'_j = \dfrac{f_{j+1} - f_j}{\Delta x}$ between any two points x_{j+1} and x_j then we get:

   $f'_j = \dfrac{(ax_{j+1} + b) - (ax_j + b)}{x_{j+1} - x_j} = a$ which is the exact solution.

4. If $f(x) = ax^2 + bx + c$ and we use the approximation $f'_j = \dfrac{f_{j+1} - f_{j-1}}{2\Delta x}$ for f_j at x_j between two points x_{j+1} and x_{j-1} then we get:

   $f'_j = \dfrac{(ax_{j+1}^2 + bx_{j+1} + c) - (ax_{j-1}^2 + bx_{j-1} + c)}{x_{j+1} - x_{j-1}} = \dfrac{a(x_j + \Delta x)^2 - a(x_j - \Delta x)^2 + 2b\Delta x}{2\Delta x}$

   $= 2ax_j + b$ which is the exact solution.