

Q1. Using Taylor series, derive a second order finite-difference approximation to $\partial_x f$ at the location x_i using a three point stencil involving f_{i-1} , f_i and f_{i+1} .

Taylor series for $f_{i\pm 1}$ at $x = x_i$ are

$$f_{i\pm 1} = f_i \pm \Delta x_{i\pm \frac{1}{2}} f'(x_i) + \frac{\Delta x_{i\pm \frac{1}{2}}^2}{2} f''(x_i) \pm \frac{\Delta x_{i\pm \frac{1}{2}}^3}{3!} f'''(x_i) + \frac{\Delta x_{i\pm \frac{1}{2}}^4}{4!} f^{(4)}(x_i) + H.O.T.$$

We pose that $f'(x_i)$ can be expressed as

$$f'(x_i) = a f_{i+1} + b f_i + c f_{i-1} + O(\Delta x^2)$$

and substitute $f_{i\pm 1}$ with their Taylor series. Collecting like terms, we see that

$$\begin{aligned} a + b + c &= 0, \\ a \frac{\Delta x_{i+\frac{1}{2}}}{2} - c \frac{\Delta x_{i-\frac{1}{2}}}{2} &= 1, \\ a \frac{\Delta x_{i+\frac{1}{2}}^2}{6} + c \frac{\Delta x_{i-\frac{1}{2}}^2}{6} &= 0. \end{aligned}$$

The solution to the last two equations is

$$\begin{aligned} a &= \left(\frac{1}{\Delta_{i-\frac{1}{2}} + \Delta_{i+\frac{1}{2}}} \right) \frac{\Delta_{i-\frac{1}{2}}}{\Delta_{i+\frac{1}{2}}} = \frac{\Delta_{i-\frac{1}{2}}^2}{(\Delta_{i-\frac{1}{2}} + \Delta_{i+\frac{1}{2}}) \Delta_{i+\frac{1}{2}} \Delta_{i-\frac{1}{2}}} \\ c &= \left(\frac{-1}{\Delta_{i-\frac{1}{2}} + \Delta_{i+\frac{1}{2}}} \right) \frac{\Delta_{i+\frac{1}{2}}}{\Delta_{i-\frac{1}{2}}} = \frac{-\Delta_{i+\frac{1}{2}}^2}{(\Delta_{i-\frac{1}{2}} + \Delta_{i+\frac{1}{2}}) \Delta_{i+\frac{1}{2}} \Delta_{i-\frac{1}{2}}} \end{aligned}$$

and using the first equation, $b = -a - c$, gives

$$b = \frac{\Delta_{i+\frac{1}{2}}^2 - \Delta_{i-\frac{1}{2}}^2}{(\Delta_{i-\frac{1}{2}} + \Delta_{i+\frac{1}{2}}) \Delta_{i+\frac{1}{2}} \Delta_{i-\frac{1}{2}}}.$$

The full expression for $\partial_x f(x_i)$ is

$$f'(x_i) \approx \frac{\Delta_{i-\frac{1}{2}}^2 f_{i+1} + (\Delta_{i+\frac{1}{2}}^2 - \Delta_{i-\frac{1}{2}}^2) f_i - \Delta_{i+\frac{1}{2}}^2 f_{i-1}}{(\Delta_{i-\frac{1}{2}} + \Delta_{i+\frac{1}{2}}) \Delta_{i+\frac{1}{2}} \Delta_{i-\frac{1}{2}}}.$$

Note that this can be written

$$f'(x_i) \approx \left(\frac{\Delta_{i-\frac{1}{2}}}{\Delta_{i-\frac{1}{2}} + \Delta_{i+\frac{1}{2}}} \right) \left(\frac{f_{i+1} - f_i}{\Delta_{i+\frac{1}{2}}} \right) + \left(\frac{\Delta_{i+\frac{1}{2}}}{\Delta_{i-\frac{1}{2}} + \Delta_{i+\frac{1}{2}}} \right) \left(\frac{f_i - f_{i-1}}{\Delta_{i-\frac{1}{2}}} \right).$$

Q2.a i) Derive the actual truncation error terms out to order Δx^2 .

$$\frac{f_{i+1} - f_i}{\Delta x} = f'(x_i) + \frac{1}{2}\Delta x f''(x_i) + \frac{1}{6}\Delta x^2 f'''(x_i) + O(\Delta x^3)$$

ii) Derive an approximation for $\partial_{xx}f$ evaluated at the same point, x_i , that uses the values f_{i-1} , f_i and f_{i+1} .

$$f''(x_i) = \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} + O(\Delta x^2 f'''')$$

iii) Substitute your approximation to $\partial_{xx}f$ from (ii) into the leading truncation term. What is the leading order truncation term and resulting scheme?

$$\frac{f_{i+1} - f_i}{\Delta x} = f'(x_i) + \frac{1}{2}\Delta x \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} + \frac{1}{6}\Delta x^2 f'''(x_i) + O(\Delta x^3)$$

or, moving the terms in f_{i-1} , f_i and f_{i+1} to the L.H.S.,

$$\frac{f_{i+1} - f_{i-1}}{2\Delta x} = f'(x_i) + \frac{1}{6}\Delta x^2 f'''(x_i) + O(\Delta x^4)$$

The largest remaining truncation term is $O(\Delta x^2)$ and so this is a centered second order difference approximation to $\partial_x f$ at $x = x_i$ (i.e. $f'(x_i)$).

Q2.b i) Derive the leading order truncation error.

As above:

$$\frac{f_{i+1} - f_{i-1}}{2\Delta x} = f'(x_i) + \frac{1}{6}\Delta x^2 f'''(x_i) + O(\Delta x^3)$$

ii) Using the stencil $(f_{i-2}, f_{i-1}, f_i, f_{i+1})$ write a finite difference approximation for $\partial_{xxx}f$.

$$f'''(x_i) = \frac{f_{i+1} - 3f_i + 3f_{i-1} - f_{i-2}}{\Delta x^3} + O(\Delta x)$$

iii) Substitute your approximation from (ii) into the leading order error term of the approximation to $\partial_x f$. This is an approximation for $\partial_x f$ of what order?

$$\frac{f_{i+1} - f_{i-1}}{2\Delta x} = f'(x_i) + \frac{1}{6}\Delta x^2 \frac{f_{i+1} - 3f_i + 3f_{i-1} - f_{i-2}}{\Delta x^3} + O(\Delta x^3)$$

or, moving the terms in f_{i-2} , f_{i-1} , f_i and f_{i+1} to the L.H.S.,

$$\frac{2f_{i+1} + 3f_i - 6f_{i-1} + f_{i-2}}{6\Delta x} = f'(x_i) + O(\Delta x^3)$$

This is a third order difference approximation to $f'(x_i)$.

Q2.c Do you see the pattern behind the methods you used in Q2.a and b. Briefly explain, how you would derive an $O(\Delta x^n)$ approximation to a finite difference expression if you were given an $O(\Delta x^{n-1})$ finite difference expression.

Replacing the leading Taylor series term in a finite difference approximation with a finite difference approximation of that term results in a higher order scheme.

Q3. i) Derive a second order expression of a similar form as before but using only the values f_{i-2} and f_{i+2} .

Literally replacing Δx with $2\Delta x$:

$$\frac{f_{i+2} - f_{i-2}}{4\Delta x} = f'(x_i) + \frac{4}{6}\Delta x^2 f'''(x_i) + O(\Delta x^4)$$

ii) Linearly combine your approximations from (i) and the former approximation to yield a $O(\Delta x^4)$ approximation for $\partial_x f$ at x_i .

$$\begin{aligned} a \left(\frac{f_{i+2} - f_{i-2}}{4\Delta x} \right) + b \left(\frac{f_{i+1} - f_{i-1}}{2\Delta x} \right) &= a \left(f'(x_i) + \frac{4}{6}\Delta x^2 f'''(x_i) \right) \\ &\quad + b \left(f'(x_i) + \frac{1}{6}\Delta x^2 f'''(x_i) \right) + O(\Delta x^4) \end{aligned}$$

To eliminate the $O(\Delta x^2)$ terms and obtain an expression for $f'(x_i)$ we must solve

$$\begin{aligned} a + b &= 1 \\ \frac{4}{6}a + \frac{1}{6}b &= 0 \end{aligned}$$

the solution to which is

$$a = \frac{-1}{3} \quad \text{and} \quad b = \frac{4}{3}.$$

The resulting $O(\Delta x^4)$ approximation to $f'(x_i)$ is

$$\frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12\Delta x} = f'(x_i) + O(\Delta x^4)$$

Q4. *i) Write down an $O(\Delta x^3)$ approximation for $F_{i+\frac{1}{2}}$ in terms of θ_{i-1} , θ_i , θ_{i+1} .*

Taylor series for θ_{i-1} , θ_i and θ_{i+1} about $x = x_{i+\frac{1}{2}}$ are:

$$\begin{aligned}\theta_{i+1} &= \theta(x_{i+\frac{1}{2}}) + \frac{\Delta x}{2}\theta'(x_{i+\frac{1}{2}}) + \frac{\Delta x^2}{2^2 \cdot 2!}\theta''(x_{i+\frac{1}{2}}) + O(\Delta x^3) \\ \theta_i &= \theta(x_{i+\frac{1}{2}}) - \frac{\Delta x}{2}\theta'(x_{i+\frac{1}{2}}) + \frac{\Delta x^2}{2^2 \cdot 2!}\theta''(x_{i+\frac{1}{2}}) + O(\Delta x^3) \\ \theta_{i-1} &= \theta(x_{i+\frac{1}{2}}) - \frac{3\Delta x}{2}\theta'(x_{i+\frac{1}{2}}) + \frac{3^2\Delta x^2}{2^2 \cdot 2!}\theta''(x_{i+\frac{1}{2}}) + O(\Delta x^3)\end{aligned}$$

We want an $O(\Delta x^3)$ approximation for $\theta(x_{i+\frac{1}{2}})$ in the form

$$a\theta_{i+1} + b\theta_i + c\theta_{i-1} = \theta(x_{i+\frac{1}{2}}) + O(\Delta x^3)$$

so

$$\begin{aligned}a + b + c &= 1 \\ a - b - 3c &= 0 \\ a + b + 9c &= 0\end{aligned}$$

First + last equations give $8c = -1$. Last two give $2a = -6c$. Difference of last two give $2b = -12c$.

$$a = \frac{3}{8} \quad ; \quad b = \frac{6}{8} \quad ; \quad c = \frac{-1}{8}$$

Third order interpolation for $\theta(x_{i+\frac{1}{2}})$ gives the stencil

$$u [c \quad b \quad a] = u \left[\frac{-1}{8} \quad \frac{6}{8} \quad \frac{3}{8} \right]$$

for $F_{i+\frac{1}{2}}$.

ii) Substitute your $O(\Delta x^3)$ expressions for $F_{i+\frac{1}{2}}$ and $F_{i-\frac{1}{2}}$ in and derive the leading order truncation error.

We need Taylor series expanded about $x = x_i$:

$$\begin{aligned}\theta_{i+1} &= \theta(x_i) + \Delta x\theta'(x_i) + \frac{\Delta x^2}{2!}\theta''(x_i) + \frac{\Delta x^3}{3!}\theta'''(x_i) + O(\Delta x^4) \\ \theta_{i-1} &= \theta(x_i) - \Delta x\theta'(x_i) + \frac{\Delta x^2}{2!}\theta''(x_i) - \frac{\Delta x^3}{3!}\theta'''(x_i) + O(\Delta x^4) \\ \theta_{i-2} &= \theta(x_i) - 2\Delta x\theta'(x_i) + \frac{2^2\Delta x^2}{2!}\theta''(x_i) - \frac{2^3\Delta x^3}{3!}\theta'''(x_i) + O(\Delta x^4)\end{aligned}$$

$$\begin{aligned}
\partial_t \theta_i &+ \frac{u}{\Delta x} [a\theta_{i+1} + (b-a)\theta_i + (c-b)\theta_{i-1} - c\theta_{i-2}] \\
&= \partial_t \theta_i + (a + (b-a) + (c-b) - c) \frac{u\theta_i}{\Delta x} \\
&\quad + (a + 0(b-a) - (c-b) + 2c)u\theta' \\
&\quad + (a + 0(b-a) + (c-b) - 2^2c) \frac{u\Delta x}{2!} \theta'' \\
&\quad + (a + 0(b-a) - (c-b) + 2^3c) \frac{u\Delta x^2}{3!} \theta''' + O(\Delta x^3) \\
&= \partial_t \theta_i + 0\theta_i + (a+b+c)u\theta' + (a-b-3c)u\Delta x\theta'' + (a+b+7c)u\Delta x^2\theta''' + O(\Delta x^3) \\
&= \partial_t \theta_i + u\theta' + 2u\Delta x^2\theta''' + O(\Delta x^3)
\end{aligned}$$

So the $O(\Delta x^2)$ remains (since $a+b-7c=10/8$) and the governing equation is only second order, not third order accurate, in Δx .

We substituted a third order approximation of the flux so why is the approximation to the governing equation not third order?

The difference approximation of $\partial_x F$

$$\partial_x F \approx \frac{F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}}{\Delta x}$$

is only second order accurate. No matter how accurate we make F , there will be a second order truncation error **unless** we can construct the truncation errors in $F_{i+\frac{1}{2}}$ and $F_{i-\frac{1}{2}}$ so as to cancel each other. As we do next...

iii) Write down the $O(\Delta x^3)$ finite difference approximation to the governing equation evaluated at x_i using the stencil $(\theta_{i-2}, \theta_{i-1}, \theta_i, \theta_{i+1})$.

$$\partial_t \theta_i + \frac{u}{\Delta x} \left[\frac{2}{6}\theta_{i+1} + \frac{3}{6}\theta_i - \theta_{i-1} + \frac{1}{6}\theta_{i-2} \right]$$

iii) Deduce an approximation for the flux $F_{i+\frac{1}{2}}$ that yields an $O(\Delta x^3)$ approximation to the linear advection problem.

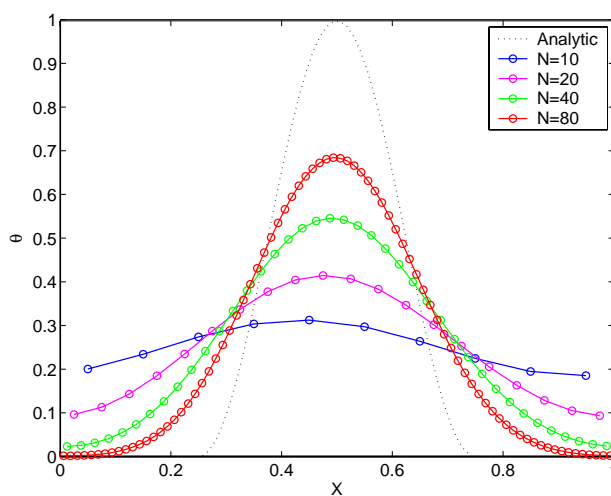
$$\left[\frac{1}{6} \quad \frac{-6}{6} \quad \frac{3}{6} \quad \frac{2}{6} \right] = [-\alpha \quad \alpha - \beta \quad \beta - \gamma \quad \gamma]$$

Solving for α , β and γ :

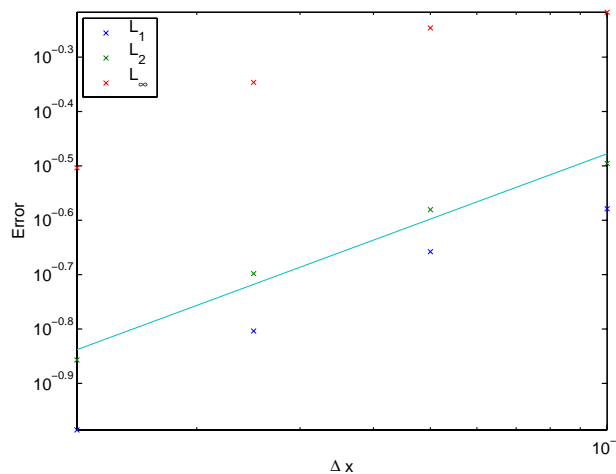
$$\alpha = \frac{-1}{6} \quad ; \quad \beta = \frac{5}{6} \quad ; \quad \gamma = \frac{2}{6}$$

Q5 (MATLAB)

i) Plot the initial conditions and solutions at time $t = 1$ for $N = 10, 20, 40, 80$.



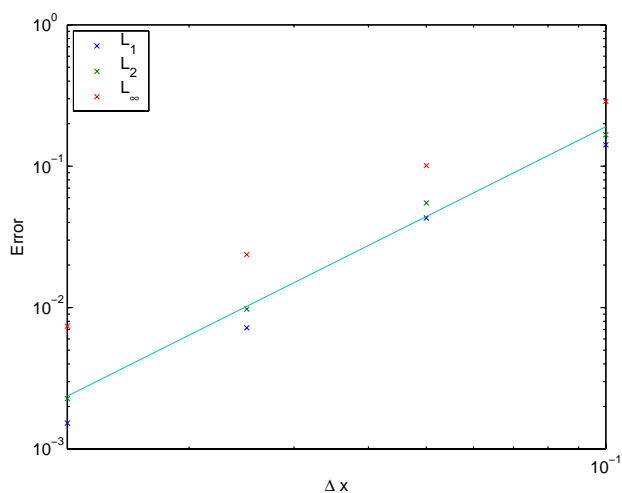
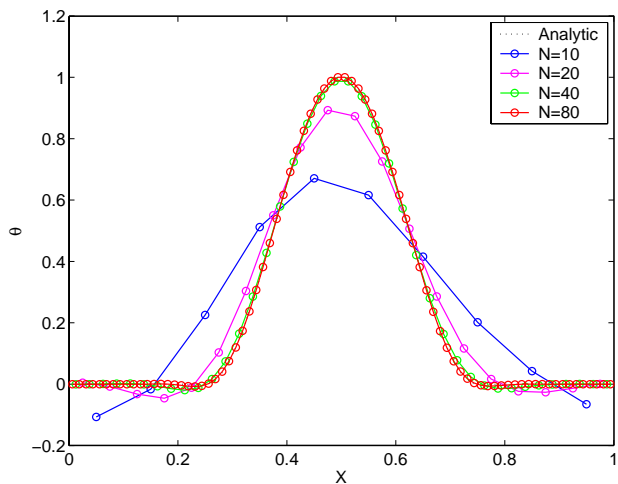
ii) At each resolution, measure the l_1 , l_2 and l_∞ norms. Plot them as a function of grid-spacing and measure the power dependence of the l_2 curve on Δx .



A fit to the l_2 -norm points gives a power of $\Delta x^{0.4}$.

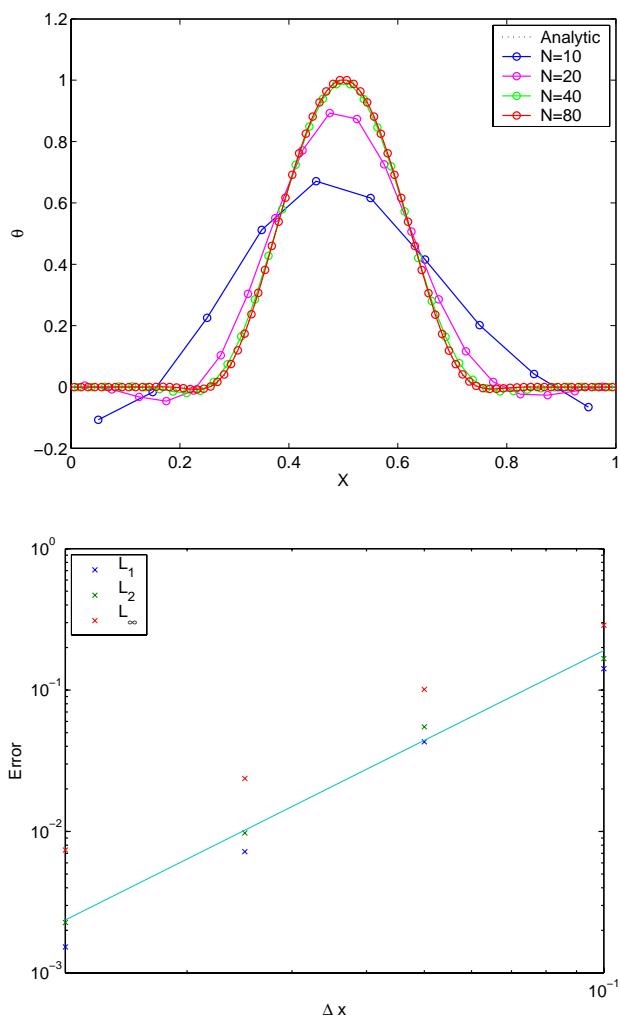
iii) Repeat (i) and (ii) using the two forms of “third” order flux in Q4.
Which is more accurate?

Third order flux (1/6 form)



A fit to the l_2 -norm points gives a power of $\Delta x^{2.1}$.

Third order flux (1/8 form)



A fit to the l_2 -norm points gives a power of $\Delta x^{1.8}$. Using $\frac{1}{6}$ form is more accurate than the $\frac{1}{8}$ form, consistent with the analysis.

iv) Why is the dependence not what you would expect, given all the effort you put into deriving the truncation errors in the previous questions?

We are using the forward time-stepping scheme which is of order Δt . Although Δt was reduced with Δx , the first order accuracy of the time differencing error dominates and higher order errors in the spatial differences.