# Discretization Methods - Exercise Sheet 1

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April 26, 2025

## Exercise 1

We want to show that the 6th order accurate central finite difference approximation is given as:

$$\left.\frac{du}{dx}\right|_{x_j} = \frac{-u_{j-3} + 9u_{j-2} - 45u_{j-1} + 45u_{j+1} - 9u_{j+2} + u_{j+3}}{60\Delta x} + \mathcal{O}(\Delta x^6). \quad (1)$$

**Derivation:** Using Taylor expansion around $x_j$, we can write the expansions for all six points:

$$u_{j\pm1} = u_j \pm \Delta x u'_j + \frac{\Delta x^2}{2}u''_j \pm \frac{\Delta x^3}{6}u'''_j + \frac{\Delta x^4}{24}u^{(4)}_j \pm \frac{\Delta x^5}{120}u^{(5)}_j + \frac{\Delta x^6}{720}u^{(6)}_j + \mathcal{O}(\Delta x^7) \quad (2)$$

$$u_{j\pm2} = u_j \pm 2\Delta x u'_j + \frac{4\Delta x^2}{2}u''_j \pm \frac{8\Delta x^3}{6}u'''_j + \frac{16\Delta x^4}{24}u^{(4)}_j \pm \frac{32\Delta x^5}{120}u^{(5)}_j + \frac{64\Delta x^6}{720}u^{(6)}_j + \mathcal{O}(\Delta x^7) \quad (3)$$

$$u_{j\pm3} = u_j \pm 3\Delta x u'_j + \frac{9\Delta x^2}{2}u''_j \pm \frac{27\Delta x^3}{6}u'''_j + \frac{81\Delta x^4}{24}u^{(4)}_j \pm \frac{243\Delta x^5}{120}u^{(5)}_j + \frac{729\Delta x^6}{720}u^{(6)}_j + \mathcal{O}(\Delta x^7) \quad (4)$$

We seek coefficients $a, b, c, d, e, f$ such that:

$$au_{j-3} + bu_{j-2} + cu_{j-1} + du_{j+1} + eu_{j+2} + fu_{j+3} = u'_j + \mathcal{O}(\Delta x^6) \quad (5)$$

This leads to the following system of equations:

$$\begin{aligned}
a + b + c + d + e + f &= 0 \quad \text{(coefficient of } u_j\text{)} \\
3a + 2b + c - d - 2e - 3f &= \frac{1}{\Delta x} \quad \text{(coefficient of } u_j'\text{)} \\
9a + 4b + c + d + 4e + 9f &= 0 \quad \text{(coefficient of } u_j''\text{)} \\
27a + 8b + c - d - 8e - 27f &= 0 \quad \text{(coefficient of } u_j'''\text{)} \\
81a + 16b + c + d + 16e + 81f &= 0 \quad \text{(coefficient of } u_j^{(4)}\text{)} \\
243a + 32b + c - d - 32e - 243f &= 0 \quad \text{(coefficient of } u_j^{(5)}\text{)}
\end{aligned}$$

Solving this system gives:

$$a = -\frac{1}{60}, \quad b = \frac{3}{20}, \quad c = -\frac{3}{4}, \quad d = \frac{3}{4}, \quad e = -\frac{3}{20}, \quad f = \frac{1}{60}$$

Substituting these coefficients back into the linear combination:

$$\begin{aligned}
u_j' &= -\frac{1}{60}u_{j-3} + \frac{3}{20}u_{j-2} - \frac{3}{4}u_{j-1} + \frac{3}{4}u_{j+1} - \frac{3}{20}u_{j+2} + \frac{1}{60}u_{j+3} + \mathcal{O}(\Delta x^6) \\
&= \frac{-u_{j-3} + 9u_{j-2} - 45u_{j-1} + 45u_{j+1} - 9u_{j+2} + u_{j+3}}{60\Delta x} + \mathcal{O}(\Delta x^6)
\end{aligned}$$

This yields the desired 6th order central difference formula.

# Exercise 2

For the linear wave problem:

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x}, \quad u(0,t) = u(2\pi, t), \quad u(x,0) = e^{ikx} \tag{6}$$

## Numerical Wave Speed

The exact solution to the wave equation is a traveling wave:

$$u(x,t) = e^{i(kx - \omega t)} \tag{7}$$

where $\omega = ck$ is the angular frequency and $k$ is the wavenumber.

When we discretize the spatial derivative using the 6th order central difference scheme:

$$\left.\frac{du}{dx}\right|_{x_j} \approx \frac{-u_{j-3} + 9u_{j-2} - 45u_{j-1} + 45u_{j+1} - 9u_{j+2} + u_{j+3}}{60\Delta x} \tag{8}$$

Substituting the exact solution at grid points:

$$\begin{aligned}\left.\frac{du}{dx}\right|_{x_j} &\approx \frac{1}{60\Delta x}\Big[ - e^{ik(x_j-3\Delta x)} + 9e^{ik(x_j-2\Delta x)} \\ &- 45e^{ik(x_j-\Delta x)} + 45e^{ik(x_j+\Delta x)} \\ &- 9e^{ik(x_j+2\Delta x)} + e^{ik(x_j+3\Delta x)}\Big] \\ &= \frac{e^{ikx_j}}{60\Delta x}\Big[ - e^{-3ik\Delta x} + 9e^{-2ik\Delta x} - 45e^{-ik\Delta x} \\ &+ 45e^{ik\Delta x} - 9e^{2ik\Delta x} + e^{3ik\Delta x}\Big]\end{aligned}$$

Using Euler's formula $e^{i\theta} = \cos\theta + i\sin\theta$, we can rewrite the expression:

$$\begin{aligned}\left.\frac{du}{dx}\right|_{x_j} &= \frac{e^{ikx_j}}{60\Delta x}\Big[2i(45\sin(k\Delta x) - 9\sin(2k\Delta x) + \sin(3k\Delta x))\Big] \\ &= \frac{ie^{ikx_j}}{30\Delta x}\Big[45\sin(k\Delta x) - 9\sin(2k\Delta x) + \sin(3k\Delta x)\Big]\end{aligned}$$

The numerical wave speed $c_3(k)$ is defined as the ratio of the numerical angular frequency to the wavenumber:

$$c_3(k) = c\frac{45\sin(k\Delta x) - 9\sin(2k\Delta x) + \sin(3k\Delta x)}{30k\Delta x} \tag{9}$$

## Phase Error

For the 6th order central difference scheme, the phase error is:

$$e_3(k) = \frac{c}{70}(k\Delta x)^6 + \mathcal{O}((k\Delta x)^8) \tag{10}$$

For a wavelength $p$ and CFL number $\nu = \frac{c\Delta t}{\Delta x}$, the phase error becomes:

$$e_3(p, \nu) = \frac{\pi\nu}{70}\left(\frac{2\pi}{p}\right)^6 \tag{11}$$

To ensure the phase error is less than $\varepsilon_p$, we need:

$$\frac{\pi\nu}{70}\left(\frac{2\pi}{p}\right)^6 \leq \varepsilon_p \tag{12}$$

This gives the minimum required points per wavelength:

$$p_3(\varepsilon_p, \nu) \geq 2\pi\sqrt[6]{\frac{\pi\nu}{70\varepsilon_p}} \tag{13}$$

The choice between different order schemes depends on the error tolerance $\varepsilon_p$ and the CFL number $\nu$:

- For $\varepsilon_p = 0.1$:
  - When $\nu > 0.06$, the 6th order scheme requires fewer points than the 2nd order scheme
  - For example, at $\nu = 0.06$:
    * 2nd order scheme requires $p_1 \approx 3.52$ points
    * 4th order scheme requires $p_2 \approx 3.15$ points
    * 6th order scheme requires $p_3 \approx 3.44$ points
- For $\varepsilon_p = 0.01$:
  - When $\nu > 0.003$, the 6th order scheme requires fewer points than the 2nd order scheme
  - For example, at $\nu = 0.003$:
    * 2nd order scheme requires $p_1 \approx 2.49$ points
    * 4th order scheme requires $p_2 \approx 2.65$ points
    * 6th order scheme requires $p_3 \approx 3.06$ points

The phase error analysis shows that:

- The 6th order scheme becomes advantageous only when $\nu$ exceeds certain thresholds.
- For $\varepsilon_p = 0.1$, the threshold is $\nu > 0.06$.
- For $\varepsilon_p = 0.01$, the threshold is $\nu > 0.003$.
- Below these thresholds, lower order schemes may require fewer points per wavelength.

# Exercise 3

**Objective:** Implement and test the Fourier differentiation matrix on $u(x) = \exp(k \sin x)$ over $x \in [0, 2\pi]$.

## Implementation

The key part of the implementation is the Fourier differentiation matrix:

```python
def fourier_differentiation_matrix(N):
    """Compute the Fourier differentiation matrix."""
    D = np.zeros((N+1, N+1))
    for i in range(N+1):
        for j in range(N+1):
            if i != j:
                D[i,j] = (-1)**(i+j) / (2 *
                    np.sin((j-i)*np.pi/(N+1)))
    return D
```

The matrix is constructed using the formula:

$$D_{ji} = \begin{cases} \frac{(-1)^{j+i}}{2\sin\left(\frac{(j-i)\pi}{N+1}\right)}, & i \neq j \\ 0, & i = j \end{cases} \tag{14}$$

## Results

The code tests the Fourier differentiation matrix for $k = 2, 4, 6, 8, 10, 12$ and finds the minimum $N$ that ensures the maximum error is less than $10^{-5}$. The results are shown in Table 1.

| $k$ | $N$ (Relative Error) | $N$ (Absolute Error) |
|---|---|---|
| 2 | 22 | 20 |
| 4 | 32 | 28 |
| 6 | 42 | 34 |
| 8 | 52 | 42 |
| 10 | 60 | 48 |
| 12 | 74 | 54 |

Table 1: Minimum $N$ values for different $k$ values

The results show that:

- The required $N$ increases with $k$, as expected.
- The relative error criterion requires more points than the absolute error criterion.