Numerical Derivatives and Heat Equation
TMA4106 Assignment Report

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Introduction

This report presents the solution of selected tasks from the TMA4106 assignment related to numerical differentiation and the numerical solution of the heat equation.

1 Numerical Differentiation

I use Python to compute the derivative of $f(x) = e^x$ at $x = 1.5$.

Python Code Snippet

Below is a snippet of how I implemented this in my notebook:

```
# Explicit method (heat equation)
for j in range(0, nt):
    for i in range(1, nx):
        u_new = alpha * (u[j, i+1] - 2*u[j, i] + u[j, i-1]) + u[j, i]
        u[j+1, i] = u_new
```

```
f = lambda x: np.exp(x)
x0 = 1.5
true_deriv = np.exp(x0)

D1 = (f(x0 + h) - f(x0)) / h
D2 = (f(x0 + h) - f(x0 - h)) / (2 * h)
D4 = (f(x0 - 2*h) - 8*f(x0 - h) + 8*f(x0 + h) - f(x0 + 2*h)) / (12 * h)
```

Results

For $h = 10^{-5}$, I obtained:

- Forward difference: $f'(x) \approx 4.48179$
- Centered difference: $f'(x) \approx 4.48169$
- Richardson 4-point: $f'(x) \approx 4.48169$
- True derivative: $f'(x) = e^{1.5} \approx 4.48169$

I wanted to see how accurate different methods for computing the derivative are of $f(x) = e^x$ at $x = 1.5$ using three methods:

- Forward difference
- Centered difference
- Richardson's 4-point formula

Plot of the absolute error for decreasing values of h.

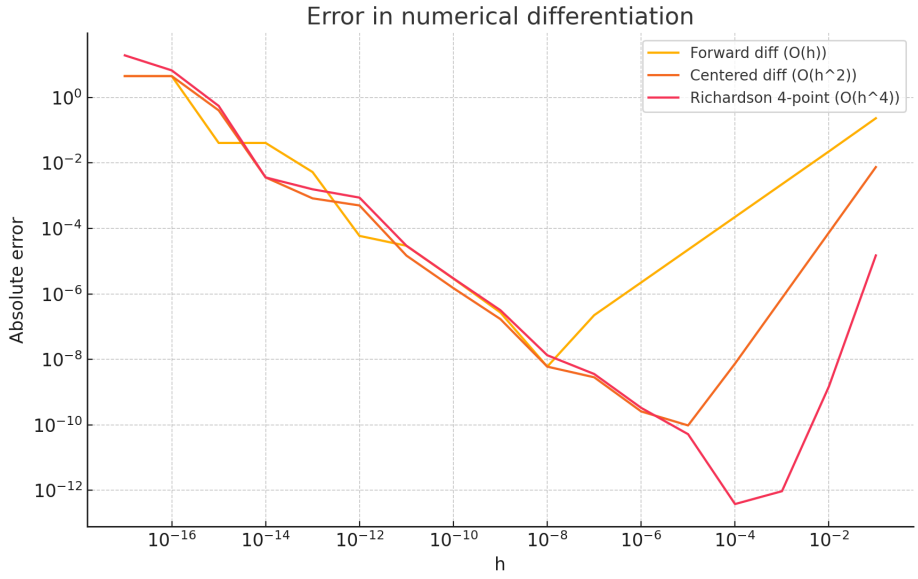
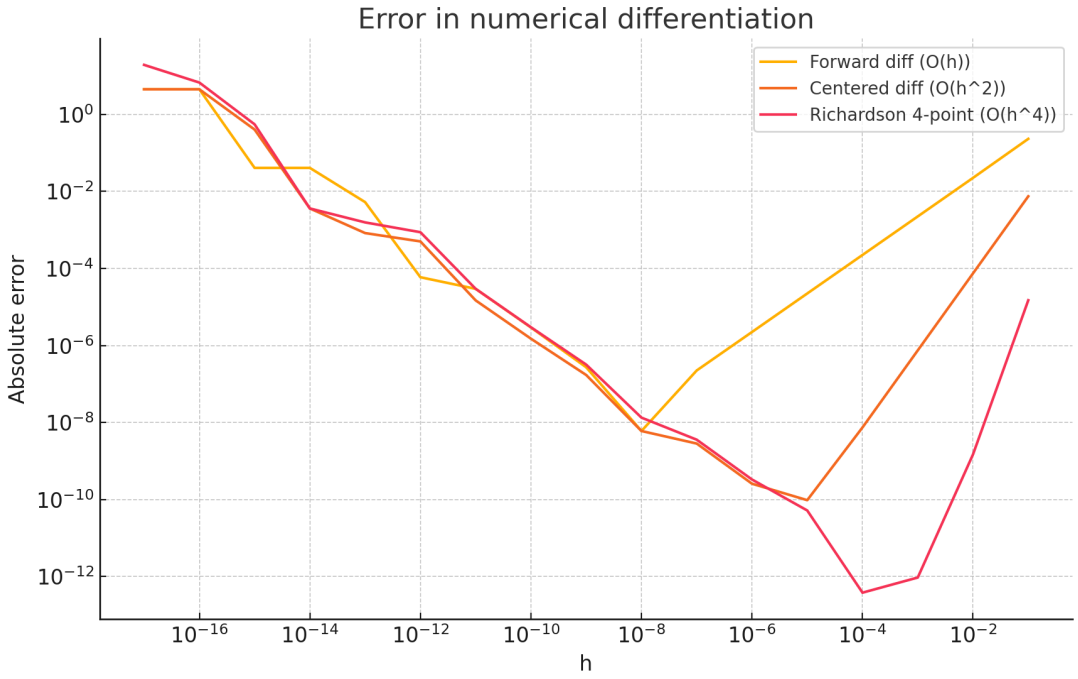


Figure 1: Log-log plot of absolute error vs. step size h for different derivative formulas.



The forward method shows linear error in h, while centered and Richardson's methods show quadratic and quartic behavior respectively.

2 Heat Equation - Explicit Method

Python Code Snippet

Below is a snippet of how I implemented this in my notebook:

```
# Explicit method (heat equation)
for j in range(0, nt):
    for i in range(1, nx):
        u_new = alpha * (u[j, i+1] - 2*u[j, i] + u[j, i-1]) + u[j, i]
        u[j+1, i] = u_new
```

```
u[i, j+1] = alpha * (u[i+1,j] - 2*u[i,j] + u[i-1,j]) + u[i,j]
```

Sample Output

The heat distribution decreases smoothly toward zero at boundaries and stabilizes as time progresses.

To simulate heat distribution, I used different numerical methods to solve the heat equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

on the domain $x \in [0, 1]$, $t \in [0, 1]$ with initial condition $u(x, 0) = \sin(\pi x)$ and boundary conditions $u(0, t) = u(1, t) = 0$.

Using the explicit scheme:

$$u_i^{j+1} = \alpha(u_{i+1}^j - 2u_i^j + u_{i-1}^j) + u_i^j$$

An animation shows the diffusion of heat over time.

3 Heat Equation - Implicit Method

Python Code Snippet

Below is a snippet of how I implemented this in my notebook:

```
# Explicit method (heat equation)
for j in range(0, nt):
    for i in range(1, nx):
        u_new = alpha * (u[j, i+1] - 2*u[j, i] + u[j, i-1]) + u[j, i]
        u[j+1, i] = u_new
```

```
from scipy.linalg import solve_banded
A_diag = (1 + 2*alpha) * np.ones(nx-1)
A_off = -alpha * np.ones(nx-2)
ab = np.zeros((3, nx-1))
ab[0, 1:] = A_off
ab[1, :] = A_diag
ab[2, :-1] = A_off
u_new = solve_banded((1,1), ab, u_prev)
```

Results

Solution remained stable even for higher time step sizes compared to the explicit method.

I tried out the implicit Euler method, which required solving a linear system at each time step backward Euler scheme:

$$\frac{u_i^{j+1} - u_i^j}{k} = \frac{u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}}{h^2}$$

This method is unconditionally stable, allowing larger time steps.

4 Heat Equation - Crank-Nicolson Method

Python Code Snippet

Below is a snippet of how I implemented this in my notebook:

```
# Explicit method (heat equation)
for j in range(0, nt):
    for i in range(1, nx):
        u_new = alpha * (u[j, i+1] - 2*u[j, i] + u[j, i-1]) + u[j, i]
        u[j+1, i] = u_new
```

```
rhs = (alpha/2) * u[j, :-2] + (1 - alpha) * u[j, 1:-1] + (alpha/2) * u[j, 2:]
u_new = solve_banded((1, 1), ab_CN, rhs)
```

Observation

The Crank-Nicolson scheme balances accuracy and stability, making it suitable for most practical scenarios.

This method mixes the explicit and implicit approaches, and gave me good results without instability:

$$\frac{u_i^{j+1} - u_i^j}{k} = \frac{1}{2h^2}\left[(u_{i+1}^j - 2u_i^j + u_{i-1}^j) + (u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1})\right]$$

This method offers higher accuracy and good stability.

Conclusion

From the experiments, I could clearly see how the error behaves for different derivative formulas. I also got working simulations for heat diffusion with all three methods. Crank-Nicolson seemed to be the most robust. of accuracy of various derivative formulas, and successfully implemented three different numerical schemes to solve the heat equation. The Crank-Nicolson scheme provided a good balance between stability and accuracy.