MSN 514 - Computational Methods for Material Science and Complex Systems

Homework 02

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I. INTRODUCTION

This report compares three methods for approximating the derivatives of a smooth, periodic function:

- **Finite-difference (FD)** methods using different stencils.
- A **Fourier-based approach** using the Fast Fourier Transform (FFT).
- A **DFT matrix method** that builds the discrete Fourier transform (DFT) directly.

The **Discrete Fourier Transform (DFT)** for a series x_n (with $n = 0, \ldots, N-1$) is defined as

$$X_k = \sum_{n=0}^{N-1} x_n \, e^{-2\pi i k n/N}, \quad k = 0, \ldots, N-1. \tag{1}$$

Its inverse gives back x_n from X_k. However, computing the DFT directly takes $\mathcal{O}(N^2)$ time, which is slow and uses much memory.

The **Fast Fourier Transform (FFT)** computes the DFT in $\mathcal{O}(N \log N)$ time and is very fast when N is a power of two. In the frequency domain, taking a derivative is simple: multiply by ik for the first derivative or by $-k^2$ for the second derivative.

Finite-difference methods estimate derivatives using nearby points. They are simple and take $\mathcal{O}(N)$ time, but their accuracy depends on the chosen stencil and is limited by truncation errors.

In this work, we compare these methods by measuring their accuracy (using a relative L_2-norm error against the true derivative) and their runtime. We also show plots of the function and its spectral data and provide error analysis for 3-, 5-, 7-, and 9-point FD stencils.

II. RESULTS

A. Function and Spectral Plots

We use the test function

$$f(x) = \exp\Big(0.5\,\cos(3\pi x) + 0.25\,\sin(5\pi x)\Big), \tag{2}$$

which is smooth and periodic. Figure 1 shows the plot of $f(x)$ and its first derivative as computed by the FFT and DFT matrix methods. The spectral derivatives match the analytic derivative well, which shows that these methods work in the frequency domain.

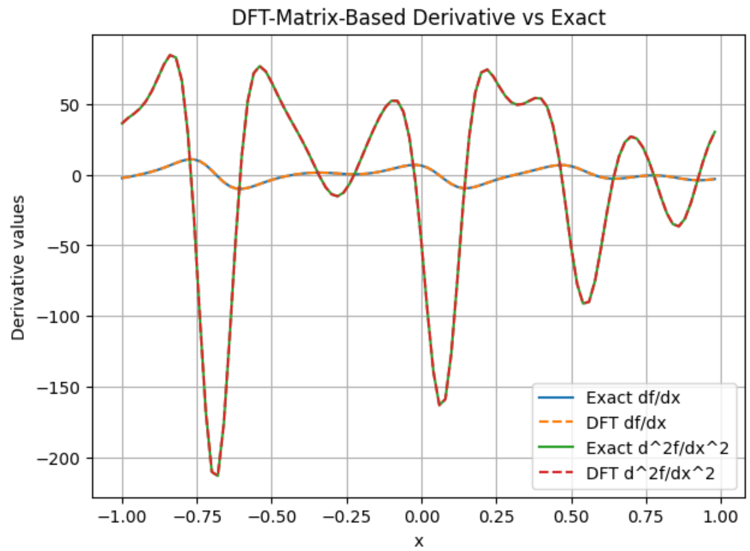

FIG. 1. The function $f(x)$ and its first derivative computed via FFT (blue dashed line) and the DFT matrix (red markers) compared with the analytic derivative (solid line).

B. Finite-Difference Stencil Error Analysis

Finite differences use a stencil (neighbors of a point) to compute derivatives. We calculated the relative L_2 error for the second derivative using 3-, 5-, 7-, and 9-point stencils. Figure 2 shows a log-log plot of the error versus the number of grid points N. In general, wider stencils give lower error but require more computation.

C. Accuracy Comparison: FD, FFT, and DFT Methods

We compare the numerical derivatives to the analytic derivatives (found using the chain rule). FD derivatives were computed with a 3-point stencil (and other stencils as above), and spectral derivatives were computed with both the FFT and the DFT matrix methods. Figure 3 shows a log-log plot of the relative L_2 error versus N for the three methods. The FFT method converges quickly, especially for smooth, periodic functions. The FD method's

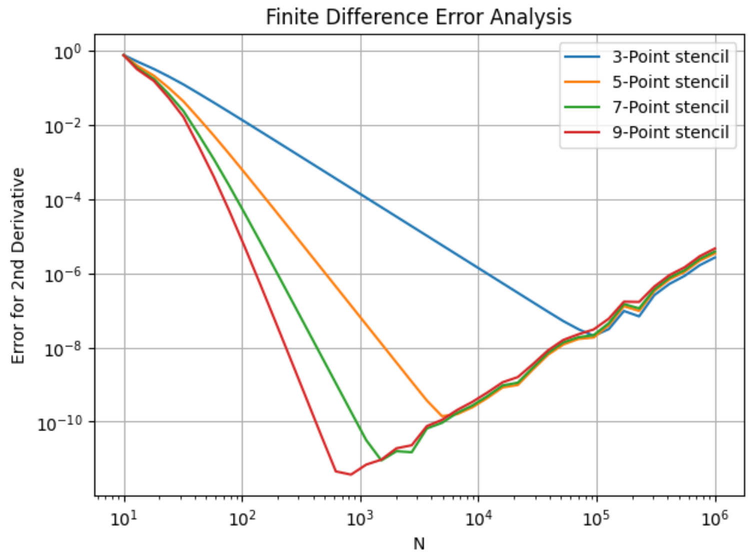

FIG. 2. Log-log plot of the relative L_2 error for the second derivative using FD methods with 3-, 5-, 7-, and 9-point stencils.

error is limited by the stencil order, and the DFT matrix method is as accurate as the FFT but takes more time.

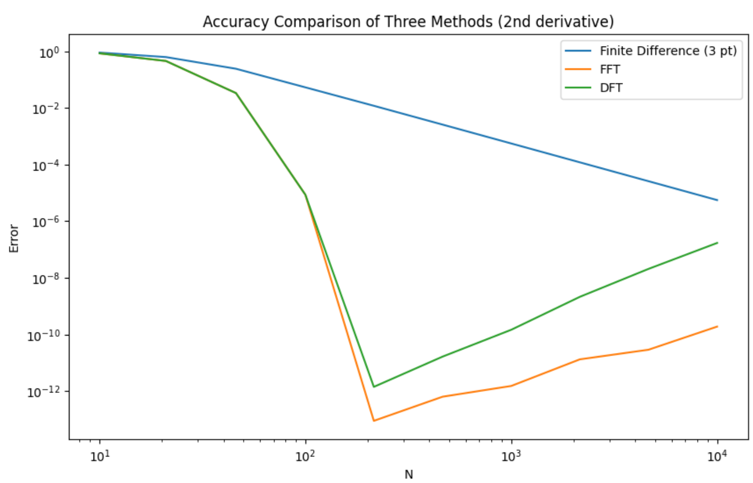

FIG. 3. Log-log plot of the relative L_2 error for the second derivative computed by FD (3-point stencil), FFT, and DFT matrix methods.

D. Runtime Analysis

We measured the time taken by each method as a function of N. The FD method runs in $\mathcal{O}(N)$, the FFT method in $\mathcal{O}(N \log N)$, and the DFT matrix method in $\mathcal{O}(N^2)$. Figure 4 shows a log-log plot of the runtime versus N. The FFT method is especially fast when N is a power of two, while the DFT matrix method becomes very slow for large N.

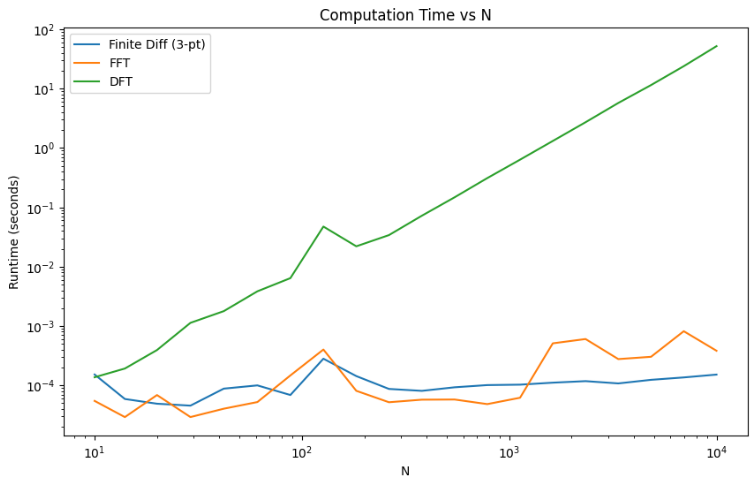

FIG. 4. Log-log plot of runtime versus N for FD, FFT, and DFT matrix methods. The FFT method performs best when $N = 2^k$.

III. CONCLUSION

We compared three ways to approximate derivatives:

- **Finite-Difference (FD):** Simple and runs in $\mathcal{O}(N)$ time, but its accuracy depends on the stencil and has truncation errors. The error analysis for 3-, 5-, 7-, and 9-point stencils shows the trade-off between accuracy and cost.
- **FFT-Based Method:** Changes the function to the frequency domain where differentiation is done by multiplying by ik. It runs in $\mathcal{O}(N \log N)$ time and is very accurate for smooth periodic functions, especially when N is a power of two.
- **DFT Matrix Method:** Directly builds the DFT matrix to compute derivatives. It is as accurate as the FFT but runs in $\mathcal{O}(N^2)$ time, which makes it less useful for large N.

Our results show that the FFT-based method is the best choice for smooth, periodic functions because it gives high accuracy and runs fast. Finite-difference methods are still useful when the problem is not periodic or when simplicity is important. The DFT matrix method is mainly useful for understanding the theory but is too slow for large problems.