# Numerical Methods for PDEs

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## 1 Introduction

This paper documents my notes in exploring numerical methods for partial differential equations. They are heavily based off of

- the 6th chapter of Haberman's Applied PDEs with Fourier Series and Boundary Value Problems (4th ed.)
- lectures from MIT's graduate-level course on Numerical Methods for Partial Differential Equations (16.920J)

## 2 Finite Differences and Truncated Taylor Series

### 2.1 Polynomial approximations

Finite differences rely fundamentally on polynomial approximations of a function $f(x)$ near $x = x_0$. If we let $x = x_0 + \Delta x$, then $\Delta x = x - x_0$. For instance, the quadratic approximation to $f(x)$ near $x_0$ is

$$f(x) \approx f(x_0) + \Delta x f'(x_0) + \frac{(\Delta x)^2}{2!} f''(x_0). \tag{1}$$

We must also consider the truncation error in these polynomial approximations, which can be obtained simply be writing the Taylor series for the function as follows:

$$f(x) \approx f(x_0) + \Delta x f'(x_0) + \ldots + \frac{(\Delta x)^n}{n!} f^{(n)}(x_0) + R_n. \tag{2}$$

The remainder term $R_n$ represents the truncation error. It is known to be of the form of the next term in the series but evaluated at a point $c_{n+1}$ such that $x_0 < c_{n+1} < x = x_0 + \Delta x$, through the Mean Value Theorem.

$$R_n = \frac{(\Delta x)^{n+1}}{(n+1)!} f^{(n+1)}(c_{n+1}). \tag{3}$$

For instance, the error in the approximation given in (1) is

$$R_1 = \frac{(\Delta x)^2}{2!} f''(c_2). \tag{4}$$

However, if $\Delta x$ is very small, we can say that the error is approximated by

$$R_1 \approx \frac{(\Delta x)^2}{2} f''(x_0). \tag{5}$$

The truncation error is then of order $O(\Delta x)^2$, meaning that $|R| \leq C(\Delta x)^2$, assuming that $f''(x)$ is bounded ($|f''(x)| < M$).

## 2.2 First derivatives

Rearranging the Taylor series, we are able to obtain an approximation for the first derivative:

$$\frac{df}{dx}(x_0) = \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x} - \frac{\Delta x}{2} \frac{d^2 f}{dx^2}(c_2). \tag{6}$$

Using this, we introduce the **forward difference**:

$$\frac{df}{dx}(x_0) \approx \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}. \tag{7}$$

If we replace $\Delta x$ with $-\Delta x$ we obtain:

$$\frac{df}{dx}(x_0) = \frac{f(x_0 - \Delta x) - f(x_0)}{-\Delta x} + \frac{\Delta x}{2} \frac{d^2 f}{dx^2}(\tilde{c_2}). \tag{8}$$

Thus, we introduce the **backward difference**:

$$\frac{df}{dx}(x_0) \approx \frac{f(x_0 - \Delta x) - f(x_0)}{-\Delta x} = \frac{f(x_0) - f(x_0 - \Delta x)}{\Delta x}. \tag{9}$$

Observe that the error in both of these approximations is of order $O(\Delta x)$. We can also average these two approximations in hopes of forming an even better approximation for $f'(x_0)$ with lower error:

$$f'(x_0) = \frac{f(x_0 + \Delta x) - f(x_0 - \Delta x)}{2\Delta x} + \frac{\Delta x}{4}(f''(\tilde{c_2}) - f''(c_2)). \tag{10}$$

To obtain a more concrete error term for this approximation, we can use the Taylor series' of $f(x_0 + \Delta x)$ and $f(x_0 - \Delta x)$:

$$f(x_0 + \Delta x) = f(x_0) + \Delta x f'(x_0) + \frac{(\Delta x)^2}{2!} f''(x_0) + \frac{(\Delta x)^3}{3!} f'''(x_0) + \ldots \tag{11}$$

$$f(x_0 - \Delta x) = f(x_0) - \Delta x f'(x_0) + \frac{(\Delta x)^2}{2!} f''(x_0) - \frac{(\Delta x)^3}{3!} f'''(x_0) + \ldots. \tag{12}$$

Thus, subtracting the (11) from (12), we obtain:

$$f(x_0+\Delta x)-f(x_0-\Delta x)=2\Delta x f'(x_0)+\frac{2}{3!}(\Delta x)^3 f'''(x_0)+\dots \tag{13}$$

$$\implies f(x_0+\Delta x)-f(x_0-\Delta x)=2\Delta x f'(x_0)+\frac{2}{3!}(\Delta x)^3 f'''(c_3) \tag{14}$$

Finally, we can rearrange for $f'(x_0)$:

$$f'(x_0)=\frac{f(x_0+\Delta x)-f(x_0-\Delta x)}{2\Delta x}-\frac{(\Delta x)^2}{6}f'''(c_3). \tag{15}$$

This leads to the **centered difference** approximation:

$$\frac{df}{dx}(x_0)\approx\frac{f(x_0+\Delta x)-f(x_0-\Delta x)}{2\Delta x}. \tag{16}$$

Observe that the truncation error in this approximation is $O(\Delta x)^2$.

## 2.3 Second derivatives

In order to find an approximation for the second derivative $f''(x_0)$, we can add (11) and (12) rather than subtracting, and rearrange for $f''(x_0)$. I will not do the calculation here as it is not particularly enlightening, but the result comes out to be

$$f''(x_0)=\frac{f(x_0+\Delta x)-2f(x_0)+f(x_0-\Delta x)}{(\Delta x)^2}-\frac{(\Delta x)^2}{12}f^{(4)}(c). \tag{17}$$

This leads to the **centered difference** approximation for the second derivative with truncation error $O(\Delta x)^2$

$$\frac{d^2f}{dx^2}(x_0)\approx\frac{f(x_0+\Delta x)-2f(x_0)+f(x_0-\Delta x)}{(\Delta x)^2}. \tag{18}$$

## 2.4 Partial derivatives

We can note that if we have a function $u(x,y)$, then $\partial u/\partial x$ is just $du/dx$, keeping $y$ constant. Using this, we can apply the forward, backward, or centered differences for partial derivatives. For instance,

$$\frac{\partial u}{\partial x}(x_0,y_0)\approx\frac{u(x_0+\Delta x,y_0)-u(x_0-\Delta x,y_0)}{2\Delta x} \tag{19}$$

using the centered difference.

As such, if we find a centered difference approximation for the second partial derivative, we can find the approximation for the Laplacian $\nabla^2 u$:

$$\begin{aligned}\nabla^2 u(x_0,y_0)\approx{}&\frac{u(x_0+\Delta x,y_0)-2u(x_0,y_0)+u(x_0-\Delta x,y_0)}{(\Delta x)^2}\\&+\frac{u(x_0,y_0+\Delta y)-2u(x_0,y_0)+u(x_0,y_0-\Delta y)}{(\Delta y)^2}.\end{aligned} \tag{20}$$

However, if we set $\Delta x = \Delta y$, then

$$\nabla^2 u(x_0, y_0) \approx \frac{\begin{aligned} u(x_0 + \Delta x, y_0) + u(x_0 - \Delta x, y_0) + u(x_0, y_0 + \Delta y) \\ + u(x_0, y_0 - \Delta y) - 4u(x_0, y_0) \end{aligned}}{(\Delta x)^2} \tag{21}$$

# 3 Heat Equation

## 3.1 Introduction

We can apply these ideas to solve the 1D heat equation without sources on a finite interval $0 < x < L$:

$$\frac{\partial u}{\partial t} = k \frac{\partial^2 u}{\partial x^2} \tag{22}$$

$$u(0, t) = 0 \tag{23}$$

$$u(L, t) = 0 \tag{24}$$

$$u(x, 0) = f(x). \tag{25}$$

## 3.2 Partial Difference Equation

If we choose a forward difference in time, and a centered difference in space, then we obtain the following approximation for the 1D heat equation:

$$\frac{u(x_0, t_0 + \Delta t) - u(x_0, t_0)}{\Delta t} \approx k \frac{u(x_0 + \Delta x, y_0) - 2u(x_0, y_0) + u(x_0 - \Delta x, y_0)}{(\Delta x)^2}. \tag{26}$$

Thus, we introduce a function $\tilde{u}(x_0, t_0)$ as the exact solution to (26), while (26) only approximates the heat equation.

Additionally, we introduce a uniform mesh $\Delta x$ and constant discretization time $\Delta t$. If we divide the rod of length $L$ into $N$ equal intervals, we have $\Delta x = L/N$. We introduce the following discretizations for space and time:

$$x_j = j\Delta x \tag{27}$$

$$t_m = m\Delta t, \tag{28}$$

for which we note that $x_N = N\Delta x = L$. We also introduce some new notation:

$$\tilde{u}(x_j, t_m) \equiv u_j^m, \tag{29}$$

such that our new partial difference equation becomes

$$\frac{u_j^{m+1} - u_j^m}{\Delta t} = k \frac{u_{j+1}^m - 2u_j^m + u_{j-1}^m}{(\Delta x)^2}, \tag{30}$$

with the initial and boundary conditions becoming

$$u_j^0 = u(x, 0) = f(x_j) \tag{31}$$

$$u_0^m = u(0, t) = 0 \tag{32}$$

$$u_N^m = u(L, t) = 0. \tag{33}$$

## 3.3 Computations

In order to compute the heat equation forward in time, we isolate for $u_j^{m+1}$:

$$u_j^{m+1} = s\left(u_{j+1}^m - 2u_j^m + u_{j-1}^m\right) + u_j^m, \tag{34}$$

$$s = k\frac{\Delta t}{(\Delta x)^2} \tag{35}$$

where $s$ is a dimensionless parameter.

## 3.4 Fourier Analysis

In order to suitably analyze our partial differential equations and the stability of their numerical schemes, it is important to define how we will use Fourier analysis.

### 3.4.1 Definition

Let $g(x)$ be some arbitrary periodic real function with period $2\pi$. Then we have

$$g(x) = \sum_{k=-\infty}^{\infty} g_k e^{ikx} \text{ ($k$ integer).} \tag{36}$$

We also have the following easily verifiable orthogonality relationship,

$$\int_0^{2\pi} e^{ikx} e^{-ik'x} dx = 2\pi\delta_{kk'}, \tag{37}$$

where $\delta_{kk'}$ is equal to 1 if $k = k'$ and 0 otherwise. Using this, we can find that the Fourier coefficients $g_k$ are of the form

$$g_k = \frac{1}{2\pi}\int_0^{2\pi} g(x)e^{-ikx} dx. \tag{38}$$

Note that for real functions, $g_k = g_{-k}^*$, where $*$ denotes the complex conjugate. Using this fact, it is easy to show that

$$g(x) = \sum_{k=0}^{\infty} a_k \cos(kx) + b_k \sin(kx), \tag{39}$$

with $a_k = g_k + g_{-k}$ and $b_k = i(g_k - g_{-k})$.

It is also of note that the smoother a function, the faster its Fourier coefficients $|g_k| \to 0$. This makes sense as larger values of $|k|$ are directly associated with more oscillatory contributions, which are intuitively much less prominent in smoother functions.

### 3.4.2 Differentiation

We can define

$$u(x) = \sum_{k=-\infty}^{\infty} u_k e^{ikx} \quad \textbf{or} \quad u(x,t) = \sum_{k=-\infty}^{\infty} u_k(t) e^{ikx}. \tag{40}$$

Then, we can see how to take partial derivatives with respect to $x$ and $t$:

$$\frac{\partial^n u}{\partial x^n} = \sum_{k=\infty}^{\infty} (ik)^n u_k e^{ikx}, \quad \frac{\partial u}{\partial t} = \sum_{k=\infty}^{\infty} \frac{du_k}{dt} e^{ikx}. \tag{41}$$

Observe that for even $n$, the $n$th partial derivative with respect to $x$ is real (as $(ik)^n$ is real), while for odd $n$ the $n$th partial derivative (with respect to $x$) is imaginary.

## 3.5 Von Neumann Stability Analysis

We analyze the stability of the finite difference scheme for the 1D heat equation obtained by using a forward difference in time and a centered difference in space, as shown in the previous section.

It is important to note that von Neumann stability analysis cannot analyze the effect of complex boundary conditions because it only analyzes the stability of the discretization itself. In order to fully analyze the stability of a discretization, you also need to make sure the discrete boundary condition is well-posed.

### 3.5.1 Continuous PDE

We first begin by understanding the mechanism behind stability analysis by using the original partial differential equation for the heat equation, or

$$\frac{\partial u}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2}. \tag{42}$$

(I'm using $\kappa$ instead of $k$ because $k$ is used with the Fourier series.)

We know that $u$ is of the form

$$u = \sum_{k=-\infty}^{\infty} u_k e^{ikx}, \tag{43}$$

with

$$u(0,t) = u(2\pi, t), \tag{44}$$

$$u_x(0,t) = u_x(2\pi, t), \tag{45}$$

$$u(x,0) = u^0(x) = \sum_{k=-\infty}^{\infty} u_k^0 e^{ikx}. \tag{46}$$

Plugging our Fourier series into (42), we have

$$\sum_{k=-\infty}^{\infty} \frac{du_k}{dt} e^{ikx} = \sum_{k=-\infty}^{\infty} -\kappa k^2 u_k e^{ikx}. \tag{47}$$

Thus, by matching our coefficients, we have

$$\frac{du_k}{dt} = -\kappa k^2 u_k. \tag{48}$$

From (46) we have that $u_k(0) = u_k^0$, so when we solve (48), we find that

$$u_k(t) = u_k^0 e^{-\kappa k^2 t} \implies u(x,t) = \sum_{k=-\infty}^{\infty} u_k^0 e^{-\kappa k^2 t} e^{ikx}. \tag{49}$$

We can immediately recognize from the $e^{-\kappa k^2 t}$ term that the initial condition dissipates over time. Additionally, there is higher decay for higher frequency Fourier modes (larger $k$), which indicates that the solution tends to become smooth over time.

### 3.5.2 Semi-Discretized PDE

We consider the semi-discretized version of the heat equation, where

$$\frac{du_j}{dt} = \kappa \frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2} \tag{50}$$

with

$$u_j = u(j\Delta x) = \sum_{k=-\infty}^{\infty} u_k e^{ikj\Delta x}. \tag{51}$$

Since we are considering a Fourier series for a discrete function, a phenomenon called aliasing can cause higher frequency waves to satisfy the function's discretized values the same way a lower frequency wave can. See this Desmos link for a visualization.

If we have a wave with $k = 1$, then a wave with $k = 1 + \frac{2\pi}{\Delta x}$ will also satisfy the discretized function values. In fact, for any value of $k$, $k' = k + \frac{2\pi}{\Delta x}$ will be the wave number for the aliased wave. (It helps to visualize the aliased waves on the unit circle to see why this might be true).

We can also see this by plugging this into our complex exponential $e^{ikj\Delta x}$:

$$e^{i\left(k + \frac{2\pi}{\Delta x}\right) j\Delta x} = e^{i2\pi j} e^{ikj\Delta x} = e^{ikj\Delta x}. \tag{52}$$

The two aliased wave numbers are mathematically equivalent.

Because of aliasing, the semi-discretized PDE can only be represented by a discrete Fourier series as opposed to continuous, and the bounds of the summation must be altered. This can be done by examining the Nyquist frequency,

$k = \pi/\Delta x$. This is the highest possible frequency of a periodic function that can be represented using discrete points. It is easy to see why this might be this case if we consider that we require at least two points per wavelength to concretely represent a periodic function. Any higher frequencies are impossible to distinguish from their lower frequency aliased counterparts.

Thus, we have $\lambda_{\min} = 2\Delta x$. Plugging this into the formula for the wave number $k = 2\pi/\lambda$, we obtain

$$k_{\mathrm{Nyq}} = \frac{2\pi}{2\Delta x} = \frac{\pi}{\Delta x}. \tag{53}$$

Since we know that the range along which we can have uniquely represented frequencies is $2\pi/\Delta x$, we can deduce that the interval of summation is $k \in [-\pi/\Delta x, \pi/\Delta x)$. This interval is chosen because every wave number inside this interval is physically resolvable, and every wave number outside this interval aliases into it. For any other interval, both physically resolvable and unresolvable wave numbers are present.

Thus, if we have $N$ grid points $N = 2\pi/\Delta x$, (50) becomes

$$\begin{aligned}\sum_{k=-\frac{N}{2}}^{\frac{N}{2}-1} \frac{du_k}{dt} e^{ikj\Delta x} &= \frac{\kappa}{\Delta x^2} \sum_{k=-\frac{N}{2}}^{\frac{N}{2}-1} u_k (e^{ik(j+1)\Delta x} + e^{ik(j-1)\Delta x} - 2e^{ikj\Delta x}) \qquad (54)\\ &= \frac{\kappa}{\Delta x^2} \sum_{k=-\frac{N}{2}}^{\frac{N}{2}-1} u_k e^{ikj\Delta x} (e^{ik\Delta x} + e^{-ik\Delta x} - 2). \qquad (55)\end{aligned}$$

By matching coefficients on both sides of the equation, we have

$$\frac{du_k}{dt} = \frac{\kappa}{\Delta x^2}(e^{ik\Delta x} + e^{-ik\Delta x} - 2)u_k. \tag{56}$$

A simple calculation shows us that

$$\frac{\kappa}{\Delta x^2}(e^{ik\Delta x} + e^{-ik\Delta x} - 2) = \frac{\kappa}{\Delta x^2}(2\cos(k\Delta x) - 2). \tag{57}$$

So,

$$\frac{du_k}{dt} = \kappa \frac{(2\cos(k\Delta x) - 2)}{\Delta x^2} u_k. \tag{58}$$

Interestingly, for $k\Delta x \ll 1$,

$$\cos(k\Delta x) \approx 1 - \frac{k^2 \Delta x^2}{2} \tag{59}$$

through its Taylor series expansion. So,

$$\frac{(2\cos(k\Delta x) - 2)}{\Delta x^2} \approx \frac{2 - k^2\Delta x^2 - 2}{\Delta x^2} = -k^2. \tag{60}$$

Thus, for sufficiently small $k\Delta x$,

$$\frac{du_k}{dt} \approx -\kappa k^2 u_k \tag{61}$$

which is exactly the same as the continuous case!

### 3.5.3 Fully Discretized PDE

We now consider the fully discretized version of the heat equation:

$$\frac{u_j^{m+1} - u_j^m}{\Delta t} = \kappa \frac{u_{j+1}^m - 2u_j^m + u_{j-1}^m}{(\Delta x)^2}. \tag{62}$$

The key difference is that instead of the $u_k$ coefficient being continuous in time, it is now discrete. Thus,

$$u_j^m = \sum_{k=-\infty}^{\infty} u_k^m e^{ikj\Delta x}. \tag{63}$$

When we substitute the Fourier series for all these terms and match coefficients, we find that

$$\frac{u_k^{m+1} - u_k^m}{\Delta t} = \frac{\kappa}{\Delta x^2}(2\cos(k\Delta x) - 2). \tag{64}$$

Isolating for $u_k^{m+1}$,

$$u_k^{m+1} = \left(1 + \frac{\kappa \Delta t}{\Delta x^2}(2\cos(k\Delta x) - 2)\right) u_k^m. \tag{65}$$

Therefore, we know that for this scheme to be stable

$$\left|1 + \frac{\kappa \Delta t}{\Delta x^2}(2\cos(k\Delta x) - 2)\right| < 1. \tag{66}$$

This condition must be valid $\forall k \in [-N/2, N/2 - 1]$. We can look at the range of the function in the absolute value signs that to find constraints for this inequality to be satisfied. First, we let

$$C = \frac{\kappa \Delta t}{\Delta x^2}. \tag{67}$$

Then, we notice that the range of the function $C(2\cos(k\Delta x) - 2)$ is $C \cdot [-4, 0]$, and our inequality becomes

$$-1 < 1 + C \cdot [-4, 0] < 1. \tag{68}$$

We deduce that $0 < C < 1/2$, so in order for this numerical scheme to be stable,

$$\frac{\kappa \Delta t}{\Delta x^2} < \frac{1}{2}. \tag{69}$$