AMATH 442 (Fall 2014 - 1149)

Numerical Solutions of Partial Differential Equations

Prof. L. Krivodonona
University of Waterloo

LaTeXer: W. Kong
http://wwkong.github.io
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These notes are currently a work in progress, and as such may be incomplete or contain errors.

Acknowledgments:

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Abstract

The purpose of these notes is to provide the reader with a secondary reference to the material covered in AMATH 442. The formal prerequisite to this course is either AMATH 351 or AMATH 350.

Errata

6-7 Assignments Biweekly

25% Assignments, 25% Midterm, 50% Final Exam

Office hours: W, Th @ 2-3pm

Midterm: Oct. 21st @ 4-5:30pm

1 Introduction

We begin with a quick review of the theoretical bases of **partial differential equations**.

1.1 Classification of 2nd Order Linear PDEs

There are 3 types of (linear) PDEs:

1. Parabolic PDEs (e.g. heat equation, diffusion equation)
   (a) Has the form $u_t = \sigma u_{xx}$ or in the multivariate case, $u_t = \sigma(u_{xx} + u_{yy} + u_{zz})$
2. Elliptic PDEs (e.g. Laplace's equation, Poisson equation)
   (a) Has the form $u_{xx} + u_{yy} = f(x, y)$ or $\Delta u = f(x, y)$
3. Hyperbolic PDEs (e.g. 1st, 2nd order wave equations)
   (a) Has the form $u_{tt} - c^2 u_{xx} = 0$ or $u_t + au_x = 0$

There are also **non-linear PDEs**:

- Burger's equation: $u_t + uu_x = 0$
- Non-linear heat equation: $u_t = (\sigma(u)u_x)_x$
- Higher-order PDEs: $u_t + uu_x = \sigma u_{xxx}$
- Mixed types

1.2 Examples of Linear PDEs

(1) Let's begin by looking at the classic **linear advection (a.k.a. wave) equation**. The basic form is

$$u_t + au_x = 0, a \in \mathbb{R}, (x, t) \in \mathbb{R} \times \mathbb{R}$$

Claim 1.1. Any $\phi(x - at)$ is a solution.

Proof. Substitution and chain rule:

$$u = \phi(x - at) \implies u_t = \phi'(x - at)(-a), u_x = \phi'(x - at) \implies -a\phi' + a\phi' = 0$$

Therefore ϕ is a solution. $\square$

With the initial condition $u(x,0) = u_0(x)$, the solution is $u = u_0(x - at)$. The PDE with the aforementioned initial condition is called the **Cauchy problem**. We can interpret the parameter a as a speed parameter.

Now suppose that we introduce a finite domain $\Omega = [\alpha, \beta]$ and **boundary conditions**. Saying $u(\beta, t) = b_{right}(t)$ might lead to contradiction since $u_0(x-at) \neq b_{right}(\beta, t)$ or $u_0 = b_{right}$ (no new information is given). Instead, we provide $u(\alpha, t) = b_{left}(t)$ if $a > 0$ and we provide $u(\beta, t) = b_{right}(t)$ if $a < 0$.[1]

Conclusion 1. Here are some conclusions regarding the above wave equation:

[1] The solution of (1) does not grow or decay over time.

[2] New extrema can be introduced only through boundary conditions.

(2) Moving on, we have the **diffusion (heat) equation**. The basic form is

$$u_t = \sigma u_{xx}, \sigma \in \mathbb{R}$$

Assume that the initial conditions (I.C.) and boundary conditions (B.C.) are such that

$$u(x,t) = \hat{u}(k,t) \sin kx$$

is a solution, with k fixed. By substitution,

$$\begin{aligned} u_t &= \hat{u}_t \sin kx \\ u_x &= k\hat{u} \cos kx \\ u_{xx} &= -k^2 \hat{u} \sin kx \end{aligned}$$

and so

$$\hat{u}_t \sin kx = -\sigma k^2 \hat{u} \sin kx \implies \hat{u}_t = -\sigma k^2 \hat{u} \implies \hat{u}(k,t) = ce^{-\sigma k^2 t} \implies u(x,t) = ce^{-\sigma k^2 t} \sin kx$$

If we set $c = 1$ then the I.C. should be

$$u(x,0) = e^{-\sigma k^2 \cdot 0} \sin kx = \sin kx$$

If the domain is $\Omega = [-1, 1]$ and $k = \pi$ then the B.C. is

$$\begin{cases} u(-1,t) &= 0 \\ u(1,t) &= 0 \end{cases}$$

Remark 1.1. Here are some remarks about the solution:

[1] If $\sigma > 0$ then $u(x,t)$ decays with time (proper heat equation) and if $\sigma < 0$ then $u(x,t)$ grows with time (inverse or backwards heat equation). For this course, we always assume that $\sigma > 0$.

[2] The larger the σ, the faster the decay with respect to time. We call σ the **diffusion coefficient**.

[3] The larger the k, the faster the decay $\implies$ high frequencies decay faster.

2 Algorithms

We now can examine some numerical algorithms for PDEs.

[1] $x = \alpha$ is called inflow while $x = \beta$ is called outflow.

2.1 Finite Difference Methods

Recall that

$$\begin{aligned} u_x &:= \lim_{\Delta x \to 0} \frac{u(x+\Delta x, t) - u(x,t)}{\Delta x} \\ \Delta^+ u &:= \frac{u(x+\Delta x, t) - u(x,t)}{\Delta x} \\ \Delta^- u &:= \frac{u(x,t) - u(x-\Delta x, t)}{\Delta x} \end{aligned}$$

where we call the last two the **1st forward difference** and **1st backward difference** respectively. By convention, $\Delta x > 0$ and $\Delta t > 0$. Note that Δx is finite which is where the name "finite difference" comes from. u_x will be approximated by $\Delta^+ u$ or $\Delta^- u$. Similarly,

$$u_t \approx \frac{u(x, t+\Delta t) - u(x,t)}{\Delta t}$$

We then introduce a discretization of space where

$$\begin{aligned} \Delta x_j &= x_{j+1} - x_j \\ \Delta t_n &= t_{n+1} - t_n \end{aligned}$$

For simplicity, assume uniform discretization. That is, $\Delta x_j = \Delta x, \Delta t_n = \Delta t$ for all j and t. In general $\Delta x \neq \Delta t$. We will use the notation

$$\begin{aligned} (x_j, t_n) &\equiv (j, n) \\ u_j^n &\equiv u(x_j, t_n) \end{aligned}$$

Finally, we denote the numerical solution as $U_j^n \approx u_j^n$. Now recall the Taylor series expansion of u about (x_j, t_n) in x:

$$\begin{aligned} u(x_j + \Delta x, t_n) &= u(x_j, t_n) + \Delta x u_x(x_j, t_n) + \frac{\Delta x^2}{2} u_{xx}(x_j, t_n) + \dots \\ u(x_j - \Delta x, t_n) &= u(x_j, t_n) - \Delta x u_x(x_j, t_n) + \frac{\Delta x^2}{2} u_{xx}(x_j, t_n) - \dots \end{aligned}$$

or more compactly,

$$\begin{aligned} u_{j+1}^n &= u_j^n + \Delta x \,(u_x)_j^n + \frac{\Delta x^2}{2}(u_{xx})_j^n + \dots \\ u_{j-1}^n &= u_j^n - \Delta x \,(u_x)_j^n + \frac{\Delta x^2}{2}(u_{xx})_j^n - \dots \end{aligned}$$

If we solve for $(u_x)_j^n$ in the first equation, then we get

$$(u_x)_j^n = \frac{u_{j+1}^n - u_j^n}{\Delta x} - \frac{\Delta x}{2}(u_{xx})_{j+\xi}^n, 0 < \xi < 1$$

by the mean value theorem. We call $\tau_j^n = -\frac{\Delta x}{2}(u_{xx})_{j+\xi}^n$ the **discretization (truncation) error**. Similarly from the second equation,

$$(u_x)_j^n = \frac{u_{j+1}^n - u_j^n}{\Delta x} \underbrace{+\frac{\Delta x}{2}(u_{xx})_{j-\xi}^n}_{\tau_j^n}, 0 < \xi < 1$$

If we subtract the two equations together, then

$$(u_x)_j^n = \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} \underbrace{-\frac{1}{6}(u_{xxx})_{j+\xi}^n \Delta x^2}_{\tau_j^n}, 0 < \xi < 1$$

We call the first term on the right side the **1st central difference**. Central difference is more accurate than forward and backward difference. More accuracy is achievable with more points x_{j+2}, x_{j+3}. Adding the two equations will give us

$$(u_{xx})_j^n = \frac{u_{j+1} - 2u_j^n + u_{j-1}^n}{\Delta x^2} - \frac{\Delta x^2}{12}(u_{xxxx})_{j+\eta}^n, 0 < \eta < 1$$

In general, higher derivatives and more accurate approximations require more points (i.e. larger **stencil**).

Using **big-O notation**, we can write:

$$\begin{aligned}
(u_x)_j^n &= \frac{u_{j+1}^n - u_j^n}{\Delta x} + O(\Delta x) \\
(u_t)_j^n &= \frac{u_j^{n+1} - u_j^n}{\Delta t} + O(\Delta t) \\
(u_{xx})_j^n &= \frac{u_{j+1} - 2u_j^n + u_{j-1}^n}{\Delta x^2} + O(\Delta x^2)
\end{aligned}$$

Example 2.1. Let's construct a finite difference (FD) scheme for the heat equation:

$$\begin{aligned}
u_t &= \sigma u_{xx}, -\infty < x < \infty \\
u(x,0) &= \phi(x)
\end{aligned}$$

We have

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \sigma \frac{u_{j+1} - 2u_j^n + u_{j-1}^n}{\Delta x^2} \implies u_j^{n+1} = ru_{j-1}^n + (1-2r)u_j^n + ru_{j+1}^n$$

where $r = \sigma \Delta t / \Delta x^2$. If we know u_j^n for all j then we can compute u_j^{n+1} for all j. We need u_j^0 so we set $u_j^0 = u(x_j, 0) = \phi(x_j)$ for all j.

Let's plug in some values. Suppose that $\sigma = 1$ and choose the I.C. such that $u_0^0 = 1, u_j^0 = 0, \forall j \neq 0$ and $\Delta x = 1, \Delta t = 1/4 \implies r = 4$. This gives us

$$u_j^{n+1} = 4u_{j-1}^n - 7u_j^n + 4u_{j+1}^n$$

From stability analysis (CS 476), you will see that:

1. u_j^n grows
2. u_j^n oscillates (+ve, -ve, +ve, -ve, ...)

Instead, let's try: $\Delta x = 1/4, \Delta t = 1/64 \implies r = 1/4$ with:

$$u_j^{n+1} = \frac{1}{4}u_{j-1}^n + \frac{1}{2}u_j^n + \frac{1}{4}u_{j+1}^n$$

This will provide reasonable results. In general, we want u_0^n to be a good approximation of u_j^n.

Definition 2.1. A scheme is **convergent** on $0 < t \leq T$ if

$$\|u^n - U^n\| \to 0$$

as $\Delta x \to 0, \Delta t \to 0, n \to \infty, n\Delta t \leq T$. Here, $\|\cdot\|$ is some norm with u^n as a vector of all the (u_j^n)'s. A scheme is **convergent of order** k if

$$\|u^n - U^n\| = O(\Delta x^k)$$

Fact 2.1. *Convergence is difficult to prove directly. Instead, we look at:*

- Stability
- Convergence

Going back to our last example, consider $\|u\|_\infty = \max_j |u_j|$. From the general equation

$$\begin{aligned} |u_j^{n+1}| &\leq |r||u_{j-1}^n| + |1-2r||u_j^n| + |r||u_{j+1}^n| \\ &\leq (|r| + |1-2r| + |r|)\|u^n\|_\infty \end{aligned}$$

If $0 < r < \frac{1}{2}$ then $|u_j^{n+1}| \leq \|u^n\|_\infty, \forall j \implies \|u^{n+1}\| \leq \|u^n\|_\infty$. If $r > \frac{1}{2}$, then

$$|r| + |1-2r| + |r| = 2r - 1 + 2r = 4r - 1 \geq 1$$

and hence

$$|u_j^{n+1}| \leq (4r-1)\|u^n\|_\infty$$

Definition 2.2. A scheme is **stable** if $\exists C > 0$ **independent** of $\Delta x, \Delta t, u^0$ such that

$$\|u^n\| \leq C\|u^0\|, \Delta x \to 0, \Delta t \to 0, n \to \infty, n\Delta t \leq T$$

Note 1. (1) We allow some growth in the solution. Don't confuse this definition of stability with stability in ODE theory.

(2) Scheme is usually stable only for fixed values of some parameters. For example, Δt as a function of Δx or r.

In our example above, we showed that it was a stable scheme for the heat equation when $r < \frac{1}{2}$.

Definition 2.3. Alternatively, if u^n, v^n are solutions with $u^0 = \phi, v^0 = \psi$ (same problem, different I.C.), then a scheme is stable if $\exists C > 0$ independent of $\Delta x, \Delta t, u^0$ such that

$$\|u^n - v^n\| \leq C\|u^0 - v^0\|, \Delta x \to 0, \Delta t \to 0, n \to \infty, n\Delta t \leq T$$

Example 2.2. Going back to heat equation, suppose we choose I.C.

$$u^0 = (..., -1, 1, -1, 1, ...) \implies u_j^0 = (-1)^\gamma$$

and hence

$$\begin{aligned} u_j^1 &= 2r(-1)^{j+1} + (1-2r)(-1)^\gamma \\ &= (-1)^\gamma(-2r + 1 - 2r) \\ &= -(4r-1)(-1)^\gamma \\ u_j^n &= (-1)^{\gamma+1}(4r-1)^n \end{aligned}$$

Taking norms, we have

$$\|u^n\|_\infty = (4r-1)^n\|u^0\|_\infty = (4r-1)^n$$

We call this **exponential growth** in the case of $r > \frac{1}{2}$. As $\Delta x, \Delta t \to 0$ with fixed T and $n \to \infty$, we have

$$\|u^n\|_\infty \to \infty$$

So with $r > \frac{1}{2}$, the results are **unstable**.

Remark 2.1. Stability for numerical methods is equivalent to **well-posedness** for PDEs:

- Solution exists given suitable I.C. and B.C.
- Solution is unique
- Solution is continuously independent on initial data

<u>How to Check your Code</u>

1. Manufacture a problem for which you know the exact solution and which you should be able to solve exactly.
   (a) In the heat equation, we could try $u(x,t) = 1$ with I.C. $u(x,0) = 1$ and B.C. $u(1,t) = 1, u(0,t) = 1$.