MATH5311 - Advanced Numerical Methods I

Taught by Wang Xiao Ping

Notes by Aaron Wang

Contents

1 September 8th, 2020

1.1 Introduction

1.1.1 Numerical Differentiation

Recall that the derivative is defined as:

$$u(x_0) = \lim_{h \to 0} \frac{u(x_0 + h) - u(x_0)}{h}.$$

Thus we can approximate the difference

Definition 1.1. Central Difference

$$u_x(x_i) = \frac{u_{i+1} - u_{i-1}}{2h}.$$

Theorem 1.2

The central difference method is second order accurate.

Proof. Using Taylor Expansion, we have:

$$u_{i+1} = u_i + u_x h + \frac{1}{2} u_{xx}.$$

$\square$

Remark 1.3 — Note that if the derivative is

1.1.2 Numerical Integration

Numerical Integration can be approximation by the **Riemann Sum**

$$\int_a^b f(x) \, dx \approx \sum_{i=1}^{N} f(x_i) \Delta x_i.$$

We can also use the **Trapezoidal Rule**, as:

$$\int_{x_i}^{x_{i+1}} \approx \frac{h}{2} \left[f(x_i) + f(x_{i+1}) \right].$$

Remark 1.4 — The above equation is approximating the curve in interval $[x_i, x_{i+1}]$ with a straight line

Thus if we add up over all intevals x_i, we'd get:

$$\int_a^b f(x) \, dx \approx \sum_{i=0}^{N-1} \frac{h}{2} \left[f(x_i) + f(x_{i+1}) \right].$$

This is **second order accurate**.

1.1.3   Simpson's Rule

1.2   Solution of ODE's

Say we have an ODE:
$$\begin{cases} \dot{x} = f(x,y) \\ x(0) = x_0 \end{cases}.$$

One simple approximation is the **Euler method**:

$$\dot{x} \approx= \frac{x^{n+1} - x^n}{\Delta t} = f(x^n, t_n).$$

with time step Δt and:
$$x^{n+1} = x^n + \Delta t f(x^n, t_n).$$

This is a first order accurate scheme.

> **Remark 1.5 —** There are some disadvantages to this method, as Δt must be chosen carefully to be stable.

The Euler method can be modified to make higher order methods, such as the **Modified Euler**
$$\begin{cases} x^* = x^n + \Delta t f(x^n, t_n) \\ x^{n+1} = x^n + \frac{\Delta t}{2}\left(f(x^n, t_n)\right) + f(x^*, t_{n+1}) \end{cases}.$$

Essentially, x^* is a predictor of the This is second order accurate.

> **Remark 1.6 —** There is also a **Runge-Katta Method**, which is a 4th order method.

1.2.1   Solving Linear System

We have a linear system:
$$Ax = b.$$

We can solve this with a variety of methods, such as
- Guassian Eliminations
- LU factorization
- Iterative methods

2   September 10th, 2020

2.1   Outline of the Course

1. Parabolic equations, 1D, 2D
2. Hyperbolic equation (1D)
3. Elliptical equation (2D)
4. Iterative methods for linear systems

2.2   Parabolic Equations in 1D

The model problem is the **heat equation** that describes heat conduction.

Definition 2.1. The **heat equation** in 1D is:

$$u_t = k u_{xx}, \quad t > 0, 0 < x < t$$

with boundary conditions

$$u(0, t) = a, \quad u(1, t) = b$$
$$u(x, 0) = u_0(x).$$

For simplicity, let's first consider $k = 1$, i.e. $u_t = u_{xx}$, and boundary conditions $u(0, t) = u(1, t) = 0$ the method will be the same.

This can be interrelated as considering a rod with unit length with some initial temperature distribution, and then observing the temperature over time.

Definition 2.2. The above heat equation has **Dirichlet boundary conditions**, meaning that they are fixed at the boundaries, i.e. specifying the temperature.

Definition 2.3. **Neumann boundary conditions** would be specifying the derivative at the boundaries, i.e.

$$u_x(0) = a, \quad u_x(1) = b.$$

Here a and b would be the heat flux at the boundaries.

2.2.1   Explicit Scheme

Like before let's discretized it by considering the uniform grid in space in time, with:

$$x_j = j\Delta x, \quad t_n = n\Delta t,$$

for $j = 0, 1, \ldots, J, \quad n = 0, 1, , \ldots$ and $\Delta x = \frac{1}{J}$. Thus we seek to approximate:

$$U_j^n \approx u(x_j, t_n).$$

The first approximation would be using an explicit method, with:

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} \approx u_t(x_j, t_n).$$

meaning we use the forward difference for the time derivative. For space derivative, we have:

$$\frac{U_{j+1}^n + U_{j-1}^n - 2U_j^n}{(\Delta x)^2} \approx u_{xx}(x_j, t_n).$$

which is derived from the central difference.

> **Remark 2.4** — Remembering Taylor expansion, this is because:
>
> $$u_{i+1} + u_{i-1} = 2u_i + u_{xx}h^2 + \frac{2}{4!}u^{(4)}h^4 + \ldots.$$
>
> $$\implies \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = u_{xx} + O(h^2).$$

Using this, we can discretize the PDE with:

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{(\Delta x)^2}.$$

Now that we have a discrete finite difference formula, we can solve it for U_j^n:

$$U_j^{n+1} = U_j^n + \frac{\Delta t}{(\Delta x)^2}\left(U_{j+1}^n - 2U_j^n + U_{j-1}^n\right).$$

Using the notation $\gamma = \frac{\Delta t}{(\Delta x)^2}$, we have:

$$U_j^{n+1} = (1 - 2\gamma)U_j^n + \gamma\left(U_{j+1}^n + U_{j-1}^n\right) \tag{1}$$

This is an **explicit scheme**, as each value at time level t_{n+1} can be independently calculated from the values at time t_n. As such, we can start with $n = 0$ and calculate for each next value of n step by step.

2.2.2   Error Analysis for Explicit Scheme

Since we are using U_j^n to approximate $u(x_j, t_n)$, if we replace U_j^n by the exact solution, the truncation error would be:

$$T_j^n = \frac{u(x_j, t_{n+1}) - u(x_j, t_n)}{\Delta t} - \frac{u(x_{j+1}, t_n) - 2u(x_j, t_n) + u(x_{j-1}, t_n)}{(\Delta x)^2} \tag{2}$$

Since this is smooth, we can use the taylor expansion, giving us:

$$\approx \frac{u_t(x_j, t_n)\Delta t + \frac{1}{2}U_{tt}(x_j, t_n)(\Delta t)^2}{\Delta t} - \frac{u_{xx}(\Delta x)^2 + \frac{2}{4!}u_{xxxx}(\Delta x)^4}{(\Delta x)^2}$$

$$= u_t + \frac{1}{2}u_{tt}(\Delta t) - u_{xx} - \frac{2}{4!}u_{xxxx}(\Delta x)^2 + \dots$$

$$= \underbrace{u_t - u_{xx}}_{=0} + \frac{1}{2}u_{tt}\Delta t - \frac{2}{4!}u_{xxxx}(\Delta x)^2 + \dots$$

$$= \frac{1}{2}u_{tt}\Delta t - \frac{2}{4!}u_{xxxx}(\Delta x)^2 + \dots.$$

Note that:

$$T^n \to 0, \quad \text{as } \Delta t \to 0, \quad (\Delta x) \to 0.$$

Since the truncation error goes to zero, this scheme is consistent. Note that this scheme is first order accurate in time and second order accurate in space. Although this scheme is consistent, this is only a necessary condition for convergence.

Definition 2.5. The scheme is **convergent** if as $\Delta t \to 0, \quad \Delta x \to 0$,
$\forall (x^*, t^*)$: $x_j \to x^*$ and $t_n \to t^*$ implies $U_j^t \to u(x^*, t^*)$

Let $e_j^n = U_j^n - u(x_j, t_n)$, meaning that convergence is equivelent to $e_j^n \to 0$ as $\Delta t \to 0$ and $\Delta x \to 0$. Rearranging 1 and 2. We have:

$$e_j^{n+1} = e_j^n + \gamma \left(e_{j+1}^n - 2e_j^n + e_{j-1}^n\right) + T_j^n \Delta t$$

$$\implies e_j^{n+1} = (1 - 2\gamma)e_j^n + \gamma e_{j+1}^n + \gamma e_{j-1}^n + T_j^n \Delta t$$

$$\implies |e_j^{n+1}| \leq |1 - 2\gamma||e_j^n| + |\gamma||e_{j+1}^n| + |\gamma||e_{j-1}^n| + |T_j^n|\Delta t$$

$$\implies |e_j^{n+1}| \leq |1 - 2\gamma|E^n + |\gamma|E^n + |\gamma|E^n + |T_j^n|\Delta t$$

where $E^n = \max_j\{|e_j^n|\}$. If $\gamma \leq \frac{1}{2}$, we have:

$$\max_j\{|e_j^{n+1}|\} \leq |1 - 2\gamma|E^n + 2|\gamma|E^n + \tilde{T}\Delta t = E^n + \tilde{T}\Delta t.$$

where $\tilde{T} = \max_{j,n}\{|T_j^n|\}$. Now we have:

$$E^{n+1} \leq E^n + \tilde{T}\Delta t \leq (E^{n-1} + \tilde{T}\Delta t) + \tilde{T}\Delta t$$

$$\leq E^{n-1} + 2\tilde{T}\Delta t$$

$$\leq \dots$$

$$\leq \underbrace{E^0}_{=0} + n\tilde{T}\Delta t$$

$$= t_F \tilde{T}$$

where $t_f = n\Delta t$ which is a constant. Since $\tilde{T} \to 0$ as $\Delta x \to 0$ and $\Delta t \to 0$ because it is consistent, we have that E^n goes to zero. Note that this means that we have the condition that:

$$\gamma = \frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{2} \implies 2\Delta t \leq (\Delta x)^2,$$

meaning that our scheme is convergent provided that $\gamma \leq \frac{1}{2}$. Next class we will consider $\gamma > \frac{1}{2}$ and show that it will not converge.