COMPUTATIONAL PDE LECTURE 17, 18, AND 19

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1. Outline of these lectures

- Cover the von Neumann stability theory of finite difference methods

2. Setup

We are trying to solve the heat equation on the whole real line with zero forcing:

$$\begin{cases} u_t(t,x) - u_{xx}(t,x) = 0, \quad t \in (0,1), x \in \mathbb{R} \\ u(0,x) = u_0(x) \end{cases} \tag{1}$$

Notice that we no longer have boundary conditions since there is no boundary!

We now consider the following numerical set up

- meshsize $h > 0$
- time stepsize $\tau > 0$
- Uniformly spaced but infinite grid: $\{x_j\}_{j\in\mathbb{Z}}$ where $x_j = jh$
- Grid function $U^{h,\tau} : \{x_j\}_{j\in\mathbb{Z}} \to \mathbb{R}$. For simplicity, we denote

$$u_j^n = U^{h,\tau}(t_n, x_j)$$

Our familiar numerical schemes for the heat equation now read

- **Forward Euler**

$$D_\tau u_j^n - D_h^2 u_j^{n-1} = 0$$

- **Backward Euler**

$$D_\tau u_j^n - D_h^2 u_j^n = 0$$

- **Crank-Nicholson**

$$D_\tau u_j^n - D_h^2 \left(\frac{u_j^n + u_j^{n-1}}{2} \right) = 0$$

where

$$D_\tau u_j^n = \frac{u_j^n - u_j^{n-1}}{\tau}, \quad D_h^2 u_j^n = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}$$

We now dig into the von Neumann theory.

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3. Symbol of an Operator

We now introduce the concept of the symbol of an operator. Let $\xi \in \mathbb{R}$. We consider a special grid function

$$v_j = e^{i\xi x_j} = e^{i\xi hj},$$

where i is the imaginary unit. You may have seen Euler's Formula before:

$$e^{i\theta} = \cos(\theta) + i\sin(\theta),$$

which will be helpful in our future calculations. Thus, we can interpret $v_j = e^{i\xi hj}$ as a grid function with oscillations like sine and cosine with frequency ξ.

Definition 3.1 (symbol)**.** Let A denote an linear map that maps grid functions to grid functions. We consider Av as an infinite matrix vector product:

$$(Au)_j = \sum_{k=-\infty}^{\infty} a_{jk}u_j$$

The **symbol** of the operator A is a function $S : \mathbb{R} \to \mathbb{C}$ such that for $\xi \in \mathbb{R}$ and $v_j = e^{i\xi hj}$, we have

$$S(\xi h)v_j = (Av)_j.$$

Remark 3.1 (interpretation of the symbol)**.** The symbol of an operator can be interpreted a few ways.

- $S(\xi h)$ is an eigenvalue of an operator A with eigenvector $v_j = e^{i\xi hj}$
- $S(\xi h)$ tells us how A acts on different frequencies ξ. For example, if $S(\xi h) = 2$, then an operator A will double the amplitude of $e^{i\xi hj}$.
- Recall that for a function defined by $f(x) = e^{i\xi x}$, we know

$$\frac{d}{dx}f(x) = if(x), \quad \frac{d^2}{dx^2}f(x) = -f(x),$$

so the second derivative of $e^{i\xi x}$ multiplies the function by -1. Essentially the symbol is an attempt to mimic these nice properties that we observe for derivatives at the discrete level.

3.1. Examples of symbols.

We now compute a few examples of symbols of operators.

- **Second finite difference** To compute the symbol of D_h^2, we write $S(\xi h)v_j = D_h^2 v_j$ and solve for $S(\xi h)$ with $v_j = e^{i\xi hj}$.

$$S(\xi h)v_j = D_h^2 v_j = \frac{v_{j+1} - 2v_j + v_{j-1}}{h^2} = \frac{e^{i\xi h(j+1)} - 2e^{i\xi hj} + e^{i\xi h(j-1)}}{h^2}$$

Recall the product property of exponentials: $e^{i\xi h(j\pm 1)} = e^{i\xi hj}e^{\pm i\xi h}$, so

$$S(\xi h)v_j = \frac{e^{i\xi hj}e^{i\xi h} - 2e^{i\xi hj} + e^{i\xi hj}e^{-i\xi h}}{h^2} = \frac{v_j}{h^2}\left(e^{i\xi h} + e^{-i\xi h} - 2\right).$$

We then use Euler's formula to simplify the complex exponentials

$$\begin{aligned} e^{i\xi h} + e^{-i\xi h} &= \cos(\xi h) + i\sin(\xi h) + \cos(-\xi h) + i\sin(-\xi h) \\ &= \cos(\xi h) + \cancel{i\sin(\xi h)} + \cos(\xi h) \cancel{- i\sin(\xi h)} \\ &= 2\cos(\xi h). \end{aligned}$$

Hence the symbol for D_h^2 is

$$S(\xi h) = \frac{2}{h^2}\left(\cos(\xi h) - 1\right).$$

- **Forward Euler Iteration** We consider the operator of A where $u_j^{n+1} = Au_j^n$ solves 1 iteration of Forward Euler. To compute the symbol of A, we write $u_j^n = v_j = e^{i\xi hj}$ and $u_j^{n+1} = S(\xi h)v_j$. The Forward Euler iteration now reads:

$$\frac{S(\xi h)v_j - v_j}{\tau} - D_h^2 v_j = 0$$

Rearranging and solving for $S(\xi h)v_j$ leads to

$$S(\xi h)v_j = v_j + \tau D_h^2 v_j$$

We now use the previous example $D_h^2 v_j = \frac{2}{h^2}\left(\cos(\xi h) - 1\right)v_j$ to simplify

$$S(\xi h)v_j = v_j + \frac{2\tau}{h^2}\left(\cos(\xi h) - 1\right)v_j$$

For simplicity of notation for the rest of the von Neumann stability lectures, I'll denote

$$\lambda = \frac{\tau}{h^2}.$$

With this notation, we have that the symbol of Forward Euler is

$$S(\xi h) = 1 + 2\lambda\left(\cos(\xi h) - 1\right)$$

3.2. **Instability of Forward Euler.** For this discussion, we consider a grid function that is as oscillatory as possible as in it switches between $+1$ and -1 at every grid point:

$$u_j^0 = (-1)^{|j|} = \cos(\pi j) = \cos(\pi j) + i\sin(\pi j) = e^{i\pi j},$$

which is the special grid function we we used to compute the symbol $S(\xi h)$ at $\xi h = \pi$. Hence, we may apply our previous work to see how Forward Euler acts on v_j. One step of Forward Euler is

$$u_j^1 = S(\xi h) u_j^0 = \left[1 + 2\lambda \left(\underbrace{\cos(\xi h)}_{=-1} - 1 \right) \right] u_j^0 = (1 - 4\lambda) u_j^0.$$

Applying n steps of Forward Euler results in

$$u_j^1 = (1 - 4\lambda)^n u_j^0 = (1 - 4\lambda)^n (-1)^{|j|}.$$

The amplitude of these oscillations grow exponentially in n if $1 - 4\lambda < -1$ or $1 - 4\lambda > -1$. This instability occurs when

$$\lambda > \frac{1}{2}.$$

In terms of h, τ, this occurs when

$$\tau > \frac{h^2}{2}.$$

Recall from previous lectures that we required that $\tau \leq \frac{h^2}{2}$ (CFL condition) was a sufficient condition for stability of Forward Euler. This discussion shows that in fact, $\tau \leq \frac{h^2}{2}$ is also a necessary condition for stability.

3.3. **Examples of symbols of implicit schemes.** To find the symbols of Backward Euler and Crank-Nicholson, we apply the same procedure as Forward Euler by replacing $u_j^{n+1} = S(\xi h) u_j^n$ and $u_j^n = v_j e^{i\xi h j}$. We then solve for $S(\xi h)$. We now go over the symbols of these schemes.

- **Backward Euler** With the mentioned substitutions, the scheme reads:

$$\frac{S(\xi h) v_j - v_j}{\tau} - D_h^2 [S(\xi h) v_j] = 0$$

  Recall the symbol of $D_h^2 v_j = \frac{2}{h^2} \big(\cos(\xi h) - 1 \big)$, so rearranging and multiplying by τ yields

$$(S(\xi h) - 1) v_j - S(\xi h) 2\lambda \big(\cos(\xi h) - 1 \big) v_j = 0.$$

  where $\lambda = \tau / h^2$ as before. We then collect terms multiplying $S(\xi h)$ and add v_j to both sides to further simplify

$$S(\xi h)[1 - 2\lambda \big(\cos(\xi h) - 1 \big)] v_j = v_j.$$

  Hence, the symbol is

$$S(\xi h) = \frac{1}{1 + 2\lambda \big(1 - \cos(\xi h) \big)}.$$

- **Crank-Nicholson** With the mentioned substitutions, the scheme reads:

$$\frac{S(\xi h)v_j - v_j}{\tau} - D_h^2\left[\frac{S(\xi h)v_j + v_j}{2}\right] = 0.$$

I'll leave the computations as an exercise. The resulting symbol is

$$S(\xi h) = \frac{1-\lambda(1-\cos(\xi h))}{1+\lambda(1-\cos(\xi h))}.$$

4. General theory

We now state the general theory and leave the proofs for a later time. We first need a few definitions. For a grid function U, we define the following norm:

$$\|U\|_{2,h} = \left(h\sum_{j=-\infty}^{\infty}|u_j|^2\right)^{1/2}.$$

We have used finite sums of this form to study discrete energy estimates. Note that if $U_j = u(x_j)$ for some $u : \mathbb{R} \to \mathbb{R}$, then

$$\|U\|_{2,h} \approx \left(\int_{-\infty}^{\infty}|u(x)|^2 dx\right)^{1/2}$$

since the sum is a Riemann sum approximation of the integral.

Theorem 4.1 (stability)**.** Let A be an operator on grid functions. We have that A is stable:

$$\|AU\|_{2,h} \leq \|U\|_{2,h}$$

if and only if the symbol of A satisfies the following bound for all $\xi \in \mathbb{R}$:

$$|S(\xi h)| \leq 1$$

4.1. **Application of general theory to time stepping schemes.** We recall the symbols of the various time stepping schemes ($\lambda = \tau/h^2$):

- **Forward Euler:**

$$S(\xi h) = 1 + 2\lambda\big(\cos(\xi h) - 1\big)$$

- **Backward Euler:**

$$S(\xi h) = \frac{1}{1+2\lambda\big(1-\cos(\xi h)\big)}.$$

- **Crank-Nicholson:**

$$S(\xi h) = \frac{1-\lambda(1-\cos(\xi h))}{1+\lambda(1-\cos(\xi h))}$$

We now determine conditions on λ to guarantee stability of these schemes.

- **Forward Euler:** We want to determine λ so that for all ξ:
$$-1 \leq 1 + 2\lambda \left(\cos(\xi h) - 1\right) \leq 1,$$
which is equivalent to requiring
$$-2 \leq 2\lambda \left(\cos(\xi h) - 1\right) \leq 0.$$
Notice that $\cos(\xi h) - 1 \leq 0$, so all we need to check is
$$-2 \leq 2\lambda \left(\cos(\xi h) - 1\right).$$
The minimum of the RHS of the above inequality is achieved for $\xi h = \pi$, so we require $-2 \leq -4\lambda$, or
$$\tau \leq \frac{h^2}{2},$$
which is the CFL condition.
- **Backward Euler:** Notice that $0 \leq 1 - \cos(\xi h) \leq 2$ and
$$1 \leq 1 + 2\lambda \left(1 - \cos(\xi h)\right) \leq 1 + 4\lambda$$
Hence, the symbol of Backward Euler can be bounded above for all ξ:
$$|S(\xi h)| = \left| \frac{1}{1 + 2\lambda \left(1 - \cos(\xi h)\right)} \right| \leq 1,$$
and Backward Euler is unconditionally stable.
- **Crank-Nicholson:** It is left as an exercise to show that the symbol of Crank-Nicholson satisfies $|S(\xi h)| \leq 1$ for all ξ and for all choices of $\lambda \geq 0$. Hence, Crank-Nicholson is unconditionally stable.

5. Comparison of Methods in High Frequency Regime

In addition to a general theory, the von Neumann method allows us to look at the behavior of methods applied to different frequencies. We now look at the behavior of these methods in the presence of high frequencies.

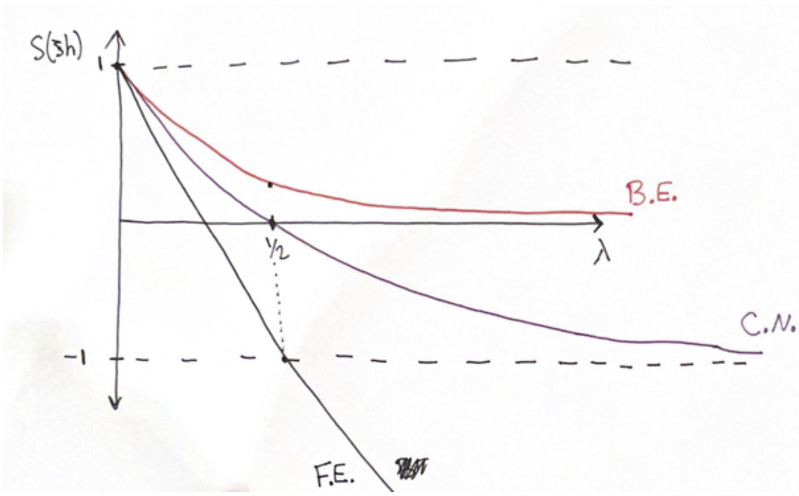
We consider a grid function that is as oscillatory as possible as in it switches between $+1$ and -1 at every grid point:
$$u_j = (-1)^{|j|} = \cos(\pi j) = \cos(\pi j) + i \sin(\pi j) = e^{i\pi j},$$
which is the special grid function we we used to compute the symbol $S(\xi h)$ at $\xi h = \pi$. The symbols of each method at $\xi h = \pi$ are

- **Forward Euler:**
$$S(\xi h) = 1 - 4\lambda$$
- **Backward Euler:**
$$S(\xi h) = \frac{1}{1 + 4\lambda}.$$

- **Crank-Nicholson:**

$$S(\xi h) = \frac{1 - 2\lambda}{1 + 2\lambda}$$

We now plot each symbol as a function of λ:



If we take τ to be relatively large compared with h^2, i.e. $\tau = h^\alpha$ for $0 \leq \alpha < 2$, then $\lambda \to \infty$ as $h \to 0$. The symbols then converge to

$$\lim_{\lambda \to \infty} S(\pi) = \begin{cases} -\infty, & \text{Forward Euler} \\ 0, & \text{Backward Euler} \\ -1, & \text{Crank-Nicholson} \end{cases}$$

These limits reveal disadvantages of each method.

- Forward Euler becomes unstable as $\lambda > 1/2$.
- Backward Euler over dissipates high frequencies as $\lambda \to \infty$
- Crank-Nicholson under dissipates high frequencies as $\lambda \to \infty$

5.1. **One method to rule them all: the θ-method.** An method that covers all the methods discussed here is the θ-method, which is

$$D_\tau u_j^n - D_h^2 \left(\theta u_j^n + (1 - \theta) u_j^{n-1} \right) = 0.$$

Note that the method reduces to FE if $\theta = 0$, B.E. if $\theta = 1$, and C.N. if $\theta = 1/2$. It is left as an exercise to check that the symbol of the θ-method is

$$S(\xi h) = \frac{1 + 2\lambda(\theta - 1)(1 - \cos(\xi h))}{1 + 2\lambda\theta(1 - \cos(\xi h))}.$$

If we look at the high frequency behavior of the θ-method, we take $\xi h = \pi$ and compute

$$S(\pi) = \frac{1 + 4\lambda(\theta - 1)}{1 + 4\lambda\theta}.$$

whose limit as $\lambda \to \infty$ is

$$\lim_{\lambda \to \infty} S(\pi) = \begin{cases} \frac{(\theta-1)}{\theta}, & \theta > 0 \\ -\infty, & \theta = 0 \end{cases}.$$

The θ parameter gives us more flexibility in tuning our method for different situations. Note that the limit is $\lim_{\lambda \to \infty} S(\pi) < -1$ if $\theta < 1/2$. As a result, we expect a CFL condition for $\theta < 1/2$. Also, one can prove the method is unconditionally stable for $\theta \geq 1/2$.