1 Diffusion Equations and Parabolic Problems

1.1 Stability Analysis

Note the Fourier transform of a function $v(x)$ is defined as

$$\hat{v}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} v(x) e^{-ikx} dx. \tag{1}$$

The inverse Fourier transform is given by

$$v(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{v}(k) e^{ikx} dk. \tag{2}$$

We first note $\hat{v}(k)$ is also called the Fourier coefficient of $v(x)$ for wave number k. We also note for any real kx that $e^{ikx} = \cos(kx) + i \sin(kx)$ by Euler's formula.

1.1.1 Differentiation and Fourier Transform

We can derive

$$\frac{d}{dx} v(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} ik \hat{v}(k) e^{ikx} dk \tag{3}$$

And we call the ik term in the integrand above the *symbol* of the differential operator d/dx.

We also note, for a function of two variables $u(x,t)$, the Fourier transform of spatial variable x is given by

$$\hat{u}(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(x,t) e^{-ikx} dx, \tag{4}$$

and its inverse is given by

$$u(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{u}(k,t) e^{ikx} dk. \tag{5}$$

Now we can try to look at the advection equation

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x},\ u(x,0) = \eta(x). \tag{6}$$

Note the Fourier transform for u w.r.t. x is $\hat{u} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(x,t)e^{-ikx}dx$, and we can see

$$\frac{\partial}{\partial t}\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{u}(k,t)e^{ikx}dk = -c\frac{\partial u}{\partial x}\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{u}(k,t)e^{ikx}dk \tag{7}$$

This is equivalent to the following

$$\int_{-\infty}^{\infty} \frac{\partial \hat{u}(k,t)}{\partial t} e^{ikx} dk = -c\int_{-\infty}^{\infty} \frac{\partial}{\partial x}(\hat{u}(k,t)e^{ikx})dk = -c\int_{-\infty}^{\infty} ik\hat{u}(k,t)e^{ikx}dk \tag{8}$$

As we have the equality of the integrands, we can write the ODE for $\hat{u}(k,t)$

as

$$\frac{\partial \hat{u}(k,t)}{\partial t} = -cik\hat{u}(k,t). \tag{9}$$

This is a first order ODE in t and we can solve it to get

$$\hat{u}(k,t) = \hat{u}(k,0)e^{-cikt} = \hat{\eta}(k)e^{-cikt}. \tag{10}$$

We also should note that the Fourier transform of the initial condition is given by $\hat{u}(k,0) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\eta(x)e^{-ikx}dx = \hat{\eta}(k)$. We can now take the inverse Fourier transform of the above (10) to get

$$u(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\hat{u}(k,0)e^{-cikt}e^{ikx}dk \tag{11}$$

This is equivalent to

$$u(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\hat{u}(k,0)e^{ik(x-ct)}dk = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\hat{\eta}(k)e^{ik(x-ct)}dk \tag{12}$$

Using change of variables $x - ct = x'$, we can write

$$u(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\hat{\eta}(k)e^{ikx'}dk = \eta(x-ct). \tag{13}$$

This is the solution to the advection equation, which means the solution is advected at a speed c from the initial condition $\eta(x)$.

Note from (10) that the solution is stable if $|e^{-cikt}| = 1$.

Note for 1d diffusion equation (infinite saptial domain):

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2},\ u(x,0) = \eta(x). \tag{14}$$

We can take the Fourier transform of the above equation to get

$$\frac{\partial \hat{u}(k,t)}{\partial t} = -\alpha k^2 \hat{u}(k,t). \tag{15}$$

This is a first order ODE in t and we can solve it to get

$$\hat{u}(k,t) = \hat{u}(k,0)e^{-\alpha k^2 t} = \hat{\eta}(k)e^{-\alpha k^2 t}. \tag{16}$$

Obviously this means

$$|\hat{u}(k,t)| = |\hat{\eta}(k)||e^{-\alpha k^2 t}|. \tag{17}$$

So in diffusion equation, the Fourier coefficient of the solution decays exponentially in time

1.1.2 Symbol for difference operators

Now we will check the *symbols* of difference operators in the finite difference method.

If x is shifted by Δx then we can see

$$\begin{aligned} u(x+\Delta x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{u}(k) e^{ik(x+\Delta x)} dk \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ik\Delta x} \hat{u}(k) e^{ikx} dk \end{aligned} \tag{18}$$

Suppose d/dx is approximated by the central difference operator

$$\begin{aligned} D_0 u(x) &= \frac{u(x+\Delta x) - u(x-\Delta x)}{2\Delta x} \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{u}(k) e^{ikx} \left(\frac{e^{ik\Delta x} - e^{-ik\Delta x}}{2\Delta x} \right) dk \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{u}(k) e^{ikx} \frac{i \sin(k\Delta x)}{\Delta x} dk \end{aligned} \tag{19}$$

The **symbol** of the above central difference operator D is given by $i\sin(k\Delta x)/\Delta x$.

Now consider:

$$\begin{aligned} \frac{i \sin(k\Delta x)}{\Delta x} &= \frac{i}{\Delta x} \left(k\Delta x - \frac{(k\Delta x)^3}{3!} + \frac{(k\Delta x)^5}{5!} - \cdots \right) \\ &= ik - \frac{ik^3 \Delta x^2}{3!} + \frac{ik^5 \Delta x^4}{5!} - \cdots \\ &= ik \left(1 - \frac{k^2 \Delta x^2}{3!} + \frac{k^4 \Delta x^4}{5!} - \cdots \right) \end{aligned} \tag{20}$$

We can see the difference between the symbol of the central difference operator and the symbol of the exact differential operator is given by $O(\Delta x^2)$, if $k\Delta x$ is small enough ($k\Delta x < 1$). In other word, it means k is considerably smaller than $1/\Delta x = N$.

We note

$$
\begin{aligned}
\frac{\partial^2 u}{\partial x^2} &= \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\right) \\
&= \frac{\partial}{\partial x}\left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \hat{u}(k)e^{ikx}dk\right) \\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \hat{u}(k)\frac{\partial}{\partial x}e^{ikx}dk \\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \hat{u}(k)(ik)e^{ikx}dk \\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} (ik)^2\hat{u}(k)e^{ikx}dk \\
&= -k^2\hat{u}(k).
\end{aligned} \tag{21}
$$

The **symbol** of the central difference operator for the second derivative is given by $-k^2$.

Now consider the central difference operator for second derivative.

$$
\begin{aligned}
D_0 u(x) &= \frac{u(x+\Delta x) - 2u(x) + u(x-\Delta x)}{\Delta x^2} \\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \hat{u}(k)e^{ikx}\left(\frac{e^{ik\Delta x} - 2 + e^{-ik\Delta x}}{\Delta x^2}\right)dk \\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \hat{u}(k)e^{ikx}\left(\frac{2\cos(k\Delta x) - 2}{\Delta x^2}\right)dk
\end{aligned} \tag{22}
$$

$$
\begin{aligned}
\frac{2\cos(k\Delta x) - 2}{\Delta x^2} &= \frac{2}{\Delta x^2}\left(\cos(k\Delta x) - 1\right) \\
&= \frac{2}{\Delta x^2}\left(1 - \frac{k^2\Delta x^2}{2!} + \frac{k^4\Delta x^4}{4!} - \cdots - 1\right) \\
&= \frac{2}{\Delta x^2}\left(-k^2\Delta x^2 + \frac{k^4\Delta x^4}{3!} - \cdots\right) \\
&= -k^2 + \frac{k^4\Delta x^2}{3!} - \cdots
\end{aligned} \tag{23}
$$

So the difference between the symbol of the central difference operator for the second derivative and the symbol of the exact differential operator is $O(\Delta x^2)$, given k is considerably small.

1.1.3 Eigengridfunction and von Neumann stability analysis

Given function in x with $e^{ix\xi}$, we notice

$$\frac{\partial}{\partial x}e^{ix\xi} = \partial_x e^{ix\xi} = i\xi e^{ix\xi},\ \partial_x^2 e^{ix\xi} = -\xi^2 e^{ix\xi}.$$

Now given grid function $W_j = e^{ijh\xi} = e^{ij\Delta x\xi}$, has the property of being an eigengridfunction of the translation-invariant finite difference operator:

$$W_{j+1} = e^{i(j+1)h\xi} = e^{ijh\xi}e^{ih\xi} = e^{ijh\xi}e^{i\xi} = W_j e^{i\xi}. \tag{24}$$

$$W_{j-1} = e^{i(j-1)h\xi} = e^{ijh\xi}e^{-ih\xi} = e^{ijh\xi}e^{-i\xi} = W_j e^{-i\xi}. \tag{25}$$

So we can see the finite difference operator for the first derivative has the symbol $i\xi$. We can also see

$$\begin{aligned} D_0 W_j &= \frac{1}{2h}(W_{j+1} - W_{j-1}) = \frac{1}{2h}(e^{i(j+1)h\xi} - e^{-i(j-1)h\xi}) \\ &= \frac{1}{2h}e^{ijh\xi}(e^{ih\xi} - e^{-ih\xi}) = \frac{i}{h}e^{ijh\xi}\sin(h\xi) = \frac{i}{h}\sin(h\xi)W_j. \end{aligned} \tag{26}$$

So W_j is an eigengridfunction of the finite difference operator D_0 for the first derivative with the symbol $i\sin(h\xi)/h$ (or we say eigenvalue).

Now consider we have grid function V_j defined at grid points $x_j = j\Delta x = jh$, for $j = 0, \pm 1, \pm 2, \ldots$. We also assume V_j is l_2 function which means

$$||V||_2 = \left(h \sum_{j=-\infty}^{\infty} |V_j|^2 \right)^{\frac{1}{2}} < \infty$$

Then we can express V_j in terms of the eigengridfunctions W_j as

$$V_j = \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} \hat{V}(\xi) e^{i\xi jh} d\xi = \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} \hat{V}(\xi) W_j d\xi. \tag{27}$$

with the Fourier coefficients $\hat{V}(\xi) = \frac{h}{\sqrt{2\pi}} \sum_{j=-\infty}^{\infty} V_j e^{-ijh\xi}$.

Parvesal's relation still holds $||\hat{V}||_2 = ||V||_2$, but using the grid norms:

$$||V||_2 = \left(h \sum_{j=-\infty}^{\infty} |V_j|^2 \right)^{1/2}, \qquad ||\hat{V}||_2 = \left(h \int_{-\pi/h}^{\pi/h} |\hat{V}(\xi)|^2 \, d\xi \right)^{1/2}.$$

Now we will discuss the von Neumann stability analysis for the finite difference method.

- It is based on the decomposition of the errors into Fourier series.
- Study growth of waves $e^{i\xi x}$
- The methods is **limited to constant coefficient linear PDEs.**
- Usually applied to the Cauchy problem (space with no boundaries $-\infty < x < \infty$ in 1D).

- Can also be applied to periodic boundary conditions.
- Note that $e^{i\xi x}$ are eigenfunctions of the differential operator ∂_x, where ξ is the wavenumber.

$$\frac{\partial}{\partial x}\left(e^{i\xi x}\right) =$$

- Then $W_j = e^{ijh\xi}$, $h = 1/(m+1)$, $j = 1, \ldots m$ is an eigenfunction of any translation-invariant finite difference operator.

- For stability, we want to show $||U^{n+1}||_2 \leq (1 + \alpha \Delta t)||U^n||_2$ for all U^n

- From Parvesal's relation, we can show $||\hat{U}^{n+1}||_2 \leq (1 + \alpha \Delta t)||\hat{U}^n||_2$ for all $\hat{U}^n$
- For a one step method, we expect to obtain $\hat{U}^{n+1}(\xi) = g(\xi)\hat{U}^n(\xi)$
  - $g(\xi)$ is called the **amplification factor**.
  - The necessary and sufficient condition for the error to remain bounded is that $|g(\xi)| \leq 1$.

1.1.4 Examples

Apply von Neumann stability analysis to

$$U_j^{n+1} = U_j^n + \frac{\Delta t}{\Delta x^2}\left(U_{j-1}^n - 2U_j^n + U_{j+1}^n\right). \tag{28}$$

and specify the amplification factor.

We work on a single wave number ξ, and set the n level grid function to $U_j^n = e^{ijh\xi}$ and expect $U_j^{n+1} = g(\xi)U_j^n = g(\xi)e^{ijh\xi}$ from the finite difference method (28). From the method in (28), we can then write

$$\begin{aligned} g(\xi)e^{ijh\xi} &= e^{ijh\xi} + \frac{\Delta t}{\Delta x^2}\left(e^{i(j-1)h\xi} - 2e^{ijh\xi} + e^{i(j+1)h\xi}\right), \\ g(\xi) &= 1 + \frac{\Delta t}{\Delta x^2}\left(e^{-ih\xi} - 2 + e^{ih\xi}\right) = 1 + 2\frac{\Delta t}{\Delta x^2}\left(\cos(h\xi) - 1\right) \end{aligned} \tag{29}$$

Example: Compute the amplification factor for Crank-Nicholson:

$$-rU_{j-1}^{n+1} + (1+2r)U_j^{n+1} - rU_{j+1}^{n+1} = rU_{j-1}^n + (1-2r)U_j^n + rU_{j+1}^n,$$

where $r = \frac{\Delta t}{2\Delta x^2}$.