

1 Z-Transform Relation to Fourier Transform

In this problem we study how the grid scaled Z-transform of the discretized solution approaches the Fourier transform of the continuous solution as the space increment $h \rightarrow 0$. Recall that if $u_j = U(jh)$, the Z-transform $\hat{u}(\xi)$ is related to the Fourier transform $\hat{U}(\kappa) = \int_{-\infty}^{\infty} U(x)e^{-ix\kappa} dx$ via

$$h\hat{u}(h\kappa) = \sum_{m=-\infty}^{\infty} \hat{U}\left(\kappa - \frac{2\pi}{h}m\right).$$

Suppose that for $\kappa \in \mathbb{R}$, $\hat{U}(\kappa)$ satisfies

- (a) $|\hat{U}(\kappa)| \leq \frac{C_r}{1+|\kappa|^r},$
- (b) $|\hat{U}(\kappa)| \leq Ce^{-\rho|\kappa|},$

where $r \geq 2$, $C_r \geq 0$, $C > 0$ and $\rho > 0$ are constants. Show that for $|\kappa| \leq \pi/h$, $|h\hat{u}(h\kappa) - \hat{U}(\kappa)|$ is bounded by

- (a) $\frac{C_r h^r}{4\pi^{r-2}}$
- (b) $\frac{2Ce^{-\rho\pi/h}}{1-e^{-2\rho\pi/h}}.$

Solution:

- (a) First, note the fact that $|k \pm \frac{2\pi}{h}m| \geq \frac{2\pi m - \pi}{h}$ and $\sum_{m=1}^{\infty} \frac{1}{(2m-1)^2} = \frac{\pi^2}{8}$. Using these facts, we achieve the first upper bound as follows:

$$\begin{aligned} |h\hat{u}(h\kappa) - \hat{U}(\kappa)| &= \left| \sum_{m=-\infty}^{\infty} \hat{U}\left(\kappa - \frac{2\pi}{h}m\right) - \hat{U}(\kappa) \right| \\ &= \left| \sum_{m \neq 0} \hat{U}\left(\kappa - \frac{2\pi}{h}m\right) \right| \\ &\leq \sum_{m \neq 0} \left| \hat{U}\left(\kappa - \frac{2\pi}{h}m\right) \right| \\ &\leq \sum_{m \neq 0} \frac{C_r}{1 + \left|\kappa - \frac{2\pi}{h}m\right|^r} \\ &\leq \sum_{m=1}^{\infty} \frac{2C_r}{1 + \left(\frac{2\pi m - \pi}{h}\right)^r} \\ &= \sum_{m=1}^{\infty} \frac{2C_r h^r}{1 + \pi^r (2m-1)^r} \\ &\leq \frac{2C_r h^r}{\pi^r} \sum_{m=1}^{\infty} \frac{1}{(2m-1)^r} \\ &\leq \frac{2C_r h^r}{\pi^r} \sum_{m=1}^{\infty} \frac{1}{(2m-1)^2} \\ &= \boxed{\frac{C_r h^r}{4\pi^{r-2}}}. \end{aligned}$$

(b) For the second upper bound, we start with the initial simplifications from the previous part as follows:

$$\begin{aligned}
 \left| h\hat{u}(h\kappa) - \hat{U}(\kappa) \right| &\leq \sum_{m \neq 0} \left| \hat{U} \left(\kappa - \frac{2\pi}{h} \right) \right| \\
 &\leq \sum_{m \neq 0} C e^{-\rho|\kappa - 2\pi m/h|} \\
 &\leq 2C \sum_{m=1}^{\infty} e^{-\rho(2\pi m - \pi)/h} \\
 &= 2C e^{\rho\pi/h} \sum_{m=1}^{\infty} \left(e^{-2\rho\pi/h} \right)^m \\
 &= \frac{2C e^{\rho\pi/h}}{1 - e^{-2\rho\pi/h}} e^{-2\rho\pi/h} \\
 &= \boxed{\frac{2C e^{-\rho\pi/h}}{1 - e^{-2\rho\pi/h}}}
 \end{aligned}$$

2 Circulant Matrix Properties

A circulant matrix is constant along diagonals with entries that "wrap around":

$$A_{jk} = \begin{cases} r_{k-j} & k \geq j, \\ r_{N+k-j} & k < j \end{cases}.$$

For convenience, we will index our matrices starting at zero. Show that $AU = U\Lambda$, with

$$U_{jk} = e^{2\pi i j k / N}, \quad \begin{pmatrix} 0 \leq j \leq N-1 \\ 0 \leq k \leq N-1 \end{pmatrix}, \quad \begin{pmatrix} \lambda_0 & & \\ & \ddots & \\ & & \lambda_{N-1} \end{pmatrix}$$

and $\lambda_k = \sum_{\ell=0}^{N-1} r_{\ell} e^{2\pi i \ell k / N}$.

Solution:

We proceed by showing that $(AU)_{jk} = (U\Lambda)_{jk}$. We compute the right hand side first:

$$\begin{aligned} (U\Lambda)_{jk} &= \lambda_k e^{2\pi i j k / N} \\ &= \sum_{\ell=0}^{N-1} r_{\ell} e^{2\pi i (\ell+j) k / N}. \end{aligned}$$

Now consider the left hand side:

$$\begin{aligned} (AU)_{jk} &= \sum_{\ell=0}^{N-1} A_{j\ell} U_{\ell k} \\ &= \sum_{\ell=0}^{N-1} A_{j\ell} e^{2\pi i \ell k / N} \end{aligned}$$

The value of $A_{j\ell}$ depends on the relationship between j and ℓ so we split up the sum into corresponding parts:

$$\begin{aligned} \sum_{\ell=0}^{N-1} A_{j\ell} e^{2\pi i \ell k / N} &= \sum_{\ell=0}^{j-1} A_{j\ell} e^{2\pi i \ell k / N} + \sum_{\ell=j}^{N-1} A_{j\ell} e^{2\pi i \ell k / N} \\ &= \sum_{\ell=0}^{j-1} r_{N+\ell-j} e^{2\pi i \ell k / N} + \sum_{\ell=j}^{N-1} r_{\ell-j} e^{2\pi i \ell k / N} \\ &= \sum_{\ell=N-j}^{N-1} r_{\ell} e^{2\pi i (\ell+j-N) k / N} + \sum_{\ell=0}^{N-j-1} r_{\ell} e^{2\pi i (\ell+j) k / N} \\ &= \sum_{\ell=N-j}^{N-1} r_{\ell} e^{2\pi i (\ell+j) k / N} + \sum_{\ell=0}^{N-j-1} r_{\ell} e^{2\pi i (\ell+j) k / N} \\ &= \sum_{\ell=0}^{N-1} r_{\ell} e^{2\pi i (\ell+j) k / N}. \end{aligned}$$

The expressions for $(AU)_{jk}$ and $(U\Lambda)_{jk}$ are indeed equal so we conclude that $AU = U\Lambda$.

3 Crank-Nicolson

Use the Crank-Nicolson scheme to solve the equation

$$u_t = \alpha u_{xx} - \beta u_x, \quad \alpha = \frac{1}{512}, \quad \beta = \frac{33}{32} \quad (\star)$$

on the interval $[0, 1]$ with periodic boundary conditions and initial conditions

$$u(x, 0) = g(x), \quad g(x) = (\sin \pi x)^{100}.$$

Solution:

For the spatial discretizations, we replace the right-hand side of (\star) by $\alpha D_x^+ D_x^- u - \beta D_x^0 u$ and then use the trapezoidal rule in time. The trapezoidal rule is the approximation $(x_{n+1} - x_n)/h \approx (f_n + f_{n+1})/2$. Applying this method yields the following finite difference:

$$D_t^+ u^n = \frac{1}{2}(\alpha D_x^+ D_x^- u^n + \alpha D_x^+ D_x^- u^{n+1} - \beta D_x^0 u^n - \beta D_x^0 u^{n+1})$$

Consider $k \in \mathbb{R}$, $M \in \mathbb{Z}$, $h = \frac{1}{M}$, and operators A, B defined as follows:

$$\begin{aligned} Au_j &= u_{j+1} - u_{j-1} \\ Bu_j &= u_{j+1} - 2u_j + u_{j-1} \end{aligned}$$

We can then rewrite the finite difference as

$$\frac{u^{n+1} - u^n}{k} = \frac{\alpha}{2h^2}(Bu^n + Bu^{n+1}) - \frac{\beta}{4h}(Au^n - Au^{n+1}).$$

We then bring the u^{n+1} terms to one side to yield an implicit update step

$$\left(I + \frac{\beta k}{4h}A - \frac{\alpha k}{2h^2}B\right)u^{n+1} = \left(I - \frac{\beta k}{4h}A + \frac{\alpha k}{2h^2}B\right)u^n$$

The last part of the scheme construction is accounting for the periodic boundary conditions. We can do this by creating a ghost node u_{-1} where $u_{-1} = u_M = u_0$. The ghost node will then slightly change the update steps for u_0 and u_{M-1} . Note that the nodes for u_0 and u_M can be treated as the same. We redefine A and B correspondingly to act on \mathbb{R}_h^M while accounting for the boundary conditions.

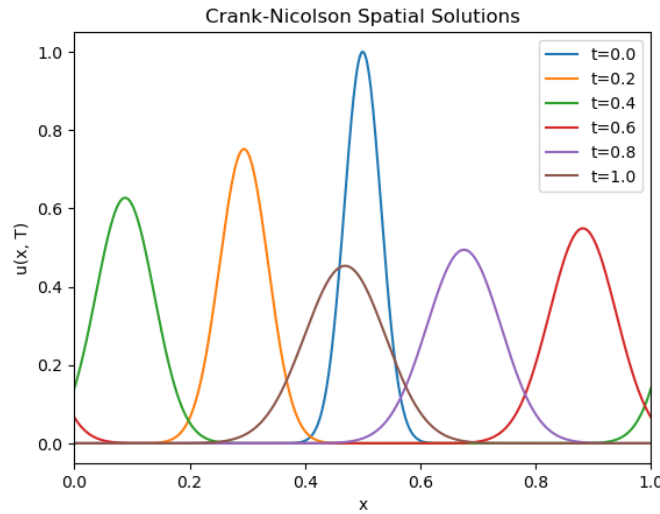
$$\begin{aligned} Au_0 &= u_1 - u_{M-1} \\ Au_{M-1} &= u_0 - u_{M-2} \\ Bu_0 &= u_1 - 2u_0 + u_{M-1} \\ Bu_{M-1} &= u_0 - 2u_{M-1} + u_{M-2} \end{aligned}$$

Shown below are the matrix representations of the operators $A, B \in \mathbb{R}_h^{M \times M}$.

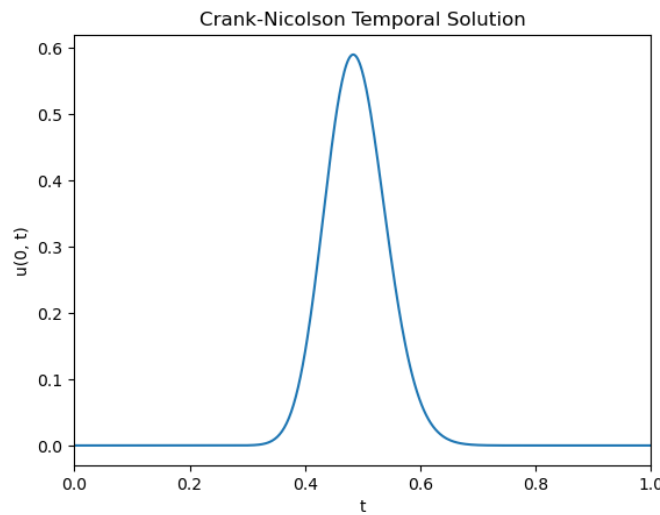
$$A = \begin{pmatrix} 0 & 1 & \cdots & 0 & -1 \\ -1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & \cdots & -1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} -2 & 1 & \cdots & 0 & 1 \\ 1 & -2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & -2 & 1 \\ 1 & 0 & \cdots & 1 & -2 \end{pmatrix}$$

We discuss results and analysis of the Crank-Nicolson scheme below.

- (a) We first solve the PDE for various time steps on the entire interval $[0, 1]$. These solutions are plotted below. Observe that the solution is both translational and dissipative.



- (b) We can gain further insights by looking at the solution trajectory over time for $u(0, t)$ where $0 \leq t \leq 1$. This is again plotted below. The translational effect is seen by the increasing and then decreasing value at $x = 0$.



- (c) The amplification factor of the scheme is found via the Z -transform of the update step. We compute this below.

$$u^{n+1} = \underbrace{\left(I + \frac{\beta k}{4h} A - \frac{\alpha k}{2h^2} B \right)^{-1} \left(I - \frac{\beta k}{4h} A + \frac{\alpha k}{2h^2} B \right)}_B u^n$$

$$\hat{u}^{n+1}(\xi) = \underbrace{\frac{1 - \frac{\beta k}{4h} G_A(\xi) + \frac{\alpha k}{2h^2} G_B(\xi)}{1 + \frac{\beta k}{4h} G_A(\xi) - \frac{\alpha k}{2h^2} G_B(\xi)}}_{G(\xi)} \hat{u}^n(\xi)$$

Here $G_A(\xi)$ and $G_B(\xi)$ are the Z -transforms of A and B , and $G(\xi)$ is the amplification factor.

$$G_A(\xi) = e^{i\xi} - e^{-i\xi} = 2i \sin \xi$$

$$G_B(\xi) = e^{i\xi} - 2 + e^{-i\xi} = 2 \cos \xi - 2 = -4 \sin^2 \frac{\xi}{2}$$

Putting these terms together, we can explicitly write the amplification factor.

$$G(\xi) = \frac{1 - \frac{2\alpha k}{h^2} \sin^2 \frac{\xi}{2} - \frac{\beta k}{2h} i \sin \xi}{1 + \frac{2\alpha k}{h^2} \sin^2 \frac{\xi}{2} + \frac{\beta k}{2h} i \sin \xi}$$

Now define variables $a = \frac{2\alpha k}{h^2} \sin^2 \frac{\xi}{2}$ and $b = \frac{\beta k}{2h} \sin \xi$. Note that $a, b \in \mathbb{R}$ and $a \geq 0$. We then plug the expressions for $G_A(\xi)$ and $G_B(\xi)$ into the earlier expression to upper bound the amplification factor.

$$\begin{aligned} |G(\xi)| &= |\hat{u}^{n+1}(\xi)| \\ &= \frac{|1 - a - bi|}{|1 + a + bi|} \\ |1 - a - bi| &= |1 - a + bi| \\ &= |1 + a + bi| \\ |G(\xi)| &\leq \frac{|1 - a - bi|}{|1 + a + bi|} \\ &= 1 \end{aligned}$$

Furthermore, $G(0) = 1$, so the upper bound is achievable on the finite interval and $\|\mathcal{B}\|_{\ell_h^2} = \|G\|_\infty = 1$. Since 1 is an upper bound for $\|\mathcal{B}\|_{\ell_h^2}$, and in fact an equality, we conclude that the scheme is **unconditionally stable**.

(d) Consider the equation $v(x, t) = u(x + \beta t, t)$. Consider the partial v_x .

$$\begin{aligned} v_t(x, t) &= \beta u_x(x + \beta t, t) + u_t(x + \beta t, t) \\ &= \beta v_x(x, t) + u_t(x + \beta t, t) \\ &= \beta v_x(x, t) + \alpha v_{xx}(x + \beta t, t) - \beta u_x(x + \beta t, t) \\ &= \cancel{\beta v_x(x, t)} + \alpha v_{xx}(x, t) - \cancel{\beta v_x(x, t)} \\ &= \alpha v_{xx}(x, t) \end{aligned}$$

This yields the following PDE: $\boxed{v_t = \alpha v_{xx}, \quad v(x, 0) = g(x)}$. The definition of $v(x, t)$ is just a shift of the x coordinate by a scalar multiple of t so it will also have periodic boundary conditions.

(e) We now derive an exact formula for $v(x, t)$. First, we expand $g(x)$ in terms of its Fourier coefficients.

$$\begin{aligned} g(x) &= (\sin \pi x)^{100} \\ &= \left(\frac{1}{2i}\right)^{100} (e^{\pi i x} - e^{-\pi i x})^{100} \\ &= \frac{1}{2^{100}} \sum_{k=0}^{100} \binom{100}{k} (-1)^{100-k} e^{2\pi i k x} e^{-100\pi i x} \\ &= \frac{1}{2^{100}} \sum_{k=-50}^{50} \binom{100}{k+50} (-1)^{k+50} e^{2\pi i k x} \end{aligned}$$

Thus, the Fourier coefficients of $g(x)$ are $c_k = \binom{100}{k+50} (-1)^{k+50} 2^{-100}$ for $-50 \leq k \leq 50$. Observe that the PDE is separable so basis elements of the solution space will be of the form $v_k(x, t) = T_k(t)X_k(x)$. By observation of the initial condition and the periodicity of $v(x, t)$, we can write the general form as

$$v(x, t) = \sum_{k=-50}^{50} c_k T_k(t) e^{2\pi i k x}$$

where each c_k is the coefficient of a basis element. We apply the PDE to an arbitrary k th term to calculate T_k since each term is in the solution space.

$$\cancel{c_k} T'_k(t) e^{2\pi i k x} = \cancel{c_k} \alpha T_k(t) (-4\pi^2 k^2) e^{2\pi i k x}$$

$$T'_k(t) = (-4\alpha\pi^2 k^2) T_k(t)$$

If we take the ansatz $T_k(t) = e^{\lambda_k t}$, we see that $\lambda_k = -4\alpha\pi^2 k^2$. Thus, the exact solution for $v(x, t)$ expressed in terms of the Fourier coefficients c_k is

$$v(x, t) = \sum_{k=-50}^{50} c_k e^{-4\alpha\pi^2 k^2 t} e^{2\pi i k x}$$

From our discussion earlier, we know $u(x, t) = v(x - \beta t, t)$, so we can recover the solution to original PDE.

$$u(x, t) = \sum_{k=-50}^{50} c_k e^{-(4\alpha\pi^2 k^2 + 2\beta\pi i k)t} e^{2\pi i k x}$$

While we could compute c_k explicitly with the exact formula found earlier, this can be computationally challenging due to floating point errors. Instead, we demonstrate an alternative approximate method. First, sample $g(x)$ on a uniform grid with $M = 128$ grid-points and apply the DFT. The DFT yields coefficients

$$\tilde{g}_k = \sum_{j=0}^{M-1} g_j e^{-2\pi i k x_j}$$

where $x_j = j/M$ are the uniform sample positions. The coefficients \tilde{g}_j relate to c_k by the following inverse transform:

$$g_j = \frac{1}{M} \sum_{k=0}^{M-1} \tilde{g}_k e^{2\pi i k x_j}.$$

However, we need coefficients between -50 and 50 . This can be done by shifting the indices cyclically. Here we assume M is even. Then,

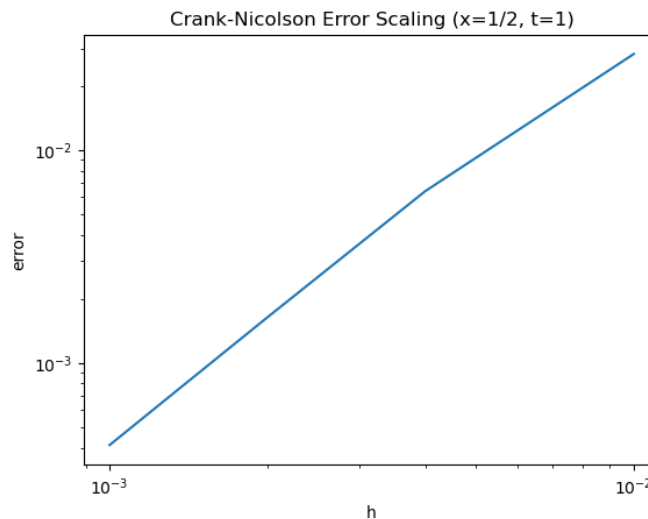
$$\begin{aligned} g_j &= \frac{1}{M} \sum_{k=0}^{M-1} \tilde{g}_k e^{2\pi i k j/M} \\ &= \frac{1}{M} \sum_{k=0}^{M-1} \tilde{g}_k e^{2\pi i (k-M) j/M} \\ &= \frac{1}{M} \sum_{k=-M/2}^{-1} \tilde{g}_{k+M} e^{2\pi i k j/M} + \frac{1}{M} \sum_{k=0}^{M/2-1} \tilde{g}_k e^{2\pi i k j/M} \end{aligned}$$

Finally, we can match terms to get approximations for the Fourier coefficients.

$$c_k = \begin{cases} \tilde{g}_{k+M}/M, & -M/2 \leq k \leq -1 \\ \tilde{g}_k/M, & 0 \leq k \leq M/2 - 1 \end{cases}$$

Note that we only need $-50 \leq k \leq 50$ so $M = 128 > 50 \times 2$ is sufficiently large. We also compute the exact solutions for c_k as a baseline by using the combinatorial formula described earlier. With the given selection for M , the corresponding relative error is less than 10^{-15} .

- (f) We can now compute $u(x, t)$ directly by using the exact form in part (e) and the DFT approximations of c_k . As an example, $u(1/2, 1) = 0.41023088876098807$.
- (g) We can now use our solution for $u(1/2, 1)$ in part (f) to compute the error of the Crank-Nicolson method and show its order of accuracy. Let the error be $e_h = |u_h(1/2, 1) - u(1/2, 1)|$ where $u_h(x, t)$ is the numerical solution from Crank-Nicolson with the refinement path $k = h$. The truncation error of the method is $O(k^2 + h^2)$ so we expect $O(h^2)$ error.



The line plot above has a slope of ≈ 2 , thus verifying the expected second order error convergence.