Chapter 3 PERIODIC GRIDS : THE DFT & FFT

Preliminary assumption throughout this chapter.

(i) Our basic periodic grid will be a subset of the interval $[0, 2\pi]$

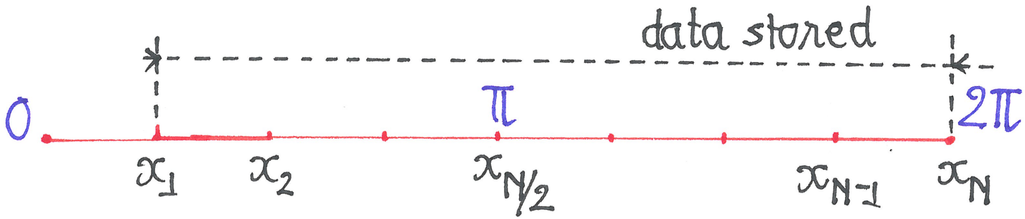
(ii) When we talk about a periodic grid, we mean that any data values on the grid come from evaluating a periodic function

(iii) Throughout the chapter, the number of grid points on a periodic grid will be even :

N is even. For examples, $N = 16, 32, 128, \ldots$

(iv) The spacing of the grid point is $\boxed{h = \frac{2\pi}{N}}$

$$\frac{\pi}{h} = \frac{N}{2}$$



We consider the Fourier Transform on the N-grid point

Physical space	discrete	bounded	: $x \in \{h, 2h, \dots, 2\pi - h, 2\pi\}$
	$\updownarrow$	$\updownarrow$	
Fourier space	bounded	discrete	: $k \in \left\{-\frac{N}{2}+1, \dots, \frac{N}{2}\right\}$

The Fourier domain is discrete as well as bounded.

(i) This is because waves [such as $\sin(kx)$ & $\cos(kx)$, or equivalently $\exp(ikx) = \sin(kx) + i\cos(kx)$] in physical space must be periodic over the interval $[0, 2\pi]$ and only waves $\exp(ikx)$ with integer wavenumbers have the required period 2π.

(ii) The mesh spacing h implies that wavenumbers differing by an integer multiple of $2\pi/h$ are distinguishable on the grid, and thus it will be enough to confine our attention to

$$k \in \left[-\frac{\pi}{h}, \frac{\pi}{h}\right]$$

Discrete Fourier Transform

$$\hat{v}_k = h \sum_{j=1}^{N} e^{-ikx_j} v_j \qquad k = -\frac{N}{2}+1, \ldots, \frac{N}{2} \qquad (\star)_1$$

Inverse Discrete Fourier Transform

$$v_j = \frac{1}{2\pi} \sum_{k=-N/2+1}^{N/2} e^{ikx_j} \hat{v}_k \qquad j = 1, \ldots, N \qquad (\star)_2$$

Exercise: Assume that we have the period grid point data $\{x_j\}_{j=1}^{N}$ and the corresponding data of function values $\{v_j\}_{j=1}^{N}$. Then we can compute $\hat{v}_k$ according to $(\star)_1$. Prove that with the data $\{\hat{v}_k\}_{k=-\frac{N}{2}+1}^{N/2}$, we can recover the values v_j by using formula $(\star)_2$.

$\Rightarrow$ That is, we need to prove: $v_j = \frac{1}{2\pi} \sum_{k=-N/2}^{N/2} e^{ikx_j} \left\{ h \sum_{m=1}^{N} e^{-ikx_m} v_m \right\}$

Spectral Differentiation : Band-limited intepolant

We need a band-limited interpolant of v on the grid points, which we obtain by evaluating the inverse discrete Fourier transform for all x rather than just x on the grid, namely only x_j.

Thus, we may use the interpolant

$$p(x) = \frac{1}{2\pi} \sum_{k=-\frac{N}{2}+1}^{N/2} e^{ikx} \hat{v}_k \qquad x \in [0, 2\pi]$$

$\Rightarrow$ Evaluating the derivative of this interpolant :

$$p'(x) = \frac{1}{2\pi} \sum_{k=-N/2+1}^{N/2-1} ik e^{ikx} \hat{v}_k + \frac{1}{2\pi} \underbrace{i \frac{N}{2} e^{iN/2 x}}_{\frac{d}{dx}\left(e^{iN/2 x}\right)} \hat{v}_{N/2}$$

Trouble Since $\exp\left(i\frac{N}{2}x\right) = \cos\left(\frac{N}{2}x\right) + i\sin\left(\frac{N}{2}x\right)$ represents a real sawtooth wave on the grid $\{x_j\}$, its derivative should be zero at the grid points, not a complex exponential

* Compute $\exp\left(i\frac{N}{2}x\right) = \cos\left(\frac{N}{2}x\right) + i\sin\left(\frac{N}{2}x\right)$ at $x_j = jh$

$$\exp\left(i\frac{N}{2}x\right)\Big|_{x\to x_j=jh} = \cos\left(\frac{N}{2}jh\right) + i\sin\left(\frac{N}{2}jh\right)$$

$$= \cos\left(\frac{\pi}{h}jh\right) + \underbrace{i\sin\left(\frac{\pi}{h}jh\right)}_{0} = \underbrace{\cos(j\pi)}_{\text{Real part}} + \underbrace{0}_{\text{Imaginary part}} = (-1)^j$$

* Compute $\frac{d}{dx}\left[e^{i\frac{N}{2}x}\right]$ at $x_j = jh$

$$\frac{d}{dx}\left[e^{i\frac{N}{2}x}\right] = \frac{N}{2}\left[-\sin\left(\frac{N}{2}x\right) + i\cos\left(\frac{N}{2}x\right)\right]$$

$$\Rightarrow \frac{d}{dx}\left[e^{i\frac{N}{2}x}\right]\Big|_{x\to x_j=jh} = \frac{N}{2}\left[\underbrace{-\sin\left(\frac{\pi}{h}jh\right)}_{0} + i\underbrace{\cos\left(\frac{\pi}{h}jh\right)}_{(-1)^j}\right] = i\frac{N}{2}(-1)^j$$

Repeat: Since $\exp\left(i\frac{N}{2}x\right) = \cos\left(\frac{N}{2}x\right) + i\sin\left(\frac{N}{2}x\right)$ represents a real, sawtooth wave on the grid, its derivative should be zero at the grid points.

Problem: The interpolant $p(x) = \frac{1}{2\pi}\sum_{k=-N/2+1}^{N/2} e^{ikx}\hat{v}_k$ treats the highest wavenumber asymmetrically.

* Modified band-limited interpolant

- We define $\widehat{v}_{-N/2} = \widehat{v}_{N/2}$
- We modify the inverse discrete Fourier transform

$$v_j = \frac{1}{2\pi} \sum_{k=-N/2}^{N/2}{}' e^{ikx_j} \widehat{v}_k \qquad (\star)_3$$

where the prime indicates that the terms $k = \pm\frac{N}{2}$ are multiplied by $1/2$. We already define $\widehat{v}_{-N/2} = \widehat{v}_{N/2}$

$$v_j = \frac{1}{2\pi}\left\{\sum_{k=-N/2+1}^{N/2-1} e^{ikx_j}\widehat{v}_k + \frac{1}{2}\left[\exp\left(i\frac{N}{2}x_j\right)\widehat{v}_{N/2} + \exp\left(-i\frac{N}{2}x_j\right)\widehat{v}_{-N/2}\right]\right\}$$

Exercise : Prove that $(\star)_3$ truly gives us the "inverse discrete Fourier transform" by experimenting with Mathematica & analytic computation.

⊕ This modification is needed just for the purpose of deriving a band-limited interpolant

* Modified band-limited interpolant (cont.)

Repeat The modified inverse discrete Fourier transform

$$v_j = \frac{1}{2\pi} \sum_{k=-N/2}^{N/2}{}' e^{ikx_j} \hat{v}_k$$

$\Longrightarrow$ The modified (appropriate) band-limit interpolant

$$p(x) = \frac{1}{2\pi} \sum_{k=-N/2}^{N/2}{}' e^{ikx} \hat{v}_k \qquad x \in \left[-\frac{\pi}{h}, \frac{\pi}{h}\right]$$

In the following we shall adopt the definition of the modified band-limited interpolant without mentioning "modified".

Exercise : We define periodic Kronecker delta function δ° as follows

$$\delta_j^\circ = \begin{cases} 1 & j \equiv 0 \pmod N \\ 0 & j \not\equiv 0 \pmod N \end{cases}$$

Prove that the band-limited interpolant of δ° is given by $\quad p(x) = \dfrac{\sin(\pi x/h)}{2\pi/h \, \tan(x/2)} = S_N(x)$

* Spectral differentiation matrix

- A periodic function v on grid points $\{x_j\}_{j=1}^{N}$ can be represented as

$$v_j = \sum_{m=1}^{N} v_m \delta_j^m \quad \Longleftrightarrow \quad v = \sum_{m=1}^{N} v_m \delta^m .$$

- Linearity of the discrete/inverse discrete Fourier Transform implies the interpolant of v is the linear combination of the interpolants of δ^m

$$p(x) = \sum_{m=1}^{N} v_m \underbrace{\left(\text{Interpolant of } \delta^m\right)}_{S_N(x-x_m)}$$

$$S_N(x-x_m) = \frac{\sin\left[\frac{\pi}{h}(x-x_m)\right]}{\frac{2\pi}{h}\tan\left[\frac{x-x_m}{2}\right]}$$

- Numerical spectral derivative

$$w_j = p'(x_j) = \sum_{m=1}^{N} v_m S_N'(x_j - x_m) = \sum_{m=1}^{N} D_{jm} v_m$$

$\Longrightarrow$ Matrix form : $\underline{w} = \underline{D}\,\underline{v}$, where $D_{jm} = S_N'(x_j - x_m)$

Repeat $\quad W_j = \sum_{m=1}^{N} v_m S_N'(x_j - x_m) = \sum_{m=1}^{N} D_{jm} v_m$

Matrix form

$$\underline{W} = \underline{D}\,\underline{v}$$

Differentiation Matrix

$\Rightarrow$ Task We need to compute the derivative of S_N at x_j

Exercise Verify the following results.

$$S_N'(x_j) = \begin{cases} 0 & j \equiv 0 \pmod N \\ \frac{1}{2}(-1)^j \cot\left(\frac{jh}{2}\right) & j \not\equiv 0 \pmod N \end{cases}$$

$$S_N''(x_j) = \begin{cases} -\frac{\pi^2}{3h^2} - \frac{1}{6} & j \equiv 0 \pmod N \\ -\frac{(-1)^j}{2\sin^2\left(\frac{jh}{2}\right)} & j \not\equiv 0 \pmod N \end{cases}$$

* Spectral differentiation matrix

$$
D_N \quad \begin{bmatrix}
0 & & & & -\frac{1}{2}\cot\frac{h}{2} \\
-\frac{1}{2}\cot\frac{h}{2} & \ddots & & & \frac{1}{2}\cot\frac{2h}{2} \\
\frac{1}{2}\cot\frac{2h}{2} & \ddots & \ddots & & -\frac{1}{2}\cot\frac{3h}{2} \\
-\frac{1}{2}\cot\frac{3h}{2} & \ddots & \ddots & & \vdots \\
\vdots & & & \ddots & \frac{1}{2}\cot\frac{h}{2} \\
\frac{1}{2}\cot\frac{h}{2} & & & & 0
\end{bmatrix}
$$

$$
D_N^{(2)} = \begin{bmatrix}
\ddots & \vdots & \ddots \\
 & -\frac{1}{2}\csc^2\left(\frac{2h}{2}\right) & \\
 & \frac{1}{2}\csc^2\left(\frac{h}{2}\right) & \\
 & -\frac{\pi^2}{3h^2} - \frac{1}{6} & \\
 & \frac{1}{2}\csc^2\left(\frac{h}{2}\right) & \\
\ddots & -\frac{1}{2}\csc^2\left(\frac{2h}{2}\right) & \ddots \\
 & \vdots &
\end{bmatrix}
$$

* Spectral differentiation scheme

There is another way of implementing the spectral derivative faster using the socalled Fast Fourier Transform. In order to compute the numerical spectral derivative $w_j = p'(x_j)$, we need $O(N^2)$ floating point multiplication operations to perform the matrix multiplication

$$\underline{w} = \underline{D}\,\underline{v}$$

However, since $\underline{D}$ has a special structure, one can implement the discrete Fourier transform & inverse discrete Fourier transform to perform the same spectral derivative with less computation effort.

Fast Fourier Transform (FFT) mentions the an algorithm to implement Discrete Fourier Transform (DFT) efficiently based on the symmetry of the summation involves in the definition of DFT.

Roughly speaking, FFT is nothing but DFT

Exercise Assume that we have the data points $\{x_j\}$ & the corresponding data of function values $\{v_j\}$. Then the following interpolant can be constructed

$$p(x) = \frac{1}{2\pi} \sum_{k=-N/2}^{N/2}{}' e^{ikx} \hat{v}_k$$

or

$$\tilde{p}(x) = \frac{1}{2\pi} \sum_{k=-N/2+1}^{N/2} e^{ikx} \hat{v}_k$$

Prove that (i) $p'(x) = ik\, p(x)$ and $\tilde{p}'(x) = ik\, p(x)$.

(ii) According to (i), the interpolant of the "derivative data" of the original hidden function v can be constructed as.

$$q(x) = \frac{1}{2\pi} \sum_{k=-N/2}^{N/2}{}' e^{ikx} \widehat{w}_k \quad \text{or} \quad \tilde{q}(x) = \frac{1}{2\pi} \sum_{k=-N/2+1}^{N/2} e^{ikx} \widehat{w}_k$$

with $\widehat{w_k} = ik\hat{v}_k \Longrightarrow$ Draw some comments/ observations

* Spectral Differentiation Scheme. (Cont.)

(A) Spectral differentiation scheme for the 1^{st} derivative.

- Given v, compute $\hat{v}$
- Define $\hat{w}_k = ik\hat{v}_k$, except $\hat{w}_{N/2} = 0$.
- Compute w from $\hat{w}$ $\Rightarrow$ w_j represents the derivative of v at x_j

<u>REMARK</u> For odd derivatives there is a symmetry and we have to set $\hat{w}_{N/2} = 0$. Alternatively we may set the wavenumber at $N/2$ to 0 in the MATLAB code. Otherwise $\hat{w}_{N/2}$ is given by the same formula as the other $\hat{w}_k$.

(B) Spectral differentiation scheme for the ν^{th} derivative

- Given v, compute $\hat{v}$
- Define $\hat{w}_k = (ik)^{\nu}\hat{v}_k$ but $\hat{w}_{N/2} = 0$ if ν is odd.
- Compute w from $\hat{w}_k$ $\Rightarrow$ w_j represents the ν^{th} derivative of v at x_j : $v^{(\nu)}(x_j)$

* A first application in solving a PDE.

Consider the variable coefficient wave equation

$$\begin{cases} u_t + c(x)\, u_x = 0. \\ c(x) = \frac{1}{5} + \sin^2(x-1) \end{cases} \qquad \text{for } x \in [0, 2\pi],\ t > 0.$$

As initial condition we take : $u(x,0) = \exp\left[-100(x-1)^2\right]$

<u>Remark</u> This initial condition is not periodic, but it is so close to zero at the ends of the interval that it can be regarded as periodic "in practice".

(A) Scheme using spectral differentiation:

$$\frac{v(x, t+\Delta t) - v(x, t+\Delta t)}{2\Delta t} = -c(x)\, D v(x,t)$$

$$\forall x \in \{\text{grid points } x_j\}$$

where D is the spectral differentiation matrix.

(B) Scheme using finite difference method

$$\frac{v(x_j, t+\Delta t) - v(x_j, t-\Delta t)}{2\Delta t} = -c(x_j)\,\frac{v(x_{j+1}, t) - v(x_{j-1}, t)}{2\Delta x} \quad \forall x_j \in \{\text{grid points}\}$$

Keep in mind the periodic boundary condition so that a fair comparision between scheme (A) and (B) can be made.

$$\begin{cases} x_{-1} = x_N \\ x_{N+1} = x_0 \end{cases}$$