

MATH 408: Computational Methods for Differential Equations

Unbounded Grids and the Semi-Discrete Fourier Transform

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Fall 2021



Outline

- 1 Unbounded Grids and the Semi-Discrete Fourier Transform
- 2 Spectral Differentiation

Our goal in the next few lessons will be to **understand and compute differentiation matrices for spectral methods**.

As with our earlier FD approach, we will get the entries of the differentiation matrices by differentiating an interpolant of samples of the solution u of our BVPs.

One of the main tools to achieve this for the **globally defined spectral methods** is the **Fourier transform**, in a few different variants:

- continuous FT (only as a starting point)
- semi-discrete FT
- discrete FT
- fast FT (as an implementation of DFT)

The Fourier Transform and its Inverse

The **Fourier transform** \hat{u} of a function u that is square-integrable on \mathbb{R} is defined as:

$$\hat{u}(\xi) = \int_{-\infty}^{\infty} e^{-i\xi x} u(x) dx, \quad \xi \in \mathbb{R}. \quad (1)$$

The FT allows us to **decompose** u into a set of **waves** \hat{u} with **wavenumbers** (or spatial frequency) ξ .

The FT \hat{u} “lives” on Fourier space (or frequency space).

The **inverse Fourier transform** lets us **reconstruct** the **signal** u from its Fourier transform \hat{u} :

$$u(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\xi x} \hat{u}(\xi) d\xi, \quad x \in \mathbb{R}. \quad (2)$$

The inverse FT u “lives” on physical space (we think “space”, but this could also be “time”).



Remark

Other popular definitions of the Fourier transform are (see Appendix E.3.1 of LeVeque's book [1])

$$\hat{u}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\xi x} u(x) dx, \quad u(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\xi x} \hat{u}(\xi) d\xi,$$

or

$$\hat{u}(\xi) = \int_{-\infty}^{\infty} e^{-2\pi i \xi x} u(x) dx, \quad u(x) = \int_{-\infty}^{\infty} e^{2\pi i \xi x} \hat{u}(\xi) d\xi.$$

Remark

Also, note that the notation \hat{u} refers to the Fourier transform of u and has nothing to do with the notation $\hat{U} = [u(x_1), u(x_2), \dots, u(x_m)]^T$ used earlier to denote a vector of values of the exact solution of an ODE.

Example

Compute the Fourier transform of the **square pulse** function

$$u(x) = \begin{cases} 1, & \text{if } -\frac{1}{2} \leq x \leq \frac{1}{2}, \\ 0, & \text{otherwise.} \end{cases}$$

The **definition of the FT**, the **definition of u** , and **Euler's formula** yield

$$\begin{aligned} \hat{u}(\xi) &= \int_{-\infty}^{\infty} e^{-i\xi x} u(x) dx \\ &= \int_{-\frac{1}{2}}^{\frac{1}{2}} e^{-i\xi x} dx \\ &= \int_{-\frac{1}{2}}^{\frac{1}{2}} [\cos(\xi x) - i \sin(\xi x)] dx \\ &= 2 \int_0^{\frac{1}{2}} \cos(\xi x) dx \\ &= 2 \frac{\sin(\xi x)}{\xi} \Big|_0^{\frac{1}{2}} = \frac{\sin\left(\frac{\xi}{2}\right)}{\frac{\xi}{2}} \quad (\text{sinc function}). \end{aligned}$$

The semi-discrete Fourier Transform and its Inverse

Let's restrict our attention to the **discrete (unbounded) physical space** $h\mathbb{Z}$, i.e., we now consider **infinitely many uniformly spaced grid points** $x_j = jh, j = \dots, -2, -1, 0, 1, 2, \dots$ (or $j \in \mathbb{Z}$).

The continuous function u is now **replaced by the (infinite) vector**

$$\mathbf{u} = [\dots, u_{-1}, u_0, u_1, \dots]^T$$

of discrete values $u_j = u(x_j), j \in \mathbb{Z}$.

We can think of the value u_j as a sample of the signal u at x_j .

Now we need the **semi-discrete Fourier transform** of \mathbf{u} given by the (continuous) function

$$\hat{u}(\xi) = h \sum_{j=-\infty}^{\infty} e^{-i\xi x_j} u_j, \quad \xi \in \left[-\frac{\pi}{h}, \frac{\pi}{h}\right], \quad (3)$$

and the **inverse semi-discrete Fourier transform**, given by the (discrete) infinite vector \mathbf{u} whose components are of the form

$$u_j = \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{i\xi x_j} \hat{u}(\xi) d\xi, \quad j \in \mathbb{Z}. \quad (4)$$

Remark

*Note that the notion of a semi-discrete Fourier transform is just a different name for a **Fourier series** based on the complex exponentials $e^{-i\xi x_j}$ with **Fourier coefficients** u_j (see Appendix).*

Aliasing

Why are we allowed to work with a **bounded Fourier space in the semi-discrete setting**?

This can be explained by the phenomenon of **aliasing**.

Aliasing arises when a **continuous function is sampled on a discrete set**.

Consider the two (continuous) complex exponential functions

$$u(x) = e^{i\xi_1 x},$$

$$v(x) = e^{i\xi_2 x}.$$

We know that $u(x) \neq v(x)$ for all $x \in \mathbb{R}$ provided $\xi_1 \neq \xi_2$.

However, if we **sample the two functions on the grid $h\mathbb{Z}$** , then we get the vectors **\mathbf{u}** and **\mathbf{v}** with values

$$u_j = e^{i\xi_1 x_j},$$

$$v_j = e^{i\xi_2 x_j}.$$

If $\xi_2 = \xi_1 + 2k\frac{\pi}{h}$ for some integer k , then

$$\begin{aligned} v_j &= e^{i\xi_2 x_j} \\ &= e^{i(\xi_1 + 2k\frac{\pi}{h})x_j} \\ &= e^{i\xi_1 x_j} \underbrace{e^{i2k\frac{\pi}{h}jh}}_{=1} = u_j \end{aligned}$$

for any j and the two (different) continuous functions u and v appear identical in their discrete samples u and v .

Thus, any complex exponential $e^{i\xi x}$ is matched on the grid $h\mathbb{Z}$ by infinitely many other complex exponentials (the **aliases** for the frequency ξ).

Therefore we can limit the representation of the Fourier variable (wavenumber) ξ to an interval of length $2\pi/h$. For reasons of symmetry we use $[-\pi/h, \pi/h]$.

Example

Let's consider two sine functions instead of complex exponentials, i.e.,

$$u(x) = \sin(\pi x),$$

$$v(x) = \sin(9\pi x).$$

Thus $\xi_1 = \pi$ and $\xi_2 = 9\pi$. Also, let $h = \frac{1}{4}$, so that $x_j = jh = \frac{j}{4}$.

Then $\xi_2 = \xi_1 + 2k\frac{\pi}{h}$ corresponds to

$$\xi_2 = \xi_1 + 2k \frac{\pi}{1/4} = \xi_1 + 8k\pi.$$

Since $\xi_1 = \pi$ and $\xi_2 = 9\pi$ we let $k = 1$ and show

$$\begin{aligned} v_j &= \sin(9\pi x_j) = \sin(\pi + 8\pi)x_j \\ &= \sin(\pi x_j) \cos(8\pi x_j) + \cos(\pi x_j) \sin(8\pi x_j) \\ &= \sin(\pi x_j) \underbrace{\cos(8\pi \frac{j}{4})}_{=1} + \cos(\pi x_j) \underbrace{\sin(8\pi \frac{j}{4})}_{=0} = u_j. \end{aligned}$$

The MATLAB script `AliasDemo.m` illustrates this aliasing phenomenon.

Band-limited Functions

To get an **interpolant** of the (infinitely many) samples u_j we can now use a continuous extension of the inverse semi-discrete Fourier transform, i.e., we define the interpolant to be the function

$$p(x) = \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{i\xi x} \hat{u}(\xi) d\xi, \quad x \in \mathbb{R}. \quad (5)$$

It is obvious (cf. (4)) from this construction that p interpolates the samples, i.e., $p(x_j) = u_j$, for any $j \in \mathbb{Z}$.

Moreover, the Fourier transform of the function p turns out to be

$$\hat{p}(\xi) = \begin{cases} \hat{u}(\xi), & \xi \in [-\pi/h, \pi/h], \\ 0, & \text{otherwise.} \end{cases}$$

This kind of function is known as a **band-limited function**, and p is called the **band-limited interpolant** of u .

Spectral Derivative

The **spectral derivative vector** \mathbf{u}' of \mathbf{u} can now be obtained by one of the following two procedures we are about to present.

Procedure #1:

- ① **Sample** the function u at the (infinite set of) discrete points $x_j \in h\mathbb{Z}$ to obtain the data vector \mathbf{u} with components u_j .
- ② **Compute the semi-discrete FT** of the data via (3):

$$\hat{u}(\xi) = h \sum_{j=-\infty}^{\infty} e^{-i\xi x_j} u_j, \quad \xi \in [-\pi/h, \pi/h].$$

- ③ Find the **band-limited interpolant** p of the data u_j via (5):

$$p(x) = \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{i\xi x} \hat{u}(\xi) d\xi, \quad x \in \mathbb{R}.$$

- ④ **Differentiate p and evaluate** at the grid points x_j .

From a computational point of view it is **better to deal with this problem in the Fourier domain.**

Note that the (continuous) **FT of the (exact) derivative u'** is given by

$$\widehat{u'}(\xi) = \int_{-\infty}^{\infty} e^{-i\xi x} u'(x) dx.$$

Applying **integration by parts** we get

$$\widehat{u'}(\xi) = e^{-i\xi x} u(x) \Big|_{-\infty}^{\infty} + i\xi \underbrace{\int_{-\infty}^{\infty} e^{-i\xi x} u(x) dx}_{=\widehat{u}(\xi)}.$$

If $u(x) \rightarrow 0$ for $x \rightarrow \pm\infty$ (which it has to for the FT of u to exist) then we see that

$$\widehat{u'}(\xi) = i\xi \widehat{u}(\xi).$$

Therefore, we obtain the spectral derivative \mathbf{u}' by **Procedure #2**:

- 1 **Sample** the function u at the (infinite set of) discrete points $x_j \in h\mathbb{Z}$ to obtain the data vector \mathbf{u} with components u_j .
- 2 **Compute the semi-discrete FT** of the data via (3):

$$\hat{u}(\xi) = h \sum_{j=-\infty}^{\infty} e^{-i\xi x_j} u_j, \quad \xi \in [-\pi/h, \pi/h].$$

- 3 **Compute the FT of the derivative** via (6):

$$\hat{u}'(\xi) = i\xi \hat{u}(\xi).$$

- 4 Find the derivative vector via **inverse semi-discrete FT** (see (4)):

$$u'_j = \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{i\xi x_j} \hat{u}'(\xi) d\xi, \quad j \in \mathbb{Z}.$$

How do we get the differentiation matrix D from these procedures?

Following Procedure #1, the **semi-discrete FT of an arbitrary sample vector u** is obtained by representing its components in terms of **shifts of (discrete) delta functions**, i.e.,

$$u_j = \sum_{k=-\infty}^{\infty} u_k \delta_{j-k}, \quad (7)$$

where the **Kronecker delta function** is defined by

$$\delta_j = \begin{cases} 1 & j = 0 \\ 0 & \text{otherwise.} \end{cases}$$

We use this approach since the **semi-discrete FT of the delta function can be computed easily**.

To find the semi-discrete FT of the delta function we recall (3), i.e.,

$$\hat{u}(\xi) = h \sum_{j=-\infty}^{\infty} e^{-i\xi x_j} u_j, \quad \xi \in \left[-\frac{\pi}{h}, \frac{\pi}{h}\right].$$

This implies

$$\begin{aligned} \hat{\delta}(\xi) &= h \sum_{j=-\infty}^{\infty} e^{-i\xi x_j} \delta_j \\ &= h e^{-i\xi x_0} = h \end{aligned}$$

for all $\xi \in [-\pi/h, \pi/h]$ since $x_0 = 0h$.

Then the **band-limited interpolant of δ** is of the form (see (5))

$$\begin{aligned}
 p(x) &= \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{i\xi x} \hat{\delta}(\xi) d\xi \\
 &= \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{i\xi x} h d\xi \\
 &= \frac{h}{\pi} \int_0^{\pi/h} \cos(\xi x) d\xi \\
 &= \frac{h}{\pi} \left. \frac{\sin(\xi x)}{x} \right|_0^{\pi/h} \\
 &= \frac{h}{\pi} \frac{\sin(\pi \frac{x}{h})}{x} = \frac{\sin(\frac{\pi x}{h})}{\frac{\pi x}{h}} = \text{sinc}\left(\frac{\pi x}{h}\right).
 \end{aligned}$$

We now calculate the **band-limited interpolant** of an arbitrary data vector **u** :

$$\begin{aligned}
 p(x) &\stackrel{(5)}{=} \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{i\xi x} \hat{u}(\xi) d\xi \\
 &\stackrel{(3)}{=} \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{i\xi x} \left[h \sum_{j=-\infty}^{\infty} e^{-i\xi x_j} u_j \right] d\xi \\
 &\stackrel{(7)}{=} \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{i\xi x} \left[h \sum_{j=-\infty}^{\infty} e^{-i\xi x_j} \sum_{k=-\infty}^{\infty} u_k \delta_{j-k} \right] d\xi.
 \end{aligned}$$

Interchanging the summation results in

$$p(x) = \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{i\xi x} \left[h \sum_{k=-\infty}^{\infty} u_k \sum_{j=-\infty}^{\infty} e^{-i\xi x_j} \delta_{j-k} \right] d\xi.$$

Now we use the **definition of the delta function** and the **same calculation as for the band-limited interpolant of the delta function** above to obtain the **final form of the band-limited interpolant of an arbitrary data vector u** :

$$\begin{aligned}
 p(x) &= \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{i\xi x} \left[h \sum_{k=-\infty}^{\infty} u_k \sum_{j=-\infty}^{\infty} e^{-i\xi x_j} \delta_{j-k} \right] d\xi \\
 &\stackrel{\text{Def.}\delta}{=} \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{i\xi x} h \sum_{k=-\infty}^{\infty} u_k e^{-i\xi x_k} d\xi \\
 &\stackrel{\text{rearrange}}{=} \sum_{k=-\infty}^{\infty} u_k \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{i\xi(x-x_k)} h d\xi \\
 &\stackrel{\text{bandlim}}{=} \sum_{k=-\infty}^{\infty} u_k \operatorname{sinc} \frac{(x-x_k)\pi}{h}.
 \end{aligned}$$

If u is a **band-limited function** then the result of this calculation is known as the **Whittaker–Shannon Sampling Theorem** and $p(x) = u(x)$, i.e., **the reconstruction is exact for all $x \in \mathbb{R}$** !

Example

Band-limited interpolation for the functions

$$u_1(x) = \begin{cases} 1, & x = 0 \\ 0, & \text{otherwise,} \end{cases}$$

$$u_2(x) = \begin{cases} 1, & |x| \leq 3 \\ 0, & \text{otherwise,} \end{cases}$$

and

$$u_3(x) = (1 - |x|/3)_+.$$

is illustrated in the MATLAB script `BandLimitedDemo.m`.

Remark

- *The accuracy of the reproduction is not very high.*
- *In particular, for $h \rightarrow 0$ we observe a Gibbs phenomenon caused by the low smoothness of the data functions.*

Calculating the Differentiation Matrix

To find the components of the derivative vector \mathbf{u}' we need to differentiate the band-limited interpolant and evaluate at the grid points.

By **linearity** this leads to

$$u'_j = p'(x_j) = \sum_{k=-\infty}^{\infty} u_k \frac{d}{dx} \left[\text{sinc} \frac{(x - x_k)\pi}{h} \right]_{x=x_j},$$

or in (infinite) matrix-vector form

$$\mathbf{u}' = \mathbf{D}\mathbf{u}$$

with the entries of \mathbf{D} given by

$$D_{jk} = \frac{d}{dx} \left[\text{sinc} \frac{(x - x_k)\pi}{h} \right]_{x=x_j}, \quad j, k = -\infty, \dots, \infty.$$

The entries in the $k = 0$ column of D are of the form (see next slide)

$$D_{j0} = \frac{d}{dx} \left[\text{sinc} \frac{x\pi}{h} \right]_{x=x_j=jh} = \begin{cases} 0, & j = 0 \\ \frac{(-1)^j}{jh}, & \text{otherwise.} \end{cases}$$

The remaining columns are up or down shifts of this column and so the matrix is a **Toeplitz matrix** of the form (see slide #18 of Notes408_15_HigherOrderMethods2ptBVPs)

$$D = \frac{1}{h} \begin{bmatrix} & & & \vdots & & \\ & \ddots & & \frac{1}{3} & & \\ & \ddots & & -\frac{1}{2} & & \\ & \ddots & & 1 & & \\ & & & 0 & & \\ & & & -1 & \ddots & \\ & & & \frac{1}{2} & \ddots & \\ & & & -\frac{1}{3} & \ddots & \\ & & & \vdots & & \end{bmatrix}.$$

The explicit formula for the derivative of the sinc function above is obtained using elementary calculations:

$$\begin{aligned}\frac{d}{dx} \left[\text{sinc} \frac{x\pi}{h} \right] &= \frac{d}{dx} \left[\frac{\sin \frac{x\pi}{h}}{\frac{x\pi}{h}} \right] \\ &= \frac{1}{x} \cos \left(\frac{x\pi}{h} \right) - \frac{h}{x^2 \pi} \sin \left(\frac{x\pi}{h} \right),\end{aligned}$$

so that

$$\begin{aligned}\frac{d}{dx} \left[\text{sinc} \frac{x\pi}{h} \right]_{x=x_j=jh} &= \frac{1}{jh} \cos(j\pi) - \frac{1}{j^2 h \pi} \sin(j\pi) \\ &= \frac{1}{jh} (-1)^j - \frac{1}{j^2 h \pi} 0.\end{aligned}$$

Working on an infinite grid is not very practical. So, next we consider periodic grids.

References I



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Finite Difference Methods for Ordinary and Partial Differential Equations.
SIAM, Philadelphia, 2007.



L. N. Trefethen.

Spectral Methods in MATLAB.
SIAM, Philadelphia, 2000.

Appendix: Complex Form of the Fourier Series

Fourier series are often expressed in terms of **complex exponentials** instead of sines and cosines.

The **main ingredient** for understanding this translation in notation is **Euler's formula**

$$e^{i\theta} = \cos \theta + i \sin \theta.$$

This, of course, implies

$$e^{-i\theta} = \cos \theta - i \sin \theta,$$

and so

$$\begin{aligned}\cos \theta &= \frac{e^{i\theta} + e^{-i\theta}}{2} \\ \sin \theta &= \frac{e^{i\theta} - e^{-i\theta}}{2i}.\end{aligned}$$

We can therefore rewrite the Fourier series

$$f(x) \sim a_0 + \sum_{n=1}^{\infty} \left[a_n \cos \frac{n\pi x}{L} + b_n \sin \frac{n\pi x}{L} \right]$$

as

$$\begin{aligned} f(x) &\sim a_0 + \sum_{n=1}^{\infty} \left[a_n \frac{e^{i\frac{n\pi x}{L}} + e^{-i\frac{n\pi x}{L}}}{2} + b_n \frac{e^{i\frac{n\pi x}{L}} - e^{-i\frac{n\pi x}{L}}}{2i} \right] \\ &= a_0 + \frac{1}{2} \sum_{n=1}^{\infty} \left[\left(a_n + \frac{b_n}{i} \right) e^{i\frac{n\pi x}{L}} + \left(a_n - \frac{b_n}{i} \right) e^{-i\frac{n\pi x}{L}} \right] \end{aligned}$$

We break this into two series and use $\frac{1}{j} = -i$ to arrive at

$$f(x) \sim a_0 + \frac{1}{2} \sum_{n=1}^{\infty} (a_n - ib_n) e^{i\frac{n\pi x}{L}} + \frac{1}{2} \sum_{n=1}^{\infty} (a_n + ib_n) e^{-i\frac{n\pi x}{L}}$$

Now we **perform an index transformation**, $n \rightarrow -n$, on the first series to get

$$f(x) \sim a_0 + \frac{1}{2} \sum_{n=-1}^{-\infty} (a_{-n} - ib_{-n}) e^{-i\frac{n\pi x}{L}} + \frac{1}{2} \sum_{n=1}^{\infty} (a_n + ib_n) e^{-i\frac{n\pi x}{L}}$$

Note that, using the **symmetries of cosine and sine**,

$$\begin{aligned} a_{-n} &= \frac{1}{L} \int_{-L}^L f(x) \cos \frac{(-n)\pi x}{L} dx = a_n \\ b_{-n} &= \frac{1}{L} \int_{-L}^L f(x) \sin \frac{(-n)\pi x}{L} dx = -b_n \end{aligned}$$

We can therefore rewrite

$$f(x) \sim a_0 + \frac{1}{2} \sum_{n=-1}^{-\infty} (a_{-n} - ib_{-n}) e^{-i \frac{n\pi x}{L}} + \frac{1}{2} \sum_{n=1}^{\infty} (a_n + ib_n) e^{-i \frac{n\pi x}{L}}$$

as

$$f(x) \sim a_0 + \frac{1}{2} \sum_{n=-1}^{-\infty} (a_n + ib_n) e^{-i \frac{n\pi x}{L}} + \frac{1}{2} \sum_{n=1}^{\infty} (a_n + ib_n) e^{-i \frac{n\pi x}{L}}$$

If we **introduce new coefficients**

$$c_0 = a_0 \quad \text{and} \quad c_n = \frac{a_n + ib_n}{2}$$

then we get the **exponential form of the Fourier series**

$$f(x) \sim \sum_{n=-\infty}^{\infty} c_n e^{-i \frac{n\pi x}{L}}$$

with **Fourier coefficients**

$$c_0 = \frac{1}{2L} \int_{-L}^L f(x) dx$$

and

$$\begin{aligned}c_n &= \frac{a_n + ib_n}{2} \\&= \frac{1}{2L} \left[\int_{-L}^L f(x) \cos \frac{n\pi x}{L} dx + i \int_{-L}^L f(x) \sin \frac{n\pi x}{L} dx \right] \\&= \frac{1}{2L} \int_{-L}^L f(x) \left[\cos \frac{n\pi x}{L} + i \sin \frac{n\pi x}{L} \right] dx \\&= \frac{1}{2L} \int_{-L}^L f(x) e^{i \frac{n\pi x}{L}} dx\end{aligned}$$

Note that this formula also gives the correct value for c_0 .

Remark

*The formula for the Fourier coefficients c_n is known as the **inverse semi-discrete Fourier transform of f** .*