MATH 408: Computational Methods for Differential Equations

Periodic Grids: The Discrete FT and Fast FT

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Outline

- Periodic Grids: The DFT and FFT
- Implementation via FFT



Periodic Grids: The DFT and FFT

We now consider the case of a bounded grid with periodic data and will explain how to find the entries in the $m \times m$ dense matrix D_m from slide #19 in Notes408_15_HigherOrderMethods2ptBVPs, i.e.,

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

For simplicity we consider the interval $[0, 2\pi]$ only, and assume we are given m (even¹) uniformly spaced grid points $x_j = jh, j = 1, ..., m$, with $h = \frac{2\pi}{m}$.

¹Formulas for odd *m* also exist, but are slightly different.

The Discrete Fourier Transform (DFT)

Let's look at the Fourier transform of the discrete and periodic data $\mathbf{u} = [u_1, \dots, u_m]^T$ with

$$u_j = u(x_j) = u(jh) = u(j\frac{2\pi}{m}), \quad j = 1, ..., m.$$

Aliasing again ensures that the Fourier domain will be bounded. Periodicity of the data implies that the Fourier domain is also discrete (since only waves e^{ikx} with integer wavenumber k have period 2π). Thus, the discrete Fourier transform (DFT) is given by

$$\hat{u}_k = h \sum_{j=1}^m e^{-ikx_j} u_j, \quad k = -\frac{m}{2} + 1, \dots, \frac{m}{2}.$$
 (1)

Remark

The (continuous) Fourier domain $[-\pi/h, \pi/h]$ used earlier now translates to the discrete domain $\{-\frac{m}{2}+1, \ldots, \frac{m}{2}\}$ since $h=\frac{2\pi}{m}$ is equivalent to $\pi/h=m/2$.

Variants of the FT used thus far

1 Fourier transform, $u \in L_2(\mathbb{R})$, arbitrary

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

Physical space: $x \in \mathbb{R}$, unbounded & continuous Fourier space: $\xi \in \mathbb{R}$, unbounded & continuous

2 Semi-discrete Fourier transform, $u \in \ell_2(\mathbb{Z})$, arbitrary

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

Physical space: $x_j \in h\mathbb{Z}$, unbounded & discrete Fourier space: $\xi \in \left[-\frac{\pi}{h}, \frac{\pi}{h}\right]$, bounded & continuous

3 Discrete Fourier Transform, \boldsymbol{u} 2π -periodic

$$\hat{u}_k = h \sum_{i=1}^m e^{-ikx_j} u_j, \quad k = -\frac{m}{2} + 1, \dots, \frac{m}{2}.$$

Physical space: $x_j \in \{h, 2h, \dots, 2\pi - h, 2\pi\}$, bounded & discrete Fourier space: $k \in \{-\frac{m}{2} + 1, \dots, \frac{m}{2}\}$, bounded & discrete



The Inverse Discrete Fourier Transform (iDFT)

The inverse discrete Fourier transform (iDFT) is defined by

$$u_j = \frac{1}{2\pi} \sum_{k=-m/2+1}^{m/2} e^{ikx_j} \hat{u}_k, \quad j = 1, \dots, m.$$
 (2)

The spectral derivative of a finite periodic data vector \boldsymbol{u} is obtained by the same procedure as before:

- Define the band-limited interpolant in terms of the iDFT.
- Represent u as a linear combination of shifts of periodic delta functions (details skipped).
- Show that band-limited interpolants for the periodic delta functions are periodic sinc functions.
- Get the band-limited interpolant for an arbitrary periodic data function in terms of periodic sinc functions.
- Differentiate periodic sinc functions to get entries of D_m .

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The band-limited interpolant of the data is given by filling in the iDFT of the data

$$p(x) = \frac{1}{2\pi} \sum_{k=-m/2}^{m/2} e^{ikx} \hat{u}_k, \quad x \in [0, 2\pi].$$
 (3)

To ensure the band-limited interpolant works properly we define $\hat{u}_{-m/2} = \hat{u}_{m/2}$, and the prime on the sum indicates that we add the first and last terms in the sum with weight $\frac{1}{2}$.

Remark

The band-limited interpolant is actually a trigonometric polynomial of degree $\frac{m}{2}$, i.e., p(x) can be written as a linear combination of

$$1, \sin(x), \cos(x), \sin(2x), \cos(2x), \dots, \sin(\frac{m}{2}x), \cos(\frac{m}{2}x).$$

We will come back to this fact when we discuss non-periodic data.

Next, we represent an arbitrary periodic data vector \boldsymbol{u} as a linear combination of shifts of periodic delta functions.

We omit the details here (they can be found in [3]).

The band-limited interpolant of the periodic delta function ends up being

$$p(x) = S_m(x) = \frac{\sin(\pi x/h)}{(2\pi/h)\tan(x/2)},$$

which is known as the periodic sinc function S_m .

Now, just as in the infinite case (see slide #22 in Notes 408_16_UnboundedGrids), the band-limited interpolant for an arbitrary periodic data function can be written as

$$p(x) = \sum_{k=1}^{m} u_k S_m(x - x_k).$$



Finally, using the same arguments and similar elementary calculations as earlier, we get the derivative of the periodic sinc function

$$S'_m(x_j) = \begin{cases} 0, & j \equiv 0 \pmod{m}, \\ \frac{1}{2}(-1)^j \cot(\frac{jh}{2}), & j \not\equiv 0 \pmod{m}. \end{cases}$$

Since

$$p'(x) = \sum_{k=1}^m u_k S'_m(x - x_k).$$

and

$$u'_{j} = p'(x_{j}) = \sum_{k=1}^{m} u_{k} S'_{m}(x_{j} - x_{k})$$

the $S'_m(x_j)$ are the entries of the m^{th} column of the Toeplitz matrix D_m .

Example

The MATLAB script SpectralDiffDemo.m illustrates the use of spectral differentiation for the not so smooth hat function and for the infinitely smooth function $u(x) = e^{\sin x}$.

Using the Fast Fourier Transform (FFT)

The most efficient computational approach is to view spectral differentiation in the Fourier domain (Procedure #2 earlier) and then implement the DFT via the fast Fourier transform (FFT).

The general outline is as follows:

- Sample the function u at the (finite set of) discrete points x_j , j = 1, ..., m to obtain the data vector u with components u_j .
- Compute the discrete Fourier transform of the (finite) data vector via (1):

$$\hat{u}_k = h \sum_{j=1}^m e^{-ikx_j} u_j, \qquad k = -\frac{m}{2} + 1, \dots, \frac{m}{2}.$$

Compute the Fourier transform of the derivative as in (6) of Notes 408_16_UnboundedGrids, i.e.,

$$\hat{u'}_k = \begin{cases} 0, & k = m/2, \\ ik\hat{u}_k, & \text{otherwise.} \end{cases}$$

Find the derivative vector via iDFT (see (2)), i.e.,

$$u'_{j} = \frac{1}{2\pi} \sum_{k=-m/2+1}^{m/2} e^{ikx_{j}} \widehat{u'}_{k}, \quad j=1,\ldots,m.$$



Remark

- Cooley and Tukey (1965) are usually given credit for discovering the FFT. However, the same algorithm was already known to Gauss in 1805 (even before Fourier completed his work on what is known today as the Fourier transform in 1822) (see [1]).
- A detailed discussion of the FFT algorithm goes beyond the scope of this course. We use the MATLAB implementations fft and ifft which are based on the current state-of-the-art FFTW algorithm (the "fastest Fourier transform in the West") developed by Matteo Frigo and Steven G. Johnson at MIT in 1998.

Example

The MATLAB script SpectralDiffFFTDemo.m is an FFT version of the earlier script SpectralDiffDemo.m. The FFT implementation is considerably faster than the implementation based on differentiation matrices. The FFT requires roughly $\mathcal{O}(m \log m)$ operations, while the differentiation matrix approach is $\mathcal{O}(m^2)$.

References I



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

L. N. Trefethen. Spectral Methods in MATLAB. SIAM, Philadelphia, 2000.

