Fundamental Concepts in Computational and Applied Mathematics

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Spectral methods

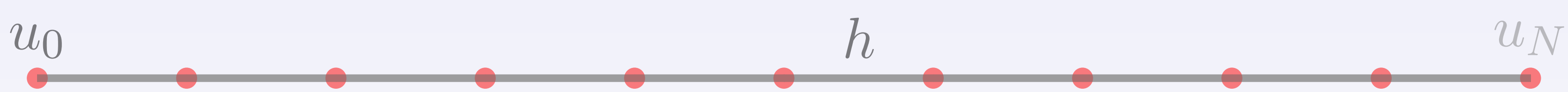
- Temporal/spatial vs frequency
- Particularly useful in problems that have periodicity or infinite domains
- Still useful if that's not the case

Motivation

- Consider the case of differentiation of a function
- One possibility is finite differences
- Another general idea: Interpolate the function of interest by a polynomial and then take derivative of polynomial
- This idea leads to the notion of a differentiation matrix

Motivation

- Consider case in 1D, on an equally spaced grid, periodic function $u(x)$
- h is the spatial discretization
- $u(0) = u(N)$



$$w'(x) = \frac{u(x_{j+1}) - u(x_{j-1})}{2h}$$

Differentiation Matrix

- A second order method can be given by the following matrix

$$D = \begin{bmatrix} 0 & 1/2 & 0 & 0 & \dots & -1/2 \\ -1/2 & 0 & 1/2 & 0 & \dots & 0 \\ 0 & -1/2 & 0 & 1/2 & \dots & 0 \\ \dots & 0 & -1/2 & 0 & \ddots & 0 \\ 0 & \dots & 0 & \ddots & 0 & 1/2 \\ 1/2 & 0 & 0 & 0 & -1/2 & 0 \end{bmatrix}$$

Note: This matrix is skew-symmetrix, Toeplitz (diagonal-constant), and circulant! All very nice properties.
The derivative is given by $w = \frac{1}{h} D \cdot u$

Spectral Method

General Principle

- Generate a high-order interpolant of your function, e.g. trigonometric polynomial
- Take the derivative of the interpolant
- Substitute this in your differential equation

Discrete Fourier Transform and Fast Fourier Transform

- The DFT is a natural extension of differentiation to a bounded, periodic grid using Fourier transforms
- The bounded physical domain implies that the Fourier domain will be discrete, i.e. the wavenumbers, k, will be integers
- The derivative in Fourier space can be computed by multiplying the transform by ik
- The FFT is a fast algorithm for computing the DFT

Discrete Fourier Transform

DFT is given by

$$\hat{X}(k) = \sum_{j=0}^{N-1} X(j) W_N^{jk}, \tag{1}$$

where

$$W_N = \exp\left(\frac{-2\pi i}{N}\right).$$

which can also be viewed as a matrix-vector multiply $F_N \cdot X$, where

$$F_N = W_N^{jk}$$

Example: N = 2, 4

Let $\omega = \exp\left(\frac{-2\pi i}{N}\right)$.

$N = 2$

$$F_2 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix},$$

$N = 4$

$$F_4 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega & \omega^2 & \omega^3 \\ 1 & \omega^2 & \omega^4 & \omega^6 \\ 1 & \omega^3 & \omega^6 & \omega^9 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -i & -1 & i \\ 1 & -1 & 1 & -1 \\ 1 & i & -1 & -i \end{bmatrix}.$$

Key Idea

One can permute the columns of F_4 so that

$$F_4\Pi_4 = \left[\begin{array}{cc|cc} 1 & 1 & 1 & 1 \\ 1 & -1 & -i & i \\ \hline 1 & 1 & -1 & -1 \\ 1 & -1 & i & -i \end{array}\right], \Pi_4 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

which is just F_4 with even-indexed columns ordered first.

Key Idea

Now notice that

$$F_4 \Pi_4 = \begin{bmatrix} F_2 & \Omega_2 F_2 \\ F_2 & -\Omega_2 F_2 \end{bmatrix},$$

where

$$\Omega_2 = \begin{bmatrix} 1 & 0 \\ 0 & -i \end{bmatrix},$$

in other words, each block of $F_4 \Pi_4$ is either F_2 or a diagonal scaling of F_2.

Some consequences

- An $N-$point DFT can be computed from two $N/2-$point DFTs!
- The complexity of the algorithm can be shown to be $\mathcal{O}(N \log N)$ vs. $\mathcal{O}(N^2)$
- Spectral methods are highly accurate for smooth functions

Summary

- Spectral methods work in Fourier (frequency) space
- The development of the FFT led to many new areas of research and applications
- Many applications in image processing, computational chemistry, Fast Poisson solvers, etc.
- Can also be used for non-periodic or non-uniform data, but that's another talk

References

- **An Algorithm for the Machine Calculation of Complex Fourier Series**, James W. Cooley and John W. Tukey, Math. Comp. 19, 297-301, 1965
- **Spectral Methods in Matlab**, Lloyd N. Trefethen, SIAM 2000.
- **Computational Frameworks for the Fast Fourier Transform**, Charles Van Loan, SIAM, 1992.