Fundamental Concepts in Computational and Applied Mathematics

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Spectral methods

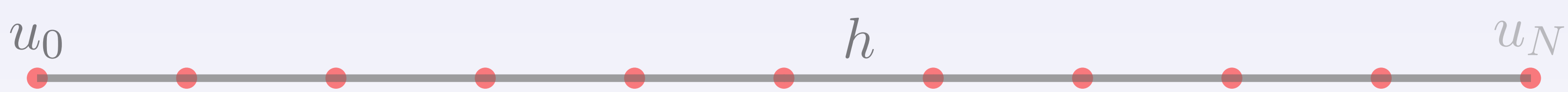
- Up until now we've been concerned with solving problems in the temporal & spatial domains
- Spectral methods transform the problem and work in the frequency domain (sometimes called phase space).
- Particularly useful in problems that have periodicity or infinite domains
- Still useful if that's not 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 a periodic function $u(x)$ in 1D, on an equally spaced grid
- 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

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

The derivative is given by $w = \frac{1}{h} D \cdot u$

Recall: This matrix is skew-symmetrix, Toeplitz (diagonal-constant), and circulant!

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

Suppose we have $X \in R^N$.
Then the DFT of X denoted by $\hat{X}(k)$ 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

$$F_N = W_N^{jk}$$

and the k are called *wave numbers*.

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

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

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

Key Idea

Now notice that for $N = 4$

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

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 and F_2 is of size $N/2$

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

FFT

Recall

$$u_j = \sum_{k=1}^{N} e^{2\pi ijk/N} \cdot w_k, \quad j = 1, \ldots, N.$$

What is the complexity for such an algorithm?

Discrete Fourier Transform (DFT) and Fast Fourier Transform (FFT)

- 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

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

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