Math 405 12: Spectral Methods

Introduction

Notice that when representing finite difference schemes with matrices, that the bandwidth gets wider as we increase the order of accuracy of our finite difference schemes:

E.g.,

$1/h^2 \times$ "1 -2 1", 2nd-order approx of Laplacian.

$1/(12h^2) \times$ "-1 16 -30 16 -1", 4th-order approx of Laplacian.

etc.

These give tri-diagonal, pentadiagonal, etc (and with fill-in in the corners for periodic BCs—*circulant matrices*).

How far can we take this? Fill the matrix completely. Gives "spectral accuracy" (better than any polynomial power of h). Example: accuracy could be 2^h. Typically very high accuracy, at least for analytic functions.

This is one approach to spectral methods, but the computations can be done more efficiently...

Fourier-based methods

Fourier series and Fourier transforms express functions of a spatial variable x in term of frequency (or wave number k)

Let $\hat{f}(k)$ be the Fourier transform of $f(x)$. Integration by parts gives nice result for n-th derivative of f:

$$\widehat{f^{(n)}(x)}(k) = (ik)^n \hat{f}(k)$$

Discrete Fourier Transform

In the discrete and bounded x case: on a grid $x = \{0, h, 2h, \ldots, 2\pi - h\}$, we have the **discrete Fourier transform**:

$$\hat{v_k} = h \sum_{j=1}^{N} \exp(-ikx_j) v_j.$$

And inverse:

$$v_k = \frac{h}{2\pi} \sum_{k=-N/2+1}^{N/2} \exp(ikx_j) \hat{v}_k.$$

This gives us a **physical domain** and a **Fourier domain**. An advantage of the Fourier/frequency domain is that we can differentiate in the Fourier domain by multiplying by (ik).

FFT

A dense $N \times N$ matrix will take $O(N^2)$ to evaluate a derivative via matrix-vector multiply.

The Fast Fourier Transform (FFT) takes $O(N \log N)$. So an algorithm for spatial derivatives is:

1) Compute FFT
2) Multiply by (ik) (or $(ik)^2$, etc)
3) Compute IFFT

Complexity: $O(N \log N)$.

Caveats: periodic boundary conditions, smooth solutions. Various issues with aliasing when doing nonlinear problems.

[demo_12_grayscott_spectral.m] Gray–Scott pattern formation combining Fourier spectral methods using the FFT with forward Euler timestepping.

In fact, we can do better using e.g., convolution-based time-stepping. See [demo_12_convolution.m].

Another demo: quasi-geostrophy movie shows cyclone/anticyclone symmetry breaking simulation using FFT-based spectral methods on the shallow-water equations.

Spectral methods on nonperiodic functions

Fourier not appropriate because of Gibbs Phenemenon (periodic extension introduces jumps).

Often Chebyshev grids used: cluster grid points near the boundaries.

[see diagram, cos of equispaced points on a semicircle.]

Chebfun

A mathematics and software project for spectral methods using "Chebyshev technology". Represents functions by (very) high-degree polynomials over Chebyshev grids.

Somewhere between numerical computing and symbolic computing. "Numerical computing with functions". Fast like numerical computing but with a "feel of symbolic computing".

Functions are expressed as high-degree polynomial interpolants. FFTs are used "under the hood" ==> fast. (Works because of equivalence between Fourier series on periodic equispaced grids and Chebyshev grids.)

One of the goals is to compute the correct answer to full 15-digit precision.

Software: http://www.chebfun.org

Mathematics: textbook: Approximation Theory and Approximation Practice.