Mathematical Models, Analysis and Simulation
Part I, Fall 2009

November 15, 2009

Homework 7: DFT and spectral methods, Max. Score 7.0, Deadline Sun, Dec. 6

1 Spectral interpolation and differentiation

Consider $L-$periodic functions f and the grid $x_k = kL/N$, $k = 0, 1, 2, \ldots, N-1$, $N = 2^m$, $m = 1, 2, \ldots$ The discrete Fourier transform (Strang Ch 4.3) establishes the correspondence between function values $f(x_j) = f_j$, DFT coefficients c_k, and the spectral interpolant Πf,

$$\Pi f(x) = \sum_{j=0}^{N-1} c_j e^{2\pi i j x/L}, \quad \Pi f(x_j) = f_j, \quad c_k = \frac{1}{N}\sum_{j=0}^{N-1} f_j e^{-2\pi i k x_j/L} \tag{*}$$

1. **(1.0)** Take

$$f(x) = e^{-M(x/L-0.3)^2}$$

on $[0, L]$ with periodic extension $f(x) = f(x+L)$ for all x. Its Fourier coefficients a_k decay,

$$a_k = \frac{1}{L}\int_0^L f(x)e^{-2\pi i k x/L}dx, \quad f(x) = \sum_{j=-\infty}^{\infty} a_j e^{2\pi i j x/L}, \quad a_j = O(j^{-p}).$$

f's "almost continuity" depends on M. What p do you expect for i) $M = 1$ and a substantially larger M, say, ii) $M = 100$? Why is this relevant for spectral computation of derivatives?

For $M = 60$, compute the DFT coefficients c_k for $N = 2^4$. Then evaluate Πf on a much denser grid, say `xpl = linspace(0,L,400)`, and plot the data and the interpolant vs. x. Note: Complex numbers!

The grid can easily be generated using the command sequence

```
x1 = linspace(0,L,N+1);
x = x1(1:N);
```

The plot can be generated conveniently using

```
plot3(x,real(f),imag(f),'o'); hold on
plot3(xpl,real(fpl),imag(fpl)); hold off
```

Comment on the suitability of Πf for differentiation.

2. **(0.5)** A better, much less wiggly interpolant can be constructed by using the interval $-N/2, \ldots, N/2-1$ instead of $0, \ldots, N-1$ of the DFT coefficients and basis function wave numbers. Look up what `fftshift` does, plot, and explain the formulas
```
fhat = fft(f);
dfhat = 2*i*pi/L*[-N/2:(N/2-1)]'.*fftshift(fhat);
df = ifft(fftshift(dfhat));
```
for computing df_k as approximations to $f'(x_k)$!

3. **(1.0)** (Hard!) Show that for real f, the formula (*) is equivalent to the DP matrix in Strang Ch 5.4 p449, and the formula on top of p 450.
Hints: i) the DFT coefficients are N-periodic, and so are the basis function values at gridpoints. Show!
ii)

$$\sum_{k=M}^{K} q^k = \frac{q^M - q^{K+1}}{1-q}, \qquad \sum_{k=-N/2}^{N/2-1} e^{iyk} = e^{-iy/2}\frac{\sin(Ny/2)}{\sin(y/2)}$$

$$\Pi f(x) = \sum_{k=0}^{N-1} \frac{1}{N}\left(\sum_{j=0}^{N-1} f_j e^{-2\pi i j x_k/L}\right) e^{2\pi i k x/L} = \sum_{j=0}^{N-1} f_j \left(\frac{1}{N}\sum_{k=0}^{N-1} e^{2\pi i k(x-x_j)/L}\right)$$

The real part of the above development produces Shannon's `psinc`. The imaginary part vanishes on all gridpoints, *but not in between.*

Let $''$ on the sum mean taking half the first and last terms. Show that symmetrizing the sum to

$$Pf(x) = \sum_{k=-N/2}^{N/2}{}'' c_k e^{2\pi i k x/L}$$

makes the imaginary part vanish, and that

$$Pf(x) = \Pi f(x) + i c_{n/2}\sin(\pi n x/L)$$

This shows how to evaluate Pf, and its derivatives at gridpoints, by FFT.

4. **(0.5)** Compute the RMS norm, $||f||_{RMS} = \sqrt{\frac{1}{N}\sum_{k=0}^{N-1}|f_k|^2}$, of the errors of derivatives at grid points with m = 3,4,5,6,7; plot in a suitable lin-log diagram and discuss the alleged exponential convergence.

2 Spectral method for First-order-in-time Named Equations

Consider the model equation

$$q_t + A(q^2)_x + Bq_x = \epsilon_2 q_{xx} + \epsilon_3 q_{xxx}, \quad 0 \le x < L, \quad t \ge 0, \quad q(x,0) = f(x) \qquad (**)$$

with $\epsilon_2 \ge 0$, f, q L-periodic, and A, B, ϵ_k constant.

2.1 Implementation (1.0)

See Strang Ch 6 p 456 and p522, and give the values of $A, B, \epsilon_2, \epsilon_3$ which give the heat, convection-diffusion, Schrödinger, Airy, Burger's, and Korteweg-deVries equations. Your task is to write a high-order method (fourth order in time, exponential order in space) for numerical solution of the initial-boundary value problem for this family of models.

Let the spectral differentiation matrix be DP. Borrowing notation from MATLAB, the semi-discretized PDE (**) becomes the system of ODEs

$$\mathbf{Q}_t = DP \times (-B\mathbf{Q} - A\mathbf{Q}. * \mathbf{Q} + DP \times (\epsilon_2\mathbf{Q} + \epsilon_3 DP \times \mathbf{Q})),$$

where

$$\mathbf{Q} = (q_0, q_1, \ldots, q_j, \ldots, q_{N-1})^T$$

The differentiations should NOT be implemented by matrix multiplication (Why?), but by `fft, fftshift`, and `ifft`, like above. Use the classical Runge-Kutta-4 scheme for the time-stepping.

2.2 The heat equation (1.5)

For $f(x) = \sin(2\pi x/L)$ the exact solution is known. Take $L = 1, \epsilon_2 = 1, m = 3, 4, 5, 6, 7$ and solve until time $T = 0.1$ and 1.

1. What is the time-step limit Δt_{max} for stability? This question may be answered either theoretically or experimentally. The RK4 stability region on the real line is approx. $[-2.8, 0]$.

2. For each m, choose a sufficiently small Δt that the error is dominated by the spatial error, and record the RMS norms of differences with the exact solution. Plot in a lin-log diagram and conclude exponential convergence (or not?)

3. For parabolic initial value problems one usually chooses implicit schemes. Explain (don't code) how to use the implicit Euler scheme. Hint: Solve the ODEs for the DFT coefficients! Transform to physical space only at the output times desired. Indeed, it is easy to compute the exact solution to this system of ODE since the matrix is diagonal. Explain!

2.3 Burgers' equation (1.5)

Take $f(x) = \sin(\pi x/L), L = 1, m = 4, 5, 6, 7$. For $\epsilon_2 > 0$ the solution is smooth for all times, but for $\epsilon_2 = 0$ it develops discontinuities after finite time, even if f is smooth.

- Determine at what time the wave breaks and the solution becomes discontinuous. You observe "wiggles" around a front when it becomes steep enough. Look up the Gibb's phenomenon and comment. Use a small $\epsilon_2 > 0$ to smooth the wiggles.

- Verify by computation the analysis for $f(x) = \delta(x - L/2)$ on Strang pp. 522-523. You may need to choose a non-zero ϵ_2 and a smooth approximation to the delta-function, like $f(x) = \alpha e^{-M(x/L-0.5)^2}$ for some suitably large M. Choose α so the approximate delta-function has mass 1, $\int_{-\infty}^{+\infty} f(x)dx = 1$.

2.4 An equation of your choice (optional, 1.0)

Choose another equation for which you find something interesting in Strang, or on the web. Solve it accurately and verify the properties.