A Pseudospectral method for periodic functions

Lab Objective: We look at a pseudospectral method with a Fourier basis, and numerically solve the advection equation using a pseudospectral discretization in space and a Runge-Kutta integration scheme in time.

Let f be a periodic function on $[0,2\pi]$. Let x_1,\ldots,x_N be N evenly spaced grid points on $[0,2\pi]$. Since f is periodic on $[0,2\pi]$, we can ignore the grid point $x_N=2\pi$. We will further assume that N is even; similar formulas can be derived for N odd. Let $h=2\pi/N$; then $\{x_0,\ldots,x_{N-1}\}=\{0,h,2h,\ldots,2\pi-h\}$.

The discrete Fourier transform (DFT) of f, denoted by \hat{f} or $\mathcal{F}(f)$, is given by

$$\hat{f}(k) = h \sum_{j=0}^{N-1} e^{-ikx_j} f(x_j)$$
 where $k = -N/2 + 1, \dots, 0, 1, \dots, N/2$.

The inverse DFT is then given by

$$f(x_j) = \frac{1}{2\pi} \sum_{k=-N/2}^{N/2} \frac{e^{ikx_j}}{c_k} \hat{f}(k), \quad j = 0, \dots, N-1,$$
(15.1)

where

$$c_k = \begin{cases} 2 & \text{if } k = -N/2 \text{ or } k = N/2, \\ 1 & \text{otherwise.} \end{cases}$$
 (15.2)

The inverse DFT can then be used to define a natural interpolant (sometimes called a band-limited interpolant) by evaluating (??) at any x rather than x_j :

$$p(x) = \frac{1}{2\pi} \sum_{k=-N/2}^{N/2} e^{ikx} \hat{f}(k).$$
 (15.3)

The interpolant for f' is then given by

$$p'(x) = \frac{1}{2\pi} \sum_{k=-N/2+1}^{N/2-1} ike^{ikx} \hat{f}(k).$$
 (15.4)

Consider the function $u(x) = \sin^2(x)\cos(x) + e^{2\sin(x+1)}$. Using (??), the derivative u' may be approximated with the following code. ¹ We note that although we only approximate u' at the Fourier grid points, (??) provides an analytic approximation of u' in the form of a trigonometric polynomial.

```
import numpy as np
from scipy.fftpack import fft, ifft
import matplotlib.pyplot as plt
N = 24
x1 = (2.*np.pi/N)*np.arange(1,N+1)
f = np.sin(x1)**2.*np.cos(x1) + np.exp(2.*np.sin(x1+1))
# This array is reordered in Python to
# accomodate the ordering inside the fft function in scipy.
k = np.concatenate(( np.arange(0,N/2) ,
                     np.array([0]) , # Because hat\{f\}'(k) at k = N/2 is zero.
                     np.arange(-N/2+1,0,1))
# Approximates the derivative using the pseudospectral method
f_hat = fft(f)
fp_hat = ((1j*k)*f_hat)
fp = np.real(ifft(fp_hat))
# Calculates the derivative analytically
x2 = np.linspace(0,2*np.pi,200)
derivative = (2.*np.sin(x2)*np.cos(x2)**2. -
                np.sin(x2)**3. +
                2*np.cos(x2+1)*np.exp(2*np.sin(x2+1))
plt.plot(x2,derivative,'-k',linewidth=2.)
plt.plot(x1,fp,'*b')
plt.savefig('spectral2_derivative.pdf')
plt.show()
```

Problem 1. Consider again the function $u(x) = \sin^2(x)\cos(x) + e^{2\sin(x+1)}$. Create a function that approximates $\frac{1}{2}u'' - u'$ on the Fourier grid points for N = 24.

The advection equation

Recall that the advection equation is given by

$$u_t + cu_x = 0 ag{15.5}$$

¹See Spectral Methods in MATLAB by Lloyd N. Trefethen. Another good reference is Chebyshev and Fourier Spectral Methods by John P. Boyd.

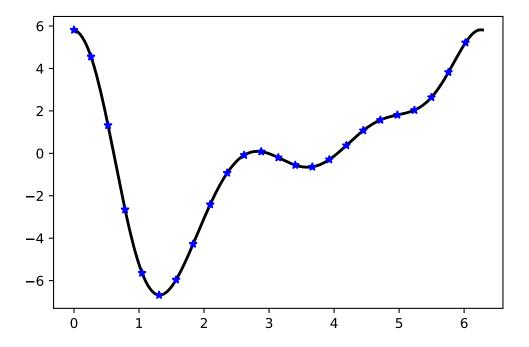


Figure 15.1: The derivative of $u(x) = \sin^2(x)\cos(x) + e^{2\sin(x+1)}$.

where c is the speed of the wave (the wave travels to the right for c > 0). We will consider the solution of the advection equation on the circle; this essentially amounts to solving the advection equation on $[0, 2\pi]$ and assuming periodic boundary conditions.

A common method for solving time-dependent PDEs is called the *method of lines*. To apply the method of lines to our problem, we use our Fourier grid points in $[0, \pi]$: given an even N, let $h = 2\pi/N$, so that $\{x_0, \ldots, x_{N-1}\} = \{0, h, 2h, \ldots, 2\pi - h\}$. By using these grid points we obtain the collection of equations

$$u_t(x_j, t) + cu_x(x_j, t) = 0, \quad t > 0, \quad j = 0, \dots N - 1.$$
 (15.6)

Let U(t) be the vector valued function given by $U(t) = (u(x_j, t))_{j=0}^{N-1}$. Let $\mathcal{F}(U)(t)$ denote the discrete Fourier transform of u(x, t) (in space), so that

$$\mathcal{F}(U)(t) = (\hat{u}(k,t))_{k=-N/2+1}^{N/2}.$$

Define \mathcal{F}^{-1} similarly. Using the pseudospectral approximation in space leads to the system of ODEs

$$U_t + \vec{c}\mathcal{F}^{-1}\left(i\vec{k}\mathcal{F}(U)\right) = 0 \tag{15.7}$$

where \vec{k} is a vector, and $\vec{k}\mathcal{F}(U)$ denotes element-wise multiplication. Similarly \vec{c} could also be a vector, if the wave speed c is allowed to vary.

Problem 2. Using a fourth order Runge-Kutta method (RK4), solve the initial value problem

$$u_t + c(x)u_x = 0, (15.8)$$

where $c(x) = .2 + \sin^2(x-1)$, and $u(x,t=0) = e^{-100(x-1)^2}$. Plot your numerical solution from t=0 to t=8 over 150 time steps and 100 x steps. Note that the initial data is nearly zero near x=0 and 2π , and so we can use the pseudospectral method. ^a Use the following code to help graph.

```
t_steps = 150  # Time steps
x_steps = 100  # x steps

''''

Your code here to set things up
''''

sol = # RK4 method. Should return a t_steps by x_steps array

X,Y = np.meshgrid(x_domain, t_domain)
fig = plt.figure()
ax = fig.add_subplot(111, projection="3d")
ax.plot_wireframe(X,Y,sol)
ax.set_zlim(0,3)
plt.show()
```

^aThis problem is solved in Spectral Methods in MATLAB using a leapfrog discretization in time.

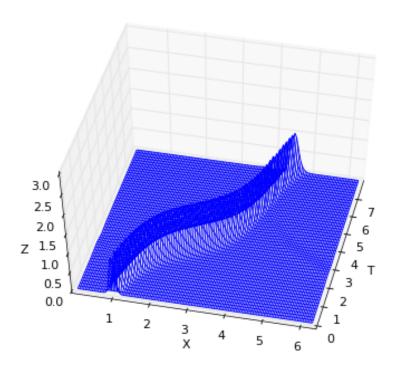


Figure 15.2: The solution of the variable speed advection equation; see Problem ??.