Spectral methods with Python

Presentation:

* Syllabus
* Objectives
* Evaluation

  50% HW

  50% Project.

= 1 =

Diferentiation Matrices.

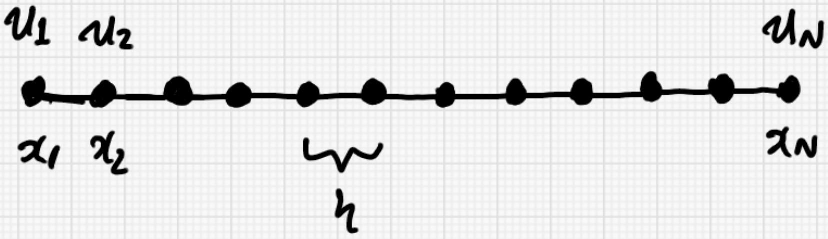
CLASS 01

Jan-16-18

Given $\{x_j\}$ and corresponding $\{u(x_j)\}$ we want approximate the derivative of u.

FIRST IDEA FINITE DIFFERENCES

Consider a uniform grid $\{x_1, \dots, x_N\}$ and $\{u_1, \dots, u_N\}$



Let $w_j \approx u'(x_j)$ and use the second-order difference approximation

$$w_j = \frac{u_{j+1} - u_{j-1}}{2h} \qquad (1.1)$$

HW01: show that this finnite difference approximation to $u'(x_j)$ is of second order

<2>

For simplicity we assume that the problem is periodic and

$$u_0 = u_N \,,\; u_1 = u_{N+1} \,, \ldots$$

then for each $j = 1, \ldots N$

$$w_j = \frac{u_{j+1} - u_{j-1}}{2h} \,,$$ that is,

for the given grid

$$w_1 = \frac{1}{2h}(u_2 - u_0) = \frac{1}{2h}(u_2 - u_N)$$

$$w_2 = \frac{1}{2h}(u_3 - u_1)$$

$$w_3 = \frac{1}{2h}(u_4 - u_2)$$

$$\vdots$$

$$\vdots$$

$$u_{N-1} = \frac{1}{2h}(u_N - u_{N-2})$$

$$u_N = \frac{1}{2h}(u_1 - u_N)$$

therefore we can represents W_j as a Matrix product

$j=1,\dots,N$

$$\begin{bmatrix} W_1 \\ W_2 \\ \vdots \\ \vdots \\ W_{N-1} \\ W_N \end{bmatrix} = \frac{1}{2h} \begin{bmatrix} 0 & 1 & \cdots & \cdots & & -1 \\ -1 & 0 & 1 & & & 0 \\ 0 & -1 & 0 & 1 & & 0 \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 0 & 1 \\ 1 & & & & -1 & 0 \end{bmatrix}$$

Results that this matrix is Toeplitz and circulant, that is

$$a_{ij} = (i-j) \pmod N.$$

HW Q2.

Consult the circulant matrix definition from

PHILIP J. DAVIS, Circulant Matrices

pg. 66.

Prove the following theorem: Let $\pi = \mathrm{circ}(0,1,0,\dots,0)$

If $A \in M_{n\times n}(\mathbb{R})$, then A is circulant iff $A\pi = \pi A$

An alternative approach to derive that

$$w_j = \frac{u_{j+1} - u_{j-1}}{2h} \quad \text{and}$$

$$\begin{pmatrix} w_1 \\ \vdots \\ \vdots \\ w_N \end{pmatrix} = \frac{1}{2h} \begin{bmatrix} 0 & 1 & & & & -1 \\ -1 & 0 & 1 & & & \\ & -1 & 0 & 1 & & \\ & & -1 & 0 & 1 & \\ & & & \ddots & \ddots & \ddots \\ & & & -1 & 0 & 1 \\ 1 & & & & -1 & 0 \end{bmatrix} \begin{bmatrix} u_1 \\ \vdots \\ \vdots \\ u_N \end{bmatrix}$$

is by the following process of local interpolation and differentiation

For $j = 1, 2, \ldots, N$

Let p_j be the unique polynomial of degree ≤ 2 with $p_j(x_{j-1}) = u_{j-1}$, $p_j(x_j) = u_j$, and $p_j(x_{j+1}) = u_{j+1}$

Set $w_j = p_j'(x_j)$

Results that for fixed j

$$p_j(x) = u_{j-1}\, a_{-1}(x) + u_j\, a_0(x) + u_{j+1}\, a_1(x)$$

where

$$a_{-1}(x) := \frac{(x-x_j)(x-x_{j+1})}{2h^2}$$

$$a_0(x) := -\frac{(x-x_{j-1})(x-x_{j+1})}{h^2}$$

$$a_1(x) := \frac{(x-x_{j-1})(x-x_j)}{2h^2}$$

HW 03.

Obtain $p_j'(x)\Big|_{x=x_j}$ to deduce

$$w_j' = \frac{u_{j+1} - u_{j-1}}{2h^2}$$

=6=

The fourth-order analogue:

For $j = 1, \dots, N$

- Let p_j be the unique polynomial of degree ≤ 4 with

$$p_j(x_{j\pm 2}) = u_{j\pm 2}$$

$$p_j(x_{j\pm 1}) = u_{j\pm 1}$$

$$p_j(x_j) = u_j$$

- Set $w_j = p_j'(x_j)$

Again, assuming periodicity of the data, we can prove that

$$(1.3)\quad \begin{pmatrix} w_1 \\ \vdots \\ w_N \end{pmatrix} = \frac{1}{h}\begin{bmatrix} & \ddots & -1/12 & & 1/12 & -2/3 \\ & \ddots & 2/3 & \ddots & & \\ & \ddots & 0 & \ddots & & \\ & \ddots & -2/3 & \ddots & & \\ -1/12 & \ddots & 1/12 & \ddots & & \\ 2/3 & -1/12 & & \ddots & & \end{bmatrix} \begin{bmatrix} u_1 \\ \vdots \\ \vdots \\ u_n \end{bmatrix}$$

Results that the matrix (1.3) is a pentadiagonal circulant matrix.

The matrices in (1.2) and (1.3) are examples of differentation matrices.

HW 05

Show that (1.3) is a circulant matrix and deduce its entries.

CE01. Convergence of fourth order finite differences.

- Open and run p01.ipynb.

This notebook ilustrates the behaviour of 1.3. We take $u(x) = e^{\sin(x)}$ over a given periodic data on the domain $[-\pi, \pi]$

The notebook compares the finitte difference approximation w_j with the exact derivative

$$e^{\sin(x_j)} \cos(x_j)$$

This is our first and last example that does not illustrate a spectral method!

Instead we ask that document (give a simple and clear explanation) about some python functions.

* coo_matrix
* norm
* semilog
* loglog

We have looked at second- and fourth-order finite differences, and this sugest tha considering higher orders will lead to circulant matrices of increasing bandwith. The idea of spectral methods is to take this process to the limit!!, at least in principle, and work with a differentiation formula of infinite order and infinite bandwidth — i.e., a dense matrix see:

B. Fornberg, On a Fourier method for the integration of hyperbolic equations, SIAM J. Numer. Anal. 12 (1975), 509 – 528

Latter we shall show that in this limit, for an infinite equi-spaced grid, one obtains the following infinite matrix

$$D := \frac{1}{h} \begin{pmatrix} & \vdots & \\ \ddots & 1/3 & \\ \ddots & -1/2 & \ddots \\ \ddots & 1 & \ddots \\ \ddots & 0 & \ddots \\ \ddots & -1 & \ddots \\ \ddots & -1/2 & \ddots \\ \ddots & -1/3 & \ddots \\ & \vdots & \end{pmatrix} \qquad (1.4)$$

This is a skew-symmetric ($D^T = -D$) doubly infinite Toeplitz matrix, also known as Laurent operator.

See P. R. Halmos, A Hilbert Space Problem Book, 2nd ed. Springer, 1974.

H. Widom Toeplitz matrices, in I. I. Hirschmann, Jr., ed., Studies in Real and Complex Analysis, Math. Assoc. Amer., 1965.

Of course, in practice one does not work with an infinite matrix.
For a finite grid, here is the desi principle for spectral collocation methods:

- Let p a single function (independent of j) such that
  $$p(x_j) = u_j \quad j = 1, \ldots, N$$
- Set $w_j = p'(x_j)$.

We are free tho chose p to fit the problem at hand. For a periodic domain, the natural choice is a trigonometric polynomial on an equi-spaced grid. For non-periodic domains, algebraic polynomials on irregular grids are the right choice, the Chebyshev methods.

In order to illustrate the performance of a Spectral method, consider the differentiation matrix of $N \times N$

$$D_N := \begin{bmatrix} & \vdots & \\ \ddots & \frac{1}{2}\cot\frac{3h}{2} & \\ \ddots & -\frac{1}{2}\cot\frac{2h}{2} & \\ \ddots & \frac{1}{2}\cot\frac{1}{2}h & \\ & 0 & \\ & -\frac{1}{2}\cot\frac{1}{2}h & \ddots \\ & \frac{1}{2}\cot h & \ddots \\ & -\frac{1}{2}\cot\frac{3}{2}h & \ddots \\ & \vdots & \end{bmatrix} \qquad (1.5)$$

Hw 05.

Show that this matrix is indeed circulant and Toeplitz.

xly notebook p02.ipynb

we use D_N instead the fourth-order finite difference.

HW06

Plot in a same figure and axis the error of bouth approximations in order to compare the performance of the spectral approximation and finite difference.