FINITE DIFFERENCE METHODS (I): INTRODUCTION

Luis Cueto-Felgueroso

1. BASIC DEFINITIONS AND NOTATION

1.1. Discretization. Grid functions.

Consider a function $u(x)$, defined on the interval $I = [0, L]$. Let us discretize I into a set of $N + 1$ uniformly spaced *nodes* $\{x_j, j = 0, \ldots, N\}$,

$$0 = x_0, x_1, \ldots, x_j, \ldots, x_{N-1}, x_N = L \tag{1}$$

with nodal coordinates $x_j = j\Delta x$, where $\Delta x = L/N$ is the (uniform) grid spacing. The above set of nodes induces a partition of the interval into a set of N subintervals $\{I_j, j = 1, \ldots, N\}$, such that

$$I = \bigcup_{j=1}^{N} I_j, \qquad I_j = [x_{j-1}, x_j] \tag{2}$$

The *grid function* $\{u_j, j = 0, \ldots, N\}$ is defined, point-wise, by the discrete values of $u(x)$ at the grid nodes, i.e. $u_j = u(x_j)$.

1.2. Discrete differentiation.

Given a grid $\{x_j, j = 0, \ldots, N\}$, and a grid function $\{u_j, j = 0, \ldots, N\}$, we are interested in computing approximations to the derivatives of $u(x)$, $\dfrac{d^m u(x)}{dx^m}$. More precisely, we want to compute grid functions $\{u_j^{(m)}, j = 0, \ldots, N\}$, such that

$$u_j^{(m)} \approx \left.\frac{d^m u(x)}{dx^m}\right|_{x=x_j} \tag{3}$$

Finite difference methods attempt to compute these approximations by expressing the discrete derivatives at the grid nodes as linear combinations of the grid function values, i.e.

$$u_j^{(m)} = \sum_{k=0}^{N} \alpha_k^{(m)} u_k \tag{4}$$

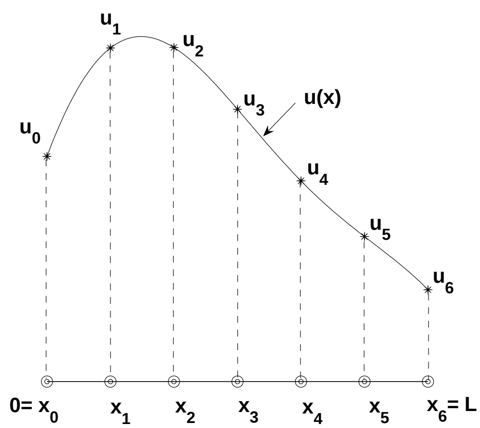

Figure 1. Finite difference grid

Note that the set of coefficients $\{\alpha_k\}$ will be different, in general, for each grid point, and therefore (4) can be written in the more general fashion

$$u_j^{(m)} = \sum_{k=0}^{N} \alpha_{jk}^{(m)} u_k \tag{5}$$

or, in matrix form,

$$\boldsymbol{u}^{(m)} = \boldsymbol{D}^{(m)} \boldsymbol{u} \tag{6}$$

where

$$\boldsymbol{u}^{(m)} = \begin{pmatrix} u_0^{(m)} \\ u_1^{(m)} \\ \vdots \\ u_{N-1}^{(m)} \\ u_N^{(m)} \end{pmatrix} \quad \boldsymbol{u} = \begin{pmatrix} u_0 \\ u_1 \\ \vdots \\ u_{N-1} \\ u_N \end{pmatrix} \tag{7}$$

and

$$\boldsymbol{D}^{(m)} = \begin{pmatrix} \alpha_{00}^{(m)} & \alpha_{01}^{(m)} & \dots & \alpha_{0N}^{(m)} \\ \alpha_{10}^{(m)} & \alpha_{11}^{(m)} & \dots & \alpha_{1N}^{(m)} \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{N0}^{(m)} & \alpha_{N1}^{(m)} & \dots & \alpha_{NN}^{(m)} \end{pmatrix} \tag{8}$$

is the *differentiation matrix*.

There are two basic considerations that must be taken into account when designing finite difference formulas. One is how many nodes, and of course which ones, will be used for the computation of a certain derivative at each grid point j. This set of “neighbor” nodes is called the *stencil* of the formula, and has a strong impact on the computational cost of applying the formula: the differentiation matrix will be less sparse, and therefore the matrix-vector operation will require more operations. On the other hand, larger stencils will allow, in general, the construction of finite differences of higher *accuracy*, which is the other fundamental design variable.

1.3. First examples

A common difference formula for the first derivative is the centered, second order formula

$$u_j' = \frac{u_{j+1} - u_{j-1}}{2\Delta x} \qquad u_j' = \left.\frac{du}{dx}\right|_{x=x_j} + O(\Delta x^2) \tag{9}$$

For the second derivative, the classical second order finite difference formula is given by

$$u_j'' = \frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2} \qquad u_j'' = \left.\frac{d^2u}{dx^2}\right|_{x=x_j} + O(\Delta x^2) \tag{10}$$

On a periodic grid, their associated differentiation matrices are

$$\boldsymbol{D}^{(1)} = \begin{pmatrix} 0 & 1 & 0 & 0 & \dots & 0 & -1 \\ -1 & 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & -1 & 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & -1 & 0 & 1 & 0 \\ 0 & 0 & \dots & 0 & -1 & 0 & 1 \\ 1 & 0 & \dots & 0 & 0 & -1 & 0 \end{pmatrix} \tag{11}$$

and

$$\boldsymbol{D}^{(2)} = \begin{pmatrix} -2 & 1 & 0 & 0 & \dots & 0 & 1 \\ 1 & -2 & 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & -2 & 1 & 0 \\ 0 & 0 & \dots & 0 & 1 & -2 & 1 \\ 1 & 0 & \dots & 0 & 0 & 1 & -2 \end{pmatrix} \tag{12}$$

Note that, in the case of periodic grids, we drop the last node of the grid. In other words, we have now N nodes $\{x_j, j = 0, \dots, N-1\}$, as

$$0 = x_0, x_1, \dots, x_j, \dots, x_{N-2}, x_{N-1} = L - \Delta x \qquad \Delta x = L/N \tag{13}$$

2. DESIGN OF FINITE DIFFERENCE APPROXIMATIONS. CONVERGENCE

2.1. Some definitions

A discrete differentiation method is *consistent* with the exact derivative if, for sufficiently smooth functions $u(x)$,

$$\left(u_j^{(m)} - \left.\frac{d^m u}{dx^m}\right|_{x=x_j} \right) \to 0 \qquad \forall j = 0, \ldots, N \tag{14}$$

when $\Delta x \to 0$. The difference between the approximate and exact derivative is called *truncation error*

$$\tau_j = u_j^{(m)} - \left.\frac{d^m u}{dx^m}\right|_{x=x_j} \qquad j = 0, \ldots, N \tag{15}$$

Finally, a finite difference formula is of *order p* if the truncation error satisfies

$$\tau_j = O(\Delta x^p) \tag{16}$$

where we define a function $f(\Delta x)$ to be $O(\Delta x^p)$, as $\Delta x \to 0$, if there exist constants C and ϵ, such that $|f(\Delta x)| < C\Delta x^p$, for all $\Delta x < \epsilon$.

2.2. Design of finite difference approximations

Given a stencil of $n = l + r + 1$ distinct nodes around each grid point j, $\{x_{j-l}, \ldots, x_j, \ldots, x_{j+r}\}$, the basic design objective is to find the coefficients $\alpha_k^{(m)}$ that maximize the order of the approximation

$$\left.\frac{d^m u}{dx^m}\right|_{x=x_j} \approx u_j^{(m)} = \sum_{k=j-l}^{j+r} \alpha_k^{(m)} u_k \tag{17}$$

2.3. Taylor series expansions

Let us derive an approximation for the second derivative at grip point j, using the stencil $\{x_{j-1}, x_j, x_{j+1}\}$. Expanding $u(x)$ in a neighborhood of x_j, we can write

$$\begin{aligned} u_{j+1} &= u_j + \Delta x u_j' + \frac{\Delta x^2}{2!} u_j'' + \frac{\Delta x^3}{3!} u_j''' + O(\Delta x^4) \\ u_{j-1} &= u_j - \Delta x u_j' + \frac{\Delta x^2}{2!} u_j'' - \frac{\Delta x^3}{3!} u_j''' + O(\Delta x^4) \end{aligned} \tag{18}$$

adding the expressions above, we arrive at

$$u_{j+1} + u_{j-1} = 2u_j + \Delta x^2 u_j'' + O(\Delta x^4) \tag{19}$$

and therefore

$$u_j'' = \frac{u_{j-1} - 2u_j + u_{j+1}}{\Delta x^2} + O(\Delta x^2) \tag{20}$$

This formula maximizes the order of the truncation error attainable with the three-point, centered stencil, and is *second order accurate*.

Increasing the stencil of the approximation in order to a 5-point formula, and matching terms in the Taylor series expansions for u_{j-2}, u_{j-1}, u_{j+1} and $u_{j+2}\}$, we would arrive at

$$u_j'' = \frac{-u_{j-2} + 16u_{j-1} - 30u_j + 16u_{j+1} - u_{j+2}}{12\Delta x^2} + O(\Delta x^4) \tag{21}$$

which is *fourth order* accurate.

2.4. Polynomial interpolation

An alternative approach, and perhaps a more convenient one from the perspective of computer implementation, is to fit a polynomial through the stencil points, and then approximate the derivatives by the derivatives of the polynomial.

Consider again a stencil of $n = l + r + 1$ nodes around grid point j, $\{x_{j-l}, \ldots, x_j, \ldots, x_{j+r}\}$. We approximate $u(x)$ *around* x_j as

$$u(x) \approx \widetilde{u}(x) = \sum_{k=j-l}^{j+r} L_k(x) u_k \tag{22}$$

where the functions $L_k(x)$ are the Lagrange polynomials

$$L_k(x) = \frac{(x - x_{j-l}) \ldots (x - x_{k-1})(x - x_{k+1}) \ldots (x - x_{j+r})}{(x_k - x_{j-l}) \ldots (x_k - x_{k-1})(x_k - x_{k+1}) \ldots (x_k - x_{j+r})} \tag{23}$$

Note that $L_k(x_i) = \delta_{ki}$, which implies that the polynomial $\widetilde{u}(x)$ interpolates the nodes. Of course, $\widetilde{u}(x)$ is a polynomial of degree $n-1$, and formally $|u(x) - \widetilde{u}(x)| = O(\Delta x^n)$ for smooth functions $u(x)$. We may approximate the derivatives of $u(x)$ as

$$\left.\frac{d^m u}{dx^m}\right|_{x=x_j} \approx \left.\frac{d^m \widetilde{u}}{dx^m}\right|_{x=x_j} = \sum_{k=j-l}^{j+r} \left.\frac{d^m L_k}{dx^m}\right|_{x=x_j} u_k \tag{24}$$

and therefore

$$\alpha_k^{(m)} = \left.\frac{d^m L_k}{dx^m}\right|_{x=x_j} \tag{25}$$

For sufficiently smooth functions $u(x)$, the approximation of the m-th derivative of $u(x)$ using a stencil comprising n points is formally of order $n - m$. In the case of *centered* formulas with uniform grid spacing, the approximation is of order $n - m + 1$ due to symmetries.

2.5. Practical consequences of the convergence order

We have seen that a p-th order finite difference approximation is such that, asymptotically (for sufficiently smooth functions $u(x)$ and small grid sizes Δx), the error ϵ behaves like

$$\epsilon = O(\Delta x^p) = O(N^{-p}) \tag{26}$$

since $\Delta x = L/N$. We still need to define suitable measures of the error for which (26) may hold. In particular, we will consider

$$\epsilon_\infty = max_j \left(\left.\frac{d^m u}{dx^m}\right|_{x=x_j} - u_j^{(m)} \right) \tag{27}$$

and

$$\epsilon_2 = \sqrt{\frac{\sum_{j=0}^{N} \left(\frac{d^m u}{dx^m}\bigg|_{x=x_j} - u_j^{(m)} \right)^2}{N+1}} \tag{28}$$

For either of these error norms, we could in principle find a constant C such that, asymptotically,

$$\epsilon = CN^{-p} \tag{29}$$

Taking logarithms in the expression above, we arrive at

$$\log \epsilon = \log C - p \log N \tag{30}$$

and thus in logarithmic scale the error decays like a straight line with slope $-p$.

3. NON-PERIODIC GRIDS: ONE-SIDED FORMULAS

The grid points located at or near the boundary require special attention, as it will not be possible, in general, to use the centered formulas derived so far. This is obviously the case for grid points lying on the boundary, but for very high-order methods, which require large stencils, the use of non-centered formulas may be required for several layers of nodes inside the domain. Assume, for example, that for interior nodes we use the fourth order centered approximation

$$u'_j = \frac{u_{j+1} - u_{j-1}}{\Delta x} + O(\Delta x^2) \tag{31}$$

In this case we only need special formulas for nodes $j = 0$ and $j = N$. In particular, for $j = 0$ we could use

$$u'_0 = \frac{-3u_0 + 4u_1 - u_2}{2\Delta x} + O(\Delta x^2) \tag{32}$$

Analogously, a second order formula for $j = N$ reads

$$u'_N = \frac{3u_N - 4u_{N-1} + u_{N-2}}{2\Delta x} + O(\Delta x^2) \tag{33}$$

4. EXAMPLES

Let us look at some practical examples of numerical differentiation. A more in-depth analysis of the practical implementation of finite difference formulas will be presented in part (II). The basic problem statement is: given the values of a certain smooth function $u(x)$, defined on an interval $I = [0, L]$, at the $N + 1$ nodes $\{x_j, j = 0, \ldots, N\}$ of a grid (i.e. given the *grid function* $\{u_j, j = 0, \ldots, N\}$), use finite difference formulas to approximate the derivatives of $u(x)$ at the nodes.

Consider for example the function (figure 2)

$$u(x) = \frac{3}{5 - 4cos^2(2x)} \qquad x \in [0, 2\pi] \tag{34}$$

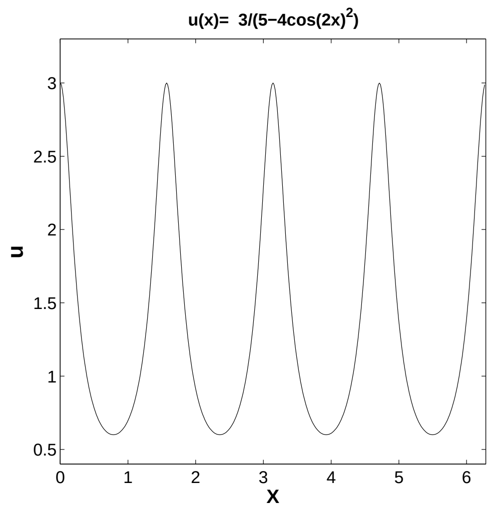

Figure 2. The function $u(x) = \dfrac{3}{5 - 4cos^2(2x)}$

which is continuous and periodic in $[0, 2\pi]$. Furthermore, all its derivatives are continuous and periodic in $[0, 2\pi]$ as well. We will study the convergence of several finite difference formulas for its first and second order derivatives. In particular, consider the second, fourth and sixth order center formulas for the *first* derivative,

$$u'_j = \frac{u_{j+1} - u_{j-1}}{2\Delta x} + O(\Delta x^2) \tag{35}$$

$$u'_j = \frac{-u_{j+2} + 8u_{j+1} - 8u_{j-1} + u_{j-2}}{12\Delta x} + O(\Delta x^4) \tag{36}$$

$$u'_j = \frac{u_{j+3} - 9u_{j+2} + 45u_{j+1} - 45u_{j-1} + 9u_{j-2} - u_{j-3}}{60\Delta x} + O(\Delta x^6) \tag{37}$$

as well as the second, fourth and sixth order center formulas for the *second* derivative,

$$u''_j = \frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2} + O(\Delta x^2) \tag{38}$$

$$u''_j = \frac{-u_{j+2} + 16u_{j+1} - 30u_j + 16u_{j-1} - u_{j-2}}{12\Delta x^2} + O(\Delta x^4) \tag{39}$$

$$u''_j = \frac{2u_{j+3} - 27u_{j+2} + 270u_{j+1} - 490u_j + 270u_{j-1} - 27u_{j-2} + 2u_{j-3}}{180\Delta x^2} + O(\Delta x^6) \tag{40}$$

In addition, we will compare the convergence of these methods with that of a spectral discretization, which uses all the grid points for the computation of the derivatives. The particular method used here will be covered later in the course, but the comparison will help understanding the limit case of increasingly high-order discretizations.

In order to have a preliminary idea of the relative accuracy of each scheme, figure 3 plots the approximate first derivative of $u(x)$, computed on a grid comprising $N = 32$ nodes, using the second and fourth order formulas (left and right, respectively). Even for this coarse grid the differences between both methods are noticeable. Figure 4 shows the convergence characteristics of the second (FD2), fourth (FD2), and sixth (FD6) order schemes, as well as the convergence of a spectral method. For this smooth function, the advantages of using higher order methods are huge. For $N = 300$ the spectral derivative is accurate to machine precision, whereas the second order method has still relative errors around 10^{-2}. Note also that the asymptotic ("straight line") behavior is only achieved for sufficiently fine grids (large N's), while for very coarse grids the error levels tend to exhibit a more "erratic" behavior.

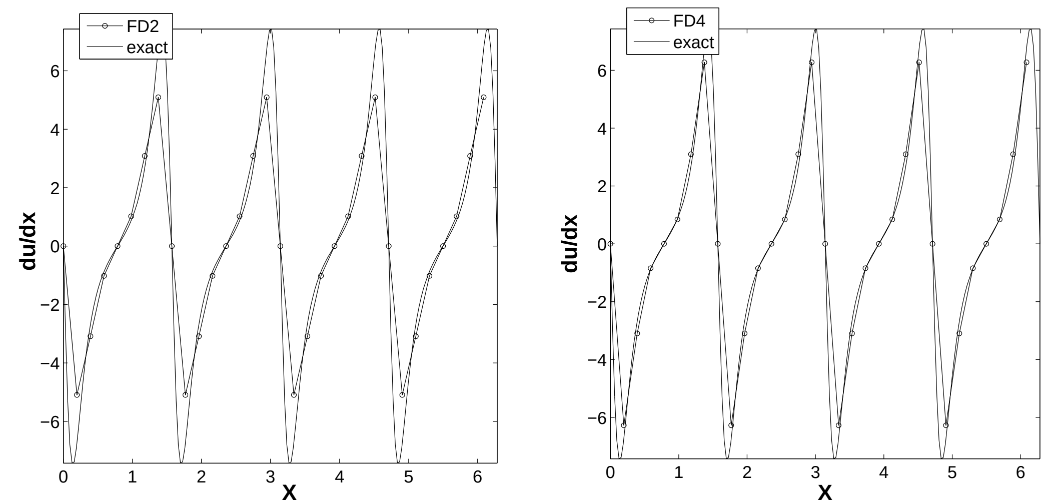

Figure 3. Approximation of the first derivative of $u(x)$ (34) using $N = 32$, points and the second and fourth order centered formulas (left and right, respectively).

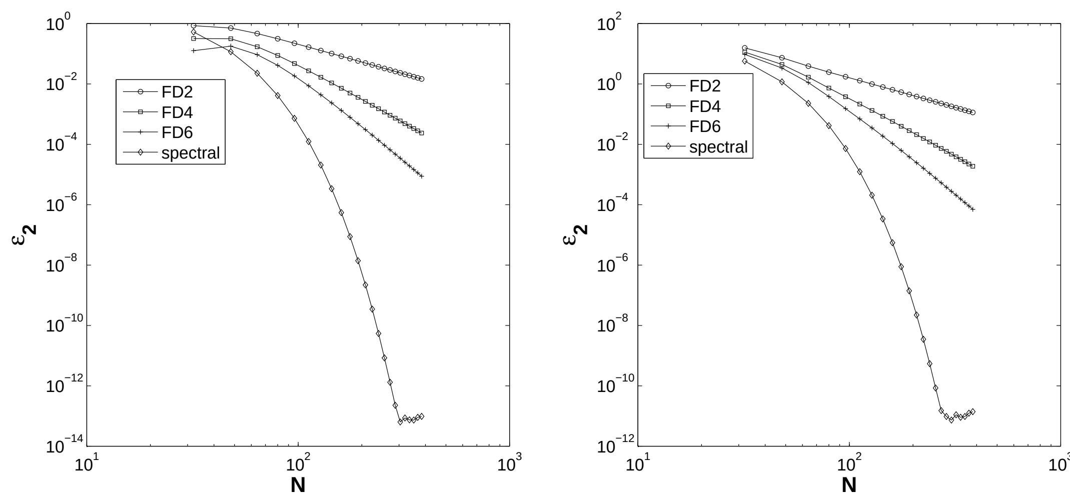

Figure 4. Convergence of finite difference approximations for smooth functions: first and second derivatives of $u(x)$ (34) (left and right, respectively).