Chapter 1 DIFFERENTIATION MATRICES

Our starting point with a basic question

Given a set of grid points $\{x_j\}$ and the corresponding function values $\{u(x_j)\}$, how can we us this data to approximate the derivative of u.

Consider a uniform grid $\{x_1, \dots, x_N\}$ with $x_{j+1} - x_j = h$ for each j, a set of corresponding data $\{u_1, \dots, u_N\}$

Let w_j denote the approximation of $u'(x_j)$, the derivative of u at x_j. The standard second-order finite difference approximation is

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

$$\boxed{\begin{aligned} u(x+h) &= u(x) + u'(x)h + O(h^2) \\ u(x-h) &= u(x) - u'(x)h + O(h^2) \\ \Rightarrow u(x+h) - u(x-h) &= 2u'(x)h + O(h^2) \end{aligned}}$$

Assumption for subsequent derivation

The problem is periodic and thus we take

$$u_0 = u_N \qquad u_1 = u_{N+1}$$

$\Rightarrow$ Differentiation matrix

$$\begin{bmatrix} w_1 \\ \vdots \\ w_N \end{bmatrix} = \frac{1}{h} \underbrace{\begin{bmatrix} 0 & 1/2 & & & -1/2 \\ -1/2 & 0 & \ddots & & \\ & & \ddots & & \\ & & & 0 & 1/2 \\ 1/2 & & & -1/2 & 0 \end{bmatrix}}_{\text{Toeplitz \& circulant matrix}} \begin{bmatrix} u_1 \\ \vdots \\ u_N \end{bmatrix}$$

Examples:

$$w_1 = (u_2 - u_0)/2h = (u_2 - u_N)/2h$$

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

$$\vdots$$

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

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

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

$$2 \leqslant j \leqslant N-1$$

* Toeplitz having constant entries along diagonals, i.e. a_{ij} depends only on $(i-j)$

* Circulant a_{ij} depends only on $(i-j)$ (mod N)

Local interpolation and differentiation

- Let p_j be the unique polynomial of degree $\leqslant 2$ with

$$p_j(x_{j-1}) = u_{j-1} \qquad p_j(x_j) = u_j \qquad p_j(x_{j+1}) = u_{j+1} \qquad (\star)$$

- Set

$$w_j = p_j'(x_j)$$

Example: Derive $p_j(x)$ according to the data $\{x_{j-1}, x_j, x_{j+1}\}$ & $\{u_{j-1}, u_j, u_{j+1}\}$

As p_j must satisfy $(\star)$, p_j can be interpolated by using Lagrange polynomials supported by such data

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

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

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

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

$$w_j = p_j'(x_j)$$

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

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

* Four-order analogue :

- Let p_j be the unique polynomial of degree $\leqslant 4$ with

$$p_j(x_{j\pm 2}) = u_{j\pm 2} \qquad p_j(x_{j\pm 1}) = u_{j\pm 1} \qquad p_j(x_j) = u_j$$

- Set $w_j = p_j'(x_j)$

$$\Longrightarrow \quad w_j = \frac{1}{h}\left[\frac{1}{12}u_{j-2} - \frac{2}{3}u_{j-1} + \frac{2}{3}u_{j+1} - \frac{1}{12}u_{j+2}\right]$$

Differentiation matrix

$$\underline{w} = \frac{1}{h}\begin{bmatrix} & & \ddots & & & 1/12 & -2/3 \\ & & \ddots & -1/12 & & & \\ & & & 2/3 & \ddots & & \\ & & \ddots & 0 & \ddots & & \\ -1/12 & & \ddots & -2/3 & \ddots & & \\ 2/3 & -1/12 & \ddots & 1/12 & \ddots & & \end{bmatrix}\underline{u}$$

It is clear that consideration of sixth, eighth- and higher-order schemes will lead to circulant matrices of increasing bandwidth. The idea behind spectral methods is to take this process to the limit, at least in principal, and work with a differentiation formula of infinite order and infinite bandwith — i.e. a dense matrix.

Design principle for spectral collocation methods

- Let p be a singl function (independent of j) such that

$$p(x_j) = u_j \qquad \text{for all } j$$

- Set

$$w_j = p'(x_j)$$

⊕ We are free to choose p to fit the problem at hand. For a periodic domain, the natural choice is a trigonometric polynomial on an equispaced grid, and the resulting Fourier methods will be our concern.

* Show output 1 for program 1
output 2 for program 2

The errors in Output 2 decrease very rapidly until such high precision is achieved that rounding errors on the computer prevent any further improvement. As N increases, the error in a finte difference or finite element scheme typically decreases like $O(N^{-m})$ for some constant m that depends on the order of approximation and the smoothness of the solution. For a spectral method, convergence at rate $O(N^{-m})$ for every m is achieved, provided the solution is indefinitely differentiable. & even faster convergence at a rate $O(c^N)$ $(0<c<1)$ is achieved if the solution is suitably analytic.