Lecture 12
APPROXIMATION OF FIRST ORDER DERIVATIVES

12.1 INTRODUCTION

Convective term in conservation equations involve first order derivatives. The simplest possible approach for discretization of these terms would be to use the approximation based on the basic definition of the derivative. In this lecture, we learn systematic procedures to obtain FD approximations based on Taylor series expansion and polynomial fitting for a generic function *f*(*x*) of a generic variable *x*.

12.2 TAYLOR SERIES EXPANSION

A continuously differentiable function *f*(*x*) can be expanded in Taylor series about $x = x_i$ as

$$f(x) = f(x_i) + (x - x_i)\left(\frac{\partial f}{\partial x}\right)_i + \frac{(x - x_i)^2}{2!}\left(\frac{\partial^2 f}{\partial x^2}\right)_i + ... + \frac{(x - x_i)^n}{n!}\left(\frac{\partial^n f}{\partial x^n}\right)_i + H \quad (12.1)$$

In series expansion, symbol *H* has been used to denote the higher order terms which have not been indicated explicitly. Thus, function values at grid points x_{i+1} and x_{i-1} can be expressed as

$$f_{i+1} \equiv f(x_{i+1}) = f(x_i) + (x_{i+1} - x_i)\left(\frac{\partial f}{\partial x}\right)_i + \frac{(x_{i+1} - x_i)^2}{2!}\left(\frac{\partial^2 f}{\partial x^2}\right)_i + H \quad (12.2)$$

$$f_{i-1} \equiv f(x_{i-1}) = f(x_i) + (x_{i-1} - x_i)\left(\frac{\partial f}{\partial x}\right)_i + \frac{(x_{i-1} - x_i)^2}{2!}\left(\frac{\partial^2 f}{\partial x^2}\right)_i + H \quad (12.3)$$

Rearrangement of Eq. (12.2) yields

$$\left(\frac{\partial f}{\partial x}\right)_i = \frac{f_{i+1} - f_i}{x_{i+1} - x_i} - \frac{(x_{i+1} - x_i)}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i + H \quad (12.4)$$

which gives us forward difference scheme (FDS) formally expressed as

$$\left(\frac{\partial f}{\partial x}\right)_i = \frac{f_{i+1} - f_i}{\Delta x_i} + O(\Delta x_i) \quad (12.5)$$

where $\Delta x_i = x_{i+1} - x_i$. Similarly, Eq. (12.3) yields the backward difference scheme (BDS) given by

$$\left(\frac{\partial f}{\partial x}\right)_i = \frac{f_i - f_{i-1}}{\Delta x_{i-1}} + O(\Delta x_{i-1}) \quad (12.6)$$

where $\Delta x_{i-1} = x_i - x_{i-1}$. Subtracting Eq. (12.3) from Eq.(12.2), we obtain the central difference scheme (CDS) given by the formula

$$\left(\frac{\partial f}{\partial x}\right)_i = \frac{f_{i+1}-f_{i-1}}{x_{i+1}-x_{i-1}} + \frac{\left(x_i - x_{i-1}\right)^2 - \left(x_{i+1}-x_i\right)^2}{2\left(x_{i+1}-x_{i-1}\right)}\left(\frac{\partial^2 f}{\partial x^2}\right)_i + H \qquad (12.7)$$

Thus, finite difference approximations based on Taylor series expansion are:

FDS: $\left(\frac{\partial f}{\partial x}\right)_i \approx \frac{f_{i+1}-f_i}{x_{i+1}-x_i}$,	Truncation Error $\sim O\left(\Delta x\right)$	
BDS: $\left(\frac{\partial f}{\partial x}\right)_i \approx \frac{f_i-f_{i-1}}{x_i-x_{i-1}}$,	Truncation Error $\sim O\left(\Delta x\right)$	
CDS: $\left(\frac{\partial f}{\partial x}\right)_i \approx \frac{f_{i+1}-f_{i-1}}{x_{i+1}-x_{i-1}}$,	Truncation Error $\sim O\left(\Delta x\right)$	on non-uniform mesh
$\left(\frac{\partial f}{\partial x}\right)_i \approx \frac{f_{i+1}-f_{i-1}}{2\Delta x}$,	Truncation Error $\sim O\left(\Delta x^2\right)$	on uniform grid

Note that the truncation error of the first order FDS or BDS is given by

$$\varepsilon_\tau \approx \frac{\Delta x}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i \qquad (12.8)$$

The truncation error of the CDS is given by

$$\left(\varepsilon_\tau\right)_{\mathrm{CDS}} = -\frac{\left(\Delta x_i\right)^2 - \left(\Delta x_{i-1}\right)^2}{2\left(\Delta x_i + \Delta x_{i-1}\right)}\left(\frac{\partial^2 f}{\partial x^2}\right)_i - \frac{\left(\Delta x_i\right)^3 + \left(\Delta x_{i-1}\right)^3}{6\left(\Delta x_i + \Delta x_{i-1}\right)}\left(\frac{\partial^3 f}{\partial x^3}\right)_i + H \qquad (12.9)$$

Thus, although the truncation error for CDS is formally of the same order as FDS or BDS, the magnitude of the truncation error for CDS is much smaller than FDS/BDS. In fact, on grid refinement, the convergence of CDS becomes second order asymptotically (Ferziger and Peric, 2003).

Further, let us substitute the value of second order derivative from Eq. (12.2) into Eq. (12.4). On rearrangement, we get

$$\left(\frac{\partial f}{\partial x}\right)_i = \frac{f_{i+1}(\Delta x_i)^2 - f_{i-1}(\Delta x_{i+1})^2 + f_i\left[(\Delta x_{i+1})^2 - (\Delta x_i)^2\right]}{\Delta x_i \Delta x_{i+1}\left(\Delta x_i + \Delta x_{i+1}\right)} - \frac{\Delta x_i \Delta x_{i+1}}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i + H \qquad (12.10)$$

which has second order accuracy on any grid (uniform or non-uniform). It reduces to the simpler form of CDS on uniform grids.

A general procedure on uniform grids

Let us define the difference approximation as (Chung, 2010)

$$\left(\frac{\partial f}{\partial x}\right)_i \approx \frac{af_i + bf_{i-1} + cf_{i+1} + df_{i-2} + ef_{i+2} + \ldots}{\Delta x} \qquad (12.11)$$

Coefficients a, b, c, d, e, …. can be determined from Taylor series expansion for the function values involved at the RHS around point x_i. We illustrate its use in the following example.

Example 12.1

Derive a three point backward difference formula on uniform grid using general procedure given by equation (12.11).

Solution

For three point backward difference formula, Eq. (12.11) takes the following form:

$$\left(\frac{\partial f}{\partial x}\right)_i \approx \frac{af_i + bf_{i-1} + cf_{i-2}}{\Delta x} \qquad \text{(i)}$$

Taylor series expansions for f_{i-1} and f_{i-2} are

$$f_{i-1} = f_i - \Delta x\left(\frac{\partial f}{\partial x}\right)_i + \frac{\Delta x^2}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i - \frac{\Delta x^3}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i + \ldots. \qquad \text{(ii)}$$

$$f_{i-2} = f_i - 2\Delta x\left(\frac{\partial f}{\partial x}\right)_i + \frac{(2\Delta x)^2}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i - \frac{(2\Delta x)^3}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i + \ldots. \qquad \text{(iii)}$$

Hence,

$$\begin{aligned}\frac{af_i + bf_{i-1} + cf_{i-2}}{\Delta x} = {} & \frac{(a+b+c)}{\Delta x} f_i - (b+2c)\left(\frac{\partial f}{\partial x}\right)_i + \frac{\Delta x}{2}(b+4c)\left(\frac{\partial^2 f}{\partial x^2}\right)_i \\ & - \frac{\Delta x^2}{6}(b+8c)\left(\frac{\partial^3 f}{\partial x^3}\right)_i + \ldots\end{aligned} \qquad \text{(iv)}$$

Equations (i) and (iv) indicate that the following three conditions must be satisfied:

$$a + b + c = 0 \qquad \text{(v)}$$
$$b + 2c = -1 \qquad \text{(vi)}$$
$$b + 4c = 0 \qquad \text{(vii)}$$

Solving Eqs. (v)-(vii), we get

$$a = 3/2, \quad b = -2, \quad c = 1/2 \qquad \text{(viii)}$$

The truncation error (TE) is given by

$$\varepsilon_\tau = \frac{\Delta x^2}{6}(b+8c)\left(\frac{\partial^3 f}{\partial x^3}\right)_i = \frac{\Delta x^2}{3}\left(\frac{\partial^3 f}{\partial x^3}\right)_i \qquad \text{(ix)}$$

Therefore, the desired three-point backward difference formula is

$$\boxed{\left(\frac{\partial f}{\partial x}\right)_i \approx \frac{3f_i - 4f_{i-1} + f_{i-2}}{2\Delta x}, \qquad \text{TE} \sim O\left(\Delta x^2\right)} \qquad \text{(x)}$$

Similarly, we can derive a three-point forward difference formula which is given by

$$\boxed{\left(\frac{\partial f}{\partial x}\right)_i \approx \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2\Delta x}, \qquad \text{TE} \sim O\left(\Delta x^2\right)} \qquad \text{(x)}$$

12.3 POLYNOMIAL FITTING

A generic function $f(x)$ can be approximated by a polynomial as

$$f(x) = a_0 + a_1 x + a_2 x^2 + ... + a_n x^n \tag{12.12}$$

or

$$f(x) = a_0 + a_1(x - x_i)x + a_2(x - x_i)^2 + ... + a_n(x - x_i)^n \tag{12.13}$$

Coefficients a_0, a_1, a_2,.., a_n are determined by fitting the interpolation curve to function values at appropriate number of points. The second form given by Eq. (12.13) is usually preferred as it directly provides the expression for derivatives at point x_i, i.e.

$$\left(\frac{\partial f}{\partial x}\right)_i = a_1, \quad \left(\frac{\partial^2 f}{\partial x^2}\right)_i = 2a_2, \quad \left(\frac{\partial^3 f}{\partial x^3}\right)_i = 6a_3, \; .... \tag{12.14}$$

The order of approximation of the resulting finite difference approximation can obtained using Taylor series expansion. The following example illustrates the use of polynomial fitting for derivation of finite difference approximation for the first order derivative.

Example 12.2

Derive a three point central difference formula on non-uniform grid using polynomial fitting at points x_{i-1}, x_i and x_{i+1}.

Solution

We can fit the following quadratic curve through three points x_{i-1}, x_i and x_{i+1}:

$$f(x) \approx a_0 + a_1(x - x_i)x + a_2(x - x_i^2) \tag{i}$$

The first order derivative at point x_i is a_1. To obtain the value of a_1, we fit the interpolation curve (i) to the function values at points x_{i-1}, x_i and x_{i+1}, which results in the following set of linear equations:

$$f_i = a_0 \tag{ii}$$

$$f_{i-1} = f_i + a_1(-\Delta x_i) + a_2(-\Delta x_i)^2 \tag{iii}$$

$$f_{i+1} = f_i + a_1(\Delta x_{i+1}) + a_2(\Delta x_{i+1})^2 \tag{iv}$$

Multiply Eq. (iv) by Δx_i^2 and subtract it from $\Delta x_{i+1}^2 \times$ Eq. (iii) to obtain

$$a_1 \Delta x_{i+1} \Delta x_i (\Delta x_i + \Delta x_{i+1}) = \Delta x_i^2 f_{i+1} - \Delta x_{i+1}^2 f_{i-1} + f_i(\Delta x_{i+1}^2 - \Delta x_i) \tag{v}$$

Rearrangement of the preceding equation gives value of coefficient a_1, and thereby an approximation for the first order derivative given by

$$\left(\frac{\partial f}{\partial x}\right)_i \equiv a_1 = \frac{\Delta x_i^2 f_{i+1} - \Delta x_{i+1}^2 f_{i-1} + f_i(\Delta x_{i+1}^2 - \Delta x_i^2)}{\Delta x_{i+1} \Delta x_i (\Delta x_i + \Delta x_{i+1})} \tag{vi}$$

The preceding formula is identical to that given by Eq. (12.10) derived earlier using Taylor series expansion. Further, on a uniform grid, $\Delta x_i = \Delta x_{i+1} = \Delta x$, Eq. (vi) (or Eq. (12.10)) reduces to the standard CDS formula

$$\left(\frac{\partial f}{\partial x}\right)_i = \frac{f_{i+1} - f_{i-1}}{2\Delta x} \tag{vii}$$

as expected.

Let us note that other polynomials, splines or shape functions can be used to approximate the function, and thereby obtain an approximate formula for the derivative. Using the procedure outlined above, we can obtain higher order approximations. For example, by fitting a cubic polynomial to four points, the following third order approximations can be obtained on a uniform grid (Ferziger and Peric, 2003):

$$\left(\frac{\partial f}{\partial x}\right)_i = \frac{2f_{i+1} + 3f_i - 6f_{i-1} + f_{i-2}}{6\Delta x} + O((\Delta x)^3) \tag{12.15}$$

$$\left(\frac{\partial f}{\partial x}\right)_i = \frac{-f_{i+2} + 6f_{i+1} - 3f_i - 2f_{i-1}}{6\Delta x} + O((\Delta x)^3) \tag{12.16}$$

The preceding approximations are third order BDS and third order FDS respectively. These schemes are very useful in convective transport problem where these are referred as *upwind difference schemes* (UDS).

In general, approximation of the first derivative obtained using polynomial fitting has the truncation error of the same order as the degree of polynomial (Ferziger and Peric, 2003).

REFERENCES

Chung, T. J. (2010). *Computational Fluid Dynamics*. 2nd Ed., Cambridge University Press, Cambridge, UK.

Ferziger, J. H. And Perić, M. (2003). *Computational Methods for Fluid Dynamics*. Springer.