Chapter 3

An Introduction to

Finite Difference Calculus

Taylor Table

Second derivative

$$\left(\frac{\partial^۲ u}{\partial x^۲}\right)_j + \frac{۱}{\Delta x^۲}(au_{j-۱} + bu_j + cu_{j+۱}) = ?$$

	u_j	$\left(\frac{\partial u}{\partial x}\right)_j \Delta x$	$\left(\frac{\partial^۲ u}{\partial x^۲}\right)_j \Delta x^۲$	$\left(\frac{\partial^۳ u}{\partial x^۳}\right)_j \Delta x^۳$	$\left(\frac{\partial^۴ u}{\partial x^۴}\right)_j \Delta x^۴$
$\left(\frac{\partial^۲ u}{\partial x^۲}\right)_j \Delta x^۲$	۰	۰	۱	۰	۰
$a \cdot u_{j-۱}$	a	$a \cdot (-۱) \cdot \frac{۱}{۱}$	$a \cdot (-۱)^۲ \cdot \frac{۱}{۲}$	$a \cdot (-۱)^۳ \cdot \frac{۱}{۶}$	$a \cdot (-۱)^۴ \cdot \frac{۱}{۲۴}$
$b \cdot u_j$	b	۰	۰	۰	۰
$c \cdot u_{j+۱}$	c	$c \cdot (۱) \cdot \frac{۱}{۱}$	$c \cdot (۱)^۲ \cdot \frac{۱}{۲}$	$c \cdot (۱)^۳ \cdot \frac{۱}{۶}$	$c \cdot (۱)^۴ \cdot \frac{۱}{۲۴}$

$$cu_{j+۱} = cu_j + c \cdot (۱) \cdot \frac{۱}{۱}\Delta x \cdot \left(\frac{\partial u}{\partial x}\right)_j + c \cdot (۱)^۲ \cdot \frac{۱}{۲}\Delta x^۲ \cdot \left(\frac{\partial^۲ u}{\partial x^۲}\right)_j$$
$$+ c \cdot (۱)^۳ \cdot \frac{۱}{۶}\Delta x^۳ \cdot \left(\frac{\partial^۳ u}{\partial x^۳}\right)_j + c \cdot (۱)^۴ \cdot \frac{۱}{۲۴}\Delta x^۴ \cdot \left(\frac{\partial^۴ u}{\partial x^۴}\right)_j$$

Taylor Table

First derivative

$$\left(\frac{\partial u}{\partial x}\right)_j + \frac{۱}{\Delta x}(au_{j-۲} + bu_{j-۱} + cu_j) = ?$$

	u_j	$\left(\frac{\partial u}{\partial x}\right)_j \Delta x$	$\left(\frac{\partial^۲ u}{\partial x^۲}\right)_j \Delta x^۲$	$\left(\frac{\partial^۳ u}{\partial x^۳}\right)_j \Delta x^۳$	$\left(\frac{\partial^۴ u}{\partial x^۴}\right)_j \Delta x^۴$
$\Delta x \cdot \left(\frac{\partial u}{\partial x}\right)_j$	۰	۱	۰	۰	۰
$a \cdot u_{j-۲}$	a	$a \cdot (-۲) \cdot \frac{۱}{۱}$	$a \cdot (-۲)^۲ \cdot \frac{۱}{۲}$	$a \cdot (-۲)^۳ \cdot \frac{۱}{۶}$	$a \cdot (-۲)^۴ \cdot \frac{۱}{۲۴}$
$b \cdot u_{j-۱}$	b	$b \cdot (-۱) \cdot \frac{۱}{۱}$	$b \cdot (-۱)^۲ \cdot \frac{۱}{۲}$	$b \cdot (-۱)^۳ \cdot \frac{۱}{۶}$	$b \cdot (-۱)^۴ \cdot \frac{۱}{۲۴}$
$c \cdot u_j$	c	۰	۰	۰	۰

Obtaining difference methods from arbitrary order

$$\left(\frac{\partial^۲ u}{\partial x^۲}\right)_j + \frac{۱}{\Delta x^۲}(au_{j-۱} + bu_j + cu_{j+۱}) = ?$$

	u_j	$\left(\frac{\partial u}{\partial x}\right)_j \Delta x$	$\left(\frac{\partial^۲ u}{\partial x^۲}\right)_j \Delta x^۲$	$\left(\frac{\partial^۳ u}{\partial x^۳}\right)_j \Delta x^۳$	$\left(\frac{\partial^۴ u}{\partial x^۴}\right)_j \Delta x^۴$
$\left(\frac{\partial^۲ u}{\partial x^۲}\right)_j \Delta x^۲$	۰	۰	۱	۰	۰
$a \cdot u_{j-۱}$	a	$a \cdot (-۱) \cdot \frac{۱}{۱}$	$a \cdot (-۱)^۲ \cdot \frac{۱}{۲}$	$a \cdot (-۱)^۳ \cdot \frac{۱}{۶}$	$a \cdot (-۱)^۴ \cdot \frac{۱}{۲۴}$
$b \cdot u_j$	b	۰	۰	۰	۰
$c \cdot u_{j+۱}$	c	$c \cdot (۱) \cdot \frac{۱}{۱}$	$c \cdot (۱)^۲ \cdot \frac{۱}{۲}$	$c \cdot (۱)^۳ \cdot \frac{۱}{۶}$	$c \cdot (۱)^۴ \cdot \frac{۱}{۲۴}$

$$\begin{bmatrix} ۱ & ۱ & ۱ \\ -۱ & ۰ & ۱ \\ ۱ & ۰ & ۱ \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} ۰ \\ ۰ \\ -۲ \end{bmatrix} \longrightarrow [a, b, c] = -[۱, -۲, ۱]$$

The columns whose summation is not zero, indicate the error value.

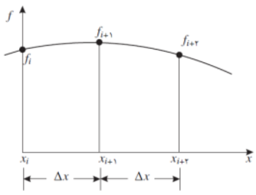
$$T.E. = \frac{۱}{\Delta x^۲}\left[\frac{a}{۲۴} + \frac{c}{۲۴}\right]\Delta x^۴ \left(\frac{\partial^۴ u}{\partial x^۴}\right)_j = -\frac{\Delta x^۲}{۱۲}\left(\frac{\partial^۴ u}{\partial x^۴}\right)_j$$

Finite Difference by Polynomials

The second procedure for approximating a derivate is to represent the function as a polynomial. The coefficients of the polynomial are computed by substitution of data (dependent variable) from a series of usually equally spaced points of the independent variable.

For example, consider a second-order polynomial (shown in the figure below):

$$f(x) = Ax^2 + Bx + C$$



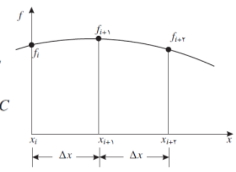
Finite Difference by Polynomials

Select the origin at x_i. Thus $x_i = 0$, $x_{i+1} = \Delta x$ and $x_{i+2} = 2\Delta x$

$$f_i = Ax_i^2 + Bx_i + C = C$$

$$f_{i+1} = Ax_{i+1}^2 + Bx_{i+1} + C = A(\Delta x)^2 + B(\Delta x) + C$$

$$f_{i+2} = Ax_{i+2}^2 + Bx_{i+2} + C = A(2\Delta x)^2 + B(2\Delta x) + C$$



From which it follows that:

$$C = f_i$$

$$B = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2\Delta x}$$

$$A = \frac{f_{i+2} - 2f_{i+1} + f_i}{2(\Delta x)^2}$$

Finite Difference by Polynomials

Now computing the first derivative

$$\frac{\partial f}{\partial x} = 2Ax + B$$

At $x_i = 0$

$$\left.\frac{\partial f}{\partial x}\right|_i = B \longrightarrow B = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2\Delta x}$$

Therefore,

$$\frac{\partial f}{\partial x} = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2\Delta x}$$

Which is identical to second-order accurate forward difference expression obtained from Taylor series.

The second derivative of function may be determined as:

$$\partial^2 f/\partial x^2 = 2A \longrightarrow A = \frac{f_{i+2} - 2f_{i+1} + f_i}{2(\Delta x)^2}$$

Finite Difference by Polynomials

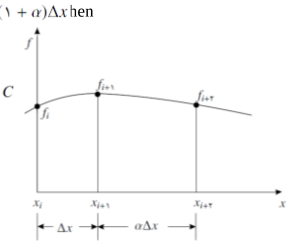
If the spacing of points i, i+1 and i+2 is not identical as shown in the figure, a finite difference approximation of the derivative is found by the same procedure.

Assume $x_i = 0$, $x_{i+1} = \Delta x$ and $x_{i+2} = (1+\alpha)\Delta x$ then

$$f_i = C$$

$$f_{i+1} = A(\Delta x)^2 + B(\Delta x) + C$$

$$f_{i+2} = A(1+\alpha)^2(\Delta x)^2 + B(1+\alpha)(\Delta x) + C$$



From which it follows that:

$$C = f_i$$

$$B = \frac{-f_{i+2} + (1+\alpha)^2 f_{i+1} - (\alpha^2 + 2\alpha) f_i}{\alpha(1+\alpha)\Delta x}$$

$$A = \frac{f_{i+2} - (1+\alpha) f_{i+1} + \alpha f_i}{\alpha(1+\alpha)(\Delta x)^2}$$

Finite Difference by Polynomials

Now computing the first derivative of function, one has

$$\frac{\partial f}{\partial x} = 2Ax + B$$

At $x_i = 0$

$$\left.\frac{\partial f}{\partial x}\right|_i = B \longrightarrow B = \frac{-f_{i+2} + (1+\alpha)^2 f_{i+1} - (\alpha^2 + 2\alpha) f_i}{\alpha(1+\alpha)\Delta x}$$

Therefore,

$$\left.\frac{\partial f}{\partial x}\right|_i = \frac{-f_{i+2} + (1+\alpha)^2 f_{i+1} - \alpha(\alpha+2) f_i}{\alpha(1+\alpha)\Delta x}$$

The second derivative of function can be determined as:

$$\partial^2 f/\partial x^2 = 2A \longrightarrow A = \frac{f_{i+2} - (1+\alpha) f_{i+1} + \alpha f_i}{\alpha(1+\alpha)(\Delta x)^2}$$

Therefore,

$$\frac{\partial^2 f}{\partial x^2} = 2\left[\frac{f_{i+2} - (1+\alpha) f_{i+1} + \alpha f_i}{\alpha(1+\alpha)(\Delta x)^2}\right]$$

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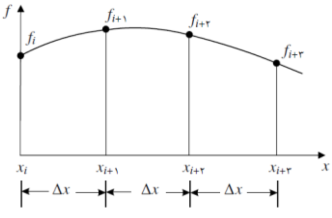
Example

Determine the approximate forward difference representation for $\partial^3 f/\partial x^3$ which is of the order Δx, by means of

A) Taylor series expansion

B) A third-degree polynomial passing through four points



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Solution

A) Taylor series expansions

$$f(x+\Delta x) = f(x) + \Delta x\frac{\partial f}{\partial x} + \frac{(\Delta x)^2}{2!}\frac{\partial^2 f}{\partial x^2} + \frac{(\Delta x)^3}{3!}\frac{\partial^3 f}{\partial x^3} + O(\Delta x)^4$$

$$f(x+2\Delta x) = f(x) + 2\Delta x\frac{\partial f}{\partial x} + \frac{(2\Delta x)^2}{2!}\frac{\partial^2 f}{\partial x^2} + \frac{(2\Delta x)^3}{3!}\frac{\partial^3 f}{\partial x^3} + O(2\Delta x)^4$$

$$f(x+3\Delta x) = f(x) + 3\Delta x\frac{\partial f}{\partial x} + \frac{(3\Delta x)^2}{2!}\frac{\partial^2 f}{\partial x^2} + \frac{(3\Delta x)^3}{3!}\frac{\partial^3 f}{\partial x^3} + O(3\Delta x)^4$$

The three simultaneous equations can be solved for $\partial^3 f/\partial x^3$

Then:

$$\frac{\partial^3 f}{\partial x^3} = \frac{f_{i+3} - 3f_{i+2} + 3f_{i+1} - f_i}{(\Delta x)^3} + O(\Delta x)$$

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Solution

B) Fitting the third-degree polynomial $f(x) = Ax^3 + Bx^2 + Cx + D$ through the four equally spaced points. One can obtain:

$$f_{i+3} = A(3\Delta x)^3 + B(3\Delta x)^2 + C(3\Delta x) + D$$
$$f_{i+2} = A(2\Delta x)^3 + B(2\Delta x)^2 + C(2\Delta x) + D$$
$$f_{i+1} = A(\Delta x)^3 + B(\Delta x)^2 + C(\Delta x) + D$$
$$f_i = D$$

From which it follows that:

$$C = \frac{2f_{i+3} - 9f_{i+2} + 18f_{i+1} - 11f_i}{6\Delta x}$$

$$B = \frac{-3f_{i+3} + 12f_{i+2} - 15f_{i+1} + 6f_i}{6(\Delta x)^2} \qquad D = f_i$$

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Solution

Now, the derivative of *f(x)* are determined as

$$\frac{\partial f}{\partial x} = 3Ax^2 + 2Bx + C, \quad \frac{\partial^2 f}{\partial x^2} = 6Ax + 2B, \quad \frac{\partial^3 f}{\partial x^3} = 6A$$

Therefore,

$$\frac{\partial^3 f}{\partial x^3} = \frac{f_{i+3} - 3f_{i+2} + 3f_{i+1} - f_i}{(\Delta x)^3} + O(\Delta x)$$

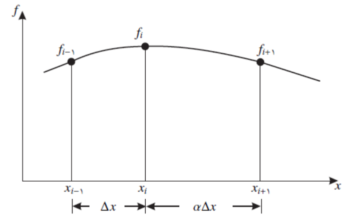
In addition, the first and second derivatives at *i*, where *x* is zero, are obtained easily as

$$\frac{\partial^2 f}{\partial x^2} = 2B = \frac{-f_{i+3} + 4f_{i+2} - 5f_{i+1} + 2f_i}{(\Delta x)^2} + O(\Delta x)^2$$

$$\frac{\partial f}{\partial x} = C = \frac{2f_{i+3} - 9f_{i+2} + 18f_{i+1} - 11f_i}{6\Delta x} + O(\Delta x)^3$$

Example

Determine a central difference approximation $\partial f/\partial x$ for the unequally spaced grid points by polynomial technique.



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Solution

The second-order polynomial is passed through the points $x_i = 0$, $x_{i+1} = \alpha \Delta x$ and $x_{i-1} = -\Delta x$

Thus,

$$f_{i-1} = A(-\Delta x)^2 + B(-\Delta x) + C$$

$$f_i = C$$

$$f_{i+1} = A(\alpha \Delta x)^2 + B(\alpha \Delta x) + C$$

Solving for the coefficients A, B and C, one finds

$$A = \frac{f_{i+1} - (\alpha + 1)f_i + \alpha f_{i-1}}{\alpha(\alpha + 1)(\Delta x)^2}$$

$$B = \frac{f_{i+1} + (\alpha^2 - 1)f_i - \alpha^2 f_{i-1}}{\alpha(\alpha + 1)(\Delta x)}$$

$$C = f_i$$

Solution

The first derivative of the function is

$$\frac{\partial f}{\partial x} = 2Ax + B$$

Which at point x_i reduces to B. Therefore,

$$\frac{\partial f}{\partial x} = \frac{f_{i+1} + (\alpha^2 - 1)f_i - \alpha^2 f_{i-1}}{\alpha(\alpha + 1)(\Delta x)} + O(\Delta x)^2$$

Note that for $\alpha = 1$ the expression reduces to $\frac{\partial f}{\partial x} = \frac{f_{i+1} - f_{i-1}}{2(\Delta x)} + O(\Delta x)^2$