A GENERAL FORMULA FOR THE NUMERICAL DIFFERENTIATION OF A FUNCTION

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Abstract. A general formula is derived of which various types of finite difference formulae for first derivatives are particular cases. Also, differentiation of the formula generates general finite difference formulae for higher derivatives.

1. Introduction

Numerical solution of a differential equation (ordinary or partial) by a finite difference method involves an approximation of the derivatives by suitable difference formulae. The accuracy of the numerical solution depends upon the number of grid points in the integration domain and upon the number of grid points used in the finite difference formulae. Derivation of the finite difference formula for the derivatives involves increasingly tedious mathematical analysis as the number of nodal points increases. Here, using Lagrange's interpolation formula, a general method is derived from which we can obtain the various types of the finite difference formulae by assigning suitable values to appropriate parameters. The general formula also facilitates the generation of finite difference formulae for higher derivatives by differentiation.

2. Analysis

An approximation to a function $f(x)$ can be obtained by using Lagrange's interpolation formula [1, p. 83]

$$f(x) = \sum_{j=0}^{n} l_j(x) f_j, \tag{2.1}$$

where f_j stands for $f(x_j)$ while $l_j(x)$ is as follows:

$$I_j(x) = \frac{\pi(x)}{(x - x_j)\,\pi'(x_j)}. \tag{2.2}$$

In the above equation, prime denotes differentiation with respect to x and

$$\pi(x) = (x - x_0)(x - x_1)\ldots(x - x_n). \tag{2.3}$$

The truncation error $E_n(x)$ in the evaluation of $f(x)$ is given by

$$E_n(x) = \frac{\pi(x)}{(n+1)!} f^{n+1}(\xi), \tag{2.4}$$

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where ξ lies in the interval $[x_0, x_n]$. Let the interval $[x_0, x_n]$ be divided into n equal subintervals of width h such that $a = x_0 < x_1 < x_2 < ... < x_n = b$, then $x_n = x_0 + nh$. Further, $f^{n+1}(\xi)$ denotes the $(n+1)^{\text{th}}$ derivative of $f(\xi)$.

By setting

$$x - x_0 = sh, x - x_1 = (s-1)h, ..., x - x_n = (s-n)h, \tag{2.5}$$

equation (2.1) may be expressed as

$$\begin{aligned} f(x) &= (-1)^n \frac{(s-1)(s-2)...(s-n)}{n!} f_0 \\ &+ (-1)^{n-1} \frac{s(s-2)(s-3)...(s-n)}{1!(n-1)!} f_1 \\ &+ (-1)^{n-2} \frac{s(s-1)(s-3)...(s-n)}{2!(n-2)!} f_2 + ... \\ &+ \frac{s(s-1)...(s-n-1)}{n!} f_n \\ &= \frac{(-1)^n}{n! a_{0n}} \left(\sum_{k=0}^{n} a_0 s^k \right) f_0 + \sum_{j=1}^{n} \left\{ \frac{(-1)^{n-j}}{j!(n-j)! a_{jn}} \left(\sum_{k=1}^{n} a_{jk} s^k \right) \right\} f_j, \end{aligned} \tag{2.6}$$

where a_{0k} $(k = 0, 1, ..., n)$ are cofactors of s^k $(k = 0, 1, 2, ..., n)$ in the determinant D, which is given as

$$D = \begin{vmatrix} s^n & s^{n-1} & s^{n-2} & \cdots & s^2 & s & 1 \\ 1 & 1 & 1 & \cdots & 1 & 1 & 1 \\ 2^n & 2^{n-1} & 2^{n-2} & \cdots & 2^2 & 2 & 1 \\ - & - & - & \cdots & - & - & - \\ - & - & - & \cdots & - & - & - \\ n^n & n^{n-1} & n^{n-2} & \cdots & n^2 & n & 1 \end{vmatrix}. \tag{2.7}$$

However, a_{jk} $(j = 1, 2, ..., n; k = 1, 2, ..., n)$ are cofactors of s^{k-1} $(k = 1, 2, ..., n)$ in the determinants which are obtained by removing the first column and the $(j+i)^{\text{th}}$ row in the determinant D.

Substituting equation (2.5) into equation (2.4), the error term E_n becomes

$$\begin{aligned} E_n &= \frac{h^{n+1}}{(n+1)!} f^{n+1}(\xi) s(s-1)(s-2)...(s-n) \\ &= \frac{h^{n+1} f^{n+1}(\xi)}{(n+1)! a_{0n}} \left(\sum_{k=0}^{n} a_{0k} s^{k+1} \right). \end{aligned} \tag{2.8}$$

From equation (2.6), the first derivative of $f(x)$ is given by

$$\begin{aligned} f'(x) &= \frac{1}{h} \left[\frac{(-1)^n}{n! a_{0n}} \left(\sum_{k=1}^{n} k a_{0k} s^{k-1} \right) f_0 \right. \\ &\left. + \sum_{j=1}^{n} \left\{ \frac{(-1)^{n-j}}{j!(n-j)! a_{jn}} \left(\sum_{k=1}^{n} k a_{jk} s^{k-1} \right) \right\} f_j \right]. \end{aligned} \tag{2.9}$$

The error of approximation in the evaluation of $f'(x)$ is as follows:

$$E'_n = \frac{h^n}{(n+1)!} \cdot \frac{f^{n+1}(\xi)}{a_{0n}} \left\{ \sum_{k=0}^{n} (k+1)\, a_{0k} s^k \right\}. \tag{2.10}$$

From equation (2.9), we can obtain $f'(x)$ at $x = x_0, x_1, x_2, ..., x_n$ for $s = 0, 1, 2, ..., n$. It should be noted that for $s = 0$, $\frac{n}{2}$ and n, equation (2.9) will give forward, central and backward difference formulae respectively. Further differentiation of equation (2.9) will give difference formulae for higher derivatives of $f(x)$.

3. Particular Cases

For $n = 1$, the determinant D reveals that $a_{00} = -1$, $a_{01} = 1$, $a_{11} = 1$ and as a result of these values, equation (2.9) gives

$$f'(x) = \frac{f_1 - f_0}{h}. \tag{3.1}$$

The error term E'_1 form equation (2.10) is obtained as $\frac{h(-1+2s)f''(\xi)}{2}$. It clearly shows that errors in the case of forward and backward difference formulae are $\frac{-hf''(\xi)}{2}$ and $\frac{hf''(\xi)}{2}$ respectively.

For $n = 2$, the determinant D is as follows:

$$\begin{vmatrix} s^2 & s & 1 \\ 1 & 1 & 1 \\ 4 & 2 & 1 \end{vmatrix}.$$

From the above determinant, we have $a_{00} = -2$, $a_{01} = 3$, $a_{02} = -1$; $a_{11} = -2, a_{12} = 1; a_{21} = -1, a_{22} = 1$. On substitution of the values of these parameters, equation (2.9) results in

$$f'(x) = \frac{[(-3+2s) f_0 + 4(1-s) f_1 + (-1+2s) f_2]}{2h}. \tag{3.2}$$

For $s = 0, 1$ and 2, the respective formulae are as follows:

$$\begin{aligned} \text{Forward difference} &= \frac{-3f_0 + 4f_1 - f_2}{2h}, \\ \text{Central difference} &= \frac{f_2 - f_0}{2h}, \\ \text{Backward difference} &= \frac{f_0 - 4f_1 + 3f_2}{2h}. \end{aligned}$$

For this case, error E'_2 from (2.10) is obtained as $\frac{(2-6s+3s^2)h^2 f'''(\xi)}{6}$. It shows that local truncation errors for the above cases are $\frac{h^2 f'''(\xi)}{3}$, $\frac{-h^2 f'''(\xi)}{6}$ and $\frac{h^2 f'''(\xi)}{3}$ respectively.

Differentiation of equation (3.2) gives readily the difference formula for second derivatives as

$$f''(x) = \frac{f_0 - 2f_1 + f_2}{h^2}. \tag{3.3}$$

When we consider $n = 3$, the determinant D takes the form

$$\begin{vmatrix} s^3 & s^2 & s & 1 \\ 1 & 1 & 1 & 1 \\ 8 & 4 & 2 & 1 \\ 27 & 9 & 3 & 1 \end{vmatrix}.$$

The above determinant implies that $a_{00} = 12$, $a_{01} = -22$, $a_{02} = 12$, $a_{03} = -2$; $a_{11} = -6$, $a_{12} = 5$, $a_{13} = -1$; $a_{21} = -6$, $a_{22} = 8$, $a_{23} = -2$, $a_{31} = -2$, $a_{32} = 3$, $a_{33} = -1$. On application of these values, formula (2.9) gives

$$f'(x) = \frac{\left(-11 + 12s - 3s^2\right) f_0 + 3\left(6 - 10s + 3s^2\right) f_1}{6h} + \frac{+3\left(-3 + 8s - 3s^2\right) f_2 + \left(2 - 6s + 3s^2\right) f_3}{6h}, \tag{3.4}$$

which yields

$$f'(x_0) = \frac{(-11f_0 + 18f_1 - 9f_2 + 2f_3)}{6h}$$

and

$$f'(x_3) = \frac{(-2f_0 + 9f_1 - 18f_2 + 11f_3)}{6h}$$

respectively for $s = 0$ and 3.

The associated error term from equation (2.10) is obtained as follows:

$$E_3' = \frac{-h^3\left(3 - 11s + 9s^2 - 2s^3\right) f^{iv}(\xi)}{12} \tag{3.5}$$

and for the above cases, the truncation errors are $\frac{-h^3 f^{iv}(\xi)}{4}$ and $\frac{h^3 f^{iv}(\xi)}{4}$ respectively.

Differentiation of equation (3.4) produces

$$f''(x) = \frac{[(2 - s) f_0 - (5 - 3s) f_1 + (4 - 3s) f_2 - (1 - s) f_3]}{h^2} \tag{3.6}$$

which, for $s = 0$ and 3, results in

$$f''(x_0) = \frac{(2f_0 - 5f_1 + 4f_2 - f_3)}{h^2}$$

and

$$f''(x_3) = \frac{(-f_0 + 4f_1 - 5f_2 + 2f_3)}{h^2}$$

respectively. Differentiation of (3.5) will give the error term for equation (3.6). Again equation (3.6) implies that

$$f'''(x) = \frac{(-f_0 + 3f_1 - 3f_2 + f_3)}{h^3}, \tag{3.7}$$

which is the difference formula for the third derivative in terms of the function at the four points.

For five point difference formulae, n is 4 and, from equation (2.7), we find that $a_{00} = 288$, $a_{01} = -600$, $a_{02} = 420$, $a_{03} = -120$, $a_{04} = 12$; $a_{11} = 48$, $a_{12} = -52$, $a_{13} = 18$, $a_{14} = -2$; $a_{21} = 72$, $a_{22} = -114$, $a_{23} = 48$, $a_{24} = -6$; $a_{31} = 48$,

$a_{32} = -84$, $a_{33} = 42$, $a_{34} = -6$; $a_{41} = 12$, $a_{42} = -22$, $a_{43} = 12$, $a_{44} = -2$. On application of these values, formula (2.9) gives

$$\begin{aligned} f'(x) &= \frac{\left(-25+35s-15s^2+2s^3\right)f_0+\left(24-52s+27s^2-4s^3\right)f_1}{12h} \\ &+\frac{2\left(6-19s+12s^2-2s^3\right)f_2+2\left(8-28s+21s^2-4s^3\right)f_3}{12h} \\ &-\frac{\left(3-11s+9s^2-2s^3\right)f_4}{12h} \end{aligned} \tag{3.8}$$

which will give forward, central and backward difference formulae in terms of five points for $s = 0, 2$ and 4 respectively. In order, they are as follows:

$$\begin{aligned} f'(x_0) &= \frac{(-25f_0+48f_1-36f_2+16f_3-3f_4)}{12h}, \\ f'(x_2) &= \frac{(f_0-8f_1+8f_3-f_4)}{12h}, \\ f'(x_4) &= \frac{(3f_0-16f_1+36f_2-48f_3+25f_4)}{12h}. \end{aligned}$$

For other values of s, i.e., 1 and 3, we can get the difference formulae for $f'(x_1)$ and $f'(x_3)$ from equation (3.8). The error of approximation associated with equation (3.8) is obtained as

$$E_4' = \frac{\left(24-100s+105s^2-40s^3+5s^4\right)h^4 f^v(\xi)}{120} \tag{3.9}$$

from equation (2.10). The above equation implies that local truncation errors corresponding to the forward, central and backward difference formulae are $\frac{h^4 f^v(\xi)}{5}$, $\frac{h^4 f^v(\xi)}{30}$ and $\frac{h^4 f^v(\xi)}{5}$ respectively.

Differentiation of equation (3.8) gives difference formulae corresponding to second derivatives as

$$\begin{aligned} f''(x) &= \frac{\left(35-30s+6s^2\right)f_0+4\left(-26+27s-6s^2\right)f_1}{12h^2} \\ &-\frac{6\left(-19+24s-6s^2\right)f_2-4\left(-14+21s-6s^2\right)f_3}{12h^2} \\ &-\frac{\left(-11+18s-6s^2\right)f_4}{12h^2}. \end{aligned} \tag{3.10}$$

For $s = 0, 2$ and 4, respective difference formulae are as follows:

$$\begin{aligned} f''(x_0) &= \frac{(35f_0-104f_1+114f_2-56f_3+11f_4)}{12h^2}, \\ f''(x_2) &= \frac{(-f_0+16f_1-30f_2+16f_3-f_4)}{12h^2}, \\ f''(x_4) &= \frac{(11f_0-56f_1+114f_2-104f_3+35f_4)}{12h^2}. \end{aligned}$$

If we differentiate equation (3.10), we have

$$\begin{aligned} f'''(x) &= \frac{(-5+2s)f_0+2(9-4s)f_1-12(2-s)f_2}{2h^3} \\ &+\frac{2(7-4s)f_3-(3-2s)f_4}{2h^3} \end{aligned} \tag{3.11}$$

from which backward, central and forward finite difference formulae can be obtained for $s = 0, 2$ and 4 respectively. A differentiation of (3.11) leads to

$$f^{iv}(x) = \frac{(f_0 - 4f_1 + 6f_2 - 4f_3 + f_4)}{h^4}, \tag{3.12}$$

which is the central difference formula for fourth derivatives of a function in terms of the function at five points. The formulation of various difference formulae for first derivatives clearly suggests that the finite difference formulae in terms of any number of points can be obtained with the help of equations (2.7) and (2.9) . The mathematical expressions resulting due to further differentiation of equation (2.9) are giving finite difference formulae for higher derivatives.

4. Conclusion

The general formula given by equation (2.9) can be used to obtain the finite difference formulae for first derivative at any point of subintervals by assigning suitable values to s and n. Finite difference formulae of higher derivatives can also be obtained by further differentiation of equation (2.9) . A scientific program of the formula (2.9) as well as its differential will facilitate the use of any finite difference formulae of desired derivatives.

References

[1] F.B. Hildebrand, *Introduction to Numerical Analysis,* Mc Graw Hill, Inc, New York (1974).

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