Finite Difference Approximation Formulae for Derivatives on Random, Asymmetric, One-Dimensional Grids

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Abstract

The approximation of derivatives on uniform grids is a fairly academic exercise encountered in most introductory numerical analysis classes. Typically the grids reach forwards, backwards, or are centered on a given point. After successfully deriving a few simple examples, one usually obtains these approximations by referring to a finite selection of common examples found in most math tables. However, grid possibilities are endless and their publication would fill infinite volumes. This paper presents a simple method that demonstrates the derivation of finite difference approximations for any derivative on any random grid scheme. The method invokes the use of Taylor series polynomials, Cramer's rule, Vandermonde matrices, and Schur polynomials.

Key Words finite difference formulae, numerical differentiation, Taylor series, Vandermonde matrix, Schur polynomials, random one-dimensional grids.

1 Introduction

Numerical differentiation is useful for approximating rates of change for data where a function is unknown. A sampling of such formulae on uniform one-dimensional grids is provided in CRC's Standard Mathematical Tables and Formulae [14]. Beyond these, pencil and paper derivations are possible. Though conceptually simple, this approach is time consuming. Several authors have developed algorithms for use in concert with computers that solve for such approximations using various uniform and non-uniform grid schemes. In an earlier work Keller and Pereyara present weight tables for derivatives of high order and accuracy on uniform grids [5]. Latter Fornberg noted isolated, systematic error's in this work and prescribed a scheme that utilizes simple recursion relations in which he reproduces corrected weight tables, again on uniform grids [3]. In both papers examples of one-sided, centered, and "half-way point" schemes are utilized. Fornberg advances his algorithms to non-uniform grids in [4]. Khan and Ohba present closed form expressions for finite difference approximations for use in digital differentiators [6, 7, 8, 9]. In these papers, data tables are produced that show derivative approximations for sample digital inputs, however, Khan and Ohba did not derive formulae to determine finite difference weights. None of the above mentioned papers provided error estimates for the approximations.

In this paper, a closed form expression is derived that can be used to approximate any order derivative to any order accuracy on uniform, non-uniform, or random one-dimensional grids. The resulting equation produces Taylor series weights as well as error estimates and works equally well for forward, backward, centered, and non-centered schemes. Approximation formulae can be obtained for random grid schemes as well with out additional computational complexity. In Section 2 a general, closed form solution is derived. In Section 3 the method is demonstrated by reproducing a five-point forward-difference approximation of the first derivative that is found in [14]. Section 4 demonstrates the method to on a four-point, non-uniform, asymmetric grid where grid-points have non-integer values.

2 A General Case

We start with a general Taylor series expansion (with error term):

$$f_a = \frac{(ah)^0}{0!} f_{_0} + \frac{(ah)^1}{1!} f_{_0}^{^{(1)}} + ... + \frac{(ah)^n}{n!} f_{_0}^{^{(n)}} + \frac{(ah)^{n+1}}{(n+1)!} f^{^{(n+1)}}(\xi), \qquad (1)$$

where a is a real number that represents the relative position from the point of interest x_0 on a one-dimensional grid and h is the grid spacing. Here $f_a = f(x_0 + ah)$. Note that if $a = 0$ and if we define $0^0 = 1$ then (1) correctly becomes $f_0 = f_0$.

Assume now that we use a random grid scheme with $r+1$ points to approximate a derivative of order $d \leq r$. The grid points are represented by real numbers a_1 through a_{r+1}. The system of Taylor series expressions generated at each grid point is:

$$\begin{array}{cccccccc}
f_{a_1} \approx & \frac{(a_1h)^0}{0!} f_{_0} & + \ldots + & \frac{(a_1h)^d}{d!} f_{_0}^{(d)} & + \ldots + & \frac{(a_1h)^r}{r!} f_{_0}^{(r)}, \\
\vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\
f_{a_d} \approx & \frac{(a_dh)^0}{0!} f_{_0} & + \ldots + & \frac{(a_dh)^d}{d!} f_{_0}^{(d)} & + \ldots + & \frac{(a_dh)^r}{r!} f_{_0}^{(r)}, \\
\vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\
f_{a_{r+1}} \approx & \frac{(a_{r+1}h)^0}{0!} f_{_0} & + \ldots + & \frac{(a_{r+1}h)^d}{d!} f_{_0}^{(d)} & + \ldots + & \frac{(a_{r+1}h)^r}{r!} f_{_0}^{(r)}.
\end{array} \qquad (2)$$

Each equation in (2) has a remainder term of the form:

$$R_i <= \frac{(a_ih)^{r+1}}{(r+1)!} f_0^{(r+1)}(\xi). \qquad (3)$$

For the time being, the remainder is omitted from the derivation. Multiplying each equations in (2) by a real number weight Ω_{a_n}:

$$
\begin{array}{llllll}
\Omega_{a_1} f_{a_1} \approx & \Omega_{a_1} \frac{(a_1 h)^0}{0!} f_0 & + \ldots + & \Omega_{a_1} \frac{(a_1 h)^d}{d!} f_0^{(d)} & + \ldots + & \Omega_{a_1} \frac{(a_1 h)^r}{r!} f_0^{(r)}, \\
\vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\
\Omega_{a_d} f_{a_d} \approx & \Omega_{a_d} \frac{(a_d h)^0}{0!} f_0 & + \ldots + & \Omega_{a_d} \frac{(a_d h)^d}{d!} f_0^{(d)} & + \ldots + & \Omega_{a_d} \frac{(a_d h)^r}{r!} f_0^{(r)}, \\
\vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\
\Omega_{a_{r+1}} f_{a_{r+1}} \approx & \Omega_{a_{r+1}} \frac{(a_{r+1} h)^0}{0!} f_0 & + \ldots + & \Omega_{a_{r+1}} \frac{(a_{r+1} h)^d}{d!} f_0^{(d)} & + \ldots + & \Omega_{a_{r+1}} \frac{(a_{r+1} h)^r}{r!} f_0^{(r)},
\end{array}
\tag{4}
$$

and summing the weighted components to obtain the $f_0^{(d)}$ yields:

$$
\begin{array}{cccccccc}
\Omega_{a_1} \frac{a_1^0}{0!} f_0 & + \ldots + & \Omega_{a_d} \frac{a_d^0}{0!} f_0 & + \ldots + & \Omega_{a_{r+1}} \frac{a_{r+1}^0}{0!} f_0 & = 0, \\
\vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\
\Omega_{a_1} \frac{a_1^d}{d!} f_0^{(d)} & + \ldots + & \Omega_{a_d} \frac{a_d^d}{d!} f_0^{(d)} & + \ldots + & \Omega_{a_{r+1}} \frac{a_{r+1}^d}{d!} f_0^{(d)} & = f_0^{(d)}, \\
\vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\
\Omega_{a_1} \frac{a_1^r}{r!} f_0^{(r)} & + \ldots + & \Omega_{a_d} \frac{a_d^r}{r!} f_0^{(r)} & + \ldots + & \Omega_{a_{r+1}} \frac{a_{r+1}^r}{r!} f_0^{(r)} & = 0,
\end{array}
\tag{5}
$$

where $f_0^{(d)}$ is the approximation of the d^{th}-derivative at x_0. Equation (5) is algebraically simplified:

$$
\begin{array}{cccccc}
\Omega_{a_1} a_1^0 & + \ldots + & \Omega_{a_d} a_d^0 & + \ldots + & \Omega_{a_{r+1}} a_{r+1}^0 & = 0, \\
\vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\
\Omega_{a_1} a_1^d & + \ldots + & \Omega_{a_d} a_d^d & + \ldots + & \Omega_{a_{r+1}} a_{r+1}^d & = \frac{d!}{h^d}, \\
\vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\
\Omega_{a_1} a_1^r & + \ldots + & \Omega_{a_d} a_d^r & + \ldots + & \Omega_{a_{r+1}} a_{r+1}^r & = 0,
\end{array}
\tag{6}
$$

and rewritten in matrix form:

$$
\begin{bmatrix}
a_1^0 & \ldots & a_d^0 & \ldots & a_{r+1}^0 \\
\vdots & \ddots & \vdots & \ddots & \vdots \\
a_1^d & \ldots & a_d^d & \ldots & a_{r+1}^d \\
\vdots & \ddots & \vdots & \ddots & \vdots \\
a_1^r & \ldots & a_d^r & \ldots & a_{r+1}^r
\end{bmatrix}
\begin{bmatrix}
\Omega_{a_1} \\ \vdots \\ \Omega_{a_d} \\ \vdots \\ \Omega_{a_{r+1}}
\end{bmatrix}
=
\begin{bmatrix}
0 \\ \vdots \\ \frac{d!}{h^d} \\ \vdots \\ 0
\end{bmatrix}.
\tag{7}
$$

Cramer's rule is applied to solve for Ω_{a_1}:

$$\Omega_{a_1} = \frac{\begin{vmatrix} 0 & \dots & a_d^0 & \dots & a_{r+1}^0 \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \frac{d!}{h^d} & \dots & a_d^d & \dots & a_{r+1}^i \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & a_d^r & \dots & a_{r+1}^r \end{vmatrix}}{\begin{vmatrix} a_1^0 & \dots & a_d^0 & \dots & a_{r+1}^0 \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ a_1^i & \dots & a_d^d & \dots & a_{r+1}^i \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ a_1^r & \dots & a_d^r & \dots & a_{r+1}^r \end{vmatrix}}. \tag{8}$$

The denominator of (8) is a Vandermonde matrix $\mathbf{V}$ whose determinant is [1, 11]:

$$\prod_{1 \le i < j \le r+1} (a_j - a_i). \tag{9}$$

Using cofactor expansion, the numerator reduces to:

$$(-1)^{(C+R)} \frac{d!}{h^d} \begin{vmatrix} a_2^0 & \dots & a_d^0 & \dots & a_{r+1}^0 \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ a_2^{d-1} & \dots & a_d^{d-1} & \dots & a_{r+1}^{d-1} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ a_2^r & \dots & a_d^r & \dots & a_{r+1}^r \end{vmatrix}. \tag{10}$$

Here $R = d + 1$ and $C = w$ where w is the value associated with the index of the weight (in this case $w = 1$ since we are solving for Ω_{a_1}).

The matrix in (10) is an initial minor $\mathbf{M}_{(R,C)}$ of the original Vandermonde matrix $\mathbf{V}$ where R and C are the numerical values of the row and column removed from the matrix. In [2, 10, 12] it was shown that:

$$\det\left(\mathbf{M}_{(R,C)}\right) = s_\lambda(a_1, .., a_{n \neq C}, ..., a_n)\det(\overline{\mathbf{V}}), \tag{11}$$

where $\overline{\mathbf{V}}$ is a Vandermonde matrix with the a_C, or in this case the a_1, term removed. The expression s_λ is a Schur polynomial where $\lambda = r - d$. A

Schur polynomial in n variables is expressed as follows:

$$\begin{aligned}
s_0(a_1,...,a_n) &= 1, \\
s_1(a_1,...,a_n) &= \sum_{i=1}^{n} a_i, \\
s_2(a_1,...,a_n) &= \sum_{1\le i<j\le n} a_i a_j, \\
s_3(a_1,...,a_n) &= \sum_{1\le i<j<k\le n} a_i a_j a_k, \\
\vdots \quad & \quad \vdots \quad \quad \vdots \\
s_n(a_1,...,a_n) &= \prod_{i=1}^{n} a_i.
\end{aligned} \tag{12}$$

From (11) we obtain the determinant of $\mathbf{M}_{(R,C)}$ for the case $R = d+1$ and $C = w$:

$$\det\left(\mathbf{M}_{(d+1,w)}\right) = s_{(r-d)}(a_1,...,a_{n\neq w},...,a_{r+1}) \prod_{\substack{1\le i<j\le r+1 \\ i,j\neq w}} (a_j - a_i). \tag{13}$$

Equations (9) through (13) are used to generate the expression for the weight:

$$\Omega_{a_w} = (-1)^{(d+w+1)} \frac{d!}{h^d} \left(\frac{\displaystyle\prod_{\substack{1\le i<j\le r+1 \\ i,j\neq w}} (a_j - a_i)}{\displaystyle\prod_{1\le i<j\le r+1} (a_j - a_i)} \right) s_{(r-d)}(a_1,...,a_{n\neq w},...,a_{r+1}). \tag{14}$$

Simplifiaction via cancelation is possible:

$$\Omega_{a_w} = (-1)^{(d+w+1)} \frac{d!}{h^d} \left(\frac{s_{(r-d)}(a_1,...,a_{n\neq w},...,a_{r+1})}{\displaystyle\prod_{1\le i\neq w\le r+1} |(a_w - a_i)|} \right). \tag{15}$$

We now consider the remainder term in (3). Using it and the calculated weights from (15) allows us to calculate a combined error expression for the approximation:

$$R = \begin{bmatrix} \Omega_{a_1} & \dots & \Omega_{a_d} & \dots & \Omega_{a_{r+1}} \end{bmatrix} \begin{bmatrix} (a_1 h)^{r+1} \\ \vdots \\ (a_d h)^{r+1} \\ \vdots \\ (a_{r+1} h)^{r+1} \end{bmatrix} \frac{f^{(r+1)}(\xi)}{(r+1)!}, \tag{16}$$

where ξ can be any value within the range of the grid points. If (16) results in a value of $R = 0$, then the next term in the Taylor series must be used to obtain a remainder, i.e.:

$$R = \begin{bmatrix} \Omega_{a_1} & \dots & \Omega_{a_d} & \dots & \Omega_{a_{r+1}} \end{bmatrix} \begin{bmatrix} (a_1 h)^{r+2} \\ \vdots \\ (a_d h)^{r+2} \\ \vdots \\ (a_{r+1} h)^{r+2} \end{bmatrix} \frac{f^{(r+2)}(\xi)}{(r+2)!}, \tag{17}$$

Equations (15) through (17) can be used to calculate finite difference weights for derivative approximation formulae of any order on simple uniform grid schemes as found in standard mathematics tables or on more complex grid schemes the are asymmetric and/or non-uniform.

3 Deriving a Classic CRC Result

The method is demonstrated by reproducing a classical result found in [14] in which we determine a five-point forward-difference approximation on a uniform grid for the first derivative. Here h is the grid spacing and $a = \{0, 1, 2, 3, 4\}$. For the first derivative we use $d = 1$. Five grid points are used and therefore $r = 4$ and $\lambda = r - d = 3$. For the first weight Ω_{a_1}, or more succinctly represented as Ω_0 for this grid scheme, $w = 1$ (Note that w represents the position in the vector and not the actual values of a). Substituting these values into (15) generates:

$$\Omega_0 = (-1)^3 \frac{1!}{h} \frac{s_3(1, 2, 3, 4)}{|(0-1)(0-2)(0-3)(0-4)|}. \tag{18}$$

Evaluating the Shcur polynomial (12) yields:

$$\Omega_0 = -\frac{1}{h} \frac{(1)(2)(3) + (1)(2)(4) + (1)(3)(4) + (2)(3)(4)}{24} = -\frac{25}{12h}. \tag{19}$$

To determine Ω_{a_2}, or in this case Ω_1, simply let $w = 2$. Equation (15) becomes:

$$\Omega_1 = (-1)^4 \frac{1!}{h} \frac{(0)(2)(3) + (0)(2)(4) + (0)(3)(4) + (2)(3)(4)}{|(1-0)(1-2)(1-3)(1-4)|} = \frac{4}{h}. \tag{20}$$

Similarly Ω_2 through Ω_4 are calculated:

$$\begin{aligned}
\Omega_2 &= (-1)^5 \frac{1!}{h} \frac{(0)(1)(3)+(0)(1)(4)+(0)(3)(4)+(1)(3)(4)}{|(2-0)(2-1)(2-3)(2-4)|} = \frac{-3}{h}, \\
\Omega_3 &= (-1)^6 \frac{1!}{h} \frac{(0)(1)(2)+(0)(1)(4)+(0)(2)(4)+(1)(2)(4)}{|(3-0)(3-1)(3-2)(3-4)|} = \frac{4}{3h}, \qquad (21) \\
\Omega_4 &= (-1)^7 \frac{1!}{h} \frac{(0)(1)(2)+(0)(1)(3)+(0)(2)(3)+(1)(2)(3)}{|(4-0)(4-1)(4-2)(4-3)|} = \frac{-1}{4h}.
\end{aligned}$$

The error term is determined using (16):

$$R = \begin{bmatrix} -\frac{25}{12h} & \frac{4}{h} & -\frac{3}{h} & \frac{4}{3h} & -\frac{1}{4h} \end{bmatrix} \begin{bmatrix} 0 \\ h^5 \\ (2h)^5 \\ (3h)^5 \\ (4h)^5 \end{bmatrix} \frac{f^{(5)}(\xi)}{5!}, \qquad (22)$$

which simplifies to:

$$R = -\frac{h^4}{5} f^{(5)}(\xi). \qquad (23)$$

Combining these results yields equation (8.3.10) of [14]:

$$f_0' = \frac{1}{12}\left(-25f_0 + 48f_1 - 36f_2 + 16f_3 - 3f_4\right) + \frac{1}{5} h^4 f^{(5)}(\xi), \qquad (24)$$

where $f_0' = f'(x_0)$ and $f_i = f(x_0 + a_i h)$. This grid scheme can also be used to generate approximations for the second through fourth derivatives. The results are stated below:

$$\begin{aligned}
f_0'' &= \tfrac{1}{12}\left(35f_0 - 104f_1 + 114f_2 - 56f_3 + 11f_4\right) - \tfrac{5}{6} h^3 f^{(5)}(\xi), \\
f_0''' &= \tfrac{1}{2}\left(-5f_0 + 18f_1 - 24f_2 + 14f_3 - 3f_4\right) + \tfrac{7}{4} h^2 f^{(5)}(\xi), \qquad (25) \\
f_0^{(4)} &= f_0 - 4f_1 + 6f_2 - 4f_3 + f_4 - 2h f^{(5)}(\xi),
\end{aligned}$$

The final equation in (25) replicates (8.3.13) of [14].

4 A Not-so-Classic Result: Four-Point Approximations for Derivatives on a Random Asymmetric Grid

This section demonstrates the versatility the procedure by extending it to a non-uniform, random, asymmetric grid. Equation (15) can be somewhat simplified by letting $h = 1$ and letting all information with regards to spacing be contained in a. Using this convention, (15) becomes:

$$\Omega_{a_w} = (-1)^{(d+w+1)} d! \left(\frac{s_{(r-d)}(a_1, ..., a_{n \neq w}, ..., a_{r+1})}{\prod\limits_{1 \leq i \neq w \leq r+1} |(a_w - a_i)|} \right). \qquad (26)$$

where $f_a = f(x_0 + a)$. The remainder expressions (16) and (17) are adjusted accordingly.

Consider the grid points $a = \{-.149, .051, .323, .410\}$ where a is represents positions relative to some point of interest. For this grid $r = 3$. We will obtain finite-difference approximation for the first derivative. Therefore $d = 1$ and $\lambda = r - d = 2$. To determine the value of the first weight $\Omega_{-.149}$ use $w = 1$. From (15) we have:

$$\Omega_{-.149} = (-1)^3 1! \frac{s_2(.051, .323, .410)}{|(-.149 - .051)(-.149 - .323)(-.149 - .410)|}, \qquad (27)$$

which, after evaluating the Schur polynomial is:

$$\Omega_{-.149} = -\frac{(.051)(.323) + (.051)(.410) + (.323)(.410)}{.0528} \approx -3.22. \qquad (28)$$

The remaining terms are similarly obtained:

$$\Omega_{.051} \approx 1.19, \quad \Omega_{.323} \approx 4.28, \quad \Omega_{.410} \approx -2.25. \qquad (29)$$

Using the calculated weights and (16), an error term is determined:

$$R = [-3.22, 1.19, 4.28, -2.25] \begin{bmatrix} -.149^4 \\ 051^4 \\ 323^4 \\ 410^4 \end{bmatrix} \frac{f^{(4)}(\xi)}{4!}, \qquad (30)$$

And therefore:

$$R \approx 7.73 * 10^{-4} f^{(4)}(\xi). \qquad (31)$$

The resulting approximation formula for the first derivative is:

$$f_0' = -3.22 f_1 + 1.19 f_2 + 4.28 f_3 - 2.25 f_4 + 7.73 * 10^{-4} f^{(4)}(\xi). \qquad (32)$$

In a similar fashion, the approximation formulae for the second and third derivatives are determined:

$$f_0'' = 29.7 f_1 - 59.8 f_2 + 55.9 f_3 - 25.8 f_4 + 4.42 * 10^{-3} f^{(4)}(\xi).$$
$$f_0''' = -114 f_1 + 307 f_2 - 537 f_3 + 344 f_4 - .159 f^{(4)}(\xi). \qquad (33)$$

To test the results, the first three derivatives for:

$$f(x) = \ln\left(\frac{1}{1+x^2}\right). \tag{34}$$

are approximated at $x = 1$. The results are summarized in the table below:

Table 1
Numerical Example
Approximation of 1st 3 Derivatives for $\ln\left(\frac{1}{1+x^2}\right)$
(Evaluated at $x = 1$)

Grid Points (Relative): {-.149, .051, .323, 410}
Grid Points (Absolute): {.851, 1.051, 1.323, 1.410}

	Approximation	Actual	|Difference|	|Remainder|
$f^{'}(1)$	-.998	-1.00	.00181	.00296
$f^{''}(1)$	.00838	0.00	.00838	.0169
$f^{'''}(1)$	.623	1.00	.377	.608

In this table, we see that the difference between actual and approximated values falls within the bounds of the Taylor series remainder. Greater accuracy or higher order derivatives are possible by increasing the number of grid points.

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