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A Mathematical Proof of Explicit Formulas for the Coefficients of Finite Difference Approximations of Second Derivatives

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ABSTRACT

Explicit formulas for the coefficients of finite difference approximations of first and higher derivatives in any order of accuracy have been presented by Khan and Ohba. They also have provided a mathematical proof of the formulas for first derivatives. In this paper, the proof is extended for second derivatives. The proof is constructed based on Taylor series, and employs some properties of Vandermonde determinant which are not found in the proof for first derivatives.

Keywords: Finite difference approximations, Taylor series, Vandermonde matrix, determinant.

1. Introduction

There are numerous phenomena in the nature which can be modeled by differential equations. In more realistic problems, the exact solutions of differential equations are sometimes difficult to find, thus a numerical approach is reasonable to use. In such cases, one needs to discretize the problem's domain and construct the approximation of the derivative terms appearing in the differential equations. This method will convert a linear (non-linear) differential equation into a system of linear (non-linear) equations, which can then be solved by a matrix algebra technique.

One of the most popular and easy-to-use numerical methods in computing the approximation of derivatives is finite difference. In this method, the domain of a function is partitioned in a number of points and the approximation formula for derivatives is obtained from Taylor series at one or more partition points (Mathews and Fink (1992)). Based on the location of the partition points used, finite difference method consists of three types, i.e. forward difference, backward difference, and central difference.

The general formula of finite difference for p-th degree of derivative and N-th order of accuracy can be generated recursively. One of the recursive algorithm was developed in Fornberg (1988) from which a table containing coefficients of forward, backwards, and central difference up to some degree of derivative and order of accuracy can be made. In practice, the recursive algorithm requires an increasingly large computational memory to compute the derivatives with higher degree and order accuracy, as it deals with a growing amount of data (partition points). To resolve this problem, one needs an explicit formula for a finite difference scheme of which the coefficients can be determined directly without recursive process.

Khan and Ohba (1999) have developed the explicit formulas for the coefficients of finite difference approximation based on Taylor series. A mathematical proof of the explicit formula for first derivative has been presented by Khan et al. (2003). In this paper, we will extend the proof of the explicit formula for second derivatives. Following the ideas in Khan et al. (2003), our proof is also constructed based on Taylor series but employs some properties of Vandermonde determinant which are not found in the proof for first derivatives.

Our presentation in this paper is organized as follows. In Section 2, we present the explicit formulas of finite difference approximations for second derivatives that will be proved. Next, in Section 3 we discuss the determinant of Vandermonde matrices which will be used in our proof. In Section 4 we derive the explicit formulas mathematically. Finally, in Section 5 we summarize our results and address current problem which is being under consideration.

2. The Explicit Formulas

By observing the solutions of equation system which is constructed based on Taylor series, Khan and Ohba (1999) gave explicit formula of finite difference approximations for second derivative of a function $f(x)$ at $x = x_0$ as follows

$$f_0'' \approx \frac{1}{T^2} \sum_k g_k f_k, \tag{1}$$

where T indicates the grid length with partition points $x_k = x_0 + kT, f_k = f(x_k)$, and the coefficient g_k and iterator k are defined based on the order and the type of the finite difference approximations as follows:

- For forward difference approximation, $k \in \{0, 1, ..., N\}$ where $N-1$ is the order of accuracy, and

$$g_k \equiv g_k^F = \begin{cases} \dfrac{(-1)^k 2N!}{k(N-k)!k!} \sum\limits_{m=1, m\neq k}^{N} \frac{1}{m}, & k = 1, 2, ..., N, \\ -\sum\limits_{m=1}^{N} g_m, & k = 0. \end{cases} \tag{2}$$

- For backward difference approximation, $k \in \{-N, -N+1, ..., -1, 0\}$ where $N-1$ is the order of accuracy, and

$$g_k \equiv g_k^B = -g_{-k}^F, \quad k = -N, -N+1, ..., -1, 0. \tag{3}$$

- For central difference approximation, $k \in \{-N, ..., -1, 0, 1, ..., N\}$ where $2N$ represents the order of accuracy, and

$$g_k \equiv g_k^C = \begin{cases} -2 \sum\limits_{m=1}^{N} g_m, & k = 0, \\ \dfrac{(-1)^{k+1} 2!(N!)^2}{k^2 (N-k)!(N+k)!}, & k = \pm 1, \pm 2, ..., \pm N. \end{cases} \tag{4}$$

Note that the explicit formula uses the sample values directly to find the derivative at a mesh point, thus it requires less computational time and storage to approximate the derivatives. As example, for order of accuracy $N - 1 = 1$ (i.e. $N = 2$), the coefficient g_k for forward difference of second derivative is

$$g_k^F = \begin{cases} 1, & k = 0, \\ -2, & k = 1, \\ 1, & k = 2, \end{cases}$$

which in turn gives

$$\begin{aligned} f_0'' &\approx \frac{1}{T^2}\left(g_0 f_0 + g_1 f_1 + g_2 f_2\right) \\ &= \frac{1}{T^2}\left(f_0 - 2f_1 + f_2\right). \end{aligned}$$

The above expression agrees with the known formula for forward difference of second derivative.

3. Determinant of Vandermonde Matrices

Determinant of Vandermonde matrices plays important role in the proof of explicit formulas of finite difference approximations. The definition of a Vandermonde matrix is provided as follows.

Definition 3.1. (Meyer (2000)) *A matrix V with size $M \times N$ of the form*

$$V_{M\times N} = \begin{bmatrix} 1 & \lambda_1 & \lambda_1^2 & \cdots & \lambda_1^{N-1} \\ 1 & \lambda_2 & \lambda_2^2 & \cdots & \lambda_2^{N-1} \\ 1 & \lambda_3 & \lambda_3^2 & \cdots & \lambda_3^{N-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \lambda_M & \lambda_M^2 & \cdots & \lambda_M^{N-1} \end{bmatrix}, \tag{5}$$

where $\lambda_i \neq \lambda_j$ for all $i \neq j$, is called Vandermonde matrix.

By applying column elementary operations and cofactor expansions at each row, the determinant $|V_{N\times N}|$ can be computed according to the following theorem.

Theorem 3.1. (Meyer (2000)) *The determinant of a Vanderrmonde matrix* *with size $N \times N$ is*

$$|V_{N\times N}| = \begin{bmatrix} 1 & \lambda_1 & \lambda_1^2 & \cdots & \lambda_1^{N-1} \\ 1 & \lambda_2 & \lambda_2^2 & \cdots & \lambda_2^{N-1} \\ 1 & \lambda_3 & \lambda_3^2 & \cdots & \lambda_3^{N-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \lambda_N & \lambda_N^2 & \cdots & \lambda_N^{N-1} \end{bmatrix} = \prod_{\substack{1<i\leq N \\ 1\leq j<N \\ j<i}} (\lambda_i - \lambda_j). \quad (6)$$

For a special case $\lambda_i = i$, where $i = 1, 2, ..., N$, the determinant of the resulting Vandermonde matrix can be written as

$$\alpha_N = \begin{vmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 2 & 2^2 & \cdots & 2^{N-1} \\ 1 & 3 & 3^2 & \cdots & 3^{N-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & N & N^2 & \cdots & N^{N-1} \end{vmatrix} = \prod_{i=1}^{N} (N-i)!. \quad (7)$$

From Theorem 3.1, we have the following corollary.

Corollary 3.1. *The determinant of a Vandermonde matrix with size $(N-1)\times(N-1)$ which is obtained by removing k-th row and second column of α_N is given by*

$$\begin{vmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 2^2 & 2^3 & \cdots & 2^{N-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & (k-1)^2 & (k-1)^3 & \cdots & (k-1)^{N-1} \\ 1 & (k+1)^2 & (k+1)^3 & \cdots & (k+1)^{N-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & N^2 & N^3 & \cdots & N^{N-1} \end{vmatrix} = \frac{N!}{k(k-1)!(N-k)!} \prod_{i=1}^{N} (N-i)! \sum_{m=1, m\neq k}^{N} \frac{1}{m}.$$

Proof. The proof follows the idea in Heineman (1929). Let a polynomial

$$P_0 x^N + P_1 x^{N-1} + \cdots + P_N = 0, \quad P_0 \neq 0, \quad (8)$$

has roots $\lambda_1, \lambda_2, ..., \lambda_N$. From Vieta's formula in Gellert (1975), we obtain

$$\frac{P_{N-1}}{P_0} = (-1)^{N-1} \sum_{m=1}^{N} \frac{\lambda_1 \lambda_2 \cdots \lambda_N}{\lambda_m}. \tag{9}$$

By substituting each root $\lambda_1, \lambda_2, ..., \lambda_N$ into Eq. (8) and then dividing the resulting equations with P_0, we arrive at the following system of equations:

$$\begin{aligned} \frac{P_1}{P_0}\lambda_1^{N-1} + \frac{P_2}{P_0}\lambda_1^{N-2} + \cdots + \frac{P_N}{P_0} &= -\lambda_1^N, \\ \frac{P_1}{P_0}\lambda_2^{N-1} + \frac{P_2}{P_0}\lambda_2^{N-2} + \cdots + \frac{P_N}{P_0} &= -\lambda_2^N, \\ &\vdots \\ \frac{P_1}{P_0}\lambda_N^{N-1} + \frac{P_2}{P_0}\lambda_N^{N-2} + \cdots + \frac{P_N}{P_0} &= -\lambda_N^N. \end{aligned} \tag{10}$$

By reversing the order of sum of terms in each equation, the system (10) can be rewritten in the matrix form as

$$\begin{bmatrix} 1 & \lambda_1 & \cdots & \lambda_1^{N-1} \\ 1 & \lambda_2 & \cdots & \lambda_2^{N-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \lambda_N & \cdots & \lambda_N^{N-1} \end{bmatrix} \begin{bmatrix} \frac{P_N}{P_0} \\ \frac{P_{N-1}}{P_0} \\ \vdots \\ \frac{P_1}{P_0} \end{bmatrix} = - \begin{bmatrix} \lambda_1^N \\ \lambda_2^N \\ \vdots \\ \lambda_N^N \end{bmatrix}. \tag{11}$$

Note that the coefficient matrix in (11) is indeed a matrix Vandermonde $V_{N\times N}$ whose determinant is given by Theorem 3.1. By using Cramer's rule, the solution for $\frac{P_{N-1}}{P_0}$ is given by

$$\frac{P_{N-1}}{P_0} = \frac{|V_{N\times N,2}|}{|V_{N\times N}|}, \tag{12}$$

where $V_{N\times N,2}$ is the matrix $V_{N\times N}$ with second column replaced by $\left[\lambda_1^N, \lambda_2^N, \cdots, \lambda_N^N\right]^T$. By applying the column interchange, the determinant $|V_{N\times N,2}|$ can be calculated as

$$|V_{N\times N,2}| \quad = \quad (-1)^{N-1}\begin{vmatrix} 1 & \lambda_1^2 & \lambda_1^3 & \cdots & \lambda_1^N \\ 1 & \lambda_2^2 & \lambda_2^3 & \cdots & \lambda_2^N \\ 1 & \lambda_3^2 & \lambda_3^3 & \cdots & \lambda_3^N \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \lambda_N^2 & \lambda_N^3 & \cdots & \lambda_N^N \end{vmatrix}. \tag{13}$$

By writing the matrix expression in (13) as

$$W_{N\times N} = \begin{bmatrix} 1 & \lambda_1^2 & \lambda_1^3 & \cdots & \lambda_1^N \\ 1 & \lambda_2^2 & \lambda_2^3 & \cdots & \lambda_2^N \\ 1 & \lambda_3^2 & \lambda_3^3 & \cdots & \lambda_3^N \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \lambda_N^2 & \lambda_N^3 & \cdots & \lambda_N^N \end{bmatrix},$$

then Eq. (12) becomes

$$\frac{P_{N-1}}{P_0} = (-1)^{N-1}\frac{|W_{N\times N}|}{|V_{N\times N}|}. \tag{14}$$

From Eqs. (9) and (14), and by Theorem 3.1, we have

$$|W_{N\times N}| \quad = \quad \prod_{\substack{1<i\le N\\ 1\le j<N\\ j<i}} (\lambda_i - \lambda_j) \sum_{m=1}^{N} \frac{\lambda_1\lambda_2\cdots\lambda_N}{\lambda_m}. \tag{15}$$

Now consider a matrix $W'_{N\times N}$ which is obtained by replacing the entries of matrix $W_{N\times N}$ with $\lambda_i = i$, where $i = 1, 2, ..., N$, i.e.

$$W'_{N\times N} = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 2^2 & 2^3 & \cdots & 2^N \\ 1 & 3^2 & 3^3 & \cdots & 3^N \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & N^2 & N^3 & \cdots & N^N \end{bmatrix}. \tag{16}$$

By comparing with Eq. (15), the determinant of matrix $W'_{N\times N}$ can be written as

$$|W'_{N\times N}| = \prod_{\substack{1<i\leq N\\ 1\leq j<N\\ j<i}} (i-j) \sum_{m=1}^{N} \frac{N!}{m}. \tag{17}$$

If the k-th row and last column of matrix $W'_{N\times N}$ are removed, the resulting determinant will be given by (17) but for $i, j, m \neq k$. By performing the product and the sum calculations, we obtain

$$\begin{aligned}
\begin{vmatrix}
1 & 1 & 1 & \cdots & 1 \\
1 & 2^2 & 2^3 & \cdots & 2^{N-1} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
1 & (k-1)^2 & (k-1)^3 & \cdots & (k-1)^{N-1} \\
1 & (k+1)^2 & (k+1)^3 & \cdots & (k+1)^{N-1} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
1 & N^2 & N^3 & \cdots & N^{N-1}
\end{vmatrix}
&= \prod_{\substack{1<i\leq N, i\neq k\\ 1\leq j<N, j\neq k\\ j<i}} (i-j) \sum_{m=1, m\neq k}^{N} \frac{N!}{km} \\
&= \frac{N!}{k(k-1)!(N-k)!} \prod_{i=1}^{N} (N-i)! \sum_{m=1, m\neq k}^{N} \frac{1}{m}.
\end{aligned}$$

which complete the proof. □

4. Proof of the Explicit Formulas

In this section, we provide a proof of the explicit formulas of finite difference approximations for second derivative as already presented in Section 2. Our proof is constructed from Taylor series, and follows the idea in Khan et al. (2003). We will first prove for the case of forward difference.

Let a function $f(x)$ be N-times differentiable $(N > 2)$ at $x = x_0$. The Taylor series for $f(x)$ at $x \approx x_0$ is

$$\begin{aligned}
f(x) &= f(x_0) + (x-x_0)f'(x_0) + \frac{(x-x_0)^2}{2!} f''(x_0) + \cdots + \frac{(x-x_0)^N}{N!} f^{(N)}(x_0) \\
&\quad + \mathcal{O}((x-x_0)^{N+1}).
\end{aligned} \tag{18}$$

If the domain of f is partitioned with grid length T and the points of partition are given by

$$x_k = x_0 + kT, \quad k = 1, 2, \cdots, N,$$

then the Taylor series (18) for $x = x_k$ can be rewritten as

$$f_k - f_0 = (kT)f_0' + \frac{(kT)^2}{2!}f_0'' + \cdots + \frac{(kT)^N}{N!}f_0^{(N)} + \mathcal{O}(T^{N+1}), \quad (19)$$

where $f_0 = f(x_0)$, $f_k = f(x_k)$ and $f_0^{(p)} = f^{(p)}(x_0)$, where p indicates the order of derivative.

After truncating up to N terms, series (19) for $k = 1, 2, ..., N$ can be expressed in a matrix form as

$$\mathbf{f} \approx A\mathbf{d}, \quad (20)$$

where

$$\begin{aligned} \mathbf{f} &= [f_1 - f_0, f_2 - f_0, \cdots, f_N - f_0]^T, \\ \mathbf{d} &= \left[f_0', f_0'', \cdots, f_0^{(N)}\right]^T, \\ A &= \begin{bmatrix} T & \frac{T^2}{2!} & \cdots & \frac{T^N}{N!} \\ 2T & \frac{(2T)^2}{2!} & \cdots & \frac{(2T)^N}{N!} \\ \vdots & \vdots & \ddots & \vdots \\ NT & \frac{(NT)^2}{2!} & \cdots & \frac{(NT)^N}{N!} \end{bmatrix}. \end{aligned}$$

By using Cramer's rule, we have

$$f_0'' \approx \frac{|A_b|}{|A|}, \quad (21)$$

where A_b is obtained by replacing the second column of matrix A with the column vector $\mathbf{f}$, i.e.

$$A_b = \begin{bmatrix} T & f_1 - f_0 & \cdots & \frac{T^N}{N!} \\ 2T & f_2 - f_0 & \cdots & \frac{(2T)^N}{N!} \\ \vdots & \vdots & \ddots & \vdots \\ NT & f_N - f_0 & \cdots & \frac{(NT)^N}{N!} \end{bmatrix}.$$

The determinants in numerator and denominator of Eq. (21) can be written without T by taking out the common terms in each column of A_b and A, i.e.

$$f_0'' \approx \frac{TT^3\cdots T^N}{TT^2T^3\cdots T^N}\frac{|A_b|_{T=1}}{|A|_{T=1}} = \frac{1}{T^2}\frac{|A_b|_{T=1}}{|A|_{T=1}}. \tag{22}$$

Next, by taking out the common terms in each row and column of $|A|_{T=1}$, and by using Vandermonde determinant as given by Eq. (7), one can easily check that $|A|_{T=1} = 1$. Thus Eq. (22) now becomes

$$f_0'' \approx \frac{1}{T^2}|A_b|_{T=1}, \tag{23}$$

Eq. (23) can be further expressed as

$$f_0'' \approx \frac{1}{T^2}\sum_{k=1}^{N} g_k(f_k - f_0) = \frac{1}{T^2}\left(\sum_{k=1}^{N} g_k f_k - \sum_{k=1}^{N} g_k f_0\right), \tag{24}$$

where g_k is the minor of $|A_b|_{T=1}$ corresponding to k-th element of second column, i.e.

$$g_k = (-1)^k \begin{vmatrix} 1 & \frac{1}{3!} & \cdots & \frac{1}{N!} \\ 2 & \frac{2^3}{3!} & \cdots & \frac{2^N}{N!} \\ \vdots & \vdots & \ddots & \vdots \\ (k-1) & \frac{(k-1)^3}{3!} & \cdots & \frac{(k-1)^N}{N!} \\ (k+1) & \frac{(k+1)^3}{3!} & \cdots & \frac{(k+1)^N}{N!} \\ \vdots & \vdots & \ddots & \vdots \\ N & \frac{N^3}{3!} & \cdots & \frac{N^N}{N!} \end{vmatrix}. \tag{25}$$

By defining

$$g_0 = -\sum_{k=1}^{N} g_k, \tag{26}$$

the expression of Eq. (24) can be simplified into

$$f_0'' \approx \frac{1}{T^2}\sum_{k=0}^{N} g_k f_k.$$

Again, by taking out the common terms in each row and column of the corresponding matrix in (25), the value of g_k for $k \neq 0$ can be calculated as

$$g_k = (-1)^k \frac{(2)(3)\cdots(N)}{(k)(3!)(4!)\cdots(N!)} \begin{vmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 2^2 & 2^3 & \cdots & 2^{N-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & (k-1)^2 & (k-1)^3 & \cdots & (k-1)^{N-1} \\ 1 & (k+1)^2 & (k+1)^3 & \cdots & (k+1)^{N-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & N^2 & N^3 & \cdots & N^{N-1} \end{vmatrix}. \tag{27}$$

Note that the determinant which appears in Eq. (27) has been given by Corollary 3.1. Thus, the value of g_k for $k = 1, 2, ..., N$ becomes

$$\begin{aligned} g_k &= (-1)^k \frac{(2^2)(3^2)\cdots(N^2)}{(k^2)(3!)(4!)\cdots(N!)} \frac{(N-1)!(N-2)!\cdots(3!)(2!)(1!)}{(k-1)!(N-k)!} \sum_{m=1, m\neq k}^{N} \frac{1}{m} \\ &= (-1)^k \frac{(2^2)(3^2)\cdots(N^2)(2!)}{(k^2)(N!)(k-1)!(N-k)!} \sum_{m=1, m\neq k}^{N} \frac{1}{m} \\ &= (-1)^k \frac{(2)(3)\cdots(N)(2)(3)\cdots(N)(2!)}{k(k!)(N-k)!N!} \sum_{m=1, m\neq k}^{N} \frac{1}{m} \\ &= \frac{(-1)^k 2N!}{k(N-k)!k!} \sum_{m=1, m\neq k}^{N} \frac{1}{m}. \end{aligned} \tag{28}$$

From Eqs. (26) and (28), we finally have

$$g_k = \begin{cases} \dfrac{(-1)^k 2N!}{k(N-k)!k!} \sum\limits_{m=1, m\neq k}^{N} \dfrac{1}{m}, & k = 1, 2, ..., N, \\ -\sum\limits_{m=1}^{N} g_m, & k = 0, \end{cases}$$

which proves the explicit formula of forward difference approximation given by (2). ■

The proof for explicit formula of backward and central difference approximations given respectively by Eqs. (3) and (4) can be performed accordingly in a similar way by simply replacing $k = -N, -N+1, ..., -1, 0$ (for backward) and $k = 0, \pm 1, \pm 2, ..., \pm N$ (for central), and then calculating the determinants of the resulting matrices.

5. Conclusion

In this paper we have proved mathematically the explicit formulas for the coefficients of finite difference approximations of second derivatives. The proof was constructed based on Taylor series from which a system of equation appears. The system was then solved by calculating the determinant of the resulting Vandermonde matrices and performing some algebraic manipulations. Khan and Ohba (1999) also provide a more general explicit formula of finite difference for the p-th derivative and the N-th order of accuracy. The mathematical proof of the latter formula is being under consideration.

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