

Numerical Computation of the p-th Derivative of a Function

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Abstract. Recently efforts have been made to compute first and second derivatives of a function numerically when its values are known in a specific interval. In the derivation mainly Chebyshev polynomials and Lagrange interpolation were used by M.T.Rashed. In this study, a generalized form is reached for the p-th derivative of a function. Thus encoding of the method on personal computer and finding solutions can be easily done. Method is applied to different examples are made and advantages and disadvantages are indicated.

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1. Introduction

It is not always possible to calculate the derivative of a function exactly. In this work the generalization of a numerical scheme is developed for the p-th derivative of a function using the technique already utilized to approximate the first and second derivatives at the endpoints of the subintervals obtained by dividing the interval $[A,B]$ into n equally spaced parts.

As is well known, Lagrange interpolation is frequently used in approximating a function if its values are known at $(n+1)$ distinct points. Lagrange interpolation is also used in this work where we attempt to approximate the p-th derivative of a function. Equation systems related to first, second and third order derivatives were obtained and expressed in matrix form and generalization of the p-th order derivative was made. Computer programmes were made to evaluate and to analyse the numerical results and to see the positive and negative aspects of the proposed method. To this end four functions each of different structure were

chosen and the numerical results up to their fourth derivatives are tabulated for comparison purposes. Approximate results are also compared on graphs with the exact values in order to give a detailed account of the method.

Results at the interior points seem to be highly satisfactory portraying errors at minimum level. It was observed that order of derivative, type of function, interval size, number of subintervals all seem to effect the relevant errors. In cases where the interval length is not too long the method gives good results up to the fourth order derivatives. Another positive aspect of the proposed method is the ease by which the algorithm can be transferred to computation media.

The paper is organized as follows. The formulation of the first derivative of a function in section 2. In section 3 the p-th derivative of a function is given. In section 4 some examples are given as some concluding remarks.

2. First derivative of a function

Lagrange interpolation of a function $y'(x)$ is given by (for further reading, see Refs. [1-4])

$$(2.1) \quad y'(x) \approx \sum_{j=0}^n y'(x_j) \ell_{j,n}(x), \quad A \leq x \leq B$$

where

$$\ell_{j,n}(x) = \prod_{\substack{k=0 \\ k \neq j}}^n \left(\frac{x - x_k}{x_j - x_k} \right), \quad x_k = A + kh, \quad h = \frac{B - A}{n} \quad \text{for } k = 0, 1, \dots, n$$

Integrating both side of (2.1) from A to x

$$(2.2) \quad y(x) - y(A) \approx \sum_{j=0}^n b_j(x) y'(x_j)$$

where

$$b_j(x) = \int_A^x \prod_{\substack{k=0 \\ k \neq j}}^n \left(\frac{t - x_k}{x_j - x_k} \right) dt$$

when suitable transformations are made

$$(2.3) \quad b_j(x) = \frac{x - A}{2} \int_{-1}^1 \prod_{\substack{k=0 \\ k \neq j}}^n \left(\frac{\frac{x - A}{2}t + \frac{x + A}{2} - x_k}{x_j - x_k} \right) dt$$

is obtained. This integration can be approximately computed using chebyshev polynomials. The infinite sum in chebyshev series is converted to a finite sum by choosing a naturel number N .

$$(2.3a) \quad b_j(x) \approx \frac{x-A}{2} \sum_{s=0}^N b_s \prod_{\substack{k=0 \\ k \neq j}}^n \left(\frac{\frac{x-A}{2}t + \frac{x+A}{2} - x_k}{x_j - x_k} \right)$$

where

$$b_s = \frac{2\delta_s}{N} \sum_{k=0}^{N''} I_k \cos\left(\frac{ks\pi}{N}\right), I_k = \begin{cases} 2, & k=0 \\ 0, & k \text{ is odd} \\ \frac{2}{1-k^2}, & k \text{ is even} \end{cases}$$

$$\delta_k = \begin{cases} 0.5, & k=0, N \\ 1, & 0 < k < N \end{cases}, t_s = \cos \frac{s\pi}{N}, \text{ for } s = 0, 1, \dots, N$$

The double prime on the N indicates that in forming the sum, the terms with subscripts $j=0$ and $j=n$ are to be halved. In (2.2) if $x=A$ is chosen, $b_j(x_0)=0, \forall j$. If we choose x by $z_i = \frac{B-A}{2} \cos\left(\frac{(i-0.45)\pi}{n}\right) + \frac{B+A}{2}$, is reached $x \neq A(\forall i)$. Hence, Eq. (2.2) becomes

$$(2.4) \quad y(z_i) - y(A) \approx \sum_{j=0}^n b_j(z_i) y'(x_j), \quad i = 0(1)n.$$

Eq. (2.4) gives the first derivative of the function $y(x)$ at points

$$x_i = A + ih, \quad h = \frac{B-A}{n}, \quad \text{for } i = 0, 1, \dots, n$$

Similarly, we can find the second derivative of a function, as in [4].

3. P-th derivative of a function

Consider the Lagrange interpolation of the p -th derivative of a function $y^{(p)}(x)$

$$y^{(p)}(x) \approx \sum_{j=0}^n y^{(p)}(x_j) \ell_{j,n}(x), \quad A \leq x \leq B$$

Integrating p times from A to x

$$y^{(p-1)}(x) - y^{(p-1)}(A) \approx \sum_{j=0}^n y^{(p)}(x_j) L_1(x)$$

$$y^{(p-2)}(x) - y^{(p-2)}(A) - (x-A)y^{(p-1)}(A) \approx \sum_{j=0}^n y^{(p)}(x_j) L_2(x)$$

$$y^{(p-3)}(x) - y^{(p-3)}(A) - (x-A)y^{(p-2)}(A) - \frac{(x-A)^2}{2}y^{(p-1)}(A)$$

$$\approx \sum_{j=0}^n y^{(p)}(x_j) L_3(x)$$

$\vdots$

$$(3.1) \quad y(x) - y(A) - \sum_{k=1}^{p-1} \frac{(x-A)^k}{k!} y^{(k)}(A) \approx \sum_{j=0}^n y^{(p)}(x_j) L_p(x)$$

where

$$L_p(x) = \int_A^x \dots (p) \dots \int_A^x \ell_{j,n}(t) \underbrace{dt \dots dt}_p = \int_A^x \frac{(x-t)^{p-1}}{(p-1)!} \ell_{j,n}(t) dt$$

When suitable transformations are made

$$L_p(x) = \frac{x-A}{2} \int_{-1}^1 \frac{\left[x - \frac{x-A}{2}t - \frac{x+A}{2} \right]^{(p-1)}}{(p-1)!} \ell_{j,n} \left(\frac{x-A}{2}t + \frac{x+A}{2} \right) dt$$

is formed. This integration can approximately be computed using Chebyshev polynomials

$$L_p(x) \approx$$

$$\frac{x-A}{2} \sum_{s=0}^N b_s \frac{\left[x - \frac{x-A}{2}t_s - \frac{x+A}{2} \right]^{(p-1)}}{(p-1)!} \prod_{\substack{k=0 \\ k \neq j}}^n \left(\frac{\frac{x-A}{2}t_s + \frac{x+A}{2} - x_k}{x_j - x_k} \right)$$

Let $x = B$ in (3.1)

$$\begin{aligned}
& \frac{y^{(p-1)}(A)}{(p-1)!} = \\
(3.2) \quad & = \frac{1}{(B-A)^{p-1}} \left[y(B) - y(A) - \sum_{k=1}^{p-2} \frac{(B-A)^k}{k!} y^{(k)}(A) - \sum_{j=0}^n y^{(p)}(x_j) L_p(B) \right]
\end{aligned}$$

Substitute (3.2) in to (3.1)

$$\begin{aligned}
& y(x) - y(A) - \sum_{k=1}^{p-2} \frac{(x-A)^k}{k!} y^{(k)}(A) - \\
& \frac{(x-A)^{p-1}}{(B-A)^{p-1}} \left[y(B) - y(A) - \sum_{k=1}^{p-2} \frac{(B-A)^k}{k!} y^{(k)}(A) - \sum_{j=0}^n y^{(p)}(x_j) L_p(B) \right] \\
& = \sum_{j=0}^n y^{(p)}(x_j) L_p(x)
\end{aligned}$$

When, suitable arrangements are done we reach at the generalized form

$$\begin{aligned}
& y(x) - y(A) - \frac{(x-A)^{(p-1)}}{(B-A)^{(p-1)}} [y(B) - y(A)] - \\
& \sum_{k=1}^{p-2} \frac{y^{(k)}(A)}{k!} \left[(x-A)^k - \frac{(x-A)^{(p-1)}}{(B-A)^{(p-k-1)}} \right] \\
(3.3) \quad & \approx \sum_{j=0}^n \left(\left[L_p(x) - \frac{(x-A)^{(p-1)}}{(B-A)^{(p-1)}} L_p(B) \right] y^{(p)}(x_j) \right)
\end{aligned}$$

Equation (3.3) may be written in the form $D = T^{-1}Y$. Where

$$\begin{aligned}
c_1 &= y(z_0) - y(A) - \frac{(z_0-A)^{(p-1)}}{(B-A)^{(p-1)}} [y(B) - y(A)] \\
c_2 &= y(z_1) - y(A) - \frac{(z_1-A)^{(p-1)}}{(B-A)^{(p-1)}} [y(B) - y(A)] \\
&\vdots \\
c_n &= y(z_n) - y(A) - \frac{(z_n-A)^{(p-1)}}{(B-A)^{(p-1)}} [y(B) - y(A)]
\end{aligned}$$

$$Y = \begin{bmatrix} c_1 - \sum_{k=1}^{p-2} \frac{y^{(k)}(A) \left[(z_0 - A)^k - \frac{(z_0 - A)^{(p-1)}}{(B - A)^{(p-k-1)}} \right]}{k!} \\ c_2 - \sum_{k=1}^{p-2} \frac{y^{(k)}(A) \left[(z_1 - A)^k - \frac{(z_1 - A)^{(p-1)}}{(B - A)^{(p-k-1)}} \right]}{k!} \\ \vdots \\ c_n - \sum_{k=1}^{p-2} \frac{y^{(k)}(A) \left[(z_n - A)^k - \frac{(z_n - A)^{(p-1)}}{(B - A)^{(p-k-1)}} \right]}{k!} \end{bmatrix}$$

$$T = \begin{bmatrix} L_p(z_0) - \frac{(z_0 - A)^{(p-1)}}{(B - A)^{(p-1)}} L_p(B) \\ L_p(z_1) - \frac{(z_1 - A)^{(p-1)}}{(B - A)^{(p-1)}} L_p(B) \\ \vdots \\ L_p(z_n) - \frac{(z_n - A)^{(p-1)}}{(B - A)^{(p-1)}} L_p(B) \end{bmatrix}$$

and

$$D = \begin{bmatrix} y^{(p)}(x_0) \\ y^{(p)}(x_1) \\ \vdots \\ y^{(p)}(x_n) \end{bmatrix}$$

The problem in using (3.1) is $L_j(x_0) = 0, \forall j$. To remove that problem we may choose x as

$$z_i = \frac{B - A}{2} \cos \left[\frac{(i - 0.45) \pi}{n} \right] + \frac{B + A}{2}, \quad i = 0(1)n.$$

4. Numerical Examples

In order to work on the numerical differentiations results made in our study some example functions were used. These functions are given below and the results obtained are tabulated in Table 4.1. The error values associated with the first, second, third and fourth derivatives of the functions in question, are shown with the symbol (σ_n) . Taking (e_n) as the difference between the calculated and the exact values. $(e_n = y_n - y_{exact})$ σ_n is calculated utilizing the formula.

$$\sigma_n = \left[\sum_{j=0}^n e_n^2(x_j) / n \right]^{1/2} \approx \left[\int_A^B e_n^2(x) dx \right]^{1/2}$$

- (1) $y(x) = (x+2)^{\log_e(x+5)}$
(2) $y(x) = x \cdot \log_e(x+3)$
(3) $y(x) = e^{\sin x}$
(4) $y(x) = 1/[5 + \sin(\frac{\pi}{2}x)]$

n	$\underline{f'(x)}$	$\underline{f''(x)}$	$\underline{f^{(3)}(x)}$	$\underline{f^{(4)}(x)}$
2	6.1D-03	3.1D-03	3.4D-01	25.2
3	9.8D-05	3.0D-05	1.8D-02	2.7D+00
4	6.1D-07	3.3D-06	1.9D-04	6.9D-02
5	4.8D-08	2.6D-07	3.9D-05	1.2D-02
6	3.3D-09	2.4D-08	4.1D-06	1.7D-03
7	2.8D-10	2.2D-09	4.9D-07	2.9D-04
8	2.2D-11	2.1D-10	5.4D-08	4.1D-05
9	1.6D-12	2.0D-10	1.1D-08	8.2D-06
10	3.2D-13	1.2D-10	8.6D-10	1.2D-05
12	4.8D-13	2.3D-10	2.0D-08	2.8D-05
15	7.0D-12	7.0D-10	1.9D-07	2.5D-04
20	7.4D-11	7.0D-08	1.2D-05	1.6D-01

Table 4.1: $f(x) = (x+2)^{\ln(x+5)}$, σ_n for $A=0, B=1.0$

n	$\underline{f'(x)}$	$\underline{f''(x)}$	$\underline{f^{(3)}(x)}$	$\underline{f^{(4)}(x)}$
2	6.8D-04	3.8D-04	1.6D-01	22.6
3	5.9D-06	7.1D-07	4.4D-03	1.3D+00
4	8.1D-09	1.6D-07	7.5D-06	7.6D-03
5	1.2D-09	7.6D-09	3.7D-06	2.5D-03
6	5.0D-11	3.8D-10	2.2D-07	2.2D-04
7	2.2D-12	5.4D-11	1.5D-08	1.4D-05
8	3.4D-13	2.4D-10	2.2D-08	4.4D-05
9	3.5D-13	3.1D-10	2.4D-08	8.6D-05
10	1.8D-13	3.9D-10	2.8D-08	1.3D-04
12	8.6D-13	3.3D-10	6.4D-08	1.4D-04
15	4.7D-12	8.9D-10	2.8D-07	1.7D-03
20	2.2D-10	6.6D-08	1.2D-05	5.6D-01

Table 4.2: $f(x) = (x+2)^{\ln(x+5)}$, σ_n for $A=0, B=0.5$

n	$\underline{f'(x)}$	$\underline{f''(x)}$	$\underline{f^{(3)}(x)}$	$\underline{f^{(4)}(x)}$
2	1.5D-03	2.4D-03	1.1D-01	6.0
3	6.7D-05	2.3D-04	1.5D-02	1.8
4	4.0D-06	2.0D-05	2.0D-03	3.9D-01
5	2.8D-07	1.6D-06	2.3D-04	7.1D-02
6	2.1D-08	1.3D-07	2.5D-05	1.1D-02
7	1.5D-09	1.0D-08	2.6D-06	1.6D-03
8	1.1D-10	8.2D-10	2.5D-07	2.0D-04
9	7.1D-12	5.4D-11	2.4D-08	2.6D-05
10	5.4D-13	1.1D-11	2.5D-09	2.1D-06
12	2.6D-13	2.2D-11	1.9D-09	4.3D-06
15	2.5D-12	2.8D-10	1.2D-08	1.4D-04
20	2.4D-11	1.4D-08	2.0D-06	3.2D-02

Table 4.3: $f(x) = x \cdot \ln(x+3), \sigma_n$ for $A=0, B=1.0$

n	$\underline{f'(x)}$	$\underline{f''(x)}$	$\underline{f^{(3)}(x)}$	$\underline{f^{(4)}(x)}$
2	3.2D-03	3.8D-03	6.4D-02	1.6
3	2.0D-04	4.8D-04	1.2D-02	6.5D-01
4	1.6D-05	5.8D-05	2.2D-03	2.0D-01
5	1.6D-06	6.7D-06	3.6D-04	5.0D-02
6	1.7D-07	7.6D-07	5.4D-05	1.1D-02
7	1.7D-08	8.4D-08	7.8D-06	2.1D-03
8	1.7D-09	9.3D-09	1.1D-06	3.9D-04
9	1.6D-10	1.0D-09	1.4D-07	6.6D-05
10	1.5D-11	1.1D-10	1.8D-08	1.1D-05
12	2.4D-13	1.1D-11	5.0D-10	8.4D-07
15	1.2D-13	2.7D-10	1.5D-08	2.2D-05
20	5.9D-11	5.9D-09	5.7D-07	2.0D-03

Table 4.4: $f(x) = x \cdot \ln(x+3), \sigma$ for $A=1.0, B=3.0$

n	$\underline{f'(x)}$	$\underline{f''(x)}$	$\underline{f^{(3)}(x)}$	$\underline{f^{(4)}(x)}$
2	4.4D-02	3.3D-02	2.9D+00	190.1
3	1.9D-03	3.4D-02	9.9D-02	52.6
4	6.9D-04	3.3D-03	2.3D-01	77.0
5	4.8D-05	5.1D-04	4.1D-02	10.3
6	7.5D-06	1.1D-04	4.5D-03	5.4
7	1.4D-06	8.4D-07	1.9D-03	1.6
8	1.7D-08	1.8D-06	7.1D-04	5.6D-02
9	1.6D-08	1.4D-07	3.9D-05	6.9D-02
10	1.1D-09	1.5D-08	4.9D-06	5.9D-03
12	1.7D-11	1.0D-10	1.1D-07	3.0D-04
15	2.6D-12	8.6D-11	4.5D-08	6.3D-05
20	2.4D-11	1.3D-08	1.8D-05	2.5D-02

Table 4.5: $f(x) = e^{\sin x}, \sigma_n$ for $A = 0, B = 1.0$

n	$\underline{f'(x)}$	$\underline{f''(x)}$	$\underline{f^{(3)}(x)}$	$\underline{f^{(4)}(x)}$
2	7.6D-04	4.9D-03	8.5D-02	2.8
3	1.3D-04	6.6D-04	3.2D-02	3.3
4	1.3D-05	2.7D-05	4.7D-03	1.4
5	3.5D-07	1.9D-05	6.2D-04	1.3D-02
6	2.4D-07	4.2D-06	3.5D-04	9.8D-02
7	4.9D-08	3.9D-07	8.4D-05	4.9D-02
8	4.2D-09	7.9D-09	7.8D-06	8.9D-03
9	6.0D-11	9.6D-09	6.6D-07	2.7D-04
10	6.8D-11	1.8D-09	3.9D-07	3.4D-04
12	1.0D-12	2.7D-12	6.2D-09	1.6D-05
15	6.0D-14	4.8D-11	2.7D-09	2.4D-05
20	2.4D-13	1.8D-09	1.4D-07	3.2D-03

Table 4.6: $f(x) = 1/\left(\sin\left[\frac{\pi x}{2}\right] + 5\right), \sigma_n$ for $A = 0, B = 1.0$

n	$f'(x)$	$f''(x)$	$f^{(3)}(x)$	$f^{(4)}(x)$
2	2.2D-04	8.6D-04	6.7D-02	7.2D+00
3	1.3D-05	2.0D-05	1.0D-02	2.8D+00
4	2.5D-07	6.6D-06	1.6D-04	2.3D-01
5	4.6D-08	8.8D-07	1.6D-04	8.7D-02
6	5.7D-09	5.0D-08	2.6D-05	2.5D-02
7	3.0D-10	8.5D-10	1.7D-06	2.8D-03
8	3.9D-12	4.0D-10	6.6D-08	1.7D-05
9	1.7D-12	3.4D-11	2.4D-08	4.8D-05
10	1.3D-13	5.9D-12	2.4D-09	9.3D-06
12	1.1D-15	1.1D-11	2.4D-09	7.9D-06
15	9.4D-14	7.2D-12	1.1D-08	5.5D-06
20	3.1D-12	1.7D-09	4.9D-07	1.5D-02

Table 4.7: $f(x) = 1/\left(\sin\left[\frac{\pi x}{2}\right] + 5\right)$, σ_n for $A = 0, B = 0.5$

5. Conclusion

The method calculates the k -th derivative of a function defined in the interval $[A, B]$ at the points $x_i = A + ih$ for $i = 0, 1, \dots, n$ where $h = \frac{B-A}{n}$.

In calculating the k -th derivative; the derivatives up to order $(k-2)$ at A are required. In other words these values are to be calculated at previous steps.

In utilizing the method at the $(k+1)$ -th step following the k -th step all calculations have to be redone. On the other hand matrix coefficients are not dependent on the function. They are uniquely determined for specific A, B, n and k values, Hence once the coefficient matrix is calculated it is re utilizable for different functions over and over again.

The method can be easily encoded on personal computers. Although increasing in values generally makes positive contributions to the results, beyond a certain specific n value error values start growing.

The increase in the order of the derivative increases the error. Especially, fifth and higher order derivatives do not give good values. It is observed in the relevant tables that especially at the two end points A and B for high order derivatives serious diversions occur.

As a conclusion, it will be fair to state that when the derivative values for a function is known at $(n+1)$ points this method is capable of approximating the derivatives of order k at equally spaced points x_i 's quite well.

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