Formulae of numerical differentiation

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Abstract

We derived the formulae of central differentiation for the finding of the first and second derivatives of functions given in discrete points, with the number of points being arbitrary. The obtained formulae for the derivative calculation do not require direct construction of the interpolating polynomial. As an example of the use of the developed method we calculated the first derivative of the function having known analytical value of the derivative. The result was examined in the limiting case of infinite number of points. We studied the spectral characteristics of the weight coefficients sequence of the numerical differentiation formulae. The performed investigation enabled one to analyze the accuracy of the numerical differentiation carried out with the use of the developed technique.

Mathematics Subject Classification: Primary 65D25; Secondary 65T50

1 Introduction

In solving many mathematical and physical problems by means of numerical methods one is often challenged to seek derivatives of various functions given in discrete points. In such cases, when it is difficult or impossible to take derivative of a function analytically one resorts to numerical differentiation.

It should be noted that there exists a great deal of formulae and techniques of numerical differentiation (see, for instance, Ref. [1]). As a rule, the function in question \( f(x) \) is replaced with the easy-to-calculate function \( \varphi(x) \) and then it is approximately supposed that \( f'(x) \approx \varphi'(x) \). The derivatives of higher orders are computed similarly. Therefore, in order to obtain numerical value of the derivative of the considered function it is necessary to indicate correctly the interpolating function \( \varphi(x) \). If the values of the function \( f(x) \) are known in \( s \) discrete points, the function \( \varphi(x) \) is usually taken as the polynomial of \( (s - 1) \)th power.

To find the derivative of functions having the intervals both quick and slow variation quasi-uniform nets are used (see Ref. [2]). This method has an ad-
vantage since constant small mesh width is unfavorable in this case, because it leads to the strong enhancement of the function values table.

The problem of the numerical differentiation accuracy is also of interest. The numerical differentiations formulae, taking into account the values of the considered function both at \( x > x_0 \) and \( x < x_0 \) (\( x_0 \) is a point where the derivative is computed), are called central differentiation formulae. For instance, the formulae based on Stirling interpolating polynomial can be included in this class. Such formulae are known to have higher accuracy compared to the formulae, using unilateral values of a function\(^1\), i.e., for instance, at \( x > x_0 \).

The range of numerical differentiation formulae based on different interpolating polynomials is limited, as a rule, to finite points of interpolation. All available formulae known at the present moment are obtained for a certain concrete limited number of interpolation points (see Refs. [3, 4]). It can be explained by the fact that the procedure of the finding of the interpolating polynomial coefficients in the case of the arbitrary number of interpolation points is quite awkward and requires formidable calculations.

It is worth mentioning that the procedure of the numerical differentiation is incorrect. Indeed, in Ref. [2] it was shown that it is possible to select such decreasing error of the function in question which results in the unlimited growth of the error in its first derivative.

Some recent publications devoted to the numerical differentiation problem should be mentioned (see, e.g., Ref. [5]). In this work the finite difference formulae for real functions on one dimensional grids with arbitrary spacing were considered.

The formulae of central differentiation for the finding of the first and the second derivatives of the functions given in \((2n + 1)\) discrete points are derived in this paper. The number of interpolation points is taken to be arbitrary. The obtained formulae for the derivatives calculation do not require direct construction of the interpolating polynomial. As an example of the use of the developed method we calculate the first derivative of the function \( y(x) = \sin x \). The obtained result is studied in the limiting case \( n \to \infty \). We examine the spectral characteristics of the weight coefficients sequence of the numerical differentiation formulae for the different number of the interpolation points. The performed analysis can be applied to the studying of the accuracy of the numerical differentiation technique developed in this work. It is found that the derived formulae of numerical differentiation have a high accuracy in a very wide range of spatial frequencies.

\(^1\)The formulae using, for example, Newton interpolating polynomial are attributed to this class of numerical differentiation formulae.
2 Formulae for approximate values of the first and the second derivatives

Without the restriction of generality we suppose that the derivative is taken in the zero point, i.e. \( x_0 = 0 \). Let us consider the function \( f(x) \) given in equidistant points \( x_m = \pm mh \), where \( m = 0, \ldots, n \) and \( h \) is the constant value. We can pass the interpolating polynomial of the 2nd power through these points

\[
P_{2n}(x) = \sum_{k=0}^{2n} c_k x^k, \tag{2.1}
\]

the values of the function in points of interpolation \( f_m = f(x_m) \) coinciding with the values of the interpolating polynomial in these points: \( P_{2n}(x_m) = f_m \). Let us define as \( d_m \) the differences of the values of the function \( f(x_m) \) in diametrically opposite points \( x_m \) and \( x_m \), i.e. \( d_m = f_m - f_m \). We can present \( d_m \) in the form

\[
d_m = 2 \sum_{k=0}^{n-1} c_{2k+1} h^{2k+1} m^{2k+1}. \tag{2.2}
\]

To find the coefficients \( c_{2k+1}, k = 0, \ldots n - 1 \), we have gotten the system of inhomogeneous linear equations with the given free terms \( d_m \). It will be shown below that this system has the single solution.

We will seek the solution of the system [Eq. (2.2)] in the following way

\[
c_{2k+1} = \frac{1}{2h^{2k+1}} \sum_{m=1}^{n} d_m \alpha_m^{(2k+1)}(n), \tag{2.3}
\]

where \( \alpha_m^{(2k+1)}(n) \) are the undetermined coefficients satisfying the condition

\[
\sum_{m=1}^{n} \alpha_m^{(2l+1)}(n)m^{2k+1} = \delta_{lk}, \quad l, k = 0, \ldots, n - 1. \tag{2.4}
\]

Thus, the system of equations [Eq. (2.2)] is reduced to the equivalent, but more simple system [Eq. (2.4)], in which for each fixed number \( k = 0, \ldots, n - 1 \) it is necessary to find the coefficients \( \alpha_m^{(2l+1)}(n) \).

Let us resolve the system of equations [Eq. (2.4)] according to the Cramer’s rule:

\[
\alpha_m^{(2l+1)}(n) = \frac{\Delta_m^{(2l+1)}(n)}{\Delta_0(n)}, \tag{2.5}
\]

where

\[
\Delta_0(n) = \begin{vmatrix}
1 & 2 & \ldots & n \\
1 & 2^3 & \ldots & n^3 \\
\vdots & \vdots & \ddots & \vdots \\
1 & 2^{2n-1} & \ldots & n^{2n-1}
\end{vmatrix} = n! \prod_{1 \leq i < j \leq n} (j^2 - i^2) \neq 0, \tag{2.6}
\]
In Eq. (2.6) we used the formula for the calculation of the Vandermonde determinant. From Eq. (2.6) it follows that the determinant of the system of equations [Eq. (2.4)] is not equal to zero, i.e. the system of equations [Eq. (2.2)] has the single solution.

The most simple expression for \( \Delta_{m}^{(2l+1)} \) is obtained in the case of \( l = 0 \) that corresponds to a calculation of the first-order derivative

\[
\Delta_{m}^{(1)}(n) = (-1)^{m+1} \left( \frac{n!}{m!} \right)^3 \prod_{1 \leq i < j \leq n} (j^2 - i^2).
\]

(2.7)

From Eq. (2.5) as well as taking into account Eqs. (2.6) and (2.7) we get the expression for the coefficients \( \alpha_{m}^{(1)}(n) \)

\[
\alpha_{m}^{(1)}(n) = \frac{1}{m \pi_{m}(n)},
\]

(2.8)

where

\[
\pi_{m}(n) = \prod_{k=1}^{n} \left( 1 - \frac{m^2}{k^2} \right).
\]

(2.9)

It should be noted that one can similarly get the expression for the coefficients \( \alpha_{m}^{(2n-1)}(n) \) which is presented in the following way

\[
\alpha_{m}^{(2n-1)}(n) = \frac{(-1)^{n+1} m}{(n!)^2 \pi_{m}(n)}.
\]

Taking into account Eqs. (2.6) and (2.8) we finally get the formula for the first derivative of the function \( f(x) \)

\[
f'(0) \approx P'_{2n}(0) = \frac{1}{2h} \sum_{m=1}^{n} \alpha_{m}^{(1)}(n)(f_{m} - f_{m}).
\]

(2.10)

The algorithm for the computation of the coefficients \( \alpha_{m}^{(1)}(n) \) is presented in the appendix A and the results for the certain concrete number of the interpolation points \( (2n + 1) \) are given in Tab. I. Note that the expression for the first derivative obtained by this method coincides with the value presented in the Refs. 3, 4 for \( n = 1, 2 \) that corresponds to three and five points of interpolation. However, technique developed in this article allows one to calculate the coefficients \( \alpha_{m}^{(1)}(n) \), and hence the first derivative, for any value of \( n \).
Similar formula can be obtained for the calculation of the second derivative.

We give without proof corresponding expression

\[ f''(0) \approx P''_{2n}(0) = 1 \frac{h^2}{n} \sum_{m=1}^{n} \alpha_{m}^{(2)}(n)(f_m - 2f(0) + f_{-m}), \]  

(2.11)

where

\[ \alpha_{m}^{(2)}(n) = \frac{1}{m^2 \pi_m(n)}, \]  

(2.12)

and the product \( \pi_m(n) \) is introduced in Eq. (2.9).

As an example of the use of the obtained central differentiation formulae we will compute the first derivative of the function \( y(x) = \sin x \) at \( x = 0 \). Let us set the value of the mesh width \( h \) equal to \( \pi/2 \). Notice that, as a rule, the less the mesh width \( h \) the more exact result numerical differentiation gives. We have chosen rather big value of \( h \). The Eq. (2.10) for this case takes the form

\[ y'(0) = \frac{2}{\pi} \sum_{m=0}^{n} (-1)^m \alpha_{2m+1}^{(1)}(n). \]  

(2.13)

In Eq. (2.13) we take that \( d_m = 0 \) if \( m \) is an even number, and \( d_m = \pm 2 \) if \( m \) is an odd number.

Let us study the obtained result in the limiting case \( n \to \infty \). First, it is necessary to calculate the value of the product \( \pi_m(n) \) within the limit \( n \to \infty \)

\[ \pi_m = \lim_{n \to \infty} \pi_m(n) = \lim_{\varepsilon \to 0} \frac{1}{1 - \left( \frac{m + \varepsilon}{m} \right)^2} \prod_{k=1}^{\infty} \left( 1 - \frac{(m + \varepsilon)^2}{k^2} \right) = \frac{(-1)^{m+1}}{2} \lim_{\varepsilon \to 0} \frac{\sin \pi \varepsilon}{\pi \varepsilon} = \frac{(-1)^{m+1}}{2} \]  

(2.14)

Here we used the known value of infinite product

\[ \prod_{k=1}^{\infty} \left( 1 - \frac{\pi^2}{k^2} \right) = \frac{\sin \pi x}{\pi x}. \]  

Table 1: Values of the coefficients \( \alpha_{m}^{(1)}(n) \).

| \( n \) | \( \alpha_{1}^{(1)}(n) \) | \( \alpha_{2}^{(1)}(n) \) | \( \alpha_{3}^{(1)}(n) \) | \( \alpha_{4}^{(1)}(n) \) | \( \alpha_{5}^{(1)}(n) \) | \( \alpha_{6}^{(1)}(n) \) |
|---|---|---|---|---|---|---|
| 1 | 1 | 0 | 0 | 0 | 0 | 0 |
| 2 | 4/3 | -1/6 | 0 | 0 | 0 | 0 |
| 3 | 3/2 | -3/10 | 1/30 | 0 | 0 | 0 |
| 4 | 8/5 | -2/5 | 8/105 | -1/140 | 0 | 0 |
| 5 | 5/3 | -10/21 | 5/42 | -5/252 | 1/630 | 0 |
| 6 | 12/7 | -15/28 | 10/63 | -1/28 | 2/385 | -1/2772 |
Using Eqs. (2.8) and (2.14), we find that the expression for the coefficients \( \alpha^{(1)}_m(n) \) within the limit \( n \to \infty \) is represented in the following way

\[
\alpha^{(1)}_m = \lim_{n \to \infty} \alpha^{(1)}_m(n) = (-1)^{m+1} \frac{2}{m}. \tag{2.15}
\]

Now it is easy to complete the studying of Eq. (2.13). Substituting the result from Eq. (2.15) to Eq. (2.13) and using the known value of infinite series we get that

\[
y'(0) = \frac{4}{\pi} \sum_{m=0}^{\infty} \frac{(-1)^m}{2m+1} = 1.
\]

Thus, it is shown that the method of the derivatives finding, developed in this paper, gives for the function \( y(x) = \sin x \) the value of the first derivative which coincides with the exact analytical one even at rather crude mesh width.

### 3 Spectral characteristics of weight coefficients sequences

In the section 2 of the present work we derived the formula for the finding of the first derivative of the function \( f(x) \) at \( x = 0 \). This result can be easily generalized for the case of the arbitrary point \( x = kh \). If we set that \( \alpha^{(1)}_{-m}(n) = -\alpha^{(1)}_m(n) \), and moreover supposing that \( \alpha^{(1)}_m(n) = 0 \) for \( m \equiv 0 \) and \( m > n \) (see Tab. 1), then in the considered case Eq. (2.10) reads as follows

\[
f'(kh) \approx P'_{2n}(kh) = \frac{1}{2h} \sum_{m} \alpha^{(1)}_{m-k}(n)f_m. \tag{3.1}
\]

Here the summing is taken over all range of the function involved: \( f(kh) \). For instance, if the values of the function are set on the limited equidistant collection of elements \( N \), then Eq. (3.1) can be rewritten in the form

\[
f'(kh) \approx \frac{1}{2h} \sum_{m=0}^{N-1} \alpha^{(1)}_{m-k}(n)f_m, \quad N \geq 2n. \tag{3.2}
\]

It is worth noticing that in Eq. (3.2) we used the periodicity condition of the weight coefficients

\[
\alpha^{(1)}_m(n) = \alpha^{(1)}_{m-N}(n).
\]

Fig. 1 presents the example of the weight coefficients of the differentiating sequence \( \alpha^{(1)}_m(1) \). Thus the first derivative computation of the function \( f(x) \) at the points \( x = kh, \ k = 0, 1, \ldots, N - 1 \), is reduced to the procedure of the calculation of the mutual correlation function between the finite sequences \( \alpha^{(1)}_m(n) \) and \( f_m \).
It is known (see, e.g., Ref. [6]) that if a function satisfies the Dirichlet conditions in the interval \((-l, l)\), then it can be expanded into the Fourier series

\[
f(x) = \sum_{k=-\infty}^{+\infty} c_k \exp \left( i \frac{\pi k}{l} x \right),
\]

(3.3)

where the expansion coefficients are presented in the way

\[
c_k = c_{-k} = \frac{1}{2l} \int_{-l}^{l} f(\xi) \exp \left( -i \frac{k\pi}{l} \xi \right) d\xi.
\]

If the first derivative \(f'(x)\) satisfies the analogous conditions as the function \(f(x)\), then the following expression will be valid

\[
f'(x) = \sum_{k=-\infty}^{+\infty} \left\{ i \frac{k\pi}{l} \right\} c_k \exp \left( i \frac{\pi k}{l} x \right),
\]

(3.4)

Therefore, form Eqs. (3.3) and (3.4) it follows that the differentiation procedure is the linear filter with the frequency characteristic: \(R_1(k) = \frac{ik(\pi/l)}{2}\).

Similarly we receive for the second derivative

\[
f''(x) = \sum_{k=-\infty}^{+\infty} \left\{ -\left( \frac{k\pi}{l} \right)^2 \right\} c_k \exp \left( i \frac{\pi k}{l} x \right),
\]

In this case the the frequency characteristic of the corresponding filter has the form: \(R_2(k) = -k^2(\pi/l)^2\).

According to Wiener-Khinchin theorem (see, e.g., Ref. [7]) the mutual correlation function between the two finite sequences can be calculated with the help of the inverse Fourier transform of the mutual spectrum of the considered sequences. Thus, if we define that

\[
\beta_1(r) = \sum_{m=0}^{N-1} \alpha_m^{(1)}(n) \exp \left( -i \frac{2\pi}{N} mr \right),
\]
Figure 2: The spectra of various sequences $\alpha_m^{(1)}(n)$ at $N = 2000$.

is the complex spectrum of the differentiating sequence $\alpha_m^{(1)}(n)$, and

$$c_r = \sum_{m=0}^{N-1} f_m \exp \left( -i \frac{2\pi}{N} mr \right),$$

is the spectrum of the function $f(x)$, then it follows from Eq. (3.2) that

$$f'(kh) = \frac{1}{2h} \sum_{r=0}^{N-1} c_r \beta_1^*(r) \exp \left( \frac{2\pi}{N} kr \right),$$

where $\beta_1^*(r)$ is the complex conjugated quantity with respect to $\beta_1(r)$.

Comparing Eqs. (3.4) and (3.5) we obtain that the accuracy of the numerical differentiation performed with the use of the various types of the sequences $\alpha_m^{(1)}(n)$ is characterized by the closeness of imaginary parts of their spectra to the linearly growing sequence $y_1(r) = 2\pi r/N$.

The spectra of the sequences $\alpha_m^{(1)}(n)$ are depicted in Fig. 2 for the various values of $n$ at $N = 2000$. It can be seen from this figure that for $n = 1$, i.e. for the sequence shown in Fig. 1 the imaginary part of the spectrum is the branch of the function $\sin(2\pi r/N)$. The linearity condition is satisfied only in the vicinity of zero and $N/2$. However, at $n = 11$ the spectrum practically does not differ from the linear one up to $r \approx N/2$. The more close to linear one is the spectrum of the sequence $\alpha_m^{(1)}(21)$.

The difference between the imaginary parts of the spectra of the sequences $\alpha_m^{(1)}(n)$ and the linearly growing sequence $y_1(r) = 2\pi r/N$ are presented in Fig. 3. The computations have been performed with the accuracy up to $10^{-15}$, thus the reliable results at $n = 11$ have been obtained for $r \gtrsim 150$, and at $n = 21$ for $r \gtrsim 300$. The presented results demonstrate the high accuracy of the numerical
differentiation carried out with the help of the sequences $\alpha_m^{(1)}(n)$ in the wide range of the spatial frequencies.

Now let us briefly consider the sequences for the calculation of the second derivative $\alpha_m^{(2)}(n)$, which are given in Eq. (2.12). Their spectral properties can be obtained in the similar manner as we have done it for the case of the sequences $\alpha_m^{(1)}(n)$ and therefore we just present the final results. The spectra of the sequences $\alpha_m^{(2)}(n)$ are shown in Fig. 4. It follows from this figure that the closeness of the corresponding spectrum to the parabola $y_2(r) = -(2\pi r/N)^2$ in the case of $n = 1$ exists only in the vicinity of zero. The spectra at $n = 11$ and $n = 21$ are close to function $y_2(r)$ in a wider range of $r$ ($r \lesssim 750$ and $r \lesssim 800$ respectively). The difference between the real parts of the spectra of the sequences $\alpha_m^{(2)}(n)$ and the parabola $y_2(r) = -(2\pi r/N)^2$ are depicted in Fig. 5 in the logarithmic scale. This figure again demonstrates the high accuracy of the second derivative computation with the use of the sequences $\alpha_m^{(2)}(n)$.

4 Conclusion

In conclusion we note that the method of central differentiation formulae finding has been developed in this article. The elaborated technique does not require direct construction of the interpolating polynomial. We have derived simple and convenient expressions for the first and the second derivatives [Eqs. (2.10) and (2.11)] of the function given in $(2n+1)$ discrete points. The number $n$ was taken to be arbitrary. In contrast to the results of the Ref. [5], where the recursion relations for the calculation of the weight coefficient being used in numerical differentiation formulae were considered, in the present work the expressions for the considered weight coefficients have been derived in the explicit form for the arbitrary number of interpolation points. As an example of the use of the
Figure 4: The spectra of various sequences $\alpha^{(2)}_{m,n}(n)$ at $N = 2000$.

Figure 5: The function $\delta_2(r) = \Re(\beta_2^*(r)) - y_2(r)$ versus $r$ for different $n$. 
developed method we have calculated the first derivative of the function $y(x) = \sin x$. The obtained result has been studied in the limiting case $n \to \infty$. We have examined the spectral characteristics of the weight coefficients sequence of the numerical differentiation formulae for the different number of the interpolation points. The performed analysis has allowed one to study the accuracy of the numerical differentiation carried out with the help of the developed method. It has been found that the derived formulae of numerical differentiation posses the high accuracy in a rather wide range of the spatial frequencies. As it has been shown in this paper, the formulae for the derivatives finding gave correct results in the case of large number of interpolation points. Thus, the developed method can be useful in lattice simulation of quantum fields [8]. To get the exact results at calculations on lattices one has to use nets with the big number of points. Derivatives which one encounters in theories of quantum fields, as a rule, do not exceed the second order. Therefore, the formulae obtained in this article could be of use in carrying out mentioned above research.

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A Algorithm for computation of weight coefficients $\alpha_{m}^{(1)}(n)$

In this appendix we present the algorithm for the computation of the coefficients $\alpha_{m}^{(1)}(n)$ on the MATLAB 6.5 programming language.

$N = 2000$; \hspace{1cm} $N$ is the size of the array

$n = 11$; \hspace{1cm} $n$ is the order of the differentiating sequence

$\alpha = \text{zeros}(1, N)$; \hspace{1cm} $\alpha$ is the array of the weight coefficients

$k_1 = 2$; $k_2 = N$;

for $m = 1 : n$

$r_1 = 1$;

for $k = 1 : n$

if $k == m$

$r_2 = 1$;

else

$r_2 = 1 - (m/k)^2$;

end

$r_1 = r_1 \times r_2$;

end

$r_1 = 1/(2 \times r_1 \times m)$;

$\alpha(1, k_1) = -r_1$; $k_1 = k_1 + 1$; \,$\alpha(1, k_2) = r_1$; $k_2 = k_2 - 1$;
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