Spectral Properties of Numerical Differentiation

Maxim Dvornikov
Department of Physics, P.O. Box 35, 40014, University of Jyväskylä, Finland*
IZMIRAN, 142190, Troitsk, Moscow region, Russia†

Abstract

We study the numerical differentiation formulae for functions given in grids with arbitrary number of nodes. We investigate the case of the infinite number of points in the formulae for the calculation of the first and the second derivatives. The spectra of the corresponding weight coefficients sequences are obtained. We examine the first derivative calculation of a function given in odd-number points and analyze the spectra of the weight coefficients sequences in the cases of both finite and infinite number of nodes. We derive the one-sided approximation for the first derivative and examine its spectral properties.

Mathematics Subject Classification: Primary 65D25; Secondary 65T50

Introduction

The problem of numerical differentiation is a long-standing issue. There are plenty of published works devoted to the generation of finite difference formulae in both one and multi dimensional lattices (see, e.g., Ref. [1]). However, many of those methods require preliminary construction of an interpolating polynomial, and hence are very awkward. Moreover, the majority of the previous techniques are valid in the case of a function given in the limited number of nodes.

The finite difference formulae for the calculation of any order derivative in a one dimensional grid with arbitrary spacing were discussed in Refs. [2, 3]. However, only recursion relations for the weight coefficients have been derived. The explicit formulas for the derivatives calculation were recently derived in Ref. [4] on the basis of the generalized Vandermonde determinant.

It should be noted that the low order derivatives (the first and the second ones) as well as equidistant lattices are of the major importance in many problems of applied mathematics and physics. The first and the second numerical derivatives in the equidistant one dimensional grid were studied in Ref. [5]. The finite difference formulae for the central derivatives of a function given on a lattice with arbitrary number of elements have been derived in that work. It is important that these formulae have been obtained in the explicit form. This method enabled one to examine the spectral properties of weight coefficients sequences as well as to analyze the accuracy of the numerical differentiation.

In the present paper we continue to study the numerical differentiation formulae for functions given in grids with arbitrary number of nodes. On the basis of the results of Ref. [5] in Sec. 1 we investigate the case of the infinite number of points in the formulae for the calculation of the first and the second derivatives. The spectra of the corresponding weight coefficients sequences are also obtained. Then, in Sec. 2 we examine the first derivative calculation of a function given in odd-number points. We also analyze the spectra of the weight coefficients sequences in the cases of both finite and infinite number of nodes. In Sec. 3 we derive the one-sided approximation for the first derivative and examine its spectral properties. It is worth noticing that the derivations of the finite difference formulae in all cases are performed for the arbitrary number of points. Finally, in Sec. 4 we resume our results.

*E-mail: dvmaxim@cc.jyu.fi
†E-mail: maxdvo@izmiran.ru
Spectral properties of the first and the second derivatives for infinite number of points

Let us study the function \( f(x) \) given in the equidistant points \( x_m = f_m \), where \( m = 0, \ldots, \pm n \). It was found in Ref. [5] that the first and the second derivatives are approximated as

\[
f'(0) \approx \frac{1}{2h} \sum_{m=1}^{n} \alpha^{(1)}_m(n)(f_m - f_{-m}).
\]

(1.1)

and

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

(1.2)

where \( h \) is the distance between nodes. The coefficients \( \alpha^{(1)}_m(n) \) and \( \alpha^{(2)}_m(n) \) can be calculated explicitly for arbitrary \( n \) (see Ref. [5]).

The spectral properties of the sequences \( \alpha^{(1)}_m(n) \) and \( \alpha^{(2)}_m(n) \) in Eqs. (1.1) and (1.2) in the case of finite number of interpolation points were carefully examined in Ref. [5]. We found out that the more points we involved in the sequence \( \alpha^{(1)}_m(n) \) the more close to linear the corresponding spectrum was. Thus the considered sequence produces more accurate first derivative of a function in the case of great number of points. As for the sequence \( \alpha^{(2)}_m(n) \), it was also shown in Ref. [5] that its spectrum approached to parabola if \( n > 1 \). We expect that the corresponding spectra will be exactly linear and parabolic ones if \( n \to \infty \).

Let us consider the spectral characteristics of the sequences \( \alpha^{(1)}_m(n) \) and \( \alpha^{(2)}_m(n) \) in the case of infinite number of interpolation points. First we remind the result for the \( \alpha^{(1)}_m(n) \) in the limit \( n \to \infty \) (see Ref. [5])

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

(1.3)

The Fourier transform of a function \( f(x) \) can be presented in the form (see, e.g., Ref. [6])

\[
c(\omega) = h \sum_{x} e^{-i\omega x} f(x) = h \sum_{m=-\infty}^{+\infty} e^{-i\omega mh} f(mh).
\]

(1.4)

The inverse Fourier transformation is given by the following expression:

\[
f(x) = \int_{-\pi/h}^{\pi/h} \frac{d\omega}{2\pi} c(\omega)e^{i\omega x}, \quad x = kh,
\]

(1.6)

and has the cutoff at high frequencies, \(|\omega| \leq \pi/h\).

Now we can calculate the spectrum of the sequence \( \alpha^{(1)}_m \),

\[
\beta_1(\omega) = h \sum_{m=-\infty}^{+\infty} e^{-i\omega mh} \alpha^{(1)}_m = -4ih \sum_{m=1}^{\infty} (-1)^{m-1} \frac{\sin(m\omega h)}{m} = -2i\omega h^2,
\]

(1.5)

where we use Eqs. (1.3) and (1.4). Note that Eq. (1.5) is valid if \( 0 \leq \omega < \pi/h \). The first derivative of the function can be expressed via the spectra \( \beta_1(\omega) \) and \( c(\omega) \),

\[
f'(x) = \frac{1}{2h} \int_{-\pi/h}^{\pi/h} \frac{d\omega}{2\pi} \beta_1^*(\omega)c(\omega)e^{i\omega x}, \quad x = kh.
\]

(1.6)

Using the result for the calculation of \( \beta_1(\omega) \) presented in Eq. (1.5) we readily find that

\[
f'(x) = \int_{-\pi/h}^{\pi/h} \frac{d\omega}{2\pi} (i\omega)c(\omega)e^{i\omega x}.
\]

(1.7)
Figure 1: The spectra of differentiating filters, (a) $\alpha_m^{(1)}$ and (b) $\alpha_m^{(2)}$, in the case of infinite number of points.

Eq. (1.7) shows that the first derivative calculation with help of the sequence $\alpha_m^{(1)}$ gives the exact value of the derivative in the case of infinite number of interpolation points for all frequencies except $\omega_{\text{max}} = \pi/h$. The fact that the first derivative computation does not give correct results at $\omega = \omega_{\text{max}}$ also follows from Fig. 1(a). However, it can be verified directly with help of Eq. (1.3) for the function $f_m = (-1)^m = \cos(\omega_{\text{max}}mh)$.

In Ref. [5] we showed that the use of the coefficients $\alpha_m^{(1)}$ give exact value for the first derivative of the function $y(x) = \sin(\omega_{\text{max}}x/2)$. However, Eq. (1.7) [see also Fig. 1(a)] indicates that this method will give the correct results not only for $\omega = \omega_{\text{max}}/2$ but also for all frequencies $\omega < \omega_{\text{max}}$.

The second derivative calculation in the case of infinite number of interpolation points can be analyzed in the similar manner as we have done it for the first derivative. The explicit form of the sequence $\alpha_m^{(2)}$ is

$$\alpha_m^{(2)} = \lim_{n \to \infty} \alpha_m^{(2)}(n) = (-1)^{m+1} \frac{2}{m^3}. $$

For the spectrum of the sequence $\alpha_m^{(2)}$ we obtain

$$\beta_2(\omega) = -\omega^2 h^3 + \frac{\pi^2}{3} h. \quad (1.8)$$

It should be noted that Eq. (1.8) is valid for all frequencies $0 \leq \omega \leq \pi/h$. The expression for the second derivative takes the form

$$f''(x) = \frac{1}{h^2} \int_{-\pi/h}^{\pi/h} \frac{d\omega}{2\pi h} \left[ \beta_2^{(2)}(\omega) - \beta_2^{(2)}(0) \right] c(\omega)e^{i\omega x} = \int_{-\pi/h}^{\pi/h} \frac{d\omega}{2\pi} (-\omega^2) c(\omega)e^{i\omega x}, \quad x = kh. \quad (1.9)$$

Eq. (1.9) demonstrates that the computation of the second derivative with the use of the sequence $\alpha_m^{(2)}$ gives the exact results in the case of infinite number of interpolation points for all frequencies even including the maximal one. The spectrum $\beta_2(\omega)$ is depicted in Fig. 1(b).

2 The first derivative computation of a function given in odd-number points

In this section we discuss the calculation of the first derivative in the case of a function given in odd-number nodes. Then we discuss the spectral properties of the derived weight coefficients sequences in the case of both finite and infinite number of nodes.
It follows from Fig. 1(a) that the computation of the first derivative gives unsatisfactory results at high frequencies near \( \omega_{\text{max}} \). In order to introduce the numerical differentiation of such rapidly oscillating functions we consider the modified sequence

\[
\alpha_{2m+1}(n) = \frac{1}{(2m + 1)\pi_m^{(1/2)}(n)}, \quad m = 0, \ldots, n-1,
\]

where

\[
\pi_m^{(1/2)}(n) = \prod_{k=0, k \neq m}^{n-1} \left( 1 - \frac{(2m + 1)^2}{(2k + 1)^2} \right),
\]

and \( \alpha_{2m}(n) = 0 \).

The coefficients in Eq. (2.1) can be formally derived if we consider the first derivative calculation of a function given in the odd-number points only

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

Note that originally the function \( f(x) \) was given in \( 2n + 1 \) points.

It is worth noticing that the results for the computation of the weights with help of Eq. (2.1) in some particular cases (namely for \( n = 3, 5, 7 \) and 9) coincide with those presented in Ref. [2] for the centered approximations at a 'half-way' point. However, the method for the central derivatives calculation elaborated in our paper enables one to get the expressions for the weight coefficients in the explicit form for any number of nodes.

We consider the spectral properties of the obtained sequence \( \alpha_m^{(1/2)}(n) \). Using the technique developed in Ref. [4] one can compute the spectrum of the sequence in question,

\[
\beta_{1/2}(r) = \sum_{m=0}^{N-1} \alpha_m^{(1/2)}(n) \exp \left( -i \frac{2\pi}{N} mr \right).
\]

The spectra of the sequences \( \alpha_m^{(1/2)}(n) \) are depicted in Fig. 2(a) for the various values of \( n \) at \( N = 2000 \). The function \( y_{1/2}(r) \) has the form...
It follows from this figure that for \( n = 1 \) the imaginary part of the spectrum is the function \( \sin(2\pi r/N) \). The linearity condition is satisfied only in the vicinity of zero and \( N/2 \). However at \( n = 10 \) linearity condition remains valid for \( r \lesssim 350 \) and \( r \gtrsim 650 \).

We examine the details of the differentiation procedure performed with help of the sequence \( \alpha_m^{(1/2)}(n) \). If a function is slowly varying, then Eq. (2.2) gives the approximate value of the first derivative. It also results from Fig. 2(a). However, if a function is rapidly oscillating (e.g., at \( \omega \lesssim \omega_{\text{max}} \)), we can consider its upper and lower envelope functions. Therefore the use of the sequence \( \alpha_m^{(1/2)}(n) \) will produce the first derivative of envelope functions since in Eq. (2.2) we calculate the sum in odd-number points only. Envelope functions can be treated as "smooth" in this case. Fig. 2(b) schematically illustrates this process.

Now let us discuss the case of infinite number of the interpolation points. We can treat the sequence \( \alpha_m^{(1/2)}(n) \) in the similar way as it was done in Ref. [5]. Indeed, proceeding to the limit \( n \to \infty \) in Eq. (2.1) we find that

\[
\alpha_{2m+1}^{(1/2)} = \lim_{n \to \infty} \alpha_{2m+1}^{(1/2)}(n) = (-1)^m \frac{4}{\pi(2m+1)^2}. \tag{2.3}
\]

In Eq. (2.3) we used the known value of infinite product,

\[
\prod_{k=0}^{\infty} \left(1 - \frac{x^2}{(2k+1)^2}\right) = \cos \left(\frac{\pi x}{2}\right).
\]

With help of Eq. (2.3) it is possible to obtain the spectrum of the sequence \( \alpha_m^{(1/2)} \)

\[
\beta_{1/2}(\omega) = -2ih \times \begin{cases} 
\omega h, & \text{if } 0 \leq \omega \leq \pi/2h, \\
(\pi - \omega)h, & \text{if } \pi/2h \leq \omega \leq \pi/h.
\end{cases} \tag{2.4}
\]

The imaginary part of the spectrum \( \beta_{1/2}(\omega) \) is presented in Fig. 3. As it follows from Eq. (2.4) (see also Fig. 3) the sequence \( \alpha_m^{(1/2)} \) performs the differentiation of a function in question if \( \omega \leq \omega_{\text{max}}/2 \), or its envelope functions if \( \omega \geq \omega_{\text{max}}/2 \). The of case \( \omega = \omega_{\text{max}}/2 \) was also considered in details in Ref. [5].

### 3 One-sided approximation for the first derivative

In this section we derive the weight coefficients for the one-sided approximation of the first derivative and then we analyze the spectral characteristics of the weight coefficients sequence. It should
be noted that the derivation of the weight coefficients is analogous to case the of the central
derivatives which was carefully examined in Ref. [5].
Without restriction of generality we suppose that we approximate the first derivative in the
zero point. Let us consider the function \( f(x) \) given in the equidistant nodes \( x_m = mh > 0 \), where
\( m = 0, \ldots, n \), and \( h \) is the constant value. We can pass the interpolating polynomial of the \( n \)th
power through these points,
\[
P_n(x) = \sum_{k=0}^{n} c_k x^k.
\]
The values of the function in the nodes \( x_m = mh \), \( f_m = f(x_m) \), should coincide with the values
of the interpolating polynomial in these points,
\[
f_m = \sum_{k=0}^{n} c_k h^k m^k. \tag{3.1}
\]
In order to find the coefficients \( c_k \), \( k = 0, \ldots, n \), we receive the system of inhomogeneous linear
equations with the given free terms \( f_m \). It will be shown below that this system has the single
solution.
We will seek the solution of the system (3.1) in the following way:
\[
c_k = \frac{1}{h^k} \sum_{m=0}^{n} f_m a_m^{(k)}(n),
\]
where \( a_m^{(k)}(n) \) are the undetermined coefficients satisfying the condition,
\[
\sum_{m=0}^{n} a_m^{(l)}(n) m^k = \delta_{lk}, \quad l, k = 0, \ldots, n. \tag{3.2}
\]
It is worth to be noted that, if we set \( k = 0 \) and \( l \neq 0 \) in Eq. (3.2), we obtain the constraint which
should be imposed on the coefficients \( a_m^{(l)}(n) \)
\[
\sum_{m=0}^{n} a_m^{(l)}(n) = 0, \quad l = 1, \ldots, n. \tag{3.3}
\]
Analogous relation between the weight coefficients was established in Ref. [2]. In deriving of
Eq. (3.3) (as well as in all subsequent similar formulae) we suppose that \( m^0 = 1 \) if \( m = 0 \).
Let us resolve the system of equations (3.2) according to the Cramer’s rule
\[
a_m^{(l)}(n) = \frac{\Delta_m^{(l)}(n)}{\Delta_0(n)}, \tag{3.4}
\]
where
\[
\Delta_0(n) = \begin{vmatrix}
1 & 1 & 1 & \ldots & 1 \\
0 & 1 & 2 & \ldots & n \\
0 & 1 & 2^2 & \ldots & n^2 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 1 & 2^n & \ldots & n^n
\end{vmatrix} = n! \prod_{1 \leq i < j \leq n} (j-i) \neq 0, \tag{3.5}
\]
and
\[
\Delta_m^{(l)}(n) = \begin{vmatrix}
1 & 1 & 1 & \ldots & 1 & 0 & 1 & \ldots & 1 \\
0 & 1 & 2 & \ldots & m-1 & 0 & m+1 & \ldots & n \\
0 & 1 & 2^2 & \ldots & (m-1)^l & 1 & (m+1)^l & \ldots & n^l \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 1 & 2^n & \ldots & (m-1)^n & 0 & (m+1)^n & \ldots & n^n
\end{vmatrix}. \tag{3.6}
\]
In Eq. (3.5) we use the formula for the calculation of the Vandermonde determinant. From Eq. (3.5) it follows that the determinant of the system of equations (3.2) is not equal to zero, i.e. the system of equations (3.1) has the single solution.

The most simple expression for $\Delta_m^{(l)}(n)$ is obtained in the case of $l = 1$ that corresponds to the calculation of the first-order derivative

$$\Delta_m^{(1)}(n) = (-1)^{m+1} \left( \frac{n!}{m!} \right)^2 \prod_{1 \leq i < j \leq n, i,j \neq m} (j - i), \quad m = 1, \ldots, n. \quad (3.7)$$

From Eq. (3.4) as well as taking into account Eqs. (3.5) and (3.7) we get the expression for the coefficients $a_m^{(1)}(n)$

$$a_m^{(1)}(n) = (-1)^{m+1} \frac{1}{m} \binom{n}{m}, \quad m = 1, \ldots, n, \quad (3.8)$$

where

$$\binom{n}{m} = \frac{n!}{m!(n-m)!}.$$

are the binomial coefficients. It is remarkable to note that the coefficient $a_1^{(1)}(n) = n$. To simplify numerical calculations (especially the analysis of the spectra of the derived sequences) Eq. (3.8) should be rewritten in the form

$$a_m^{(1)}(n) = \frac{1}{mp_m(n)}, \quad m = 1, \ldots, n,$$

where

$$p_m(n) = \prod_{k=1}^{n} \left( 1 - \frac{m}{n} \right).$$

In order to find the coefficient $a_0^{(1)}(n)$ we use Eq. (3.3) rather than compute the determinant (3.6). Thus we receive the following expression for this coefficient,

$$a_0^{(1)}(n) = - \sum_{m=1}^{n} a_m^{(1)}(n) = - \sum_{m=1}^{n} (-1)^{m+1} \frac{1}{m} \binom{n}{m} = - \sum_{m=1}^{n} \frac{1}{m}. \quad (3.9)$$

Eqs. (3.8) and (3.9) provide the weight coefficients for the one-sided approximation of the first derivative of the function $f(x)$ given in $n + 1$ equidistant nodes,

$$f'(0) \approx \frac{1}{h} \sum_{m=0}^{n} f_m a_m^{(1)}(n).$$

The results for the computation of the weights in some particular cases (namely for $n = 1, 2, \ldots, 8$) coincide with those presented in Ref. [2]. However, the technique for derivatives calculation developed in the present work allows one to obtain the expressions for the weight coefficients in the explicit form for any $n$.

Without derivation we mention that on the basis of Eqs. (3.4)-(3.6) one can find the coefficients $a_m^{(n)}(n)$ that correspond to the computation of the $n$th-order derivative

$$a_m^{(n)}(n) = (-1)^{m+n} \frac{1}{n!} \binom{n}{m}, \quad m = 0, \ldots, n. \quad (3.10)$$

It should be noted that Eq. (3.10) is consistent with Eq. (3.3).
Now we consider the spectral properties of the derived sequence $a_m^{(1)}(n)$. Using the results of the previous section (see also Ref. [5]) we readily find the expression for the spectrum of the considered sequence,

$$b_1(r) = \sum_{m=0}^{N-1} a_m^{(1)}(n) \exp\left(-i\frac{2\pi}{N}mr\right).$$

The imaginary parts, $\Im[b_1^*(r)]$, of the spectra of the sequences $a_m^{(1)}(n)$ for the various values of $n$ at $N = 2000$ as well as the linearly growing sequence $I(r) = 2\pi r/N$ are presented in Fig. 4(a). It follows from this figure that the imaginary parts are close to the linear sequence only in the vicinity of zero ($r \lesssim 200$) even at $n = 5$. It points out that the one-sided approximation of the first derivative has worse accuracy in comparison with the central derivatives. This fact was also mentioned in Ref. [7]. Therefore, the application of the sequence $a_m^{(1)}(n)$ for the calculation of the one-sided first derivative will give reliable results only for slowly varying functions.

The spectrum $b_1(r)$ has not only imaginary part, but also nonzero real part since $a_0^{(1)}(n) \neq 0$. The real parts, $\Re[b_1^*(r)]$, of the spectra of the sequences $a_m^{(1)}(n)$ for the various values of $n$ at $N = 2000$ as well as the constant sequence $R(r) = 0$ are shown in Fig. 4(b). It can be seen from this figure that the real parts of the spectra are close to zero if $r \lesssim 100$ at $n = 1$, and if $r \lesssim 300$ at $n = 3$ and $n = 5$. The deviation from zero is especially great if $r \gtrsim 700$ at $n = 3$, and if $r \gtrsim 500$ at $n = 5$. Such a behavior of the real parts of the spectra also reveals the limited level of accuracy of the one-sided first derivative.

## 4 Conclusion

In conclusion we note that in our paper we have studied the numerical differentiation formulae for functions given on grids with arbitrary number of nodes. In Sec. 1 we have investigated the case of the infinite number of points in the formulae for the calculation of the first and the second derivatives. The spectra of the corresponding weight coefficients sequences have been obtained. It has been revealed that the calculation of the first derivative with help of the derived formulae gave reliable results for all spatial frequencies except $\omega_{\text{max}}$. As for the calculation of the second derivative we have shown that the corresponding formulae were valid for all spatial frequencies including $\omega_{\text{max}}$. In Sec. 2 we have examined the first derivative calculation of a function given in odd-number points. We have also analyzed the spectra of the weight coefficients sequences in the cases of both finite and infinite number of nodes. It has been found out that the obtained formulae
perform the differentiation of the considered function if $\omega \leq \omega_{\text{max}}/2$, and its envelope functions if $\omega \geq \omega_{\text{max}}/2$. In Sec. 3 we have derived the one-sided approximation for the first derivative and examined its spectral properties. The accuracy of the one-sided first derivative has been discussed. On the basis of the spectral properties of the weight coefficients sequences it has been shown that the accuracy of the one-sided approximation for the first derivative was essentially lower compared to the computation of the central derivatives. This our result is in agreement with previous works (see, e.g. Ref. [7]). Nevertheless, the obtained one-sided first derivative formulae could be of use in solving differential equations by means of numerical methods. It is also possible to apply the elaborated technique of the numerical differentiation in construction of quantum field theory models of unified interactions.

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