THEORETICAL ANALYSES ON DISCRETE FORMULAE OF DIRECTIONAL DIFFERENTIALS IN THE FINITE POINT METHOD∗

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Abstract
For the five-point discrete formulae of directional derivatives in the finite point method, overcoming the challenge resulted from scattered point sets and making full use of the explicit expressions and accuracy of the formulae, this paper obtains a number of theoretical results: (1) a concise expression with definite meaning of the complicated directional difference coefficient matrix is presented, which characterizes the correlation between coefficients and the connection between coefficients and scattered geometric characteristics; (2) various expressions of the discriminant function for the solvability of numerical differentials along with the estimation of its lower bound are given, which are the bases for selecting neighboring points and making analysis; (3) the estimations of combinatorial elements and of each element in the directional difference coefficient matrix are put out, which exclude the existence of singularity. Finally, the theoretical analysis results are verified by numerical calculations.

The results of this paper have strong regularity, which lay the foundation for further research on the finite point method for solving partial differential equations.

Key words: Finite point method, Finite difference, Scattered point distribution, Discrete directional differentials, Theoretical analysis.

1. Introduction
The finite difference method for solving partial differential equations (PDEs) (see, e.g., [1–4]) was originated in the 1920s, which was constructed on regular grids in computational domains. Due to the limitation of computational problems and conditions at that time, the computational scale was often small, and the complexity was not high, so the method could solve problems effectively. However, with the emergence of large and complex problems, the traditional finite difference method on regular grids was facing enormous challenges. To settle the matter, [1] and [5] proposed the method of dividing irregular mesh regions into regular sub-regions, respectively. [6] considered the finite difference method on irregular sub-regions with restricted topology. For irregular grids, [7] proposed a finite difference method with six-point stencils earlier, which could give approximations up to second-order derivatives, but was often troubled by singularity or ill-conditioning of numerical differentials.

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Thereafter, to overcome the singularity, some scholars proposed the generalized finite difference method by enlarging stencils [8–10], which enhanced the computational capability of the finite difference method on irregular grids to a certain extent [11,12]. With insight into the finite difference method, it is not difficult to find from the discrete process that it has properties of meshless methods.

In recent years, many efforts have been devoted to generalize the traditional difference method on scattered point sets. Most of them are based on a large number of neighboring points to fit derivatives [13–16], while there are also a few jobs in which a small number of neighbors are employed [17–19], however, none of them can address the issue of singularity or ill-conditioning of numerical derivatives at the fundamental level. In addition, many scholars have studied the difference method based on radial basis function (RBF) [20–24], which can be also viewed as a generalization of the traditional difference method.

To sum up, these works on scattered point sets undoubtedly improve the computational ability of the difference method, whereas scattered point sets also bring great difficulties to the theoretical analysis of related methods. Compared with its wide applications, theoretical results of meshless finite difference method are far from enough, especially for discrete analyses of PDEs. At present, the few existing works are often limited on discrete points with special distributions or on them only with a small number of discrete points near the boundary being irregular [25, 26].

The finite point method [27] to be studied in this paper is the finite difference method based on scattered point sets in irregular regions. In this method, only a few neighboring points are required to give the discretization of differential operators with higher accuracy. For example, in the two-dimensional case, given a discrete point, only 5 neighbors are demanded to obtain second-order approximations for first-order derivatives and first-order approximations for second-order derivatives. Above all, based on the analysis of the solvability conditions of numerical derivatives, the method of selecting neighboring points is presented, and the software module is formed, which can overcome the singularity problem of numerical derivatives fundamentally. The explicit expression of derivative approximation is also derived, by which some important theoretical results, such as convergence analysis for Poisson equation on scattered point sets [28] and the compatibility of nonlinear diffusion operators [29] are obtained, moreover, by which two-dimensional three-temperature energy equations in high temperature plasma physics have also been successfully solved numerically [29]. This paper aims at making a detailed analysis to give estimations of the numerical discrete formulae of directional derivatives on scattered point sets, including the lower bound of absolute value of the discriminant function for the solvability of numerical derivatives and the bounds of a series of coefficients. These theoretical results are the key bases for further developing the theoretical research of relevant methods.

The rest of the paper is arranged as follows: Section 2 gives some basic denotations; Section 3 discusses the structure of the directional difference coefficient matrix; Section 4 presents a variety of expressions and estimations of the discriminant function for the solvability of numerical differentials; Section 5 puts out analyses and estimation results of the directional difference coefficient matrix; Section 6 validates the theoretical results by numerical examples. Finally, the conclusions are drawn in Section 7.
2. Preliminaries

To simplify presentation, we introduce some denotations and definitions as defined in [27,28]. Let us denote by

- $i$ the index of point $(x_i, y_i)$ and “$O$” a specific point $(x_0, y_0)$;
- $\vec{l}_j$ the $j$th directional vector from $O$ and $\vec{e}_j$ the corresponding unit vector;
- $h_i$ the distance between point “$O$” and $i$;
- $u_i = u(x_i, y_i)$ the function value of $u(x, y)$ at point $i$;

We also have the following:

- $\langle i \, j \, k \rangle := \frac{1}{2} \begin{vmatrix} x_i - x_k & y_i - y_k \\ x_j - x_k & y_j - y_k \end{vmatrix}$, namely the algebraic area of triangle spanned by the points $i$, $j$ and $k$.
- $\langle i \, j \rangle := \langle i \, j \, O \rangle$, i.e., $k$ is a special point as “$O$” in the expression $\langle i \, j \, k \rangle$.
- $\langle i \, j \rangle_0 = \frac{1}{2} \sin(\vec{e}_i, \vec{e}_j)$, i.e., a special case of $\langle i \, j \rangle$ as $h_i = h_j = 1$, where $(\vec{e}_i, \vec{e}_j)$ denotes the anticlockwise angle between $\vec{e}_i$ and $\vec{e}_j$.
- $\langle i \, j \rangle_0 = \frac{1}{2} \cos(\vec{e}_i, \vec{e}_j)$.

Obviously, for any indices $i$, $j$, $k$, $l$, $m$, the following properties hold.

Property 2.1.

\[
\langle i \, j \rangle = -\langle j \, i \rangle,
\]
\[
\langle j \, k \rangle (l \, m) = \langle j \, l \rangle (k \, m) + \langle j \, m \rangle (l \, k).
\]

In this paper, we also follow the definition of the operation for indices as defined in [27].

Definition 2.1. (Algorithm ⃝) Given $i$, $j$, $k$ ($k \geq 3$) positive integers, an addition of $i$ and $j$ with period of $k$ is defined by

\[
i \, \hat{\,} \, j = 1 + (i + j - 1) \pmod{k},
\]

where $(i + j - 1) \pmod{k}$ represents the remainder of $(i + j - 1)$ modulo $k$.

3. The Structure of Directional Difference Coefficient Matrix

3.1. The discrete formulae of directional differentials on scattered point distributions

On the 2D scattered point sets, suppose that a point $O(x_0, y_0)$ with its five neighbors $(x_i, y_i)$ ($i = 1, \ldots, 5$), and their corresponding function values $u_i$ ($i = 0, 1, \ldots, 5$) are available. Here, the order of the indices is free (see Fig. 3.1).

Let $I = \{1, 2, 3, 4, 5\}$ be an index set, the discrete formulae for $\frac{\partial u}{\partial x}$, $\frac{\partial^2 u}{\partial x^2}$ ($\forall i \in I$) at the point “$O$” are obtained with second-order and first-order accuracy ([27]), respectively, the method for selecting neighboring points is designed, and the solvability of numerical derivatives is analyzed. To facilitate further research, we require a thorough understanding of the variation of coefficients
in expressions, especially give estimations to the variation bounds, so as to avoid singularity or oscillation caused by the scattered point sets in computing differentials. To this end, we first reconstruct the expressions of \( \frac{\partial u}{\partial l_i} \) and \( \frac{\partial^2 u}{\partial l_i^2} \) (\( \forall i \in I \)) into concise and easy-to-analyze forms.

For any \( i \in I \), denote by

\[
\begin{align*}
\Delta u_i &= u_i - u_0, \\
\delta u_i &= \Delta u_i / h_i, \\
\Delta_\sigma u_i &= \frac{1}{m_i} \sum_{j=1}^{5} a_{ij} \Delta u_j, \\
\delta^{(1)}_\sigma u_i &= \Delta_\sigma u_i / h_i, \\
\delta^{(2)}_\sigma u_i &= (\delta u_i - \delta^{(1)}_\sigma u_i) / (h_i / 2),
\end{align*}
\]

where \( a_{ij} (\forall i, j \in I) \) are elements of the matrix \( A \) concretely expressed by

\[
A = (a_{ij})_{5 \times 5} =
\begin{pmatrix}
\end{pmatrix}
\]

Here, \( A \) is called the directional difference coefficient matrix, \( \Delta_\sigma u_i \), \( \delta^{(1)}_\sigma u_i \), and \( \delta^{(2)}_\sigma u_i \) are called the compound difference, the compound first-order difference quotient, and the compound second-order difference quotient in the \( i \)-direction, respectively, and

\[
m_i = (23)(41)(1 \ 2 \ 5)(3 \ 4 \ 5) - (12)(34)(2 \ 3 \ 5)(4 \ 1 \ 5)
\]

is called the discriminant function for the solvability of numerical differentials. It appears in the denominators of the expressions of \( \frac{\partial u}{\partial l_i} \), \( \frac{\partial^2 u}{\partial l_i^2} \) (\( \forall i \in I \)), and becomes an important basis for selecting neighboring points. In the next section, we will present its multiple expressions and estimations of its bounds.
In above expressions, to approximate \( \frac{\partial u}{\partial \rightarrow l_i} \), \( \delta u_i \) employs a single neighboring point, and consequently has first-order accuracy, while \( \delta^{(1)} u \), formed by the informations of five neighbors has second-order accuracy. Meanwhile, as for the approximation to \( \frac{\partial u}{\partial \rightarrow l_i^2} \), \( \delta^{(2)}_\sigma u_i \) has first-order accuracy.

Denote by \( \Delta U = (\Delta u_1, \ldots, \Delta u_5)^T \), \( \delta U = (\delta u_1, \ldots, \delta u_5)^T \), and \( H = \text{diag}(h_1, h_2, \ldots, h_5) \).

Hence by [27] one has
\[
\Delta \sigma U = \frac{1}{m_t} A \cdot \Delta U,
\]
\[
\delta^{(1)} \sigma U = \tilde{A} \cdot \delta U,
\]
\[
\delta^{(2)} \sigma U = H^{-1} B \cdot \delta U,
\]
where
\[
\tilde{A} = \frac{1}{m_t} H^{-1} AH,
\]
\[
B = 2(E - \tilde{A}),
\]
where \( E \) denotes the unit matrix.

Obviously, the directional difference coefficient matrix \( A \) is the basis of discussing \( \tilde{A} \) and \( B \), namely, the compound first-order difference quotient and the compound second-order difference quotient. Let
\[
\frac{\partial u}{\partial L} = \left( \frac{\partial u}{\partial l_1}, \ldots, \frac{\partial u}{\partial l_5} \right)^T,
\]
\[
\frac{\partial^2 u}{\partial L^2} = \left( \frac{\partial^2 u}{\partial l_1^2}, \ldots, \frac{\partial^2 u}{\partial l_5^2} \right)^T.
\]

Then, the five-point formulæ of numerical differentials presented in [27] can be rewritten as the following theorem.

**Theorem 3.1.** Given point \( O \) and its five neighboring points numbered \( 1, \ldots, 5 \), the first-order and the second-order directional derivatives of the smooth function \( u(x, y) \) at the point \( O \) can be approximated with the second-order truncation error and first-order truncation error as
\[
\frac{\partial u}{\partial L} = \delta^{(1)}_\sigma U + O(h_M^2),
\]
\[
\frac{\partial^2 u}{\partial L^2} = \delta^{(2)}_\sigma U + O(h_M),
\]
respectively, under the so-called solvability condition, i.e., \( m_t \neq 0 \), where
\[
h_M = \max_{1 \leq i \leq 5} h_i,
\]
and \( m_t \) is as given by (3.2).

By (3.7), it is obvious to see that the properties of the coefficient matrix \( \tilde{A} \) of the compound first-order difference quotient will easily lead to those of the coefficient matrix \( B \) of the compound second-order difference quotient. As a result, this paper discusses only the properties of the matrix \( \tilde{A} \). In the next section, we first consider the expression of the difference coefficient matrix \( A \) which is closely related to the matrix \( \tilde{A} \).
3.2. Analytical expressions of the matrix $A$

(1) In the numerical formulae of directional differentials, the coefficients of $\Delta u_i$ ($i = 1, \ldots, 5$) are essentially related to ten independent geometry quantities, which are the coordinates of five neighboring points, namely,

$$x_1, y_1; x_2, y_2; x_3, y_3; x_4, y_4; x_5, y_5.$$ 

We consider these ten quantities replaced by ten independent algebraic areas, which are

$$\langle 1 \ 2 \rangle, \langle 2 \ 3 \rangle, \langle 3 \ 4 \rangle, \langle 4 \ 5 \rangle, \langle 5 \ 1 \rangle; \langle 1 \ 3 \rangle, \langle 2 \ 4 \rangle, \langle 3 \ 5 \rangle, \langle 4 \ 1 \rangle, \langle 5 \ 2 \rangle.$$ 

Here we neglect the difference between two quantities resulted from swapping two indices, since $\langle i \ j \rangle = -\langle j \ i \rangle$. In the later discussion, we will refer to $\langle i \ j \rangle$ or $\langle j \ i \rangle$ on request.

In the numerical formula of $\frac{\partial u}{\partial - \rightarrow l_i}$, how much contribution does each $\Delta u_j$ make? In other words, for any index $i$, how much correlation does other index $j$ have with it? For this problem, we will give the answer in the following discussion.

For any index $i$, classify the ten algebraic areas mentioned above into two groups: one is related to $i$; the other is unrelated to $i$. Take the index “1” for example, the quantities related to “1” are $\langle 1 \ 2 \rangle, \langle 1 \ 3 \rangle, \langle 1 \ 4 \rangle, \langle 1 \ 5 \rangle$ (see Fig. 3.2 (left)), and those unrelated to “1” are $\langle 2 \ 3 \rangle, \langle 3 \ 4 \rangle, \langle 4 \ 5 \rangle, \langle 5 \ 2 \rangle, \langle 2 \ 4 \rangle, \langle 3 \ 5 \rangle$ (see Fig. 3.2 (right)). Two groups of algebraic areas play different roles in numerical formulae.

![Fig. 3.2. Left: the areas related to the index “1”; right: the areas unrelated to the index “1”.

(2) For a given index $i$ ($i \in I$), we call

$$f_{ij} = \langle i \ j \rangle, \quad \forall j \in I$$

as the $j$th direct correlation factor of the index $i$, and call the vector

$$F_i = ( f_{i1} \ f_{i2} \ f_{i3} \ f_{i4} \ f_{i5} )^T, \quad \forall i \in I$$

as the direct correlation vector of the index $i$. Moreover, the matrix

$$F = \begin{pmatrix}
F_1^T \\
F_2^T \\
\vdots \\
F_5^T
\end{pmatrix} = 
\begin{pmatrix}
f_{11} & f_{12} & f_{13} & f_{14} & f_{15} \\
f_{21} & f_{22} & f_{23} & f_{24} & f_{25} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
f_{51} & f_{52} & f_{53} & f_{54} & f_{55}
\end{pmatrix}
= 
\begin{pmatrix}
0 & \langle 1 \ 2 \rangle & \langle 1 \ 3 \rangle & \langle 1 \ 4 \rangle & \langle 1 \ 5 \rangle \\
\langle 2 \ 1 \rangle & 0 & \langle 2 \ 3 \rangle & \langle 2 \ 4 \rangle & \langle 2 \ 5 \rangle \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\langle 5 \ 1 \rangle & \langle 5 \ 2 \rangle & \langle 5 \ 3 \rangle & \langle 5 \ 4 \rangle & 0
\end{pmatrix}$$

is called the direct correlation matrix. It is obvious that $F$ is an anti-symmetric matrix, namely,

$$F = -F^T.$$
To discuss the algebraic areas not including the index $i$, we first consider a special case. Suppose that two of the five neighbors of the central point $O$, say, “1” and “2”, along with the point $O$ are collinear (see Fig. 3.3), then (3.8) and (3.9) read as

$$
\frac{\partial u}{\partial l_1} = \frac{\partial u}{\partial l_2} = \frac{1}{m_1} \left( h_2^2 \Delta u_1 - h_1^2 \Delta u_2 \right) + O(h_M^2),
$$

$$
\frac{\partial^2 u}{\partial l_1^2} = \frac{\partial^2 u}{\partial l_2^2} = \frac{2}{m_1} \left( h_2 \Delta u_1 + h_1 \Delta u_2 \right) + O(h_M),
$$

where $m_1 = h_1 h_2 (h_1 + h_2)$, and $h_M$ is as given in Theorem 3.1.

Fig. 3.3. Special point distribution. Left: 1D case; right: 2D case.

These formulae coincide with those in the one dimensional case, which means if three points are collinear, then the formulae for first-order numerical differentials with second-order accuracy and those for second-order numerical differentials with first-order accuracy can be derived along the line determined by the three points. It shows in this special case that points “3”, “4”, and “5” do not play any role in computing $\frac{\partial u}{\partial l_1}$, $\frac{\partial u}{\partial l_2}$ and $\frac{\partial^2 u}{\partial l_1^2}$, $\frac{\partial^2 u}{\partial l_2^2}$, since $(1 \ 2) = 0$. If “1” and “3”, or “2” and “3”, along with the point $O$ are collinear, we have similar results. This motivates us that how much points “4” and “5” contribute to computing $\frac{\partial u}{\partial l_i}$, $\frac{\partial^2 u}{\partial l_i^2} (i = 1, 2, 3)$ depends upon $(1 \ 2)$, $(1 \ 3)$, and $(2 \ 3)$ simultaneously.

Based on these analyses, $\forall i, j \in I$, we introduce new quantities as follows:

$$
\begin{align*}
g_{ij} &= \text{sgn}(j - i)(-1)^{i+j} \langle k_1, k_2 \rangle \langle k_3, k_4 \rangle \langle k_5, k_6 \rangle, \\
g_{ij} &= 0, \quad k_1 < k_2 < k_3, \quad k_i \in I \setminus \{i, j\}, \quad i = 1, 2, 3, \quad i \neq j.
\end{align*}
$$

We call $g_{ij}$ as the $j$th indirect correlation factor of the index $i$. It is obvious that

$$
g_{ij} = -g_{ji}.
$$

Define a vector as

$$
G_i = \left( g_{i1}, g_{i2}, g_{i3}, g_{i4}, g_{i5} \right)^T, \quad \forall i \in I.
$$

We call $G_i (i = 1, \ldots, 5)$ as the indirect correlation vector of the index $i$. Obviously, the index $i$ is not included in this vector expression. Define a matrix as

$$
G = \begin{pmatrix}
G_1^T \\
G_2^T \\
\vdots \\
G_5^T
\end{pmatrix} =
\begin{pmatrix}
g_{11} & g_{12} & g_{13} & g_{14} & g_{15} \\
g_{21} & g_{22} & g_{23} & g_{24} & g_{25} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
g_{51} & g_{52} & g_{53} & g_{54} & g_{55}
\end{pmatrix} =
\begin{pmatrix}
0 & g_{12} & g_{13} & g_{14} & g_{15} \\
g_{21} & 0 & g_{23} & g_{24} & g_{25} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
g_{51} & g_{52} & g_{53} & g_{54} & 0
\end{pmatrix}.
$$
We call $G$ as the **indirect correlation matrix**, and easily find it being an anti-symmetric matrix, namely

$$G = -G^T.$$  

(4) According to the analyses above, it is not difficult to give a new expression of the matrix $A$ as defined in (3.1) as follows

$$a_{ij} = F_i^T G_j, \quad \forall i, j \in I,$$

that is,

$$A = \begin{pmatrix}
F_1^T G_1 & F_1^T G_2 & \ldots & F_1^T G_5 \\
\vdots & \vdots & \ddots & \vdots \\
F_5^T G_1 & F_5^T G_2 & \ldots & F_5^T G_5
\end{pmatrix},$$

or

$$A = FG^T. \quad (3.11)$$

(5) Let $\overline{h}$ be the geometric average of $h_i$, $\forall i \in I$, that is,

$$\overline{h} = (h_1 b_2 \ldots h_5)^{1/5}.$$  

Note that, in the following fractions

$$\frac{a_{ij}}{m_t} = \frac{F_i^T G_j}{m_t}, \quad \forall i, j \in I,$$

numerators and denominators have a common factor $\overline{h}^3$. Separating this factor will facilitate relevant discussion.

To this end, we first denote by

$$\lambda_i = \frac{h_i}{\overline{h}}, \quad \forall i \in I, \quad \Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_5),$$

$$F_0 = \begin{pmatrix}
(1 1)_0 & (1 2)_0 & (1 3)_0 & (1 4)_0 & (1 5)_0 \\
(2 1)_0 & (2 2)_0 & (2 3)_0 & (2 4)_0 & (2 5)_0 \\
\vdots & \vdots & \ddots & \vdots \\
(5 1)_0 & (5 2)_0 & (5 3)_0 & (5 4)_0 & (5 5)_0
\end{pmatrix},$$

then, we have

$$F = \overline{h}^2 \Lambda F_0 \Lambda. \quad (3.12)$$

For the same sake, denote by

$$g_{ij0} = \text{sgn}(j - i)(-1)^{i+j} \langle k_1, k_2 \rangle_0 \langle k_3 \rangle_0 \langle k_4 \rangle_0 \langle k_5 \rangle_0,$$

$$g_{ij0} = 0, \quad k_1 < k_2 < k_3, \quad k_l \in I \setminus \{i, j\}, \quad i \neq j,$$

$$g_{ij0} = \begin{pmatrix}
g_{110} & g_{120} & g_{130} & g_{140} & g_{150} \\
g_{210} & g_{220} & g_{230} & g_{240} & g_{250} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
g_{510} & g_{520} & g_{530} & g_{540} & g_{550}
\end{pmatrix},$$
Then, we have

$$G = \frac{h^6}{6} \Lambda^{-2} G_0 \Lambda^{-2}. \quad (3.13)$$

By (3.12) and (3.13), we have

$$A = \frac{h^8}{8} \Lambda A_\lambda \Lambda^{-2},$$

where

$$A_\lambda = F_0 \Lambda^{-1} G_0^T.$$

**Remark 3.1.** 1. \(\{F_i, \forall i \in I\}\) and \(\{G_i, \forall i \in I\}\) are two vectors corresponding to different kinds of indices, of which the elements are \(f_{ij}\) and \(g_{ij}\) (\(\forall i, j \in I\)), respectively. The indices of the former are \(i, j\), while those of the latter are \(I \setminus \{i, j\}\), namely, the indices of them are complementary. As aforesaid, they reflect different geometry characteristics of the scattered point sets. After the element \(a_{ij}\) is factorized into \(F_i\) and \(G_j\), the rows and columns of \(A = (F_i^T G_j)_{5 \times 5}\) have strong correlation and regularity, which supports to make discrete analysis on PDEs by the FPM.

2. The indices in the formulae of the first-order difference quotient (3.8) and the second-order difference quotient (3.9) can be freely permutated, that means, after indices are permuted, the formulae still hold. For example, for two orders of the indices as illustrated in Fig. 3.4, both formulae hold.

![Fig. 3.4. Point O and its five neighbors.](image)

For convenience to discussion and analysis, the anticlockwise order of indices is usually employed (as shown in Fig. 3.4 (left)), and the angles between adjacent directions are denoted by \(\theta_1, \theta_2, \theta_3, \theta_4, \theta_5\) in turn, which is called an ordinary order, and is also the default order in the later discussion.

### 4. Expressions and Estimations of the Discriminant Function for the Solvability of Numerical Differentials

The discriminant function for the solvability of numerical differentials plays key roles in designing methods for selecting neighboring points. The paper [27] presents the method for selecting neighboring points. The corresponding software module is developed hereafter and applied to practical computation for solving PDEs by the FPM [29]. To deepen related research, this section makes further analysis to the discriminant function. In later discussion, hypotheses on angles are demanded in terms of different cases. We first state the fundamental hypothesis.

**Hypothesis I.** In the ordinary order, \(\forall i \in I\), suppose that the angles \(\theta_i\) satisfy the following conditions:
4.1. Expressions of the discriminant function $m_t$

As aforesaid, the discriminant function $m_t$ is an important function with respect to indices, and has multiple expressions in different forms. These expressions will play an important role in simplifying problems in different discussions.

(1) Expressions of $m_t$ composed of two terms

For

$$m_t = (23)(41)(125)(345) - (12)(34)(235)(415),$$

by exchanging two indices freely, the sign of $m_t$ will change while its absolute value remains unchanged. For instance, exchanging indices “3” and “5”, then one has


It is obvious that corresponding to five neighbors 1,2,3,4,5, there are ten expressions of this type. They correspond to the actual five directions, expressed in ten different orders of 1,2,3,4,5. For example, as shown in Fig. 3.4, they are two of them.

(2) Expressions of $m_t$ composed of ten terms

By expanding $(125)$, $(345)$, $(235)$ and $(415)$ in previous expressions, and by properties of algebraic areas, it is not difficult to have

$$+ (45)(12)(23)(13)$$

$$= \sum_{i,j=1}^{5} f_{ij} g_{ij}.$$  \hspace{1cm} (4.1)

Note that $f_{ij} g_{ij} = f_{ji} g_{ji}$, one has

$$m_t = \frac{1}{2} \sum_{i,j=1}^{5} f_{ij} g_{ij} = \frac{1}{2} \sum_{k=1}^{5} F_k^T G_k.$$

Similar to factorizing $A$ into $F$ and $G$, $m_t$ is also factorized into $F$ and $G$. The factorization means that $m_t$ is half of the sum of all elements of the matrix $(f_{ij} g_{ij})_{5 \times 5}$. It is easy to know, under the Hypothesis I, each term in (4.1) is nonnegative, and there must exist one positive term at least, so an important property as follows is obtained.

**Property 4.1. Under the Hypothesis I,**

$$m_t > 0.$$
(3) **The expression of** $m_t$ **separating** $\mathbf{h}^8$

If reform $(i \; j \; k)$ as

$$(i \; j \; k) = (i \; j) + (j \; k) + (k \; i)$$

$$= (i \; j)_{0}h_{j}h_{j} + (j \; k)_{0}h_{j}h_{k} + (k \; i)_{0}h_{k}h_{i}$$

$$= h^{2}\lambda_{i}\lambda_{j}\lambda_{k}(i \; j)_{0}\lambda_{k}^{-1} + (j \; k)_{0}\lambda_{j}^{-1} + (k \; i)_{0}\lambda_{j}^{-1}$$

where

$$(i \; j \; k)_{\lambda} = (i \; j)_{0}\lambda_{k}^{-1} + (j \; k)_{0}\lambda_{j}^{-1} + (k \; i)_{0}\lambda_{j}^{-1},$$

then by (3.2), and note that $\prod_{i=1}^{5}\lambda_{i} = 1$, $m_t$ can be rewritten as

$$m_t = \mathbf{h}^8 m_{\lambda},$$

where

$$m_{\lambda} = \langle 2 \; 3 \; 0 \; 4 \; 1 \rangle_{0}(1 \; 2 \; 5)_{\lambda}(3 \; 4 \; 5)_{\lambda} - (1 \; 2)_{0}(3 \; 4)_{0}(2 \; 3 \; 5)_{\lambda}(4 \; 1 \; 5)_{0}$$

If all steplengths are equal, namely, $\lambda_{i} = 1 (\forall i \in I)$, the discussion will be simplified. In this case, denote $m_{\lambda}$ by $m_{\lambda_{0}}$. Hence, we get the following theorem.

**Theorem 4.1.** Under the Hypothesis 1, if $h_{i} = \mathbf{h}, \forall i \in I$, then it follows

$$m_{\lambda_{0}} = 4\prod_{i=1}^{5}\left(\sin\frac{\theta_{i}}{2}\sin\frac{1}{2}(\theta_{i} + \theta_{i+1})\right).$$  \hspace{1cm} (4.2)

**Proof.** As all steplengths are equal, $\lambda_{i} = 1, \forall i \in I$, which consequently lead to

$$m_{\lambda_{0}} = \langle 2 \; 3 \; 0 \; 4 \; 1 \rangle_{0}(1 \; 2 \; 5)_{0}(3 \; 4 \; 5)_{0} - (1 \; 2)_{0}(3 \; 4)_{0}(2 \; 3 \; 5)_{0}(4 \; 1 \; 5)_{0}$$

$$= \frac{1}{16}\left[\sin\theta_{2}\sin(\theta_{4}+\theta_{5})(\sin\theta_{1}+\sin\theta_{5}-\sin(\theta_{1}+\theta_{5}))(\sin\theta_{3}+\sin\theta_{4}-\sin(\theta_{3}+\theta_{4}))\right.$$\n
$$+\sin\theta_{1}\sin\theta_{3}(\sin\theta_{2}+\sin(\theta_{3}+\theta_{4})+\sin(\theta_{1}+\theta_{5}))(\sin\theta_{4}+\sin\theta_{5}-\sin(\theta_{4}+\theta_{5}))\right].$$

Note that, for any $\alpha$, $\beta$, there is

$$\sin\alpha + \sin\beta - \sin(\alpha + \beta) = 4\sin\frac{\alpha}{2}\sin\frac{\beta}{2}\sin\frac{\alpha + \beta}{2}.$$ 

Hence by simplification, one gets

$$m_{\lambda_{0}} = 4\prod_{i=1}^{5}\sin\frac{\theta_{i}}{2}\sin\frac{1}{2}(\theta_{3} + \theta_{4})\sin\frac{1}{2}(\theta_{4} + \theta_{5})\sin\frac{1}{2}(\theta_{5} + \theta_{1})$$

$$\cdot \left(\cos\frac{\theta_{2}}{2}\cos\frac{\theta_{4} + \theta_{5}}{2} + \cos\frac{\theta_{1}}{2}\cos\frac{\theta_{3}}{2}\right).$$

Further combining with

$$\cos\frac{\theta_{2}}{2}\cos\frac{\theta_{4} + \theta_{5}}{2} + \cos\frac{\theta_{1}}{2}\cos\frac{\theta_{3}}{2} = \sin\frac{1}{2}(\theta_{1} + \theta_{2})\sin\frac{1}{2}(\theta_{2} + \theta_{3}),$$

one obtains (4.2).
4.2. Estimations of the discriminant function $m_t$

We first consider the case of even steplength.

By (4.2), it is easy to have $m_{\lambda_0} > 0$ under the Hypothesis I. Furthermore, we concern about which distributions of $\theta_i$ ($i = 1, \ldots, 5$) can maximize the value of $m_{\lambda_0}$?

Let $\theta_5 = 2\pi - \theta_1 - \theta_2 - \theta_3 - \theta_4$, and view $m_{\lambda_0}$ as the function with respect to $\theta_1, \theta_2, \theta_3, \theta_4$. We first discuss the change of $m_{\lambda_0}$ with $\theta_1$. It is obvious that

$$m_{\lambda_0} = 4 \sin \frac{\theta_2}{2} \sin \frac{\theta_3}{2} \sin \frac{\theta_4}{2} \sin \frac{1}{2} (\theta_2 + \theta_3) \sin \frac{1}{2} (\theta_3 + \theta_4) \sin \frac{1}{2} (\theta_2 + \theta_3 + \theta_4),$$

where

$$m_{\lambda_0}^* = \sin \frac{\theta_1}{2} \sin \frac{\theta_2}{2} \sin \frac{1}{2} (\theta_1 + \theta_2) \sin \frac{1}{2} (\theta_1 + \theta_3)$$

$$= \sin \frac{\theta_1}{2} \sin \frac{1}{2} (\theta_1 + \theta_2) \sin \frac{1}{2} (\theta_1 + \theta_2 + \theta_3) \sin \frac{1}{2} (\theta_1 + \theta_2 + \theta_3 + \theta_4).$$

Computing the derivative of $\ln m_{\lambda_0}^*$ results in

$$\frac{d(\ln m_{\lambda_0}^*)}{d\theta_1} = \frac{1}{2} \left( \cot \frac{\theta_1}{2} \cot \frac{\theta_1 + \theta_2}{2} + \cot \frac{\theta_1 + \theta_2 + \theta_3}{2} + \cot \frac{\theta_1 + \theta_2 + \theta_3 + \theta_4}{2} \right).$$

It is obvious that $d(\ln m_{\lambda_0}^*)/d\theta_1$ is a monotone decreasing function with respect to $\theta_1$, and it has a single zero point, hence, $\ln m_{\lambda_0}^*$, namely, $m_{\lambda_0}^*$ has a maximum point. Similar results are derived for $\theta_2, \theta_3, \theta_4, \theta_5$. So we can conclude, when $\theta_i = \frac{2}{5}\pi$ ($i = 1, \ldots, 5$), $m_{\lambda_0}$ attains the maximum.

By using $\sin \frac{2}{5}\pi = \frac{1}{4} \sqrt{10 + 2\sqrt{5}}$, $\sin \frac{3}{5}\pi = \frac{1}{4} \sqrt{10 - 2\sqrt{5}}$, one obtains

$$\max m_{\lambda_0} = 4 \left( \frac{1}{4} \sqrt{10 - 2\sqrt{5}} \right)^5 \left( \frac{1}{4} \sqrt{10 + 2\sqrt{5}} \right)^5 = \frac{25}{256} \sqrt{5} \approx 0.2184.$$  

Here, 0.2184 makes sense of the basic quantity of $m_t$, which is the value of $m_t$ when the step size is 1 and each angle is $\frac{2}{5}\pi$. When the angles are uneven, the value of $m_{\lambda_0}$ can be estimated by (4.2). In the next section, we will use (4.2) and the expression of $a_{ij}$ to estimate $\tilde{a}_{ij}$.

For the case of uneven steplengths, it is not difficult by the expression with ten terms (4.1) to have the following estimation of $m_t$.

**Theorem 4.2.** Under the Hypothesis I, the discriminant function $m_t$ satisfies the estimation as follows

$$m_t \geq H^{10} h_M^{-2} m_{\lambda_0},$$

where $h_M$ is as defined in (3.10).

5. The Bound of Difference Quotient Coefficient Matrix

5.1. The estimation of combinatorial coefficients

By the expression (3.6) of the compound first-order difference quotient matrix $\tilde{A}$, it is easy to have

$$\tilde{A} = \frac{1}{m_t} \Lambda^{-1} A \Lambda.$$  

(5.1)
Moreover, for a given \( i \), one has
\[
\tilde{A}_0 = \frac{1}{m_{\lambda_0}}A_{\lambda_0},
\] (5.2)
where \( \tilde{A}_0 \) and \( A_{\lambda_0} \) denote \( \tilde{A} \) and \( A_{\lambda} \) in the case of even steplength, respectively.

The element \( \tilde{a}_{ij} \) of the matrix \( \tilde{A} \) is a fraction, which has complex expression. Although its structure has been analyzed and understood, there is no in-depth understanding of its magnitude. Hence, we must give estimation to \( \tilde{a}_{ij} \).

The following theorem puts out the estimation of the combination of the difference quotient coefficients \( \tilde{a}_{ij} \) (\( i, j \in I \)).

**Theorem 5.1.** Under the Hypothesis I, the difference quotient coefficients \( \tilde{a}_{ij} \) of the five-point formulae with second-order accuracy satisfy the following equalities
\[
\sum_{j=1}^{5} \langle j \rangle_0 \tilde{a}_{ij} = \langle i \rangle_0, \quad \forall k, \ i \in I.
\] (5.3)
Moreover, for a given \( i \), only two of the five equations of \( k = 1, \ldots, 5 \) are independent.

**Proof.** Take \( i = 1 \) for illustration. By the expression (3.4) of the compound first-order difference quotient, one has
\[
\delta^{(1)}_0 u_1 = \tilde{a}_{11} \delta u_1 + \tilde{a}_{12} \delta u_2 + \tilde{a}_{13} \delta u_3 + \tilde{a}_{14} \delta u_4 + \tilde{a}_{15} \delta u_5.
\] (5.4)
Using
\[
\langle 4 \rangle_0 \delta u_3 + \langle 5 \rangle_0 \delta u_4 + \langle 3 \rangle_0 \delta u_5 = O(h_M)
\] (5.5)
to eliminate \( \delta u_5 \) in (5.4), and noticing the Hypothesis I, \( \langle 3 \rangle_0 \) does not vanish, hence one has
\[
\delta^{(1)}_0 u_1 = \tilde{a}_{11} \delta u_1 + \tilde{a}_{12} \delta u_2 + \frac{1}{\langle 3 \rangle_0} (\langle 3 \rangle_0 \tilde{a}_{13} - \langle 4 \rangle_0 \tilde{a}_{15}) \delta u_3
\]
\[
+ \frac{1}{\langle 3 \rangle_0} (\langle 5 \rangle_0 \tilde{a}_{14} - \langle 3 \rangle_0 \tilde{a}_{15}) \delta u_4 + O(h_M).
\] (5.6)
Similarly, using
\[
\langle 3 \rangle_0 \delta u_2 + \langle 4 \rangle_0 \delta u_4 + \langle 2 \rangle_0 \delta u_5 = O(h_M)
\] (5.7)
to eliminate \( \delta u_4 \) in (5.6), and noticing the Hypothesis I, \( \langle 2 \rangle_0 \) does not vanish, so one has
\[
\delta^{(1)}_0 u_1 = \delta u_1 + (\tilde{a}_{11} - 1) \delta u_1 + \frac{1}{\langle 2 \rangle_0} (\langle 2 \rangle_0 (\tilde{a}_{12} - \langle 3 \rangle_0 \tilde{a}_{14} + \langle 5 \rangle_0 \tilde{a}_{15}) \delta u_2
\]
\[
+ \frac{1}{\langle 2 \rangle_0 (\langle 3 \rangle_0)} (\langle 2 \rangle_0 (\tilde{a}_{13} - \langle 4 \rangle_0 \tilde{a}_{15} - \langle 2 \rangle_0 (\langle 3 \rangle_0 \tilde{a}_{14} - \langle 5 \rangle_0 \tilde{a}_{15})) \delta u_3 + O(h_M).
\] (5.8)
Further using
\[
\langle 2 \rangle_0 \delta u_1 + \langle 3 \rangle_0 \delta u_2 + \langle 1 \rangle_0 \delta u_3 = O(h_M)
\] (5.9)
to eliminate the second term in the right-hand side of (5.8), one obtains
\[
\delta^{(1)}_0 u_1 = \delta u_1 + \frac{1}{\langle 2 \rangle_0 (\langle 3 \rangle_0)} (\langle 3 \rangle_0 \langle 1 \rangle_0 (\tilde{a}_{11} - \tilde{a}_{13} + \langle 3 \rangle_0 \tilde{a}_{14} - \langle 5 \rangle_0 \tilde{a}_{15}) \delta u_2
\]
\[
+ \langle 3 \rangle_0 \tilde{a}_{15}) \delta u_2 + \langle 3 \rangle_0 \langle 1 \rangle_0 (\tilde{a}_{11} - \tilde{a}_{13} + \langle 2 \rangle_0 (\langle 3 \rangle_0 \tilde{a}_{14} - \langle 5 \rangle_0 \tilde{a}_{15}) \delta u_3 + O(h_M).
\] (5.10)
As noticing that
\[ \langle 4 \ 2 \rangle_0 \langle 5 \ 3 \rangle_0 = \langle 4 \ 5 \rangle_0 \langle 2 \ 3 \rangle_0 + \langle 3 \ 4 \rangle_0 \langle 2 \ 5 \rangle_0, \]
one gets
\[ \delta_{u_1}^{(1)} = \delta u_1 + \frac{1}{(2 \ 3)_0} \left\{ [3 \ 1]_0 \lambda (1 - \tilde{a}_{11}) + (2 \ 3)_0 \tilde{a}_{12} - (3 \ 4)_0 \tilde{a}_{14} + (5 \ 3)_0 \tilde{a}_{15} \right\} \delta u_2 \]
\[ + \left\{ (2 \ 3)_0 (1 - \tilde{a}_{11}) + (2 \ 3)_0 \tilde{a}_{13} - (4 \ 2)_0 \tilde{a}_{14} + (2 \ 5)_0 \tilde{a}_{15} \right\} \delta u_3 + O(h_M). \]  
(5.11)

Since \( \delta u_1, \delta_{u_1}^{(1)} \) are corresponding first-order and second-order approximations to \( \frac{\partial u}{\partial t} \) at the point “O”, it follows that
\[ \delta_{u_1}^{(1)} = \delta u_1 + O(h_M). \]  
(5.12)

Hence, the coefficients of \( \delta u_2 \) and \( \delta u_3 \) in (5.11) must vanish, that is,
\[ \langle 2 \ 3 \rangle_0 \tilde{a}_{11} + \langle 4 \ 2 \rangle_0 \tilde{a}_{12} + \langle 5 \ 3 \rangle_0 \tilde{a}_{14} = \langle 2 \ 3 \rangle_0 \tilde{a}_{13} + \langle 4 \ 2 \rangle_0 \tilde{a}_{14} + \langle 5 \ 3 \rangle_0 \tilde{a}_{15} = \langle 2 \ 3 \rangle_0 \tilde{a}_{11} + \langle 4 \ 2 \rangle_0 \tilde{a}_{12} + \langle 5 \ 3 \rangle_0 \tilde{a}_{15} = \langle 2 \ 3 \rangle_0 \tilde{a}_{11} + \langle 4 \ 2 \rangle_0 \tilde{a}_{12} + \langle 5 \ 3 \rangle_0 \tilde{a}_{15} = 0. \]  
(5.13)

As \( \langle 2 \ 2 \rangle_0 = 0, \langle 3 \ 3 \rangle_0 = 0 \), these two equations can be reformulated as
\[ \sum_{j=1}^{5} (j \ k) \tilde{a}_{1j} = \langle 1 \ k \rangle_0, \quad k = 2, 3. \]  
(5.15)

By combining (5.13) and (5.14), it is not difficult to derive the following equations
\[ \sum_{j=1}^{5} (j \ k) \tilde{a}_{1j} = \langle 1 \ k \rangle_0, \quad k = 1, 4, 5. \]  
(5.16)

It is obvious that only two of above five equations are independent. For \( \delta_{u_2}^{(1)}, \delta_{u_3}^{(1)}, \delta_{u_4}^{(1)}, \delta_{u_5}^{(1)} \), we can derive the similar results, which complete the proof. \( \square \)

The theorem restricts the combination of \( \tilde{a}_{ij} \). In particular, when \( \lambda_i = 1 \ (i = 1, \ldots, 5) \), i.e., even steplength, further conclusions can be drawn.

**Theorem 5.2.** Under the Hypothesis I and the case of even steplength, the first-order difference quotient coefficients in the five-point formulae with second-order accuracy satisfy the following equations:
\[ \sum_{j=1}^{5} \tilde{a}_{ij0} = 0, \quad \forall i \in I. \]

\[ \sum_{j=1}^{5} \tilde{a}_{ij0} = \frac{1}{m_{\lambda_0}} \sum_{j=1}^{5} \sum_{k=1}^{5} f_{1k0} g_{jk0} = \frac{1}{m_{\lambda_0}} \sum_{k=1}^{5} f_{1k0} \left( \sum_{j=1}^{5} g_{jk0} \right). \]

(5.17)

When \( k = 1 \), one gets
\[ \sum_{j=1}^{5} g_{j10} = \langle 3 \ 4 \rangle_0 (4 \ 5)_0 (5 \ 3)_0 - (4 \ 5)_0 (5 \ 2)_0 (2 \ 4)_0 + (5 \ 2)_0 (2 \ 3)_0 (3 \ 5)_0 - (2 \ 3)_0 (3 \ 4)_0 (4 \ 2)_0 \]
\[ = (5 \ 3)_0 (3 \ 4)_0 (4 \ 5)_0 - (5 \ 2)_0 (2 \ 3)_0 - (2 \ 4)_0 (4 \ 5)_0 (5 \ 2)_0 - (2 \ 3)_0 (3 \ 4)_0. \]  
(5.18)
Simplifying above equation gives

\[ \sum_{j=1}^{5} g_{j0} = \langle 5 \cdot 3 \rangle_0 \sin(\theta_2 + \theta_3) \sin(\theta_2 + \theta_4) + \langle 2 \cdot 4 \rangle_0 \sin(\theta_1 + \theta_4) \sin(\theta_2 + \theta_4) = 0. \] (5.19)

Similar deductions can be done to obtain

\[ \sum_{j=1}^{5} g_{jk0} = 0, \quad 2 \leq k \leq 5. \]

Hence one obtains

\[ \sum_{j=1}^{5} \tilde{a}_{1j0} = 0. \]

It can be also proved that

\[ \sum_{j=1}^{5} \tilde{a}_{ij0} = 0, \quad 2 \leq i \leq 5. \]

So the theorem is proved. \( \square \)

The theorem can be also regarded as a generalization of the one-dimensional case of even steplength.

5.2. Estimation of coefficient in the discrete formulae of directional differentials

Next, we will give estimation to each \( \tilde{a}_{ij} (\forall i, j \in I) \). Here, we firstly give hypotheses to the angles.

**Hypothesis II.** In the ordinary order, \( \forall i \in I \), suppose that \( \theta_i \) satisfies

1. \( \theta_i \geq \frac{\pi}{4} \);
2. \( \theta_i + \theta_i \circ \underline{5} \leq \pi. \)

Under above hypotheses, one easily has

\[ \theta_i \leq \frac{3}{4} \pi, \quad \forall i \in I. \]

First of all, we will estimate \( \tilde{a}_{ij0} \) in the case of even steplength, which is the most basic case.

5.2.1. The case of even steplength

Suppose that the Hypothesis II holds for the angles in the ordinary order. From the expression of \( \tilde{a}_{ij0} \), it is obvious that there are

\[ \tilde{a}_{ij0} \geq 0, \quad j = i, \ i \circ 1, \ i \circ 4, \]

\[ \tilde{a}_{ij0} \leq 0, \quad j = i \circ 2, \ i \circ 3. \]

That is, \( \tilde{a}_{i00} \) is nonnegative, and the coefficients corresponding to two directions adjacent to \( \overrightarrow{l_i} \) are also nonnegative, while the coefficients corresponding to two directions far from \( \overrightarrow{l_i} \) are nonpositive.
For convenience of later deduction, denote by

$$\varphi_i = \frac{\theta_i}{2}, \ \forall i \in I.$$  

Obviously, we are concerned with the upper bound of $$|\tilde{a}_{ij0}|$$ on the following region

$$\omega_0 = \left\{ \varphi_i, \ i = 1, \ldots, 5 \mid \varphi_i \geq \frac{\pi}{8}; \varphi_i + \varphi_{i+1} \leq \frac{\pi}{2} \sum_{i=1}^{5} \varphi_i = \pi \right\}.$$  

In this regard, there is the following theorem.

**Theorem 5.3.** Under the Hypothesis II, $$\forall i, j \in I$$, there are estimations of $$|\tilde{a}_{ij0}|$$ on the region $$\omega_0$$ as follows

$$|\tilde{a}_{ij0}| \leq \begin{cases} 
\frac{1}{2}, & j = i, \\
\frac{\sqrt{2}}{2}, & j \neq i,
\end{cases} \quad (5.20)$$

and there must exist a subset of $$\omega_0$$ to make equalities hold.

**Proof.** Just a proof of $$i = 1$$ is enough.  

(1) Firstly, by simplification, the expression of $$|\tilde{a}_{110}|$$ is obtained as follows

$$|\tilde{a}_{110}| = \frac{1}{4} \frac{\cos \varphi_2 \cos(2\varphi_5 + \varphi_4) + \cos \varphi_4 \cos(2\varphi_1 + \varphi_2)}{\sin \varphi_1 \sin \varphi_5 \sin(\varphi_1 + \varphi_2) \sin(\varphi_4 + \varphi_5)}. \quad (5.21)$$

Denote by

$$\varphi_1 + \varphi_2 = \varphi_{12}, \quad \varphi_4 + \varphi_5 = \varphi_{45}.$$  

It is obvious that $$\varphi_1, \varphi_5, \varphi_{12}, \varphi_{45}$$ are independent variables, hence (5.21) can be reformed as

$$|\tilde{a}_{110}| = \frac{1}{4} \frac{\cos(\varphi_{12} - \varphi_1) \cos(\varphi_{45} + \varphi_5) + \cos(\varphi_{45} - \varphi_5) \cos(\varphi_{12} + \varphi_1)}{\sin \varphi_1 \sin \varphi_5 \sin \varphi_{12} \sin \varphi_{45}}. \quad (5.22)$$

By simple operation, and noticing the condition of angle distributions, one easily obtains

$$\frac{\partial |\tilde{a}_{110}|}{\partial \varphi_1} \geq 0, \quad \frac{\partial |\tilde{a}_{110}|}{\partial \varphi_5} \geq 0, \quad \frac{\partial |\tilde{a}_{110}|}{\partial \varphi_{12}} \geq 0, \quad \frac{\partial |\tilde{a}_{110}|}{\partial \varphi_{45}} \geq 0.$$  

Hence, to maximize $$|\tilde{a}_{110}|$$, $$\varphi_1, \varphi_5, \varphi_{12}, \varphi_{45}$$ or $$\varphi_1, \varphi_2, \varphi_4, \varphi_5$$ should be as large as possible, which implies that $$\varphi_3$$ should be as small as possible, that is,

$$\varphi_3 = \frac{\pi}{8}.$$  

Note the Hypothesis II, one consequently has

$$\varphi_{12} + \varphi_{45} = \frac{7}{8}\pi,$$

and

$$\varphi_{12} \geq \frac{3}{8}\pi, \quad \varphi_{45} \geq \frac{3}{8}\pi.$$
As $\varphi_3$ has been decided, there are three independent variables $\varphi_1, \varphi_5, \varphi_{12}$ being remained, then (5.22) can be rewritten as

$$
|\tilde{a}_{110}| = -\frac{1}{4} \frac{\cos(\varphi_{12} - \varphi_1) \cos(\frac{7}{8}\pi - \varphi_{12} + \varphi_5) + \cos(\frac{7}{8}\pi - \varphi_{12} - \varphi_5) \cos(\varphi_{12} + \varphi_1)}{\sin \varphi_1 \sin \varphi_5 \sin \varphi_{12} \sin(\frac{7}{8}\pi - \varphi_{12})}. \quad (5.23)
$$

It is easy to get

$$
\frac{\partial |\tilde{a}_{110}|}{\partial \varphi_1} \geq 0, \quad \frac{\partial |\tilde{a}_{110}|}{\partial \varphi_5} \geq 0,
$$

with the following two cases:

- **Case I.** If $\frac{3}{8}\pi \leq \varphi_{12} \leq \frac{7}{16}\pi$, then $\frac{\partial |\tilde{a}_{110}|}{\partial \varphi_1} \leq 0$.

- **Case II.** If $\frac{7}{16}\pi \leq \varphi_{12} \leq \frac{\pi}{2}$, then $\frac{\partial |\tilde{a}_{110}|}{\partial \varphi_1} \geq 0$.

For Case I, $|\tilde{a}_{110}|$ attains the maximum at $\varphi_{12} = \frac{3}{8}\pi$. If $\varphi_1$ and $\varphi_5$ are supposed to be parametric angles, then the corresponding five angles can be expressed in turn by

$$
\varphi_1, \quad \frac{3}{8}\pi - \varphi_1, \quad \frac{\pi}{8}, \quad \frac{\pi}{2} - \varphi_5, \quad \varphi_5.
$$

For the Case II, $|\tilde{a}_{110}|$ attains the maximum at $\varphi_{12} = \frac{\pi}{2}$. If $\varphi_1$ and $\varphi_5$ are supposed to be parametric angles, then the corresponding five angles can be expressed in turn by

$$
\varphi_1, \quad \frac{\pi}{2} - \varphi_1, \quad \frac{\pi}{8}, \quad \frac{3}{8}\pi - \varphi_5, \quad \varphi_5.
$$

Substituting above two distributions of five angles into (5.21), it is not difficult for both of them to have $|\tilde{a}_{110}| = \frac{1}{2}$, that is

$$
\max_{\omega_0} |\tilde{a}_{110}| = \frac{1}{2}.
$$

(2) Note that

$$
|\tilde{a}_{120}| = \frac{1}{2} \frac{\cos(\varphi_1 + \varphi_2) \cos(\varphi_4 + \varphi_5) \cos \varphi_5}{\sin \varphi_1 \sin \varphi_2 \sin(\varphi_2 + \varphi_3) \sin(\varphi_5 + \varphi_1)}. \quad (5.24)
$$

Take $\varphi_1, \varphi_2, \varphi_4, \varphi_5 \in \omega_0$ as independent variables, then one has

$$
|\tilde{a}_{120}| = \frac{1}{2} \frac{\cos(\varphi_1 + \varphi_2) \cos(\varphi_4 + \varphi_5) \cos \varphi_5}{\sin \varphi_1 \sin \varphi_2 \sin(\varphi_1 + \varphi_2 + \varphi_3) \sin(\varphi_5 + \varphi_1)}. \quad (5.25)
$$

It is easy to prove that

$$
\frac{\partial |\tilde{a}_{120}|}{\partial \varphi_i} \leq 0, \quad i = 1, 2, 4, 5.
$$

Hence, to maximize $|\tilde{a}_{120}|$, $\varphi_1, \varphi_2, \varphi_4, \varphi_5$ should be as small as possible, namely, $\varphi_3$ should be as large as possible, so it should be taken as

$$
\varphi_3 = \frac{3}{8}\pi.
$$

Note again the definition of $\omega_0$, it is not hard to come up with

$$
\varphi_2 = \varphi_4 = \frac{\pi}{8}.
$$
If \( \varphi_1 \) is supposed to be the parametric angle, then to maximize \(|\tilde{a}_{120}|\), the five angles should have the following distribution

\[
\varphi_1, \, \frac{\pi}{8}, \, \frac{3\pi}{8}, \, \frac{5\pi}{8}, \, \frac{7\pi}{8} - \varphi_1.
\]

Substituting above distribution of five angles into (5.24) and by operation results in

\[
|\tilde{a}_{120}| = \frac{1}{2} \sin\left(\frac{\pi}{4} + 2\varphi_1\right) \sin\frac{\pi}{4}.
\]

(5.26)

It is obvious that \(|\tilde{a}_{120}|\) attains the maximum at \( \varphi_1 = \frac{\pi}{8} \), which gives

\[
\max_{\omega_0} |\tilde{a}_{120}| = \frac{\sqrt{2}}{2}.
\]

(3) Note that

\[
|\tilde{a}_{130}| = \frac{1}{2} \cos \varphi_1 \cos \varphi_5 \cos (\varphi_4 + \varphi_5) \sin \varphi_3 \sin (\varphi_3 + \varphi_4) \sin (\varphi_3 + \varphi_4 + \varphi_5) \sin (\varphi_1 + \varphi_2) .
\]

(5.27)

Take \( \varphi_{12} = \varphi_1 + \varphi_2, \, \varphi_2, \, \varphi_4, \, \varphi_5 \) as four independent variables, then \(|\tilde{a}_{130}|\) can be expressed by

\[
|\tilde{a}_{130}| = \frac{1}{2} \cos (\varphi_{12} - \varphi_2) \cos \varphi_5 \cos (\varphi_4 + \varphi_5) \sin (\varphi_{12} + \varphi_4 + \varphi_5) \sin (\varphi_{12} + \varphi_5) \sin \varphi_{12}. 
\]

(5.28)

It is easy to obtain by operation that

\[
\frac{\partial |\tilde{a}_{130}|}{\partial \varphi_i} \leq 0, \quad i = 2, 4, 5.
\]

On the basis of analysis, \(|\tilde{a}_{130}|\) is sure to attain the maximum at \( \varphi_2 = \varphi_4 = \varphi_5 = \frac{\pi}{8} \), which leads to

\[
|\tilde{a}_{130}| = \frac{1}{2} \cos (\varphi_{12} - \frac{\pi}{8}) \cos \frac{\pi}{8} \cos \frac{\pi}{8} \sin (\varphi_{12} + \frac{\pi}{8}) \sin (\varphi_{12} + \frac{\pi}{8}) \sin \varphi_{12}. 
\]

(5.29)

Besides, by the definition of \( \omega_0 \), it is easy to have \( \varphi_{12} \in [\frac{3\pi}{8}, \frac{5\pi}{8}] \).

By operation, it is not difficult to prove that \( |\tilde{a}_{130}| \) in (5.29) is monotone decreasing with respect to \( \varphi_{12} \) on \([\frac{3\pi}{8}, \frac{5\pi}{8}]\), hence \(|\tilde{a}_{130}|\) attains the maximum at \( \varphi_{12} = \frac{3\pi}{8} \), and

\[
\max_{\omega_0} |\tilde{a}_{130}| = \frac{\sqrt{2}}{2}.
\]

(4) Estimations of \( \tilde{a}_{140} \) and \( \tilde{a}_{150} \) are similar to those of \( \tilde{a}_{130} \) and \( \tilde{a}_{120} \), since they have similar expressions. The conclusions can be also drawn by their adjacent relationship with \( \tilde{l}_1 \). \( \Box \)

### 5.2.2. The case of uneven steplength

In the pentagon formed by connecting the five neighbors of the point “O” in sequence, given a vertex “j” and its two adjacent vertices “i” and “k” (see Fig. 5.1), we will discuss \((i \, j \, k)\).
In the case of even steplength, the corner of \("j\) must be convex, and \(\langle i \ j \ k \rangle_0\) shown as the shadow area can be expressed by

\[
\langle i \ j \ k \rangle_0 = \langle i \ j \rangle_0 - \langle i \ k \rangle_0
\]

where

\[
\langle i \ j \rangle_0 + \langle j \ k \rangle_0 = \sin \frac{\theta_i + \theta_j}{2} \cos \frac{\theta_i - \theta_j}{2}.
\]

Therefore one gets

\[
\langle i \ j \ k \rangle_0 = \eta(\theta_i, \theta_j)(\langle i \ j \rangle_0 + \langle j \ k \rangle_0),
\]

where

\[
\eta(\theta_i, \theta_j) = 2 \sin \frac{\theta_i}{2} \sin \frac{\theta_j}{2} \cos \frac{1}{2} (\theta_i - \theta_j).
\]

In the case of uneven steplength, the corners of the pentagon may be convex or concave. In order to make a concise estimation to \(|\tilde{a}_{ij}|\), for \(\langle i \ j \ k \rangle\) at such corners, it may be assumed as follows.

**Hypothesis III.**

\[
|\langle i \ j \ k \rangle| \leq \eta(\theta_i, \theta_j)(\langle i \ j \rangle + \langle j \ k \rangle).
\]

Hence, we obtain the following theorem.

**Theorem 5.4.** Under the Hypotheses II and III, \(\forall i,j \in I, |\tilde{a}_{ij}|\) has the following estimation on the region \(\omega_0\)

\[
|\tilde{a}_{ij}| \leq \begin{cases} \frac{1}{2} h_M^2, & j = i, \\ \frac{\sqrt{2}}{2} h_M^2 h_m, & j \neq i, \end{cases}
\]

where \(h_M\) is as defined in (3.10), and \(h_m = \min_{i \in I} h_i\).
Proof. Here is a proof for $i = 1$.

(1) By the property of algebraic areas, one knows that exchanging the indices “2” and “4” in the expression of $a_{11}$ changes only its sign, hence $a_{11}$ can be rewritten as

$$a_{11} = \langle 2 \ 3 \rangle \langle 4 \ 1 \rangle \langle 3 \ 5 \rangle \langle 2 \ 4 \ 5 \rangle + \langle 1 \ 3 \rangle \langle 2 \ 4 \rangle \langle 5 \ 3 \ 5 \rangle,$$

which leads to

$$|a_{11}| \leq h_{1}h_{2}h_{3}h_{4}h_{5}\langle 2 \ 3 \rangle_{0}\langle 4 \ 1 \rangle_{0}\langle 3 \ 5 \rangle_{0}h_{2}h_{4}h_{5}\left(\frac{(2 \ 4)_{0}}{h_{5}} + \frac{(4 \ 5)_{0}}{h_{2}} + \frac{(5 \ 2)_{0}}{h_{4}}\right)$$

$$+ h_{1}h_{2}h_{3}h_{4}h_{5}\langle 1 \ 3 \rangle_{0}\langle 2 \ 4 \rangle_{0}\langle 5 \ 3 \rangle_{0}h_{2}h_{3}h_{5}\left(\frac{(2 \ 3)_{0}}{h_{5}} + \frac{(3 \ 5)_{0}}{h_{2}} + \frac{(5 \ 2)_{0}}{h_{3}}\right)$$

$$\leq \frac{h_{10}}{h_{1}}h_{1}^{-1}h_{m}^{-1}\langle 2 \ 3 \rangle_{0}\langle 4 \ 1 \rangle_{0}\langle 3 \ 5 \rangle_{0}\langle 2 \ 4 \ 5 \rangle_{0} + \langle 1 \ 3 \rangle_{0}\langle 2 \ 4 \rangle_{0}\langle 5 \ 3 \rangle_{0}\langle 2 \ 3 \ 5 \rangle_{0}$$

$$= \frac{h_{10}}{h_{1}}h_{1}^{-1}h_{m}^{-1}|a_{110}|.$$

(5.34)

Moreover by (5.1), (5.2), and the estimation of $m_{t}$ in Theorem 4.2, it is easy to prove

$$|\tilde{a}_{11}| = \frac{1}{m_{t}}|a_{11}| \leq \frac{h_{2}^{2}}{h_{1}h_{m}}|\tilde{a}_{110}|.$$

(5.35)

Hence by Theorem 5.3, one derives

$$|\tilde{a}_{11}| \leq \frac{1}{2}\frac{h_{2}^{2}}{h_{1}h_{m}}.$$

(5.36)

(2) By the Hypothesis III, there is

$$|a_{12}| = |\langle 1 \ 3 \rangle\langle 1 \ 4 \rangle\langle 5 \ 3 \ 4 \ 5 \rangle|$$

$$\leq h_{1}h_{2}h_{4}h_{5}\langle 1 \ 3 \rangle_{0}\langle 1 \ 4 \rangle_{0}\langle 1 \ 5 \rangle_{0}|\eta(\theta_{3}, \theta_{4})(\langle 3 \ 4 \rangle + \langle 4 \ 5 \rangle).$$

(5.37)

Further noticing (5.30), one easily proves

$$|a_{12}| \leq h_{1}^{3}h_{2}^{3}h_{4}^{2}h_{5}^{2}h_{m}^{-1}|a_{120}|,$$

which consequently results in

$$|\tilde{a}_{12}| = \frac{h_{2}}{m_{t}h_{1}}|a_{12}| \leq \frac{\sqrt{2}}{2}\frac{h_{2}^{2}}{h_{2}h_{m}}.$$n

(5.39)

(3) By noting that

$$|a_{13}| = |\langle 1 \ 2 \rangle\langle 1 \ 4 \rangle\langle 1 \ 5 \rangle\langle 2 \ 4 \ 5 \rangle|$$

$$= h_{1}^{3}h_{2}^{3}h_{2}^{2}h_{5}\langle 1 \ 2 \rangle_{0}\langle 1 \ 4 \rangle_{0}\langle 1 \ 5 \rangle_{0}\left(\frac{(2 \ 4)_{0}}{h_{5}} + \frac{(4 \ 5)_{0}}{h_{2}} + \frac{(5 \ 2)_{0}}{h_{4}}\right)$$

$$\leq h_{1}^{3}h_{2}^{3}h_{2}^{2}h_{5}^{2}h_{m}^{-1}|a_{130}|,$$

(5.40)

one easily gets

$$|\tilde{a}_{13}| = \frac{h_{3}}{m_{t}h_{1}}|a_{13}| \leq \frac{\sqrt{2}}{2}\frac{h_{3}^{2}}{h_{3}h_{m}}.$$

(5.41)

(4) The estimations of $\tilde{a}_{14}$ and $\tilde{a}_{15}$ are similar to those of $\tilde{a}_{13}$ and $\tilde{a}_{12}$, respectively. $\square$
6. Numerical Examples

In this section, numerical examples of discrete formulae of directional differentials are given for the cases of even steplength and the nontrivial cases of uneven steplength. According to aforesaid analyses, it is easy to obtain the compound first-order difference quotients as follows

\[ \delta_{\sigma}^{(1)} u_i = \sum_{j=1}^{5} \tilde{a}_{ij} \delta u_j, \quad \forall i \in I. \]

**Example 6.1.** The cases of even steplength.

![Fig. 6.1. Special distribution I (left) and II (right).](image)

(1) As shown in Fig. 6.1, the left figure illustrates the case of even angle and even steplength, which is the most basic case in the discretization of directional differentials. It is obvious that only presenting the discretization to \( \frac{\partial u}{\partial l_1} \) at point \( O \) is enough. The relevant results are shown in Table 6.1.

<table>
<thead>
<tr>
<th>( j )</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>( \sum_{j=1}^{5} \tilde{a}_{ij} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \tilde{a}_{1j} )</td>
<td>0</td>
<td>( \frac{\sqrt{5} - 1}{10} )</td>
<td>( -\frac{\sqrt{5} + 1}{10} )</td>
<td>( -\frac{\sqrt{5} + 1}{10} )</td>
<td>( \frac{\sqrt{5} + 1}{10} )</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 6.1 shows that the coefficients of numerical differentials satisfy the relevant estimations as given in the former section, and

- In the expression of \( \delta_{\sigma}^{(1)} u_1 \), the coefficient \( \tilde{a}_{11} \) is the most important term. Hence, one can assert that the major contribution to \( \delta_{\sigma}^{(1)} u_1 \) should be \( \tilde{a}_{1i} \delta u_i \).

- In above expression, it holds \( \sum_{j=1}^{5} \tilde{a}_{1j} = 0 \), which coincides with the case of even steplength in one dimension.

(2) As shown in Fig. 6.1, the right figure illustrates another case of even steplength, in which the uneven angles between adjacent directions are exhibited. The relevant results are shown in Table 6.2.

Table 6.2 shows that the coefficients of numerical differentials satisfy the relevant estimations as given in the former section, and
In the expression of $\delta_{\sigma}^{(1)} u_1$, the coefficient $\tilde{a}_{12}$ attains the maximum, which is in good agreement with analysis in Theorem 5.3. In fact, since $\tilde{a}_{12}$ is the contribution of the point “2” to $\frac{\partial}{\partial l_1}$, it is not difficult to see from geometric intuition that the more the point “2” approaches to $l_1$, the more it contributes. Limited by the conditions of angles, the minimum of $\theta_1$ has to be $\pi/4$.

In consideration of the contribution to the positive direction of $l_1$, the most important points are “2” and “5”. By the Hypothesis II, if the contribution of the point “2” is large, then that of the point “5” should be small. Limited by the conditions of angles, the maximum of $\theta_5$ has to be $\pi/2$. This happens to be the distribution II as illustrated in the right figure of Fig. 6.1.

**Example 6.2.** The distribution formed by the vertexes of a square, which is the regular distribution in general (see Fig. 6.2).

This is the special case of a uneven steplength distribution, which is also the distribution applicable to the classical finite difference method. Table 6.3 displays the numerical results of $\delta_{\sigma}^{(1)} u_1$ and $\delta_{\sigma}^{(1)} u_5$. The results corresponding to the points 2, 3 and 4 are similar to those of the point 1, and hence are neglected here. The results show that the coefficients of numerical differentials satisfy the relevant estimations as given in the former section, and

- $\delta_{\sigma}^{(1)} u_1$ can be viewed as the same as that of the one dimensional case, which needs only the neighbors “1” and “3”, but is irrelevant to the points “2”, “4” and “5”.
- $\delta_{\sigma}^{(1)} u_5$ is determined by the values of points “1”, “2”, “3” and “4”, but is irrelevant to the point “5”.

**Example 6.3.** A scattered point distribution on an irregular geometric domain is illustrated in Fig. 6.3 (left). For all points satisfying conditions of angles, compute corresponding coefficients of the difference quotients $\delta_{\sigma}^{(1)} u_i$, $\forall i \in I$, and evaluate the maximum of the absolute values.
Table 6.3: Coefficients of difference quotients on the distribution III.

<table>
<thead>
<tr>
<th>j</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \tilde{a}_{1j} )</td>
<td>( \frac{1}{2} )</td>
<td>0</td>
<td>(-\frac{1}{2} )</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>( \tilde{a}_{5j} )</td>
<td>( 2^{-3/2} )</td>
<td>(-2^{-3/2} )</td>
<td>(-2^{-3/2} )</td>
<td>( 2^{-3/2} )</td>
<td>0</td>
</tr>
</tbody>
</table>

\( (\approx 0.3536) \)\( (\approx -0.3536) \)\( (\approx -0.3536) \)\( (\approx 0.3536) \)

Fig. 6.3. Scattered point distribution (left) and local magnification (right).

Obviously, this is a general case of uneven steplength. Table 6.4 displays \( \tilde{a}_{1j} \) and \( \tilde{a}_{5j} \), \( j = 1, \ldots, 5 \) at the point where the maximum is obtained. Fig. 6.3 (right) shows the point “O” and its neighbors “1, 2, ..., 5” (marked by large bold circles) in a local magnified figure. Table 6.4 shows that the coefficients of numerical differentials satisfy the relevant estimations as given in the former section.

Table 6.4: Examples of coefficients of difference quotients on some scattered point distribution.

<table>
<thead>
<tr>
<th>j</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \tilde{a}_{1j} )</td>
<td>0.6784</td>
<td>3.3567e-2</td>
<td>-0.2280</td>
<td>-0.1072</td>
<td>2.3682e-2</td>
</tr>
<tr>
<td>( \tilde{a}_{5j} )</td>
<td>6.8231e-2</td>
<td>-0.3374</td>
<td>-0.1761</td>
<td>0.1382</td>
<td>0.5526</td>
</tr>
</tbody>
</table>

7. Concluding Remarks

As known to all, establishing rigorous finite difference method on scattered point set is undoubtedly a challenging task, however, to meet requirements of solving large and complex scientific computing problems, it is necessary to face up to the difficulties and carry out relevant research. Over the past decade, the authors have made some progress in this field. The results of theoretical analysis of the discrete formulae of directional derivatives in this paper give us a deeper understanding of the finite point method, and are of great significance for further research in this field.

(1) As for the structure of the directional difference coefficient matrix, a concise expression with clear meaning is given, which represents the correlation between different coefficients and
its relationship with the geometric characteristics of scattered points, and reveals its essential characteristics. At the same time, it also provides an effective analytical approach for the study of discretizing PDEs on scattered point sets.

(2) The research on the discriminant function \( m_t \) provides not only the basis for selecting neighboring points, but also the space for relevant scholars to choose different expressions of \( m_t \) in terms of the discrete problems in different studies, so as to facilitate the effective analysis.

(3) For the difference quotient approximation of directional derivatives, corresponding estimations are satisfactory. Above all, they exclude the existence of singularity and alleviate people’s worries about the possibility of numerical instability.

The results of this paper are the bases for further research on the finite point method of PDEs.

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