

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

Guixia Lv¹⁾ and Longjun Shen

*Laboratory of Computational Physics, Institute of Applied Physics and Computational Mathematics,
P. O. Box 8009-26, Beijing 100088, China
Email: lv_guixia@iapcm.ac.cn, shenlj@iapcm.ac.cn*

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.

Mathematics subject classification: 65D25, 65N06, 65N35.

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.

* Received December 21, 2019 / Revised version received April 18, 2020 / Accepted May 12, 2020 /
Published online June 18, 2021 /

¹⁾ Corresponding author

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 $\langle i j k \rangle$.
- $\langle i j \rangle_0 = \frac{1}{2} \sin(\widehat{\vec{e}_i, \vec{e}_j})$, i.e., a special case of $\langle i j \rangle$ as $h_i = h_j = 1$, where $\widehat{\vec{e}_i, \vec{e}_j}$ denotes the anticlockwise angle between \vec{e}_i and \vec{e}_j .
- $\langle \bar{i} \bar{j} \rangle_0 = \frac{1}{2} \cos(\widehat{\vec{e}_i, \vec{e}_j})$.

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

Property 2.1.

$$\begin{aligned} \langle i j \rangle &= -\langle j i \rangle, \\ \langle j k \rangle \langle l m \rangle &= \langle j l \rangle \langle k m \rangle + \langle j m \rangle \langle l k \rangle. \end{aligned}$$

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

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

$$i \textcircled{\mathbb{K}} j = 1 + (i + j - 1) \pmod{k},$$

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) ($i = 1, \dots, 5$), and their corresponding function values u_i ($i = 0, 1, \dots, 5$) 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 $\frac{\partial u}{\partial l_i}$, $\frac{\partial^2 u}{\partial l_i^2}$ ($\forall i \in I$) 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.

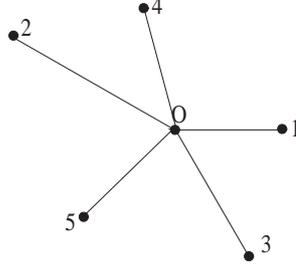


Fig. 3.1. Point O and its five neighbors.

For any $i \in I$, denote by

$$\begin{aligned}\Delta u_i &= u_i - u_0, \\ \delta u_i &= \Delta u_i / h_i, \\ \Delta_\sigma u_i &= \frac{1}{m_t} \sum_{j=1}^5 a_{ij} \Delta u_j, \\ \delta_\sigma^{(1)} u_i &= \Delta_\sigma u_i / h_i, \\ \delta_\sigma^{(2)} u_i &= (\delta u_i - \delta_\sigma^{(1)} u_i) / (h_i / 2),\end{aligned}$$

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

$$\mathbf{A} = (a_{ij})_{5 \times 5} = \begin{pmatrix} \langle 12 \rangle \langle 34 \rangle \langle 35 \rangle \langle 245 \rangle & \langle 13 \rangle \langle 14 \rangle \langle 15 \rangle \langle 345 \rangle & -\langle 12 \rangle \langle 14 \rangle \langle 15 \rangle \langle 245 \rangle & \langle 12 \rangle \langle 13 \rangle \langle 15 \rangle \langle 235 \rangle & -\langle 12 \rangle \langle 13 \rangle \langle 14 \rangle \langle 234 \rangle \\ -\langle 13 \rangle \langle 24 \rangle \langle 25 \rangle \langle 345 \rangle & \langle 23 \rangle \langle 45 \rangle \langle 41 \rangle \langle 351 \rangle & \langle 24 \rangle \langle 25 \rangle \langle 21 \rangle \langle 451 \rangle & -\langle 23 \rangle \langle 25 \rangle \langle 21 \rangle \langle 351 \rangle & \langle 23 \rangle \langle 24 \rangle \langle 21 \rangle \langle 341 \rangle \\ -\langle 23 \rangle \langle 24 \rangle \langle 25 \rangle \langle 345 \rangle & -\langle 24 \rangle \langle 35 \rangle \langle 31 \rangle \langle 451 \rangle & \langle 34 \rangle \langle 51 \rangle \langle 52 \rangle \langle 412 \rangle & -\langle 35 \rangle \langle 41 \rangle \langle 42 \rangle \langle 512 \rangle & \langle 35 \rangle \langle 31 \rangle \langle 32 \rangle \langle 512 \rangle & -\langle 34 \rangle \langle 31 \rangle \langle 32 \rangle \langle 412 \rangle \\ \langle 32 \rangle \langle 34 \rangle \langle 35 \rangle \langle 245 \rangle & -\langle 34 \rangle \langle 35 \rangle \langle 31 \rangle \langle 451 \rangle & -\langle 45 \rangle \langle 41 \rangle \langle 42 \rangle \langle 512 \rangle & \langle 45 \rangle \langle 12 \rangle \langle 13 \rangle \langle 523 \rangle & \langle 41 \rangle \langle 42 \rangle \langle 43 \rangle \langle 123 \rangle \\ -\langle 42 \rangle \langle 43 \rangle \langle 45 \rangle \langle 235 \rangle & \langle 43 \rangle \langle 45 \rangle \langle 41 \rangle \langle 351 \rangle & -\langle 54 \rangle \langle 51 \rangle \langle 52 \rangle \langle 412 \rangle & -\langle 41 \rangle \langle 52 \rangle \langle 53 \rangle \langle 123 \rangle & \langle 51 \rangle \langle 23 \rangle \langle 24 \rangle \langle 134 \rangle \\ \langle 52 \rangle \langle 53 \rangle \langle 54 \rangle \langle 234 \rangle & -\langle 53 \rangle \langle 54 \rangle \langle 51 \rangle \langle 341 \rangle & \langle 54 \rangle \langle 51 \rangle \langle 52 \rangle \langle 412 \rangle & -\langle 51 \rangle \langle 52 \rangle \langle 53 \rangle \langle 123 \rangle & -\langle 52 \rangle \langle 13 \rangle \langle 14 \rangle \langle 234 \rangle \end{pmatrix}. \quad (3.1)$$

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

$$m_t = \langle 23 \rangle \langle 41 \rangle \langle 125 \rangle \langle 345 \rangle - \langle 12 \rangle \langle 34 \rangle \langle 235 \rangle \langle 415 \rangle \quad (3.2)$$

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 $\frac{\partial u}{\partial \vec{l}_i}$, δu_i employs a single neighboring point, and consequently has first-order accuracy, while $\delta_\sigma^{(1)} u_i$ formed by the informations of five neighbors has second-order accuracy. Meanwhile, as for the approximation to $\frac{\partial u^2}{\partial \vec{l}_i^2}$, $\delta_\sigma^{(2)} u_i$ has first-order accuracy.

Denote by $\Delta \mathbf{U} = (\Delta u_1, \dots, \Delta u_5)^T$, $\delta \mathbf{U} = (\delta u_1, \dots, \delta u_5)^T$, and $\mathbf{H} = \text{diag}(h_1, h_2, \dots, h_5)$. Hence by [27] one has

$$\Delta_\sigma \mathbf{U} = \frac{1}{m_t} \mathbf{A} \cdot \Delta \mathbf{U}, \quad (3.3)$$

$$\delta_\sigma^{(1)} \mathbf{U} = \tilde{\mathbf{A}} \cdot \delta \mathbf{U}, \quad (3.4)$$

$$\delta_\sigma^{(2)} \mathbf{U} = \mathbf{H}^{-1} \mathbf{B} \cdot \delta \mathbf{U}, \quad (3.5)$$

where

$$\tilde{\mathbf{A}} = \frac{1}{m_t} \mathbf{H}^{-1} \mathbf{A} \mathbf{H}, \quad (3.6)$$

$$\mathbf{B} = 2(\mathbf{E} - \tilde{\mathbf{A}}), \quad (3.7)$$

where \mathbf{E} denotes the unit matrix.

Obviously, the directional difference coefficient matrix A is the basis of discussing $\tilde{\mathbf{A}}$ and \mathbf{B} , namely, the compound first-order difference quotient and the compound second-order difference quotient. Let

$$\begin{aligned} \frac{\partial u}{\partial \mathbf{L}} &= \left(\frac{\partial u}{\partial \vec{l}_1}, \dots, \frac{\partial u}{\partial \vec{l}_5} \right)^T, \\ \frac{\partial^2 u}{\partial \mathbf{L}^2} &= \left(\frac{\partial^2 u}{\partial \vec{l}_1^2}, \dots, \frac{\partial^2 u}{\partial \vec{l}_5^2} \right)^T. \end{aligned}$$

Then, the five-point formulae 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 $1, \dots, 5$, 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*

$$\frac{\partial u}{\partial \mathbf{L}} = \delta_\sigma^{(1)} \mathbf{U} + O(h_M^2), \quad (3.8)$$

and

$$\frac{\partial^2 u}{\partial \mathbf{L}^2} = \delta_\sigma^{(2)} \mathbf{U} + O(h_M), \quad (3.9)$$

respectively, under the so-called solvability condition, i.e., $m_t \neq 0$, where

$$h_M = \max_{1 \leq i \leq 5} h_i, \quad (3.10)$$

and m_t is as given by (3.2).

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

3.2. Analytical expressions of the matrix A

(1) In the numerical formulae of directional differentials, the coefficients of Δu_i ($i = 1, \dots, 5$) 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 $\frac{\partial u}{\partial l_i}$, how much contribution does each Δu_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 $\langle 1\ 2 \rangle, \langle 1\ 3 \rangle, \langle 1\ 4 \rangle$, and $\langle 1\ 5 \rangle$ (see Fig. 3.2 (left)), and those unrelated to “1” are $\langle 2\ 3 \rangle, \langle 3\ 4 \rangle, \langle 4\ 5 \rangle, \langle 5\ 2 \rangle, \langle 2\ 4 \rangle$, and $\langle 3\ 5 \rangle$ (see Fig. 3.2 (right)). Two groups of algebraic areas play different roles in numerical formulae.

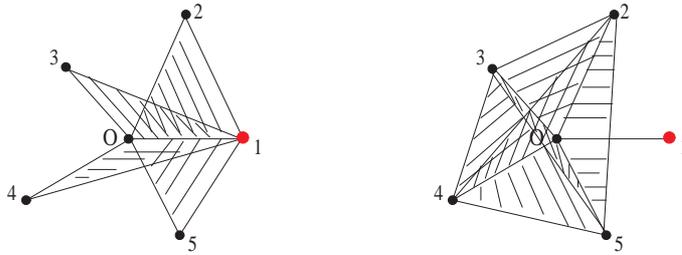


Fig. 3.2. Left: the areas related to the index “1”; right: the areas unrelated to the index “1”.

(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

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

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

$$\mathbf{F} = \begin{pmatrix} \mathbf{F}_1^T \\ \mathbf{F}_2^T \\ \vdots \\ \mathbf{F}_5^T \end{pmatrix} = \begin{pmatrix} f_{11} & f_{12} & f_{13} & f_{14} & f_{15} \\ f_{21} & f_{22} & f_{23} & f_{24} & f_{25} \\ & & \vdots & & \\ f_{51} & f_{52} & f_{53} & f_{54} & f_{55} \end{pmatrix} = \begin{pmatrix} 0 & \langle 1\ 2 \rangle & \langle 1\ 3 \rangle & \langle 1\ 4 \rangle & \langle 1\ 5 \rangle \\ \langle 2\ 1 \rangle & 0 & \langle 2\ 3 \rangle & \langle 2\ 4 \rangle & \langle 2\ 5 \rangle \\ & & \vdots & & \\ \langle 5\ 1 \rangle & \langle 5\ 2 \rangle & \langle 5\ 3 \rangle & \langle 5\ 4 \rangle & 0 \end{pmatrix}$$

is called the **direct correlation matrix**. It is obvious that \mathbf{F} is an anti-symmetric matrix, namely,

$$\mathbf{F} = -\mathbf{F}^T.$$

(3) 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

$$\begin{aligned} \frac{\partial u}{\partial \vec{l}_1} &= -\frac{\partial u}{\partial \vec{l}_2} = \frac{1}{m_1}(h_2^2 \Delta u_1 - h_1^2 \Delta u_2) + O(h_M^2), \\ \frac{\partial^2 u}{\partial \vec{l}_1^2} &= \frac{\partial^2 u}{\partial \vec{l}_2^2} = \frac{2}{m_1}(h_2 \Delta u_1 + h_1 \Delta u_2) + O(h_M), \end{aligned}$$

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

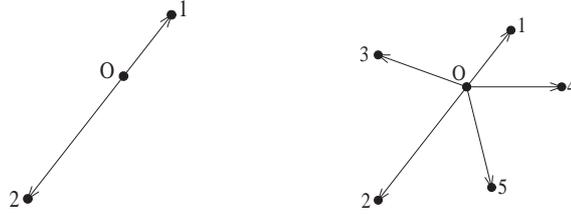


Fig. 3.3. Special point distribution. Left: 1D case; right: 2D case.

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 $\frac{\partial u}{\partial \vec{l}_1}$, $\frac{\partial u}{\partial \vec{l}_2}$ and $\frac{\partial^2 u}{\partial \vec{l}_1^2}$, $\frac{\partial^2 u}{\partial \vec{l}_2^2}$, since $\langle 1\ 2 \rangle = 0$. 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 $\frac{\partial u}{\partial \vec{l}_i}$, $\frac{\partial^2 u}{\partial \vec{l}_i^2}$ ($i = 1, 2, 3$) depends upon $\langle 1\ 2 \rangle$, $\langle 1\ 3 \rangle$, and $\langle 2\ 3 \rangle$ simultaneously.

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

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

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

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

We call $\mathbf{G}_i (i = 1, \dots, 5)$ as the **indirect correlation vector** of the index i . Obviously, the index i is not included in this vector expression. Define a matrix as

$$\mathbf{G} = \begin{pmatrix} \mathbf{G}_1^T \\ \mathbf{G}_2^T \\ \vdots \\ \mathbf{G}_5^T \end{pmatrix} = \begin{pmatrix} g_{11} & g_{12} & g_{13} & g_{14} & g_{15} \\ g_{21} & g_{22} & g_{23} & g_{24} & g_{25} \\ & & \vdots & & \\ g_{51} & g_{52} & g_{53} & g_{54} & g_{55} \end{pmatrix} = \begin{pmatrix} 0 & g_{12} & g_{13} & g_{14} & g_{15} \\ g_{21} & 0 & g_{23} & g_{24} & g_{25} \\ & & \vdots & & \\ g_{51} & g_{52} & g_{53} & g_{54} & 0 \end{pmatrix}.$$

We call G as the **indirect correlation matrix**, and easily find it being an anti-symmetric matrix, namely

$$\mathbf{G} = -\mathbf{G}^T.$$

(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

$$a_{ij} = \mathbf{F}_i^T \mathbf{G}_j, \quad \forall i, j \in I,$$

that is,

$$\mathbf{A} = \begin{pmatrix} \mathbf{F}_1^T \mathbf{G}_1 & \mathbf{F}_1^T \mathbf{G}_2 & \dots & \mathbf{F}_1^T \mathbf{G}_5 \\ \dots & \dots & \dots & \dots \\ \mathbf{F}_5^T \mathbf{G}_1 & \mathbf{F}_5^T \mathbf{G}_2 & \dots & \mathbf{F}_5^T \mathbf{G}_5 \end{pmatrix},$$

or

$$\mathbf{A} = \mathbf{F} \mathbf{G}^T. \quad (3.11)$$

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

$$\bar{h} = (h_1 h_2 \dots h_5)^{1/5}.$$

Note that, in the following fractions

$$\frac{a_{ij}}{m_t} = \frac{\mathbf{F}_i^T \mathbf{G}_j}{m_t}, \quad \forall i, j \in I,$$

numerators and denominators have a common factor \bar{h}^8 . Separating this factor will facilitate relevant discussion.

To this end, we first denote by

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

$$\mathbf{F}_0 = \begin{pmatrix} \langle 1 \ 1 \rangle_0 & \langle 1 \ 2 \rangle_0 & \langle 1 \ 3 \rangle_0 & \langle 1 \ 4 \rangle_0 & \langle 1 \ 5 \rangle_0 \\ \langle 2 \ 1 \rangle_0 & \langle 2 \ 2 \rangle_0 & \langle 2 \ 3 \rangle_0 & \langle 2 \ 4 \rangle_0 & \langle 2 \ 5 \rangle_0 \\ & & \vdots & & \\ \langle 5 \ 1 \rangle_0 & \langle 5 \ 2 \rangle_0 & \langle 5 \ 3 \rangle_0 & \langle 5 \ 4 \rangle_0 & \langle 5 \ 5 \rangle_0 \end{pmatrix},$$

then, we have

$$\mathbf{F} = \bar{h}^2 \mathbf{\Lambda} \mathbf{F}_0 \mathbf{\Lambda}. \quad (3.12)$$

For the same sake, denote by

$$\begin{cases} g_{ij0} = \text{sgn}(j-i)(-1)^{i+j}\langle k_1, k_2 \rangle_0 \langle k_2, k_3 \rangle_0 \langle k_3, k_1 \rangle_0, \\ \quad k_1 < k_2 < k_3, k_l \in I \setminus \{i, j\}, l = 1, 2, 3, & i \neq j, \\ g_{ij0} = 0, & i = j, \end{cases}$$

$$\mathbf{G}_0 = \begin{pmatrix} g_{110} & g_{120} & g_{130} & g_{140} & g_{150} \\ g_{210} & g_{220} & g_{230} & g_{240} & g_{250} \\ & & \vdots & & \\ g_{510} & g_{520} & g_{530} & g_{540} & g_{550} \end{pmatrix}.$$

Then, we have

$$\mathbf{G} = \bar{h}^6 \mathbf{\Lambda}^{-2} \mathbf{G}_0 \mathbf{\Lambda}^{-2}. \quad (3.13)$$

By (3.12) and (3.13), we have

$$\mathbf{A} = \bar{h}^8 \mathbf{\Lambda} \mathbf{A}_\lambda \mathbf{\Lambda}^{-2},$$

where

$$\mathbf{A}_\lambda = \mathbf{F}_0 \mathbf{\Lambda}^{-1} \mathbf{G}_0^T.$$

Remark 3.1. 1. $\{\mathbf{F}_i, \forall i \in I\}$ and $\{\mathbf{G}_i, \forall i \in I\}$ 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 \mathbf{F}_i and \mathbf{G}_j , the rows and columns of $A = (\mathbf{F}_i^T \mathbf{G}_j)_{5 \times 5}$ 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 permuted, 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.

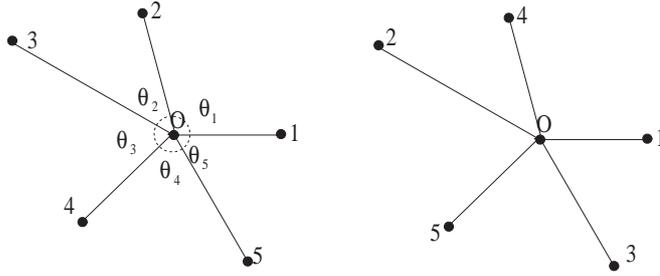


Fig. 3.4. Point O and its five neighbors.

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 θ_i satisfy the following conditions:

- (1) $\theta_i > 0$;
- (2) $\theta_i + \theta_{i \oplus 1} \leq \pi$.

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

$$m_t = \langle 23 \rangle \langle 41 \rangle \langle 125 \rangle \langle 345 \rangle - \langle 12 \rangle \langle 34 \rangle \langle 235 \rangle \langle 415 \rangle,$$

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

$$m_t = -\langle 25 \rangle \langle 41 \rangle \langle 123 \rangle \langle 543 \rangle + \langle 12 \rangle \langle 54 \rangle \langle 253 \rangle \langle 413 \rangle.$$

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 $\langle 125 \rangle$, $\langle 345 \rangle$, $\langle 235 \rangle$ and $\langle 415 \rangle$ in previous expressions, and by properties of algebraic areas, it is not difficult to have

$$\begin{aligned} m_t &= \langle 12 \rangle \langle 34 \rangle \langle 45 \rangle \langle 35 \rangle + \langle 13 \rangle \langle 24 \rangle \langle 45 \rangle \langle 52 \rangle + \langle 41 \rangle \langle 23 \rangle \langle 35 \rangle \langle 52 \rangle \\ &\quad + \langle 51 \rangle \langle 23 \rangle \langle 34 \rangle \langle 24 \rangle + \langle 23 \rangle \langle 45 \rangle \langle 51 \rangle \langle 41 \rangle + \langle 24 \rangle \langle 51 \rangle \langle 13 \rangle \langle 35 \rangle \\ &\quad + \langle 52 \rangle \langle 34 \rangle \langle 41 \rangle \langle 13 \rangle + \langle 34 \rangle \langle 51 \rangle \langle 12 \rangle \langle 52 \rangle + \langle 35 \rangle \langle 12 \rangle \langle 24 \rangle \langle 41 \rangle \\ &\quad + \langle 45 \rangle \langle 12 \rangle \langle 23 \rangle \langle 13 \rangle \\ &= \sum_{\substack{i,j=1 \\ i < j}}^5 f_{ij} g_{ij}. \end{aligned} \tag{4.1}$$

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

$$m_t = \frac{1}{2} \sum_{i,j=1}^5 f_{ij} g_{ij} = \frac{1}{2} \sum_{k=1}^5 \mathbf{F}_k^T \mathbf{G}_k.$$

Similar to factorizing \mathbf{A} into \mathbf{F} and \mathbf{G} , m_t is also factorized into \mathbf{F} and \mathbf{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 \bar{h}^8

If reform $\langle i j k \rangle$ as

$$\begin{aligned} \langle i j k \rangle &= \langle i j \rangle + \langle j k \rangle + \langle k i \rangle \\ &= \langle i j \rangle_0 h_i h_j + \langle j k \rangle_0 h_j h_k + \langle k i \rangle_0 h_k h_i \\ &= \bar{h}^2 \lambda_i \lambda_j \lambda_k (\langle i j \rangle_0 \lambda_k^{-1} + \langle j k \rangle_0 \lambda_i^{-1} + \langle k i \rangle_0 \lambda_j^{-1}) \\ &= \bar{h}^2 \lambda_i \lambda_j \lambda_k \langle i j k \rangle_\lambda, \end{aligned}$$

where

$$\langle i j k \rangle_\lambda = \langle i j \rangle_0 \lambda_k^{-1} + \langle j k \rangle_0 \lambda_i^{-1} + \langle k i \rangle_0 \lambda_j^{-1},$$

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

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

where

$$m_\lambda = \langle 2 3 \rangle_0 \langle 4 1 \rangle_0 \langle 1 2 5 \rangle_\lambda \langle 3 4 5 \rangle_\lambda - \langle 1 2 \rangle_0 \langle 3 4 \rangle_0 \langle 2 3 5 \rangle_\lambda \langle 4 1 5 \rangle_\lambda.$$

If all steplengths are equal, namely, $\lambda_i = 1 (\forall i \in I)$, the discussion will be simplified. In this case, denote m_λ by m_{λ_0} . Hence, we get the following theorem.

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

$$m_{\lambda_0} = 4 \prod_{i=1}^5 \left(\sin \frac{\theta_i}{2} \sin \frac{1}{2} (\theta_i + \theta_{i \oplus 1}) \right). \quad (4.2)$$

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

$$\begin{aligned} m_{\lambda_0} &= \langle 2 3 \rangle_0 \langle 4 1 \rangle_0 \langle 1 2 5 \rangle_0 \langle 3 4 5 \rangle_0 - \langle 1 2 \rangle_0 \langle 3 4 \rangle_0 \langle 2 3 5 \rangle_0 \langle 4 1 5 \rangle_0 \\ &= \frac{1}{16} \left[\sin \theta_2 \sin(\theta_4 + \theta_5) (\sin \theta_1 + \sin \theta_5 - \sin(\theta_1 + \theta_5)) (\sin \theta_3 + \sin \theta_4 - \sin(\theta_3 + \theta_4)) \right. \\ &\quad \left. + \sin \theta_1 \sin \theta_3 (\sin \theta_2 + \sin(\theta_3 + \theta_4) + \sin(\theta_1 + \theta_5)) (\sin \theta_4 + \sin \theta_5 - \sin(\theta_4 + \theta_5)) \right]. \end{aligned}$$

Note that, for any α, β , 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). \square

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 θ_i ($i = 1, \dots, 5$) can maximize the value of m_{λ_0} ?

Let $\theta_5 = 2\pi - \theta_1 - \theta_2 - \theta_3 - \theta_4$, and view m_{λ_0} as the function with respect to $\theta_1, \theta_2, \theta_3, \theta_4$. We first discuss the change of m_{λ_0} with θ_1 . It is obvious that

$$m_{\lambda_0} = 4 \sin \frac{\theta_2}{2} \sin \frac{\theta_3}{2} \sin \frac{\theta_4}{2} \sin \frac{1}{2}(\theta_2 + \theta_3) \sin \frac{1}{2}(\theta_3 + \theta_4) \sin \frac{1}{2}(\theta_2 + \theta_3 + \theta_4) m_{\lambda_0}^*, \quad (4.3)$$

where

$$m_{\lambda_0}^* = \sin \frac{\theta_1}{2} \sin \frac{\theta_5}{2} \sin \frac{1}{2}(\theta_1 + \theta_2) \sin \frac{1}{2}(\theta_4 + \theta_5) \\ = \sin \frac{\theta_1}{2} \sin \frac{1}{2}(\theta_1 + \theta_2) \sin \frac{1}{2}(\theta_1 + \theta_2 + \theta_3) \sin \frac{1}{2}(\theta_1 + \theta_2 + \theta_3 + \theta_4). \quad (4.4)$$

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

$$\frac{d(\ln m_{\lambda_0}^*)}{d\theta_1} = \frac{1}{2} \left(\cot \frac{\theta_1}{2} + \cot \frac{1}{2}(\theta_1 + \theta_2) + \cot \frac{1}{2}(\theta_1 + \theta_2 + \theta_3) + \cot \frac{1}{2}(\theta_1 + \theta_2 + \theta_3 + \theta_4) \right). \quad (4.5)$$

It is obvious that $d(\ln m_{\lambda_0}^*)/d\theta_1$ is a monotone decreasing function with respect to θ_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 $\theta_i = \frac{2}{5}\pi$ ($i = 1, \dots, 5$), m_{λ_0} attains the maximum.

By using $\sin \frac{2}{5}\pi = \frac{1}{4}\sqrt{10 + 2\sqrt{5}}$, $\sin \frac{\pi}{5} = \frac{1}{4}\sqrt{10 - 2\sqrt{5}}$, 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_{λ_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*

$$m_t \geq \bar{h}^{10} h_M^{-2} m_{\lambda_0}, \quad (4.6)$$

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 $\tilde{\mathbf{A}}$, it is easy to have

$$\tilde{\mathbf{A}} = \frac{1}{m_t} \mathbf{\Lambda}^{-1} \mathbf{A} \mathbf{\Lambda}. \quad (5.1)$$

Specially, in the case of even steplength, as $\mathbf{\Lambda}$ is a unit matrix, one has

$$\tilde{\mathbf{A}}_0 = \frac{1}{m_{\lambda_0}} \mathbf{A}_{\lambda_0}, \quad (5.2)$$

where $\tilde{\mathbf{A}}_0$, \mathbf{A}_{λ_0} denote $\tilde{\mathbf{A}}$, \mathbf{A}_λ in the case of even steplength, respectively.

The element \tilde{a}_{ij} of the matrix $\tilde{\mathbf{A}}$ 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*

$$\sum_{j=1}^5 \langle j \ k \rangle_0 \tilde{a}_{ij} = \langle i \ k \rangle_0, \quad \forall k, i \in I. \quad (5.3)$$

Moreover, for a given i , only two of the five equations of $k = 1, \dots, 5$ are independent.

Proof. Take $i = 1$ for illustration. By the expression (3.4) of the compound first-order difference quotient, one has

$$\delta_\sigma^{(1)} u_1 = \tilde{a}_{11} \delta u_1 + \tilde{a}_{12} \delta u_2 + \tilde{a}_{13} \delta u_3 + \tilde{a}_{14} \delta u_4 + \tilde{a}_{15} \delta u_5. \quad (5.4)$$

Using

$$\langle 4 \ 5 \rangle_0 \delta u_3 + \langle 5 \ 3 \rangle_0 \delta u_4 + \langle 3 \ 4 \rangle_0 \delta u_5 = O(h_M) \quad (5.5)$$

to eliminate δu_5 in (5.4), and noticing the Hypothesis I, $\langle 3 \ 4 \rangle_0$ does not vanish, hence one has

$$\begin{aligned} \delta_\sigma^{(1)} u_1 &= \tilde{a}_{11} \delta u_1 + \tilde{a}_{12} \delta u_2 + \frac{1}{\langle 3 \ 4 \rangle_0} (\langle 3 \ 4 \rangle_0 \tilde{a}_{13} - \langle 4 \ 5 \rangle_0 \tilde{a}_{15}) \delta u_3 \\ &\quad + \frac{1}{\langle 3 \ 4 \rangle_0} (\langle 3 \ 4 \rangle_0 \tilde{a}_{14} - \langle 5 \ 3 \rangle_0 \tilde{a}_{15}) \delta u_4 + O(h_M). \end{aligned} \quad (5.6)$$

Similarly, using

$$\langle 3 \ 4 \rangle_0 \delta u_2 + \langle 4 \ 2 \rangle_0 \delta u_3 + \langle 2 \ 3 \rangle_0 \delta u_4 = O(h_M) \quad (5.7)$$

to eliminate δu_4 in (5.6), and noticing the Hypothesis I, $\langle 2\ 3 \rangle_0$ does not vanish, so one has

$$\begin{aligned} \delta_\sigma^{(1)} u_1 &= \delta u_1 + (\tilde{a}_{11} - 1)\delta u_1 + \frac{1}{\langle 2\ 3 \rangle_0} [\langle 2\ 3 \rangle_0 \tilde{a}_{12} - \langle 3\ 4 \rangle_0 \tilde{a}_{14} + \langle 5\ 3 \rangle_0 \tilde{a}_{15}] \delta u_2 \\ &\quad + \frac{1}{\langle 2\ 3 \rangle_0 \langle 3\ 4 \rangle_0} [\langle 2\ 3 \rangle_0 (\langle 3\ 4 \rangle_0 \tilde{a}_{13} - \langle 4\ 5 \rangle_0 \tilde{a}_{15}) - \langle 4\ 2 \rangle_0 (\langle 3\ 4 \rangle_0 \tilde{a}_{14} - \langle 5\ 3 \rangle_0 \tilde{a}_{15})] \delta u_3 + O(h_M). \end{aligned} \quad (5.8)$$

Further using

$$\langle 2\ 3 \rangle_0 \delta u_1 + \langle 3\ 1 \rangle_0 \delta u_2 + \langle 1\ 2 \rangle_0 \delta u_3 = O(h_M) \quad (5.9)$$

to eliminate the second term in the right-hand side of (5.8), one obtains

$$\begin{aligned} \delta_\sigma^{(1)} u_1 &= \delta u_1 + \frac{1}{\langle 2\ 3 \rangle_0 \langle 3\ 4 \rangle_0} \{ [\langle 3\ 4 \rangle_0 \langle 3\ 1 \rangle_0 (1 - \tilde{a}_{11}) + \langle 3\ 4 \rangle_0 (\langle 2\ 3 \rangle_0 \tilde{a}_{12} - \langle 3\ 4 \rangle_0 \tilde{a}_{14} \\ &\quad + \langle 5\ 3 \rangle_0 \tilde{a}_{15})] \delta u_2 + [\langle 3\ 4 \rangle_0 \langle 1\ 2 \rangle_0 (1 - \tilde{a}_{11}) + \langle 2\ 3 \rangle_0 (\langle 3\ 4 \rangle_0 \tilde{a}_{13} - \langle 4\ 5 \rangle_0 \tilde{a}_{15}) \\ &\quad - \langle 4\ 2 \rangle_0 (\langle 3\ 4 \rangle_0 \tilde{a}_{14} - \langle 5\ 3 \rangle_0 \tilde{a}_{15})] \delta u_3 \} + O(h_M). \end{aligned} \quad (5.10)$$

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

$$\begin{aligned} \delta_\sigma^{(1)} u_1 &= \delta u_1 + \frac{1}{\langle 2\ 3 \rangle_0} \{ [\langle 3\ 1 \rangle_0 (1 - \tilde{a}_{11}) + \langle 2\ 3 \rangle_0 \tilde{a}_{12} - \langle 3\ 4 \rangle_0 \tilde{a}_{14} + \langle 5\ 3 \rangle_0 \tilde{a}_{15}] \delta u_2 \\ &\quad + [\langle 1\ 2 \rangle_0 (1 - \tilde{a}_{11}) + \langle 2\ 3 \rangle_0 \tilde{a}_{13} - \langle 4\ 2 \rangle_0 \tilde{a}_{14} + \langle 2\ 5 \rangle_0 \tilde{a}_{15}] \delta u_3 \} + O(h_M). \end{aligned} \quad (5.11)$$

Since $\delta u_1, \delta_\sigma^{(1)} u_1$ are corresponding first-order and second-order approximations to $\frac{\partial u}{\partial t_1}$ at the point “O”, it follows that

$$\delta_\sigma^{(1)} u_1 = \delta u_1 + O(h_M). \quad (5.12)$$

Hence, the coefficients of δu_2 and δu_3 in (5.11) must vanish, that is,

$$\langle 1\ 2 \rangle_0 \tilde{a}_{11} + \langle 3\ 2 \rangle_0 \tilde{a}_{13} + \langle 4\ 2 \rangle_0 \tilde{a}_{14} + \langle 5\ 2 \rangle_0 \tilde{a}_{15} = \langle 1\ 2 \rangle_0, \quad (5.13)$$

$$\langle 1\ 3 \rangle_0 \tilde{a}_{11} + \langle 2\ 3 \rangle_0 \tilde{a}_{12} + \langle 4\ 3 \rangle_0 \tilde{a}_{14} + \langle 5\ 3 \rangle_0 \tilde{a}_{15} = \langle 1\ 3 \rangle_0. \quad (5.14)$$

As $\langle 2\ 2 \rangle_0 = 0, \langle 3\ 3 \rangle_0 = 0$, these two equations can be reformed as

$$\sum_{j=1}^5 \langle j\ k \rangle_0 \tilde{a}_{1j} = \langle 1\ k \rangle_0, \quad k = 2, 3. \quad (5.15)$$

By combining (5.13) and (5.14), it is not difficult to derive the following equations

$$\sum_{j=1}^5 \langle j\ k \rangle_0 \tilde{a}_{1j} = \langle 1\ k \rangle_0, \quad k = 1, 4, 5. \quad (5.16)$$

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

The theorem restricts the combination of \tilde{a}_{ij} . In particular, when $\lambda_i = 1$ ($i = 1, \dots, 5$), 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:*

$$\sum_{j=1}^5 \tilde{a}_{ij0} = 0, \quad \forall i \in I.$$

Proof. Also take $i = 1$ as example. By the Property 4.1, it is easy to get $m_{\lambda_0} \neq 0$, hence one has

$$\sum_{j=1}^5 \tilde{a}_{1j0} = \frac{1}{m_{\lambda_0}} \sum_{j=1}^5 \sum_{k=1}^5 f_{1k0} g_{jk0} = \frac{1}{m_{\lambda_0}} \sum_{k=1}^5 f_{1k0} \left(\sum_{j=1}^5 g_{jk0} \right). \quad (5.17)$$

When $k = 1$, one gets

$$\begin{aligned} \sum_{j=1}^5 g_{j10} &= \langle 34 \rangle_0 \langle 45 \rangle_0 \langle 53 \rangle_0 - \langle 45 \rangle_0 \langle 52 \rangle_0 \langle 24 \rangle_0 + \langle 52 \rangle_0 \langle 23 \rangle_0 \langle 35 \rangle_0 - \langle 23 \rangle_0 \langle 34 \rangle_0 \langle 42 \rangle_0 \\ &= \langle 53 \rangle_0 (\langle 34 \rangle_0 \langle 45 \rangle_0 - \langle 52 \rangle_0 \langle 23 \rangle_0) - \langle 24 \rangle_0 (\langle 45 \rangle_0 \langle 52 \rangle_0 - \langle 23 \rangle_0 \langle 34 \rangle_0). \end{aligned} \quad (5.18)$$

Simplifying above equation gives

$$\sum_{j=1}^5 g_{j10} = \langle 53 \rangle_0 \sin(\theta_2 + \theta_3) \sin(\theta_2 + \theta_4) + \langle 24 \rangle_0 \sin(\theta_3 + \theta_4) \sin(\theta_2 + \theta_4) = 0. \quad (5.19)$$

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 θ_i satisfies

- (1) $\theta_i \geq \frac{\pi}{4}$;
- (2) $\theta_i + \theta_{i \oplus 1} \leq \pi$.

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

$$\begin{aligned}\tilde{a}_{ij0} &\geq 0, & j = i, i \textcircled{5}1, i \textcircled{5}4, \\ \tilde{a}_{ij0} &\leq 0, & j = i \textcircled{5}2, i \textcircled{5}3.\end{aligned}$$

That is, \tilde{a}_{ii0} is nonnegative, and the coefficients corresponding to two directions adjacent to \vec{l}_i are also nonnegative, while the coefficients corresponding to two directions far from \vec{l}_i are nonpositive.

For convenience of later deduction, denote by

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

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

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

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 ω_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 ω_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 φ_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 φ_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 $\frac{\partial |\tilde{a}_{110}|}{\partial \varphi_{12}} \leq 0$;

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

For Case I, $|\tilde{a}_{110}|$ attains the maximum at $\varphi_{12} = \frac{3}{8}\pi$. If φ_1 and φ_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 φ_1 and φ_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

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

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, φ_3 should be as large as possible, so it should be taken as

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

Note again the definition of ω_0 , it is not hard to come up with

$$\varphi_2 = \varphi_4 = \frac{\pi}{8}.$$

If φ_1 is supposed to be the parametric angle, then to maximize $|\tilde{a}_{120}|$, the five angles should have the following distribution

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

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

$$|\tilde{a}_{120}| = \frac{1}{2} \frac{\sin(\frac{\pi}{4} + 2\varphi_1)}{\sin \frac{\pi}{4}}. \quad (5.26)$$

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

$$|\tilde{a}_{130}| = \frac{1}{2} \frac{\cos \varphi_1 \cos \varphi_5 \cos(\varphi_4 + \varphi_5)}{\sin \varphi_2 \sin \varphi_3 \sin(\varphi_3 + \varphi_4) \sin(\varphi_1 + \varphi_2)}. \quad (5.27)$$

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

$$|\tilde{a}_{130}| = \frac{1}{2} \frac{\cos(\varphi_{12} - \varphi_2) \cos \varphi_5 \cos(\varphi_4 + \varphi_5)}{\sin \varphi_2 \sin(\varphi_{12} + \varphi_4 + \varphi_5) \sin(\varphi_{12} + \varphi_5) \sin \varphi_{12}}. \quad (5.28)$$

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

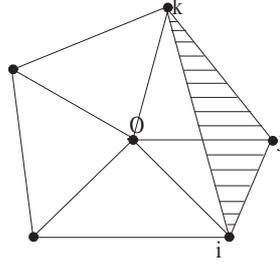
$$|\tilde{a}_{130}| = \frac{1}{2} \frac{\cos(\varphi_{12} - \frac{\pi}{8}) \cos \frac{\pi}{8} \cos \frac{\pi}{4}}{\sin \frac{\pi}{8} \sin(\varphi_{12} + \frac{\pi}{4}) \sin(\varphi_{12} + \frac{\pi}{8}) \sin \varphi_{12}}. \quad (5.29)$$

Besides, by the definition of ω_0 , it is easy to have $\varphi_{12} \in [\frac{3}{8}\pi, \frac{\pi}{2}]$.

By operation, it is not difficult to prove that $|\tilde{a}_{130}|$ in (5.29) is monotone decreasing with respect to φ_{12} on $[\frac{3}{8}\pi, \frac{\pi}{2}]$, hence $|\tilde{a}_{130}|$ attains the maximum at $\varphi_{12} = \frac{3}{8}\pi$, 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 \vec{l}_1 . \square


 Fig. 5.1. Point O and its five neighbors.

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 $\langle i j k \rangle$.

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

$$\begin{aligned} \langle i j k \rangle_0 &= \langle i j \rangle_0 + \langle j k \rangle_0 - \langle i k \rangle_0 \\ &= \frac{1}{2} (\sin \theta_i + \sin \theta_j - \sin(\theta_i + \theta_j)) \\ &= 2 \sin \frac{\theta_i}{2} \sin \frac{\theta_j}{2} \sin \frac{\theta_i + \theta_j}{2}, \end{aligned}$$

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

$$\langle i j k \rangle_0 = \eta(\theta_i, \theta_j)(\langle i j \rangle_0 + \langle j k \rangle_0), \quad (5.30)$$

where

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

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.

$$|\langle i j k \rangle| \leq \eta(\theta_i, \theta_j)(\langle i j \rangle + \langle j k \rangle). \quad (5.31)$$

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 ω_0

$$|\tilde{a}_{ij}| \leq \begin{cases} \frac{1}{2} \frac{h_M^2}{h_i h_m}, & j = i, \\ \frac{\sqrt{2}}{2} \frac{h_M^2}{h_j h_m}, & j \neq i, \end{cases} \quad (5.32)$$

where h_M is as defined in (3.10), and $h_m = \min_{\forall l \in I} h_l$.

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

$$a_{11} = \langle 2\ 3 \rangle \langle 4\ 1 \rangle \langle 3\ 5 \rangle \langle 2\ 4\ 5 \rangle + \langle 1\ 3 \rangle \langle 2\ 4 \rangle \langle 4\ 5 \rangle \langle 2\ 3\ 5 \rangle, \quad (5.33)$$

which leads to

$$\begin{aligned} |a_{11}| &\leq h_1 h_2 h_3^2 h_4 h_5 \langle 2\ 3 \rangle_0 \langle 4\ 1 \rangle_0 \langle 3\ 5 \rangle_0 h_2 h_4 h_5 \left(\frac{\langle 2\ 4 \rangle_0}{h_5} + \frac{\langle 4\ 5 \rangle_0}{h_2} + \frac{\langle 5\ 2 \rangle_0}{h_4} \right) \\ &\quad + h_1 h_2 h_3 h_4^2 h_5 \langle 1\ 3 \rangle_0 \langle 2\ 4 \rangle_0 \langle 4\ 5 \rangle_0 h_2 h_3 h_5 \left(\frac{\langle 2\ 3 \rangle_0}{h_5} + \frac{\langle 3\ 5 \rangle_0}{h_2} + \frac{\langle 5\ 2 \rangle_0}{h_3} \right) \\ &\leq \bar{h}^{10} h_1^{-1} h_m^{-1} (\langle 2\ 3 \rangle_0 \langle 4\ 1 \rangle_0 \langle 3\ 5 \rangle_0 \langle 2\ 4\ 5 \rangle_0 + \langle 1\ 3 \rangle_0 \langle 2\ 4 \rangle_0 \langle 4\ 5 \rangle_0 \langle 2\ 3\ 5 \rangle_0) \\ &= \bar{h}^{10} h_1^{-1} h_m^{-1} |a_{110}|. \end{aligned} \quad (5.34)$$

Moreover by (5.1), (5.2), and the estimation of m_t in Theorem 4.2, it is easy to prove

$$|\tilde{a}_{11}| = \frac{1}{m_t} |a_{11}| \leq \frac{h_M^2}{h_1 h_m} |\tilde{a}_{110}|. \quad (5.35)$$

Hence by Theorem 5.3, one derives

$$|\tilde{a}_{11}| \leq \frac{1}{2} \frac{h_M^2}{h_1 h_m}. \quad (5.36)$$

(2) By the Hypothesis III, there is

$$\begin{aligned} |a_{12}| &= |\langle 1\ 3 \rangle \langle 1\ 4 \rangle \langle 1\ 5 \rangle \langle 3\ 4\ 5 \rangle| \\ &\leq h_1^3 h_3 h_4 h_5 |\langle 1\ 3 \rangle_0 \langle 1\ 4 \rangle_0 \langle 1\ 5 \rangle_0| \cdot \eta(\theta_3, \theta_4) (\langle 3\ 4 \rangle + \langle 4\ 5 \rangle). \end{aligned} \quad (5.37)$$

Further noticing (5.30), one easily proves

$$|a_{12}| \leq h_1^3 h_3^2 h_4^2 h_5^2 h_m^{-1} |a_{120}|, \quad (5.38)$$

which consequently results in

$$|\tilde{a}_{12}| = \frac{1}{m_t} \frac{h_2}{h_1} |a_{12}| \leq \frac{\sqrt{2}}{2} \frac{h_M^2}{h_2 h_m}. \quad (5.39)$$

(3) By noting that

$$\begin{aligned} |a_{13}| &= |\langle 1\ 2 \rangle \langle 1\ 4 \rangle \langle 1\ 5 \rangle \langle 2\ 4\ 5 \rangle| \\ &= h_1^3 h_2^2 h_4^2 h_5^2 \left| \langle 1\ 2 \rangle_0 \langle 1\ 4 \rangle_0 \langle 1\ 5 \rangle_0 \left(\frac{\langle 2\ 4 \rangle_0}{h_5} + \frac{\langle 4\ 5 \rangle_0}{h_2} + \frac{\langle 5\ 2 \rangle_0}{h_4} \right) \right| \\ &\leq h_1^3 h_2^2 h_4^2 h_5^2 h_m^{-1} |a_{130}|, \end{aligned} \quad (5.40)$$

one easily gets

$$|\tilde{a}_{13}| = \frac{1}{m_t} \frac{h_3}{h_1} |a_{13}| \leq \frac{\sqrt{2}}{2} \frac{h_M^2}{h_3 h_m}. \quad (5.41)$$

(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.

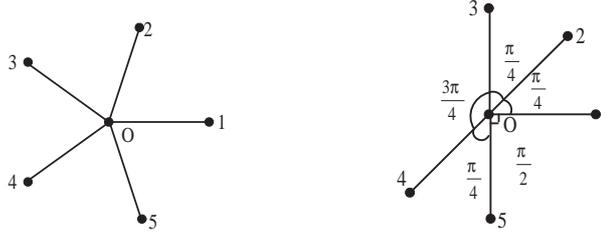


Fig. 6.1. Special distribution I (left) and II (right).

(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 6.1: Coefficients of difference quotients on the distribution I.

j	1	2	3	4	5	$\sum_{j=1}^5$
\tilde{a}_{1j}	$\frac{2}{5}$ (= 0.4)	$\frac{\sqrt{5}-1}{10}$ (≈ 0.1236)	$-\frac{\sqrt{5}+1}{10}$ (≈ -0.3236)	$-\frac{\sqrt{5}+1}{10}$ (≈ -0.3236)	$\frac{\sqrt{5}-1}{10}$ (≈ 0.1236)	0

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 $\delta_{\sigma}^{(1)}u_i$ should be $\tilde{a}_{ii}\delta u_i$.
- 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

Table 6.2: Coefficients of difference quotients on the distribution II.

j	1	2	3	4	5	$\sum_{j=1}^5$
\tilde{a}_{1j}	0	$\frac{\sqrt{2}}{2}$	$-\frac{1}{2}$	$-\frac{\sqrt{2}}{2}$	$\frac{1}{2}$	0

- 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 \vec{l}_1 , the more it contributes. Limited by the conditions of angles, the minimum of θ_1 has to be $\pi/4$.
- In consideration of the contribution to the positive direction of \vec{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 θ_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).

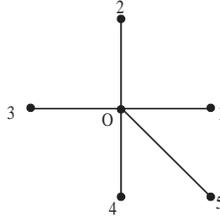


Fig. 6.2. Special distribution III.

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.

j	1	2	3	4	5
\tilde{a}_{1j}	1/2	0	-1/2	0	0
\tilde{a}_{5j}	$2^{-3/2}$ (≈ 0.3536)	$-2^{-3/2}$ (≈ -0.3536)	$-2^{-3/2}$ (≈ -0.3536)	$2^{-3/2}$ (≈ 0.3536)	0

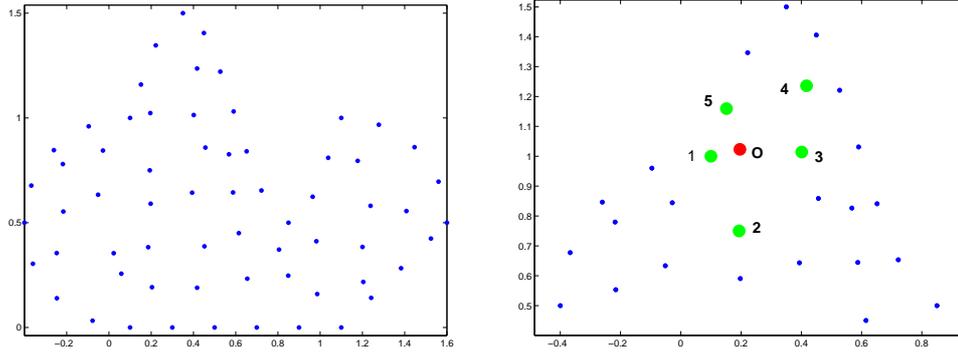


Fig. 6.3. Scattered point distribution (left) and local magnification (right).

Obviously, this is a general case of uneven steplength. Table 6.4 displays \tilde{a}_{1j} and \tilde{a}_{5j} , $j = 1, \dots, 5$ 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.

j	1	2	3	4	5
\tilde{a}_{1j}	0.6784	3.3567e-2	-0.2280	-0.1072	2.3682e-2
\tilde{a}_{5j}	6.8231e-2	-0.3374	-0.1761	0.1382	0.5526

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.

Acknowledgments. This project was supported by the National Natural Science Foundation of China (11671049), the Foundation of LCP, and the CAEP Foundation (CX2019026).

References

- [1] G.E. Forsythe and W.R. Wasow, *Finite Difference Methods for Partial Differential Equations*, Wiley, New York, 1960.
- [2] R.D. Richtmyer and K.W. Morton, *Difference Methods for Initial Value Problems*, Wiley-Interscience, New York, 1967.
- [3] A.A. Samarskii, *The Theory of Finite Difference Schemes*, (In Russian), Nauka Publishers, Moscow, 1977.
- [4] Y.L. Zhou, *Applications of Discrete Functional Analysis to the Finite Difference Method*, Intern. Acad. Publishers, 1990.
- [5] R.H. MacNeal, An asymmetrical finite difference network, *Appl. Math.*, **11** (1953), 295–310.
- [6] W.H. Frey, Flexible finite-difference stencils from isoparametric finite elements, *Int. J. Numer. Meth. Eng.*, **12** (1978), 229–235.
- [7] P.S. Jenson, Finite difference technique for variable grids, *Comput. Struct.*, **2** (1972), 17–29.
- [8] N. Perrone and R. Kao, A general finite difference method for arbitrary meshes, *Comput. Struct.*, **5** (1975), 45–58.
- [9] T. Liszka and J. Orkisz, The finite difference method at arbitrary irregular grids and its application in applied mechanics, *Comput. Struct.*, **11** (1980), 83–95.
- [10] K.C. Chung, A generalized finite difference method for heat transfer problems of irregular geometries, *Numer. Heat Transfer, Part A: Applications*, **4** (1981), 345–357.
- [11] J.J. Benito, F. Ureña and L. Gavete, Influence of several factors in the generalized finite difference method, *Appl. Math. Model.*, **25** (2001), 1039–1053.
- [12] J.J. Benito, F. Ureña and L. Gavete, Solving parabolic and hyperbolic equations by the generalized finite difference method, *J. Comp. Appl. Math.*, **209**:2 (2007), 208–233.
- [13] E. Oñate, S. Idelsohn, O.C. Zienkiewicz and R.L. Taylor, A finite point method in computing mechanics application to convective transport and fluid flow, *Internat. J. Numer. Methods Engrg.*, **39** (1996), 3839–3866.
- [14] D. Sridar and N. Balakrishnan, An upwind finite difference scheme for meshless solvers, *J. Comput. Phys.*, **189** (2003), 1–29.
- [15] L. Gavete, F. Ureña, J.J. Benito, A. García, M. Ureña and E. Salet, Solving second order non-linear elliptic partial differential equations using generalized finite difference method, *J. Comput. Appl. Math.*, **318** (2017), 378–387.

- [16] Y. Gu, J. Lei, C.M. Fan and X.Q. He, The generalized finite difference method for an inverse time-dependent source problem associated with three-dimensional heat equation, *Eng. Anal. Bound Elem.*, **91** (2018), 73–81.
- [17] G.M.J. Payre, Influence graphs and the generalized finite difference method, *Comput. Methods Appl. Mech. Engrg.*, **196** (2007), 1933–1945.
- [18] B. Seibold, Minimal positive stencils in meshfree finite difference methods for the Poisson equation, *Comput. Methods Appl. Mech. Engrg.*, **198**:3–4 (2008), 592–601.
- [19] A. Kamyabi, V. Kermani and M. Kamyabi, Improvements to the meshless generalized finite difference method, *Eng. Anal. Bound Elem.*, **99** (2019), 233–243.
- [20] G. Wright and B. Fornberg, Scattered node compact finite difference-type formulas generated from radial basis functions, *J. Comput. Phys.*, **212**:1 (2006), 99–123.
- [21] E. Larsson, E. Lehto, A. Heryudono and B. Fornberg, Stable computation of differentiation matrices and scattered node stencils based on Gaussian radial basis functions, *SIAM J. Sci. Comput.*, **35**:4 (2013), 2096–2119.
- [22] B. Fornberg and N. Flyer, Solving PDEs with radial basis functions, *Acta Numer.*, **24** (2015), 215–258.
- [23] D.T. Oanh, O. Davylov and H.X. Phu, Adaptive RBF-FD method for elliptic problems with point singularities in 2D, *Appl. Math. Comput.*, **313** (2017), 474–497.
- [24] V. Bayona, B. Fornberg, N. Flyer and G.A. Barnett, on the role of polynomials in RBF-FD approximations: II. Numerical solution of elliptic PDEs, *J. Comput. Phys.*, **332** (2017), 257–273.
- [25] D.W. Kim and W.K. Liu, Maximum principle and convergence analysis for the meshfree point collocation method, *SIAM J. Numer. Anal.*, **44** (2006), 515–539.
- [26] G. Yoon and C. Min, Analyses on the finite difference method by Gibou et al. for Poisson equation, *J. Comput. Phys.*, **288** (2015), 184–194.
- [27] L.J. Shen, G.X. Lv and Z.J. Shen, A finite point method based on directional differences, *SIAM J. Numer. Anal.*, **47** (2009), 2224–2242.
- [28] G.X. Lv, S.K. Sun and L.J. Shen, Discrete maximum principle and convergence of Poisson problem for the finite point method, *J. Comp. Math.*, **35**:3 (2017), 245–264.
- [29] G.X. Lv and L.J. Shen, The finite point method for solving the 2-D 3-T diffusion equations, *Commun. Comp. Phys.*, **26**:2 (2019), 413–433.