HIGHER DIMENSIONAL NUMERICAL QUADRATURE

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ABSTRACT

This thesis contains a study of higher dimensional numerical quadrature, especially two dimensional Gregory quadrature.

In Chapter I we discuss the problem of approximation and integration, the reasons why numerical quadrature has been developed and review some important numerical quadrature formulas.

Chapter II contains some fundamental concepts, including some useful notations on higher dimensions, barycentric coordinates, homogeneous representation of polynomials, the Newton-Cotes polynomials, and integration and differentiation in barycentric coordinates.

In Chapter III we present a generalization of Newton-Cotes quadrature to higher dimensions over k-simplices. Our generalization is based on the properties of the Newton-Cotes lattice and the Newton-Cotes polynomials. A rather complete list (up to 13th order) of two dimensional Newton-Cotes quadrature formulas over triangles as well as some three dimensional Newton-Cotes quadrature formulas over tetrahedra are given.

In Chapter IV we apply the concept of the hexagonal k-partition of unity, developed by Professor P.O. Frederickson, to construct some two dimensional Gregory quadrature formulas. The general derivation of an mth order Gregory quadrature formula over a plane region with piece-wise linear boundary is given. Particularly, the Gregory quadrature formulas of the first three

orders over some special regions are computed.

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CHAPTER I

INTRODUCTION TO NUMERICAL QUADRATURE

1.1 APPROXIMATION AND INTEGRATION

Let Ω be a compact set in $\mathbb{R}^n$, and let $G[\Omega]$ be a linear space of real continuous functions on Ω. It may be $C[\Omega]$, the space of all real continuous functions on Ω, but usually is not. Denote by $I : G[\Omega] \to \mathbb{R}$ the linear operator

$$I(f) = \int_\Omega f(X)dX. \qquad (1.1.1)$$

Even in one dimension, where some elementary functions have elementary anti-derivative, it is necessary to consider approximations to the operator I because not all functions can be integrated in closed form. Even when integration in closed form is possible, it may not be advantageous, for one must use tables of special functions in the end, and these are only approximate. Another reason we develop the rules for approximate integration is to allow us to integrate a function given only at a finite number of points. Additionally, in recent years it has become possible to force a computer to perform a lot of calculations in a rather short time, and approximate integration may be both faster and more accurate than integration using paper and pencil and tables of special functions.

We will consider numerical quadrature (which we sometimes call numerical integration, or mechanical quadrature or approximate integration) of the form

$$I_k(f) = \sum_i^k a_i f(X_i), \qquad (1.1.2)$$

with $$I(f) = I_k(f) + R(f). \qquad (1.1.3)$$

Here I_k is also a linear operator on $G[\Omega]$. We will say that I_k is a numerical quadrature of *order* $k+1$ if $R(f) = 0$ for all $f \in \mathcal{P}^k$, the set of all polynomials in X, of degree less than or equal to k.

The basic problem of numerical quadrature is concerned with choosing the coefficients a_i (and the lattice points X_i), so that $I_k(f)$ will be a close approximation to $I(f)$ for a large class (a subclass of $G[\Omega]$) of functions f. "How to choose these coefficients a_i?" is a question naturally asked. We will find some answers in the next two sections.

If we have several formulas (several sets of a_i), then we always wish to know how accurate each formula is, which one is better, and how to compare them. Thus, a measure of errors is necessary. Usually, we measure the errors in terms of norms or seminorms. A *norm* $||\cdot||$ on a linear space L is a functional such that, for all $f \in L$, $g \in L$ and $\alpha \in \mathbb{R}$,

$$||f|| \geq 0, \qquad (1.1.4)$$

$$||f|| = 0, \text{ only if } f = 0, \qquad (1.1.5)$$

$$||\alpha f|| = |\alpha| \; ||f|| , \tag{1.1.6}$$

and

$$||f+g|| \leq ||f|| + ||g|| . \tag{1.1.7}$$

If (1.1.5) is not satisfied, then $||\cdot||$ is called a *seminorm*, and we will always denote it by $|\cdot|$.

Given any $f \varepsilon G[\Omega]$ and $1 \leq p < \infty$, define

$$||f||_p = \left(\int_\Omega |f|^p\right)^{1/p}$$

and

$$|f|_{m,p} = \left(\int_\Omega \sum_{|i|=m} |D^i f|^p\right)^{1/p}; \tag{1.1.8}$$

and for $p = \infty$, we define

$$||f||_p = \sup_{x\varepsilon\Omega} |f(x)|,$$

and

$$|f|_{m,p} = \sup_{x\varepsilon\Omega} \sum_{|i|=m} |D^i f| . \tag{1.1.9}$$

Then it is clear $||\cdot||_p$ is a norm on $G[\Omega]$, while $|\cdot|_{m,p}$ is a seminorm, and we refer to $|\cdot|_{m,p}$ as the m<u>th</u> *order* L_p-*Sobolev seminorm*. In particular, if $\Omega \subseteq \mathbb{R}$, then for $p = \infty$, $|f|_{m,p} = \left(\int_\Omega^p |f^{(m)}(x)|^p\right)^{1/p}$ and $|f|_{m,\infty} = \sup_{x\varepsilon\Omega} \left|f^{(m)}(x)\right|$, for $p \neq \infty$.

1.2 ONE DIMENSIONAL NUMERICAL QUADRATURE

Many types of one dimensional numerical quadrature are given in the standard text books on numerical analysis, such as those by Conte and deBoor [3], Davis and Rabinowitz [5], Fröberg [7], Hildebrand [11], Isaacson and Keller [15], Ralston [21] and others. In this section, we will only discuss three types of formulas: Gregory type, Newton-Cotes type and Gaussian type. Other types of formulas, the reader can find from the above references or other books or papers. In particular, we will not discuss minimum norm quadrature as discussed by Sard [22] and others.

(I) *Newton-Cotes formulas (closed type)*

There are many derivations of this type of formula. We only show two of them, algebraic and interpolatory. Let f be a function defined on the interval $[a,b]$. For simplicity, we assume $[a,b] = [0,1]$. The formula over an arbitrary interval $[c,d]$ can be obtained by multiplying a constant $1/(d-c)$ times the coefficients a_i (for $[a,b]$). Let $a = x_0 < x_1 < \ldots < x_k = b$ and $x_i - x_{i-1} = \frac{b-a}{k}$, $i = 1,2,\ldots,k$. Let

$$I(f) = \int_a^b f(x)dx, \tag{1.2.1}$$

$$NC_k(f) = \sum_{i=0}^{k} a_i f(x_i), \tag{1.2.2}$$

and

$$I(f) = NC_k(f) + R(f). \tag{1.2.3}$$

(A) *Algebraic Derivation*

Let $f = x^j$. Then (1.2.2) becomes

$$\sum_{i=0}^{k} a_i x_i^{\,j} = \frac{1}{j+1}, \qquad (1.2.4)$$

for $j = 0,1,\ldots,k$.

This linear system has a unique solution if the coefficient matrix $(x_i^{\,j})$ is non-singular. Let $M = (x_i^{\,j})$, then the determinant of M is called a *Vandermonde determinant* (see [15]) and it can be easily evaluated to yield,

$$\det M = \prod_{j=0}^{k-1} \left(\prod_{i=j+1}^{k} (x_i - x_j) \right).$$

This shows M is non-singular.

(B) *Interpolatory Derivation*

Let $P_i^k(x) = \prod_{\substack{j \neq i \\ j=0}}^{k} \frac{x - x_j}{x_i - x_j}$, and we call this the *k-degree Newton-Cotes polynomial*. (Sometimes, we also call this the *Lagrangian interpolation polynomial*.) We note that $I(P_i^k(x)) = NC_k(P_i^k(x)) = \sum_{j=0}^{k} a_j P_i^k(x_j) = \sum_{j=0}^{k} a_j \delta_j^i = a_i$. (This is the way we compute the coefficients, a_i.) For example, when $k = 1$, this is the *trapezoidal* rule with $a_0 = a_1 = \frac{1}{2}$, and when $k = 2$, this is the *Simpson's* formula with $a_0 = a_2 = \frac{1}{6}$ and $a_1 = \frac{4}{6}$. Denote by T and S the trapezoidal rule and the Simpson's formula respectively. The errors of these are bounded by

$$|R_T(f)| \le \frac{h}{4}(b-a)\ |f|_{1,\infty},$$

$$\text{or} \quad \le \frac{h^2}{12}(b-a)\ |f|_{2,\infty}; \tag{1.2.5}$$

$$\text{and } |R_s(f)| \le \frac{h^3}{72}(b-a)\ |f|_{3,\infty},$$

$$\text{or} \quad \le \frac{h^4}{180}(b-a)\ |f|_{4,\infty}, \tag{1.2.6}$$

$$\text{or} \quad \le \frac{h^4}{72}(b-a)\ |f|_{4,1}.$$

Note that these formulas (1.2.5) and (1.2.6) can be obtained by computing the Peano kernal and applying the Peano Theorem. See Peano [17], Sard [22], and Davis and Rabinowitz [5, pp. 108-112].

(II) *Newton-Cotes formula (open type)*

In the derivation of the Newton-Cotes formula, we consider the two end points a and b, and the formula is referred to as the *Newton-Cotes formula* of *closed type*. An *open type formula* is obtained when these two end points are not used. (Sometimes, we also call this the *Steffensen's* formula. See Davis and Rabinowitz [5, p. 32].) Formulas of open type are used for the integration of ordinary differential equations. Let $ONC_{k-2}(f) = \sum_{i=1}^{k-1} a_i f(x_i)$. Then, when

$k = 3, \quad a_1 = a_2 = \frac{3}{2}$ and $|R(f)| \le \frac{3}{4} h^2(b-a) \, |f|_{2,\infty}$,

$k = 4, \quad a_1 = a_3 = \frac{8}{3}$ and $a_2 = -\frac{4}{3}$ and $|R(f)| \le \frac{14}{45} h^4(b-a)$
$|f|_{4,\infty}$,

$k = 5, \quad a_1 = a_4 = \frac{55}{24}$ and $a_3 = a_2 = \frac{5}{24}$ and $|R(f)| \le \frac{95}{144} h^4$
$(b-a) \, |f|_{4,\infty}$.

(See Davis and Rabinowitz [5, p. 32].)

(III) *Gregory type formula*

This type formula can be computed by several different methods. We may refer to the recent paper of Phillips [19] and the standard texts such as those by Fröberg [7], Hildebrand [11], Ralston [21] and others. Frederickson in [6] defines a k-partition of unity and derives the formula using this concept.

Denote $f(x_j)$ by f_j. Then let

$$\int_a^b f(x) = \sum_{j=0}^{m} a_j f_j + R(f),$$

$$= \sum_{i=0}^{k-1} b_i (f_i + f_{m-i}) + \sum_{j=1}^{m-1} f_j + R(f). \qquad (1.2.7)$$

We may write G_k for the set of coefficients $\{a_i\} =$ $\{b_0, 1+b_1, \ldots, 1+b_{k-1}, 1, 1, \ldots, 1, 1+b_{m-k+1}, \ldots, 1+b_{m-1}, b_m\}$, where

$b_i = b_{m-i}$, $i = 0,1,\ldots,k-1$. Note that the set G_k represents the kth order Gregory formula. For example, when $k = 1,2,3$, they are

$$G_1 = \left\{\frac{1}{2}, 1, \ldots, 1, \frac{1}{2}\right\},$$

$$G_2 = \left\{\frac{5}{12}, \frac{13}{12}, 1, \ldots, 1, \frac{13}{12}, \frac{5}{12}\right\},$$

and
$$G_3 = \left\{\frac{3}{8}, \frac{7}{6}, \frac{23}{24}, 1, \ldots, 1, \frac{23}{24}, \frac{7}{6}, \frac{3}{8}\right\}$$

respectively.

Note that G_1 is the trapezoidal rule; and G_3 is exact on $\mathcal{P}^3(x)$. Moreover, the error of $f \in C^3[a,b]$ is bounded by

$$|R_{G3}(f)| \leq \frac{h^3}{192}\left(1 + \frac{20}{3}h\right)\|f\|_{3,\infty}. \qquad (1.2.8)$$

We observe that G_3 is nearly three times better than S on $C^3[a,b]$ by (1.2.6) and (1.2.8), for h small. It is not as good as S on $C^4[a,b]$, as evaluation of the Peano error estimate shows.

(IV) *Gaussian type formula*

This is a rather different type formula from the above two. The basic idea is to find a formula including the coefficients a_i and the lattice points x_i (for a given number of lattice points), which is optimal; that is to find an integer m and a formula such that m is the largest integer for which there exists a formula that is exact on $\mathcal{P}^m(x)$. There are many different derivations. For example, the orthogonal polynomial derivation, the algebraic derivation, and the continued fraction derivation.

Let $[a,b] = [-1,1]$, and let $x_i \in [-1,1]$, $i = 0,1,\ldots,k-1$, be distinct. Let $F(x) = \prod_{j=0}^{k-1} (x-x_j)$, then for any $f(x) \in \mathcal{P}^m(x)$, we have

$$f(x) = \sum_{i=0}^{k-1} f(x_i)P_{i(x)}^{k-1} + \sum_{j=0}^{m-k} \alpha_j x^i F(x), \tag{1.2.9}$$

since $\left(f(x) - \sum_{i=0}^{k-1} f(x_i)P_{i(x)}^{k-1}\right)/F(x)$ is a polynomial of degree at most $m-k$ and hence of the form $\sum_{j=0}^{m-k} \alpha_j x^j$. See Fröberg [7, p. 182]. It follows that

$$a_i = \int_{-1}^{1} P_{i(x)}^{k-1} dx, \tag{1.2.10}$$

$$\text{and} \quad R(f) = \sum_{j=0}^{m-k} \alpha_j \int_{-1}^{1} x^j F(x)dx, \tag{1.2.11}$$

by (1.1.2) and (1.1.3) when $n = 1$. We may choose x_i in such a way that $R(f) = 0$ if $f \in \mathcal{P}^{2k-1}(x)$. That is

$$\int_{-1}^{1} x^j F(x)dx = 0, \quad \text{if} \quad j < k. \tag{1.2.12}$$

But this is true if and only if $F(x) = \lambda P_k(x)$ for some $\lambda \neq 0$, where $P_k(x)$ is the Legendre polynomial of degree k. Thus the points x_i are the roots of P_k. (See Fröberg [7, pp. 185-186].)

1.3 HIGHER DIMENSIONAL NUMERICAL QUADRATURE

As we mentioned in section 1.2, we can find easily most of the one dimensional numerical quadrature formulas in the books on numerical analysis, but only a few of these books contain anything on higher dimensional numerical quadrature. The only book on higher dimensional numerical quadrature is by Stroud [25], and we refer to it frequently. Stroud also provides a rather complete bibliography at the end of his book. From the bibliography in [25] we conclude that before 1953, only about 40 papers had appeared. By 1973, just two decades later, about 400 papers had appeared. Thus, most of the work on this subject has been done in the past two decades. The reasons for delay of this subject may be due to the large variety of regions for integration, and the large size of computations. Since high speed computers have been developed, this last difficulty is no longer so important.

One type of formula in higher dimensions can be constructed easily by taking combinations or products of formulas for regions of lower dimensions. But it is not possible to construct the product formulas for any arbitrary region. We only can construct these formulas for some special regions; for instance, the n-cube, the n-sphere, and so forth. For more details, the reader should consult [25, Chapter 2]. In the following, we will discuss some non-product methods for constructing formulas, including Newton-Cotes formulas, Gregory formulas and Gaussian formulas.

(I) *Newton-Cotes type formula*

One type of region in $\mathbb{R}^k$ for k-dimensional Newton-Cotes quadrature is the k-simplex. We will define the k-simplex and the k-dimensional Newton-Cotes quadrature on the k-simplex in Chapter 2 and Chapter 3 respectively. Our generalization of Newton-Cotes quadrature to higher dimensions is based on the Newton-Cotes lattice and the Newton-Cotes polynomials, which we will define in Chapter 2. The coefficients of the quadrature are represented in terms of Stirling numbers. For more details, see Chapter 3. Sylvester [29] and Nicolaides [14] also worked on this type of formula; Sylvester gave a derivation similar to ours, but on a more complicated path, and he also gave some examples for Newton-Cotes quadrature of closed type as well as open type in two and three dimensions. We will review and discuss [29] in Chapter 3.

(II) *Gregory type formula*

We will define a hexagonal k-partition of unity ϕ on $\mathbb{R}^2$ and derive the m<u>th</u> order Gregory type quadrature by using this ϕ, in Chapter 4. The regions we will consider are the plane regions with piece-wise linear boundary. We will discuss these in detail in Chapter 4. Sobolev and some other Russian authors have developed the theory of *formulas with a regular boundary layer* in recent years. The formulas they construct agree in some cases with ours.

(III) *Gaussian type formula*

Radon was the first person to construct integration formulas in higher dimensions by using the theory of orthogonal polynomials. Recently, some other authors, like Stroud, Davis, Peirce, Tyler, Hammer etc. also had obtained some additional results about integration formulas and orthogonal polynomials.

In [20], Radon constructs seven point fifth order formulas on a plane region by finding three linearly independent third order orthogonal polynomials which have seven common zeros. If these zeros are distinct, then they are the lattice points for the formulas. For example, when he takes the unit square $\{(x,y) : -1 \le x,y \le 1\}$, the lattice points he finds are $(0,0)$, $(0,\pm t)$ and $(\pm r,\pm s)$, where $r = \sqrt{\frac{3}{5}}$, $s = \sqrt{\frac{1}{3}}$ and $t = \sqrt{\frac{14}{15}}$, with coefficients $\frac{8}{7}$, $\frac{20}{63}$, $\frac{5}{9}$ respectively. Note that these lattice points are the six vertices of a regular hexagon of side $\sqrt{\frac{14}{15}}$ with center $(0,0)$.

In [30], Tyler also computes some formulas of this type, for example, he has an eight point fifth order formula on the rectangle with (vertices $(\pm a,\pm b)$ and) $\{x_i\} = \left\{\left(\pm \frac{\sqrt{7}}{3} a, \pm \frac{\sqrt{7}}{3} b\right), \left(\pm\sqrt{\frac{7}{15}}\, a, 0\right), \left(0, \pm\sqrt{\frac{7}{15}}\, b\right)\right\}$ and $\{a_i\} = \frac{1}{4ab} \cdot \left\{\frac{9}{49}, \frac{40}{49}, \frac{40}{49}\right\}$.

Stroud [26] constructs the second order formulas with $n+1$ points for some regions in $\mathbb{R}^n$. For example if the plane region is the unit square, then the lattice $\{x_i\} = \left\{\left(\sqrt{\frac{2}{3}}, 0\right), \left(-\sqrt{\frac{1}{6}}, \sqrt{\frac{1}{2}}\right), \left(-\sqrt{\frac{1}{6}}, -\sqrt{\frac{1}{2}}\right)\right\}$ with coefficients $\left\{\frac{4}{3}, \frac{4}{3}, \frac{4}{3}\right\}$; or $\{x_i\} = \left\{(1,1), \left(\frac{1}{3}, \frac{-2}{3}\right), \left(\frac{-5}{9}, \frac{2}{9}\right)\right\}$ with coefficients $\left\{\frac{4}{7}, \frac{3}{2}, \frac{27}{14}\right\}$; or $\{x_i\} = \left\{\left(1, \frac{4}{3}\right), \left(-\frac{1}{3}, 0\right), (1,-1)\right\}$ with coefficients $\left\{\frac{3}{7}, 3, \frac{4}{7}\right\}$. He also constructs the third order formulas with $2n$ points for some regions in $\mathbb{R}^n$. In [27], Stroud gives some fifth order formulas with $n^2 + n + 2$ points for some regions in $\mathbb{R}^n$. In [28], he gives a rather complete theory of Gaussian type formula.

CHAPTER II

BASIC CONCEPTS

2.1 PRELIMINARY NOTATIONS

Let us denote by $\mathbb{R}^{k+1}$ Euclidean (k+1) dimensional space, with elements $X = (x_0, x_1, \ldots, x_k)$. We will refer to an element $i = (i_0, i_1, \ldots, i_k) \in \mathbb{N}^{k+1} \subseteq \mathbb{R}^{k+1}$, as an index vector, where $\mathbb{N}$ denotes the set of natural numbers $\{0,1,2,\ldots\}$.

The following notations are useful:

(N1) For $X = (x_0 x_1, \ldots, x_k) \in \mathbb{R}^{k+1}$ and $i = (i_0, i_1, \ldots, i_k) \in \mathbb{N}^{k+1}$, define

$$X^i = x_0^{i_0} x_1^{i_1} \ldots x_k^{i_k} .$$

(N2) Define

$$X^{(i)} = x_0^{(i_0)} x_1^{(i_1)} \ldots x_k^{(i_k)}$$

where $X \in \mathbb{R}^{k+1}$, $i \in \mathbb{N}^{k+1}$ and $x_j^{(i_j)} = \prod_{\ell=0}^{i_j - 1} (x_j - \ell)$, $j = 0,1,2,\ldots,k$ is the i_jth *factorial polynomial* in x_j.

(N3) Define

$$S_j^{(i)} = S_{j_0}^{(i_0)} S_{j_1}^{(i_1)} \ldots S_{j_k}^{(i_k)},$$

where $i, j \in \mathbb{N}^{k+1}$ and $S_{j_\ell}^{(i_\ell)}$, $\ell = 0,1,2,\ldots,k$ is the j_ℓth *Stirling number of the first kind and order* i_ℓ.

(N4) For $\mathbf{i},\mathbf{j} \in \mathbb{N}^{k+1}$, define

$$|\mathbf{i}| = \sum_{j=0}^{k} i_j$$

and
$$\sum_{\mathbf{j}=0}^{\mathbf{i}} = \sum_{j_1=0}^{i_0} \sum_{j_1=0}^{i_1} \cdots \sum_{j_k=0}^{i_k} .$$

In the notations $\sum_{|\mathbf{i}|=n}$ and $\sum_{|\mathbf{i}|\le n}$, the summations are restricted to non-negative integers.

In particular, (N1)-(N4) are related by:

<u>Lemma 2.1.1</u> $$X^{(\mathbf{i})} = \sum_{\mathbf{j}=0}^{\mathbf{i}} S_{\mathbf{j}}^{(\mathbf{i})} X^{\mathbf{j}} \qquad (2.1.1)$$

<u>Proof</u> $$X^{(\mathbf{i})} = x_0^{(i_0)} x_1^{(i_1)} \cdots x_k^{(i_k)}$$

$$= \left(\sum_{j_0=0}^{i_0} S_{j_0}^{(i_0)} X_0^{j_0}\right)\left(\sum_{j_1=0}^{i_1} S_{j_1}^{(i_1)} X_1^{j_1}\right) \cdots \left(\sum_{j_k=0}^{i_k} S_{j_k}^{(i_k)} X_k^{j_k}\right)$$

$$= \sum_{j_0=0}^{i_0} \sum_{j_1=0}^{i_1} \cdots \sum_{j_k=0}^{i_k} S_{j_0}^{(i_0)} S_{j_1}^{(i_1)} \cdots S_{j_k}^{(i_k)} X_0^{j_0} X_1^{j_1} \cdots X_k^{j_k}$$

$$= \sum_{\mathbf{j}=0}^{\mathbf{i}} S_{\mathbf{j}}^{(\mathbf{i})} X^{\mathbf{j}} .$$

We will also use the elements $\mathbf{i} \in \mathbb{N}^{k+1}$ as subscripts, thus $\{X_{\mathbf{i}}\}$ will denote a collection of points in $\mathbb{R}^{k+1}$ as $\mathbf{i}$

ranges over a given subset of $\mathbb{N}^{k+1}$; and $\{a_i\}$ will denote a collection of scalars.

Moreover,

(N5) Define $i! = i_0!i_1!\ldots i_k!$

where $i = (i_0, i_1, \ldots, i_k) \in \mathbb{N}^{k+1}$.

(N6) For $i \in \mathbb{N}^{k+1}$, $r \in \mathbb{N}$, define the *multinomial coefficient* by

$$\binom{r}{i} = \begin{cases} \frac{r!}{i!}, & \text{if } r = |i|, \\ 0, & \text{otherwise}. \end{cases}$$

(N7) $\mathcal{P}^m(X)$ denotes the set of all polynomials of degree less than or equal to m, in $k+1$ variables $x_0, x_1, \ldots, x_k$; the space spanned by $\{X^i : |i| \leq m\}$.

2.2 BARYCENTRIC COORDINATES

In the previous section, we had defined the notations for $\mathbb{R}^{k+1}$. For elements in $\mathbb{R}^k$, they work precisely the same as those in $\mathbb{R}^{k+1}$. Denote by $\overline{X}$ the elements in $\mathbb{R}^k$, and by X the elements in $\mathbb{R}^{k+1}$. A special subset $\mathbf{A}^k = \{\boldsymbol{\alpha} = (\alpha_0, \alpha_1, \ldots, \alpha_k),$ $\alpha_0 = 1 - \sum_{i=1}^{k} \alpha_i\}$ of $\mathbb{R}^{k+1}$ will also be used in this section and the following sections.

In this section, the concept of barycentric coordinates will be treated.

Suppose that A, B and C are three non-colinear points in the plane. Every point Q in the convex hull of A, B and C

can be represented as

$$Q = \alpha A + \beta B + \gamma C, \tag{2.2.1}$$

for a unique triple of non-negative real numbers (α,β,γ) satisfying

$$\alpha+\beta+\gamma = 1. \tag{2.2.2}$$

<u>Definition 2.2.1</u> *Given three non-colinear points* A,B *and* C *in the plane, define the barycentric coordinates with respect to* A, B *and* C, *of an arbitrary point* $Q \in R^2$ *to be the unique triple* (α,β,γ) *in* A^2 *satisfying* (2.2.1).

We observe that α,β and γ are illustrated in Figure 2.2.1.

$$\alpha(A) = \beta(B) = \gamma(C) = 1, \tag{2.2.3}$$

$$\text{and} \quad \alpha(BC) = \beta(AC) = \gamma(AB) = 0. \tag{2.2.4}$$

Graphically, α,β and γ are

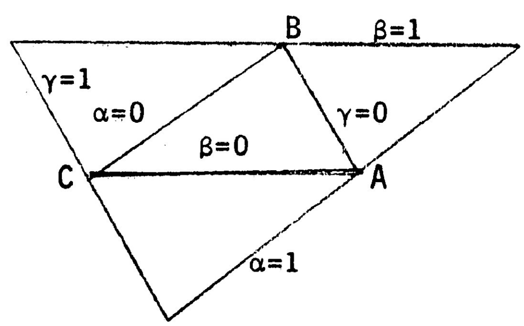


Figure 2.2.1

The barycentric coordinate system is one generalization of the usual orthogonal x-y coordinate system, since we may take $\alpha = x$, $\beta = y$ and $\gamma = 1-x-y$.

More generally, suppose $A_0, A_1, \ldots,$ and A_k are $(k+1)$ *affine independent* points in $\mathbb{R}^k$. *A k-simplex* $\mathbb{D}^k$ *with vertices* $A_0, A_1, \ldots$ *and* A_k, *is the convex hull of these* $(k+1)$ *points.* Every point $Q \in \mathbb{D}^k$ can be represented as

$$Q = \sum_{i=0}^{k} \alpha_i A_i \tag{2.2.5}$$

for a unique $(k+1)$-tuple of non-negative real numbers $(\alpha_0, \alpha_1, \ldots, \alpha_k)$ satisfying

$$\sum_{i=0}^{k} \alpha_i = 1 \tag{2.2.6}$$

Definition 2.2.2 *Given* $k+1$ *affine-independent points* $A_0, A_1, \cdots$ *and* A_k *in* $\mathbb{R}^k$, *define the barycentric coordinates with respect to* A_0, A_1 $\ldots$ *and* A_k, *for an arbitrary point* $Q \in R^k$ *to be the unique* $(k+1)$-*tuple* $(\alpha_0, \alpha_1, \ldots \alpha_k)$ *in* A^k *satisfying* (2.2.5) *and* (2.2.6).

We will develop some basic differentiation operators in barycentric coordinates in Section 2.5, and thus another treatment of barycentric coordinates is introduced. Let A_i, $i = 0,1,\ldots,k$ be $(k+1)$ affine independent points in $\mathbb{R}^k$ (and hence these $(k+1)$ points form an affine basis in $\mathbb{R}^k$). Denote by $\langle A,B \rangle$ the inner product of two vectors A and B. For $i = 0,1,\ldots,k$, define

$$A_i' = \sum_{s \neq i} \omega(i,s)(A_i - A_s) \tag{2.2.7}$$

where the coefficients $\omega(i,s)$ are chosen to satisfy the following k equations:

$$\sum_{s \neq i} \langle A_i - A_r, A_i - A_s \rangle \, \omega(i,s) = 1, \tag{2.2.8}$$

for $r = 0,1,\ldots,i-1,i+1,\ldots,k$.

The linear system (2.2.8) has a unique solution, since the k vectors $A_i - A_r$ are linearly independent, if and only if the $k+1$ vectors A_j, $j = 0,1,\ldots,k$ are affine independent. Then

$$\langle A_i', A_i - A_r \rangle = 1 - \delta_i^r. \tag{2.2.9}$$

It follows immediately that

$$\langle A_i', A_s - A_r \rangle = (\delta_i^s - \delta_i^r). \tag{2.2.10}$$

For $i = 0,1,\ldots,k$, $t \neq i$ and $\overline{X} \in \mathbb{R}^k$, define

$$\langle A_i', \overline{X} - A_t \rangle = \alpha_i. \tag{2.2.11}$$

Now, we want to show that

$$\sum_{i=0}^{k} \langle A_i', \overline{X} - A_t \rangle \, A_i = \overline{X}, \tag{2.2.12}$$

and

$$\sum_{i=0}^{k} \langle A_i', \overline{X} - A_t \rangle = 1. \tag{2.2.13}$$

It is clear that they are true for $\overline{X} = A_r$, $r = 0,1,\ldots,k$. But A_r,

$r = 0,1,\ldots,k$ are $(k+1)$ affine-independent points in $\mathbb{R}^k$, that is they form an affine basis in $\mathbb{R}^k$, and hence (2.2.12) and (2.2.13) are true for all $\bar{X} \in \mathbb{R}^k$. Therefore, (2.2.11) satisfies (2.2.5) and (2.2.6), and the $(k+1)$-tuple $(\alpha_0,\alpha_1,\ldots,\alpha_k)$ is the barycentric coordinate for the point $\bar{X}$ in $\mathbb{R}^k$. Particularly, when $k = 2$, we simply write A, B and C for A_1 A_2 and A_0, and α, β and γ for α_1, α_2 and α_0 respectively.

2.3 HOMOGENEOUS REPRESENTATION OF POLYNOMIALS

In the previous section, we had defined the barycentric coordinates $\boldsymbol{\alpha}$ in $\mathbb{R}^k$. We will show in this section that the set $HBB = \{\boldsymbol{\alpha}^{i} : i \in \mathbb{N}^{k+1}, |i| = n\}$ forms a basis for $\mathcal{P}^n(\mathbb{R}^k)$.

Lemma 2.3.1 *The set* HBB *forms a basis for* $\mathcal{P}^n(\mathbb{R}^k)$.

Proof

We observe that the set $BB = \{\bar{\boldsymbol{\alpha}}^{\bar{i}} : \bar{i} \in \mathbb{N}^k, |\bar{i}| \le n\}$, $\bar{\boldsymbol{\alpha}} = (\alpha_1, \alpha_2, \ldots, \alpha_k)$, is a basis for $\mathcal{P}^n(\mathbb{R}^k)$. Thus, to prove that HBB is a basis, it is sufficient to prove that HBB $\Leftrightarrow$ BB. For $\boldsymbol{\alpha}^{i} \in HBB$, we have

$$\begin{aligned}
\boldsymbol{\alpha}^{i} &= \bar{\boldsymbol{\alpha}}^{\bar{i}}\, \boldsymbol{\alpha}_0^{i_0} = \bar{\boldsymbol{\alpha}}^{\bar{i}}(1-|\bar{\boldsymbol{\alpha}}|)^{i_0} \\
&= \bar{\boldsymbol{\alpha}}^{\bar{i}} \sum_{\bar{j}} \binom{i_0}{j} (-\bar{\boldsymbol{\alpha}})^{\bar{j}} \\
&= \sum_{\bar{j}} (-1)^{|\bar{j}|} \binom{i_0}{j} \bar{\boldsymbol{\alpha}}^{\bar{i}+\bar{j}} \qquad (2.3.1)
\end{aligned}$$

where $i = (i_0, \bar{i})$, $j = (j_0, \bar{j})$ and $|\bar{i}+\bar{j}| = |\bar{i}|+|\bar{j}| \le n$. This implies HBB $\Rightarrow$ BB. On the other hand, if $\bar{\boldsymbol{\alpha}}^{\bar{i}} \in BB$, then

$$\begin{aligned}
\bar{\boldsymbol{\alpha}}^{\bar{i}} &= \bar{\boldsymbol{\alpha}}^{\bar{i}}\, |\boldsymbol{\alpha}|^{n-|\bar{i}|} \\
&= \bar{\boldsymbol{\alpha}}^{\bar{i}} \sum_{j} \binom{n-|\bar{i}|}{j} \boldsymbol{\alpha}^{j} \\
&= \sum_{j} \binom{n-|\bar{i}|}{j} \boldsymbol{\alpha}^{i'+j} \qquad (2.3.2)
\end{aligned}$$

where $\mathbf{i}' = (0,\bar{\mathbf{i}})$ and $|\mathbf{i}'+\mathbf{j}| = |\bar{\mathbf{i}}|+|\mathbf{j}| = n$.

Hence HBB $\Leftrightarrow$ BB. This shows HBB is a basis for $\mathcal{P}^n(\mathbb{R}^k)$.

We call the basis HBB the *homogeneous barycentric basis* for $\mathcal{P}^n(\mathbb{R}^k)$. Suppose that P is a polynomial in $\mathcal{P}^n(\mathbb{R}^k)$. Then P can be represented uniquely by

$$P = \sum_{|\mathbf{i}|=n} a_{\mathbf{i}} \boldsymbol{\alpha}^{\mathbf{i}}. \tag{2.3.3}$$

We call this representation of P the *homogeneous barycentric representation* of P.

2.4 NEWTON-COTES POLYNOMIALS AND INTERPOLATION

Let $\mathbb{D}^k$ be a k-simplex in $\mathbb{R}^k$ with vertices A_i, $i = 0,1,\ldots,k$, and let $\boldsymbol{\alpha} = (\alpha_0,\alpha_1,\ldots,\alpha_k)$ be the barycentric coordinates with respect to this k-simplex. Let $\mathbb{H}_i$, $i=0,1,\ldots,k$ be the hyperplane which contains the k vertices A_j, $j = 0,1\ldots,i-1,i+1,\ldots k$, of $\mathbb{D}^k$. Denote by $\mathbb{H}_{i,j}$, $i = 0,1,\ldots,k$, $j = 0,1,\ldots,n$, the hyperplane which is parallel to $\mathbb{H}_i$ and such that the distance from A_i to $\mathbb{H}_{i,j}$ is $\left|1 - \frac{j}{n}\right| d_i$, where d_i is the distance from A_i to $\mathbb{H}_i$. Note that $\mathbb{H}_{i,0} = \mathbb{H}_i$, $i = 0,1,\ldots,k$. Denote by $\mathbb{L}n$ the set of points at which these hyperplanes $\mathbb{H}_{i,j}$ intersect, and we call this the n^{th} *degree Newton-Cotes lattice* for the k-simplex $\mathbb{D}^k$ (while Nicolaides [14] calls this the nth *order principal lattice* for $\mathbb{D}^k$). There are $\binom{n+k}{k}$ points in $\mathbb{L}n$ (this can be shown by induction on k); and for each point $\frac{\mathbf{i}}{n} \in \mathbb{L}n$, there is a polynomial of degree n with the form

$$P^n_{\mathbf{i}}(\boldsymbol{\alpha}) = \frac{1}{\mathbf{i}!} (n\boldsymbol{\alpha})^{(\mathbf{i})}. \tag{2.4.1}$$

We call these polynomials the nth *degree Newton-Cotes polynomials* on $\mathbb{D}^k$. Note that

$$P_i^n\left(\frac{j}{n}\right) = \delta_j^i \qquad (2.4.2)$$

for all $\frac{j}{n} \varepsilon \mathbb{L}n$. Here, δ_j^i is defined by 1, if the vectors i, j, are equal and 0 otherwise.

Lemma 2.4.1 *The set of polynomials* P_i^n, $i/n \varepsilon \mathbb{L}n$ *given in* (2.4.1) *forms a basis for* $\mathcal{P}^n(\alpha)$.

Proof

We know that the number of P_i^n is $\begin{pmatrix} n+k \\ k \end{pmatrix}$. Thus, to prove this set is a basis for $\mathcal{P}^n(\alpha)$, it is sufficient to prove that these polynomials are linearly independent (since the BB of Lemma 2.3.1 has $\begin{matrix} n+k \\ k \end{matrix}$ members). Suppose that

$$\sum_{\frac{i}{n}\varepsilon\mathbb{L}n} C_i P_i^n(\alpha) = 0 \qquad (2.4.3)$$

This means (2.4.3) is identically equal to zero for all $\alpha \varepsilon \mathbb{A}^k$. In particular, take $\alpha = \frac{j}{n} \varepsilon \mathbb{L}n$, then (2.4.3) becomes

$$0+\ldots+0+C_j P_j^n\left(\frac{j}{n}\right) +0\ldots+0 = C_j = 0,$$

hence $C_i = 0$ for all $\frac{i}{n} \varepsilon \mathbb{L}n$. This proves the lemma.

We call this basis the nth *degree Newton-Cotes basis* (NCB) for $\mathcal{P}^n(\mathbb{R}^k)$. In particular, when $k = 1,2$, the NCB is simply the

Lagragian basis and the *triangular basis* for $\mathcal{P}^n(\mathbb{R})$ and $\mathcal{P}^n(\mathbb{R}^2)$ respectively.

We can now give an easy constructive proof for the interpolation theorem for which Nicolaides [14] provides a long proof.

Theorem 2.4.1 *(Interpolation Theorem) Given any function* f *on the* k*-simplex* $\mathbb{D}^k$, *there is exactly one polynomial* $P \in \mathcal{P}^n(\mathbb{R}^k)$ *which interpolates* f *on the* n<u>th</u> *degree Newton-Cotes Lattice* $\mathbb{L}n$.

Proof

Let $P(\alpha) = \sum_{\frac{i}{n}\in\mathbb{L}n} f\left(\frac{i}{n}\right) P_i^n(\alpha)$. Then it is obvious that $p(\alpha)$ is a polynomial of degree n, and $p\left(\frac{i}{n}\right) = 0+\ldots+0+f\left(\frac{i}{n}\right)p_i^n\left(\frac{i}{n}\right) +\ldots+0 = f\left(\frac{i}{n}\right)$. From Lemma 2.4.1, we know that $\{P_i^n : \frac{i}{n} \in \mathbb{L}n\}$ is a basis for $\mathcal{P}^n(\mathbb{R}^k)$, thus every polynomial in $\mathcal{P}^n(\mathbb{R}^k)$ can be represented uniquely in terms of this basis, and hence $P(\alpha)$ is unique.

2.5 INTEGRATION AND DIFFERENTIATION IN BARYCENTRIC COORDINATES

In this section, we will develop two formulas for integrating monomials $\alpha^i\beta^i\gamma^\ell$ and α^i over any arbitrary triangle and simplex respectively; and some basic differentiation operators, for example ∇f and Δf, in barycentric coordinates.

Let κ denote the area of an arbitrary triangle ABC in the plane and let α, β and γ be the barycentric coordinates with respect to triangle ABC. Let i, j, ℓ denote any three non-negative integers.

<u>Lemma 2.5.1</u> $$\iint_{ABC} \alpha^i \beta^j \gamma^\ell \, d\kappa = \frac{i!\,j!\,\ell!\,2!}{(i+j+\ell+2)!}\,\kappa \tag{2.5.1}$$

<u>Proof</u>

We begin by using an affine transformation to map the triangle ABC into the triangle (1,0), (0,1), (0,0). The Jacobian of this transformation is $\frac{1}{2\kappa}$. Thus, it is sufficient to prove the formula for this special triangle, or to prove that

$$\int_0^1 \int_0^{1-\alpha} \alpha^i \beta^j (1-\alpha-\beta)^\ell \, d\beta \, d\alpha = \frac{i!\,j!\,\ell!}{(i+j+\ell+2)!}. \tag{2.5.2}$$

Let $$h(\mu, j, \ell) = \int_0^\mu \beta^j (\mu-\beta)^\ell \, d\beta \tag{2.5.3}$$

where $\mu = 1-\alpha$.

Then, integrating by parts, we have

$$h(\mu, j, \ell) = \frac{j}{\ell+1} h(\mu, j-1, \ell+1) \tag{2.5.4}$$

Repeating this procedure $(j-1)$ times,

$$h(\mu, j, \ell) = \frac{j!\,\ell!}{(j+\ell)!} h(\mu, 0, j+\ell)$$

$$= \frac{j!\ell!}{(j+\ell)!} \int_0^{\mu} (\mu-\beta)^{j+\ell} d\beta$$

$$= \frac{j!\ell!}{(j+\ell+1)!} \mu^{j+\ell+1}. \qquad (2.5.5)$$

Now, the formula becomes,

$$\int_0^1 \int_0^{1-\alpha} \alpha^i \beta^j (1-\alpha-\beta)^{\ell} d\beta d\alpha = \frac{j!\ell!}{(j+\ell+1)!} \int_0^1 \alpha^i (1-\alpha)^{j+\ell+1} \, d\alpha$$

$$= \frac{j!\ell!}{(j+\ell+1)!} h(1,i,j+\ell+1)$$

$$= \frac{j!\ell!i!}{(i+j+\ell+2)!}, \qquad (2.5.6)$$

using formula (2.5.5) a second time. Thus, the Lemma is proved.

In particular, we have

P	1	α	α^2	$\alpha\beta$	α^3	$\alpha^2\beta$	$\alpha\beta\gamma$	α^4	$\alpha^3\beta$	$\alpha^2\beta^2$	$\alpha^2\beta\gamma$
$\frac{1}{\kappa}\iint_{ABC} P$	1	$\frac{1}{3}$	$\frac{1}{6}$	$\frac{1}{12}$	$\frac{1}{10}$	$\frac{1}{30}$	$\frac{1}{60}$	$\frac{1}{15}$	$\frac{1}{60}$	$\frac{1}{90}$	$\frac{1}{180}$

Table 2.5.1

Let $\mathbb{V}$ denote the volume of an arbitrary k-simplex $\mathbb{D}^k$ in R^k with the barycentric coordinates $\boldsymbol{\alpha} = (\alpha_0, \alpha_1, \ldots, \alpha_k)$. Let $\mathbf{i} = (i_0, i_1, i_2, \ldots, i_k)$ denote any $(k+1)$ non-negative integers.

<u>Lemma 2.5.2</u> $$\iint\cdots\int_{\mathbb{D}^k} \boldsymbol{\alpha}^{\mathbf{i}} d\mathbf{V} = \frac{\mathbf{i}!k!}{(|\mathbf{i}|+k)!} \times \mathbf{V} \qquad (2.5.7)$$

<u>Proof</u>

Use an affine transformation to map the k-simplex $\mathbb{D}^k$ into the simplex with vertices $(1,0,\ldots,0)$, $(0,1,0,\ldots,0)$, $\ldots,(0,0,\ldots,0,1)$ and $(0,0,\ldots,0)$. The Jacobian of this transformation is $\frac{1}{k!\mathbf{V}}$. Thus, it is sufficient to prove the formula for this special simplex, or to prove

$$\int_0^1 \int_0^{1-\alpha_0} \cdots \int_0^{1-\sum_{i=0}^{k-3}\alpha_i} \int_0^{1-\mu} \alpha_0^{i_0}\cdots\alpha_{k-1}^{i_{k-1}}(\mu-\alpha_{k-1})^{i_k} d\alpha_{k-1} d\alpha_{k-2}\cdots d\alpha_0$$

$$= \frac{\mathbf{i}!}{(|\mathbf{i}|+k)!}, \qquad (2.5.8)$$

where $\mu = 1 - \sum_{i=0}^{k-2} \alpha_i$.

We will prove this by induction. For $n = 2$, this is simply the previously proved Lemma. Suppose this formula has been proved for $k-1$. Then

$$\int_0^1 \int_0^{1-\alpha_0} \cdots \int^{1-\sum_{i=0}^{k-3}\alpha_i} \int_0^{1-\mu} \alpha_0^{i_0}\cdots\alpha_{k-1}^{i_{k-1}}(\mu-\alpha_{k-1})^{i_k} \; d\alpha_{k-1}\cdots d\alpha_0$$

$$= \int^1\int_0^{1-\alpha_0} \cdots \int_0^{1-\sum_{i=0}^{k-3}\alpha_i} \alpha_0^{i_0}\cdots\alpha_{k-2}^{i_{k-2}} h(\mu,i_{k-1},i_k) d\alpha_{k-2}\cdots d\alpha_0$$

$$= \frac{i_{k-1}!\,i_k!}{(i_{k-1}+i_k+1)!}\int_0^1\int_0^{1-\alpha_0}\cdots\int_0^{1-\sum_{i=0}^{k-3}\alpha_i}\alpha_0^{i_0}\cdots\alpha_{k-2}^{i_{k-2}}\left(1-\sum_{i=0}^{k-2}\alpha_i\right)^{i_{k-1}+i_k+1} d\alpha_{k-2}\cdots d\alpha_0$$

$$= \frac{i_{k-1}!\,i_k!}{(i_{k-1}+i_k+1)!}\times\frac{i_0!\cdots i_{k-2}!\,(i_{k-1}+i_k+1)!}{(i_0+\cdots+i_{k-1}+i_k+1+k-1)!}$$

$$= \frac{i!}{(|i|+k)!}\ ,$$

by formula (2.5.5) and induction hypothesis. Hence, the formula is true for all k, and the proof is completed.

Suppose Ω is an open subset of $\mathbb{R}^k$ and $f : \mathbb{R}^k \to \mathbb{R}^j$. Then the *differential* of f at X in Ω, is a linear transformation $df(X) : \mathbb{R}^k \to \mathbb{R}^j$, such that $||f(X+U)-f(X)-df(X)U|| = \theta(U)$, that is, such that for all $\varepsilon > 0$, there exists an $\delta > 0$, such that $||f(X+U)-f(X)-df(X)U|| < \varepsilon||U||$ if $||U|| < \delta$. When $j = 1$, then there is a vector ∇f in $\mathbb{R}^i$, such that $\langle df(X)U\rangle = \langle U\cdot\nabla f\rangle$, and we call ∇f the *gradient* of f. (Note that the *Laplacian* Δf of f is defined by $\Delta f = \nabla^2 f = \nabla(\nabla f)$.)

The operators (∇f and Δf) in this section will only be discussed in two dimensions. Let ABC be an arbitrary triangle on the plane. Let α, β and γ be the barycentric coordinages with respect to this triangle. Then, when $k = 2$, (2.2.10) and (2.2.11) become,

$$\langle A', A-C\rangle = \langle A', A-B\rangle = 1,$$
$$\langle A', B-C\rangle = \langle A', C-B\rangle = 0, \qquad (2.5.9)$$
$$\langle A', \overline{X}-C\rangle = \langle A', \overline{X}-B\rangle = \alpha(\overline{X}),\ \overline{X} \in \mathbb{R}^2.$$

Similarly, for B' and C'.

Since $\alpha(\overline{X})$ is linear, we have

$$\alpha(\overline{X}) = \alpha(C) + \langle\nabla\alpha, \overline{X}-C\rangle = \langle A', \overline{X}-C\rangle,$$

that is $\nabla\alpha = A'$.

Since $\nabla\alpha^i\beta^j\gamma^\ell = i\alpha^{i-1}\beta^j\gamma^\ell A' + j\alpha^i\beta^{j-1}\gamma^\ell B' + \ell\alpha^i\beta^j\gamma^{\ell-1}C'$, and $\Delta\alpha^i\beta^j\gamma^\ell = \nabla\cdot\nabla\alpha^i\beta^j\gamma^\ell$, therefore we have

$$\begin{aligned}\Delta\alpha^i\beta^j\gamma^\ell &= [i(i-1)\alpha^{i-2}\beta^j\gamma^\ell A' + ij\alpha^{i-1}\beta^{j-1}\gamma^\ell B' + i\ell\alpha^{i-1}\beta^j\gamma^{\ell-1}C']A' \\ &+ [ij\alpha^{i-1}\beta^{j-1}\gamma^\ell A' + j(j-1)\alpha^i\beta^{j-2}\gamma^\ell B' + j\ell\alpha^i\beta^{j-1}\gamma^{\ell-1}C']B' \\ &+ [i\ell\alpha^{i-1}\beta^j\gamma^{\ell-1}A' + j\ell\alpha^i\beta^{j-1}\gamma^{\ell-1}B' + \ell(\ell-1)\alpha^i\beta^j\gamma^{\ell-2}C']C' \\ &= [i(i-1)\alpha^{i-2}\beta^j\gamma^\ell\|A'\|^2 + j(j-1)\alpha^i\beta^{j-2}\gamma^\ell\|B'\|^2 + \ell(\ell-1) \\ &\qquad \alpha^i\beta^j\gamma^{\ell-2}\|C'\|^2] \\ &+ [2ij\alpha^{i-1}\beta^{j-1}\gamma^\ell A'B' + 2i\ell\alpha^{i-1}\beta^j\gamma^{\ell-1}A'C' + 2j\ell\alpha^i\beta^{j-1}\gamma^{\ell-1}B'C'].\end{aligned}$$

(2.5.11)

In particular, if ABC is the equilateral triangle of side h, then

$$\|A'\|^2 = \|B'\|^2 = \|C'\|^2 = \frac{4}{3h^2},$$
$$\text{and} \qquad A'B' = A'C' = B'C' = -\frac{2}{3h^2}. \qquad (2.5.12)$$

Thus (2.6.11) becomes

$$\Delta\alpha^i\beta^j\gamma^\ell = \frac{4}{3h^2}\,[i(i-1)\alpha^{i-2}\beta^j\gamma^\ell + j(j-1)\alpha^i\beta^{j-2}\gamma^\ell + \ell(\ell-1)\alpha^i\beta^j\gamma^{\ell-2}$$
$$-ij\alpha^{i-1}\beta^{j-1}\gamma^\ell - i\ell\alpha^{i-1}\beta^j\gamma^{\ell-1} - \ell j\alpha^i\beta^{j-1}\gamma^{\ell-1}]. \qquad (2.5.13)$$

The following table shows the values of ΔP for $P = \alpha^i\beta^j\gamma^\ell$, $0 \le i+j+\ell \le 4$ and $h = 1$, for an equilateral triangle.

P	1	α	α^2	$\alpha\beta$	α^3	$\alpha^2\beta$	$\alpha\beta\gamma$	α^4	$\alpha^3\beta$	$\alpha^2\beta^2$	$\alpha^2\beta\gamma$
ΔP	0	0	$\frac{8}{3}$	$-\frac{4}{3}$	8α	$\frac{8}{3}(\beta-\alpha)$	$-\frac{4}{3}$	$16\alpha^2$	$4(2\alpha\beta-\alpha^2)$	$\frac{8}{3}(\alpha-\beta)^2$	$\frac{4}{3}(2\beta\gamma-2\alpha\gamma-2\alpha\beta-\alpha^2)$

Table 2.5.2

CHAPTER III

HIGHER DIMENSIONAL NEWTON-COTES QUADRATURE

One dimensional Newton-Cotes quadrature as well as other one dimensional quadrature formulas have been generalized to higher dimensions. Our region in $\mathbb{R}^k$ for k-dimensional Newton-Cotes quadrature is the k-simplex. The generalization is naturally obtained by making use of the nice property of the Newton-Cotes polynomials.

3.1 DEFINITION, DERIVATION AND EXAMPLES

In this section, we will define k-dimensional Newton-Cotes quadrature over k-simplex in $\mathbb{R}^k$, and derive the Newton-Cotes coefficients by using explicit intergration formulas for the Newton-Cotes polynomials. Finally, we will give some examples.

Let $\mathbb{D}^k$ be a k-simplex in $\mathbb{R}^k$ with barycentric coordinates $\boldsymbol{\alpha} = (\alpha_0, \alpha_1, \ldots, \alpha_k)$ and let $\mathbb{L}n$ be the nth degree Newton-Cotes lattice for $\mathbb{D}^k$. For any continuous function f defined on this simplex, we let

$$I(f) = \int_{\mathbb{D}^k} f(\boldsymbol{\alpha})d\boldsymbol{\alpha}, \tag{3.1.1}$$

$$In(f) = \sum_{\frac{\mathbf{i}}{n}\in\mathbb{L}n} a_{\mathbf{i}} f_{\mathbf{i}}, \tag{3.1.2}$$

and $$I(f) = In(f)+R(f), \tag{3.1.3}$$

where $f_i = f\left(\frac{i}{n}\right)$.

The expression in (3.1.2) is called the k-*dimensional Newton-Cotes quadrature of order* n+1 with respect to $\mathbb{D}^k$, and the coefficients a_i are called the (n+1)st *order Newton-Cotes coefficients,* if $R(f) = 0$ for $f \in \mathcal{P}^n$.

Lemma 3.1.1 *The Newton-Cotes coefficient* a_i *in* (3.1.2) *has the following representation:*

$$a_i = \frac{1}{i!} \sum_{j=0}^{i} n^j \mathbf{S}_j^{(i)} \frac{j!k!}{(|j|+k)!} \times \mathbf{V} \tag{3.1.4}$$

where V *is defined in* P.25.

Proof

If f is the Newton-Cotes polynomial P_i^n (which is given in (2.4.1)) then $f_i\left(\frac{j}{n}\right) = \delta_j^i$, and hence

$$I(P_i^n) = \sum_{\frac{j}{n}\in L n} a_j \delta_j^i = a_i .$$

Using Lemma (2.5.1), formulas (2.4.1), (3.1.1) and (3.1.2), we have

$$a_i = \int_{\mathbb{D}^k} P_i^n(\alpha)\, d\alpha$$

$$= \frac{1}{i!} \int_{\mathbb{D}^k} (n\alpha)^i\, d\alpha$$

$$= \frac{1}{\mathbf{i}!} \sum_{\mathbf{j}=0}^{\mathbf{i}} S_{\mathbf{j}}^{(\mathbf{i})} \int_{D^k} \mathbf{n}^{\mathbf{j}} \boldsymbol{\alpha}^{\mathbf{j}} d\boldsymbol{\alpha}$$

$$= \frac{1}{\mathbf{i}!} \sum_{\mathbf{j}=0}^{\mathbf{i}} \mathbf{n}^{\mathbf{j}} S_{\mathbf{j}}^{(\mathbf{i})} \frac{\mathbf{j}!k!}{(|\mathbf{j}|+k)!} \times \mathbf{V}.$$

This completes the proof.

We observe that there are $\binom{n+k}{n}$ coefficients $a_{\mathbf{i}}$ in (3.1.4), for given n; and $a_{\mathbf{i}'} = a_{\mathbf{i}}$, if $\mathbf{i}'$ is a permutation of $\mathbf{i}$. In particular, when $k = 1$, $a_{\mathbf{i}}$ are simply (one dimensional) Newton-Cotes Coefficients, which give the trapezoidal rule when $n = 1$ and Simpson's rule when $n = 2$. When $k = 2$ and 3, the following two tables show these.

n	$\mathbf{i}$	$d \times a_{\mathbf{i}}$	d
1	1,0,0	1	3
2	2,0,0 1,0,0	0 1	1 3
3	3,0,0 2,1,0 1,1,1	1 3 9	30 40 20
4	4,0,0 3,1,0 2,2,0 2,1,1	0 4 -1 8	1 45 45 45
5	5,0,0 4,1,0 3,2,0 3,1,1 2,2,1	11 25 25 25 25	1008 1008 1008 126 1008

6	6,0,0	0	1
	5,1,0	3	70
	4,2,0	-9	280
	4,1,1	3	35
	3,3,0	8	105
	3,2,1	3	35
	2,2,2	-9	140
7	7,0,0	167	32400
	6,1,0	2989	259200
	5,2,0	3577	259200
	5,1,1	16121	129600
	4,3,0	539	51840
	4,2,1	-343	12960
	3,3,1	4459	25920
	3,2,2	343	25920
8	8,0,0	0	1
	7,1,0	368	14175
	6,2,0	-52	1575
	6,1,1	704	14175
	5,3,0	1136	14175
	5,2,1	832	14175
	4,4,0	-361	4725
	4,3,1	32	675
	4,2,2	-1448	14175
	3,3,2	1472	14175
9	9,0,0	173	59136
	8,1,0	783	123200
	7,2,0	351	35200
	7,1,1	5589	61600
	6,3,0	2073	985600
	6,2,1	-10449	197120
	5,4,0	8937	985600
	5,3,1	46413	246400
	5,2,2	2187	70400
	4,4,1	[illegible]	1925
	4,3,2	-30861	985600
	3,3,3	3789	17600
10	10,0,0	0	1
	9,1,0	5315	299376
	8,2,0	-685	21384
	8,1,1	9475	299376
	7,3,0	545	6237
	7,2,1	175	3564
	6,4,0	-2665	21384

	6,3,1	2675	149688
	6,2,2	-10075	74844
	5,5,0	5213	33264
	5,4,1	12995	299376
	5,3,2	23465	149688
	4,4,2	-2225	10692
	4,3,3	4225	74844
11	11,0,0	112601869691	60684263640000
	10,1,0	427251287	110335024800
	9,2,0	293140085533	35307207936000
	9,1,1	855139549	11887948800
	8,3,0	-330209	82555200
	8,2,1	-185146093	2641766400
	7,4,0	166165549	11887948800
	7,3,1	1316243203	5943974400
	7,2,2	121572209	1981324800
	6,5,0	-46343	16982784000
	6,4,1	-284191127	1132185600
	6,3,2	-164310619	1698278400
	5,5,1	989706311	2830464000
	5,4,2	3563087	226437120
	5,3,3	17011511	53071200
	4,4,4	-16449829	106142400
12	12,0,0	0	1
	11,1,0	1042	79625
	10,2,0	-53737	1751750
	10,1,1	18608	875875
	9,3,0	150382	1576575
	9,2,1	324	7007
	8,4,0	-1248201	7007000
	8,3,1	-8952	875875
	8,2,2	-13347	79625
	7,5,0	241068	875875
	7,4,1	56256	875875
	7,3,2	209136	875875
	6,6,0	-2416112	7882875
	6,5,1	8208	875875
	6,4,2	-328401	875875
	6,3,3	-378944	7882875
	5,5,2	329256	875875
	5,4,3	130512	875875
	4,4,4	-286581	700700

Table 3.1.1 Triangular Newton-Cotes Coefficients

n	i	$d\times a_i$	d
1	1,0,0,0	1	4
2	2,0,0,0 1,1,0,0	-1 1	20 5
3	3,0,0,0 2,1,0,0 1,1,1,0	1 0 9	40 40 40

Table 3.1.2 Newton-Cotes Coefficients on the Tetrahedra

3.2 REVIEW AND DISCUSSION

There are several papers which have been written on the generalizations of Newton-Cotes quadrature to higher dimensional cases as we mentioned in section 1.2. In this section, we will discuss and review the paper [29] of Sylvester.

For a given k-simplex $\mathbb{D}^k$ in $\mathbb{R}^k$, with vertices A_i, $i = 0,1,\ldots,k$, Sylvester defines the simplex coordinates $\boldsymbol{\alpha} = (\alpha_0,\alpha_1,\ldots,\alpha_k)$ (we call them the barycentric coordinates) of an arbitrary point Q in $\mathbb{D}^k$ (we define $\boldsymbol{\alpha}$ for any point Q in $\mathbb{R}^k$) in terms of the volumes of sub-simplices $\mathbb{D}_i^k$ and k-simplex $\mathbb{D}^k$. That is, he defines

$$\alpha_i = \frac{V_i}{V}, \quad i = 0,1,2,\ldots,k,$$

where $\mathbb{D}_i^k$ is a sub-simplex in $\mathbb{R}^k$, with vertices A_j, $j = 0,1,\ldots,i-1,i+1,\ldots,k$ and the point Q; and V_i, $i = 0,1,\ldots,k$ and

V are the volumes of these simplices respectively. It is clear that $\sum_{i=0}^{k} \alpha_i = 1$, since the sum of the volumes of all sub-simplices $\mathbb{D}_i^k$, $i = 0,1,\ldots,k$ is equal to the total volume of $\mathbb{D}^k$. In most cases, the volumes of simplices in $\mathbb{R}^k$ are not easy to compute. But, we know that the ratio of V_i and V is simply the ratio of two distances from Q and A_i to the (k-1)-simplex with vertices A_j, $j = 0,1,\ldots,i-1,i+1,\ldots,k$.

Sylvester does not mention the Newton-Cotes lattice $\mathbb{L}n$ for $\mathcal{P}^n(\mathbb{R}^k)$; and his way of defining the interpolation polynomials (we call them the Newton-Cotes polynomials) is not clear. Finally, he applies the identity given in [2] to compute the coefficients. We represent the Newton-Cotes polynomial as the product of factorial polynomials, and compute the Newton-Cotes coefficients in terms of Stirling numbers. Sylvester does not have a formula this explicit. In his paper, he lists two tables of examples of close type Newton-Cotes formulas as well as the open type ones for triangles and tetrahedra.

CHAPTER IV

TWO DIMENSIONAL GREGORY QUADRATURE

Our generalization of Gregory type quadrature to two dimensions is based on a special partition of unity, namely hexagonal k-partition of unity which we will define first, the regions we will consider are the plane regions with piece-wise linear boundary.

4.1 HEXAGONAL k-PARTITIONS OF UNITY

In this section, we will define a hexagonal k-partition of unity and give some examples of it. In the later sections, we will see how they work for the derivation of two dimensional Gregory type quadrature.

Suppose the plane $\mathbb{R}^2$ is triangularly partitioned into a regular (i.e. equilateral) triangular grid of side h. Let Γ be the set of vertices of all triangles. Let H be a basic hexagon of side h with center C and vertices $C+h\omega_s$, $s = 1,2,\ldots,6$, in Γ. For simplicity, we assume that C is the origin O of the plane. Denote by $\mathrm{sym}(H)$ the set of all symmetries of H, that is, $\mathrm{sym}(H)$ is the set of affine transformations which maps $\mathbb{R}^2$ into itself, and permutes the vertices of H.

Definition 4.1.1 *A function* $\phi : \mathbb{R}^2 \to \mathbb{R}$ *is said to be a hexagonal k-partition of unity if it satisfies the following four conditions:*

$$\sum_{Y \in \Gamma} \phi(X-Y) = 1, \tag{4.1.1}$$

$$\int_{\mathbb{R}^2} P(X)\phi(X)dX = P(0)\,\frac{\sqrt{3}}{2}\,h^2, \quad p \in \mathcal{P}^k(\mathbb{R}^2), \tag{4.1.2}$$

$$\phi(ZX) = \phi(X), \quad Z \in \mathrm{sym}(H), \tag{4.1.3}$$

$$\mathrm{supp}(\phi) \subseteq H, \tag{4.1.4}$$

where $\mathrm{supp}(\phi)$ = the support of ϕ.

Thus, the function ϕ by (4.1.3) is symmetric with respect to the symmetries of H.

We can easily find some examples of hexagonal k-partitions. For example, $\phi = -\frac{1}{2} + \frac{5}{2}\gamma$ (where α, β and γ are the barycentric coordinates with respect to ABC, one of the six triangles of the hexagon H with center C) is a hexagonal 3-partition, and hence also is a hexagonal 1-partition.

4.2 FORMULAS OVER GENERAL REGIONS

We are familar with (one dimensional) first, second and third order Gregory quadrature formulas G_1, G_2 and G_3 respectively. They are given in Section 1.2.

Suppose we have a hexagonal k-partition of unity ϕ. Let Ω be an arbitrary plane region with piece-wise linear boundary. Then a mth order Gregory type quadrature can be derived on this region provided $m \leq k$ and Ω is large enough to contain a regular triangle of side $(m-1)h$ with vertices in Γ. We also expect that the resulting quadrature formulas will in some cases agree with the formulas constructed by using the methods of Sobolev [23,24].

From now on, the following notation (concept) will be used: if we say that the intersection of two polygons A and B of Ω (A or B may be equal to Ω) is empty, that is $A \cap B = \Phi$, we mean that if $A \cap B = \bigcup_{i=1}^{n} T_i$, with $T_\ell \cap T_j = \Phi$ for $\ell \neq j$, where T_i is either an equilateral triangle of side h or a subtriangle of an equilateral triangle of side h, then $n = 0$. Let $W = \{Y \varepsilon \Gamma : (Y+H) \cap \Omega = \Phi\}$, where $Y+H$ is a hexagon of side h with center Y, and let $V = Y \cap \Omega$. In particular, if Ω is a plane region that can be partitioned completely into an equilateral triangular grid of side h, then $V = W$. Now if f is a continuous function on Ω, then by (4.1.1) to (4.1.4), we have

$$\iint_\Omega f(X)dX = \iint_\Omega f(X) \sum_{Y \varepsilon W} \phi(X-Y)dX \qquad (4.2.1.a)$$

$$= \sum_{Y \varepsilon W} \iint_\Omega f(X)\phi(X-Y)dX$$

$$= \sum_{Y \varepsilon W} \left[\sum_{Z \varepsilon V} b(Z,Y)f(Z)+R_Y(f)\right] \qquad (4.2.1.b)$$

$$= \sum_{Y \varepsilon W} \left[\sum_{X \varepsilon V} b(X,Y)f(X)+R_Y(f)\right] \qquad (4.2.1.c)$$

$$= \sum_{Y \varepsilon W} \sum_{X \varepsilon V} b(X,Y)f(X)+R(f)$$

$$= \sum_{X \varepsilon V} a(X)f(X)+R(f) \qquad (4.2.1)$$

where $a(X) = \sum_{Y \in W} b(X,Y)$ (4.2.2)

and $R(f) = \sum_{Y \in W} R_Y(f)$. (4.2.2.a)

We note that, in (4.2.1.a), $\sum_{Y \in W} \phi(X-Y) = 1$, this is because $1 = \sum_{Y \in \Gamma} \phi(X-Y) = \sum_{Y \in \Gamma \setminus W} \phi(X-Y) + \sum_{Y \in W} \phi(X-Y)$ and $(H+X) \cap (H+X-Y) = \Phi$, for $Y \in \Gamma \setminus W$, where $(H+X)$ and $(H+X-Y)$ are hexagons of side h with centers X and $X-Y$ respectively, and hence by (4.1.4) $\phi(X-Y) = 0$, for $Y \in \Gamma \setminus W$. We will construct $b(Z,Y)$ in (4.2.1.b) so that (4.2.1.b) is true, in particular, we will construct $b(Z,Y)$ in (4.2.1.b) (or $b(Z,Y)$ in (4.2.1.c)) so that $R_Y(f) = 0$ (and hence $R(f) = 0$) if $f \in \mathcal{P}^{m-1}$ for some $m \leq k$ in $\mathbb{N}$, and such that for each $Y \in W$, $b(X,Y)$ is non-zero for only a small number of points X which are close to Y.

Now, the problem is how to determine the coefficients $a(X)$, $X \in V$. Particularly, if the hexagon $X+mH$ of side mh with center X, is contained entirely in Ω for a given point X in V, then $a(X) = \frac{\sqrt{3}}{2} h^2$, this is because we may consider $\Omega = X+mH$, and in this case $V = W = \{W\}$, and hence

$$\frac{\sqrt{3}}{2} h^2 = \iint_{X+mH} f(Z)dZ$$

$$= \iint_{X+mH} f(Z)\phi(Z-X)dZ$$

$$= b(X,X)f(X)$$

$$= a(X)f(X)$$

if $f \in \mathcal{P}^{m-1}$.

The set of points X in W without the above property $(a(X) = \frac{\sqrt{3}}{2} h^2)$ is referred to as the *regular boundary layer* of Ω. Now for any $X \in V$, $a(X)$ is given by formula (4.2.2). Hence, the problem becomes to determine the values of $b(X,Y)$. The values of $b(X,Y)$ should be found so that

$$\left.\begin{aligned} b(X,Y) &= \sum_{T\in\tau} b^T(X,Y) \\ \text{and} \qquad \iint_T f(X)\phi(X,Y)dX &= \sum_{X\in V} f(X)b^T(X,Y) \end{aligned}\right\} \qquad (4.2.3)$$

for all $Y \in W$, all $f \in \mathcal{P}^{m-1}$ and τ is one of triangular partitions (a triangular partition is a collection of triangles which is a partition) of $(Y+H) \cap \Omega$. For each $Y \in W$, the second sum in (4.2.3) is only taken over a small number of points X in V which are close to Y (since for all other X, $b^T(X,Y) = 0$, and this is because of our choice of k-hexagonal partition $\emptyset$). We will see (later on) how $b^T(X,Y)$ is defined and why τ is introduced when the actual computation of $b(X,Y)$ (and hence $a(X)$) is computed.

Let $V^i = \{X \in V : X+H \subseteq \Omega\}$ and $V^b = V \setminus V^i$. For a point Y in W, if $(Y+H) \cap \Omega = Y+H$, then $Y \in V^i$ and $b(X,Y) = \frac{\sqrt{3}}{2} h^2 \times \delta_Y^X$, for $X \in V$ (the same reason as $a(X) = \frac{\sqrt{3}}{2} h^2$, see above). Otherwise $Y \in V^b$ or $Y \in W \setminus V$. Suppose Y is a point in W and the center of the hexagon $Y+H$. Let T be one of the six triangles of $Y+H$, such that $T \cap \Omega \neq \emptyset$, and let α, β and γ be the barycentric coordinates with respect to this triangle. Let V_Y^m be a $(m-1)$th degree Newton-Cotes lattice of points in V which are close to Y. Then, there exists a set of Newton-Cotes polynomials $P_X(\alpha,\beta,\gamma)$ of degree m-1 on this V_Y^m. (Note that for each triangle T with the above properties, there corresponds a V_Y^m and a set of polynomials P_X on this V_Y^m.) For example, if Y is the vertex of a 60° angle of Ω such that $(Y+H)\cap\Omega = ABY$ is a regular triangle of side h, as shown in Figure 4.2.1, then when m = 1,2,3, V_Y^m are {Y}, {Y,A,B} and $\{Y,A,B,X_1,X_2,X_3\}$ respectively. Usually, the set V_Y^m is not unique and sometimes it does not contain the point

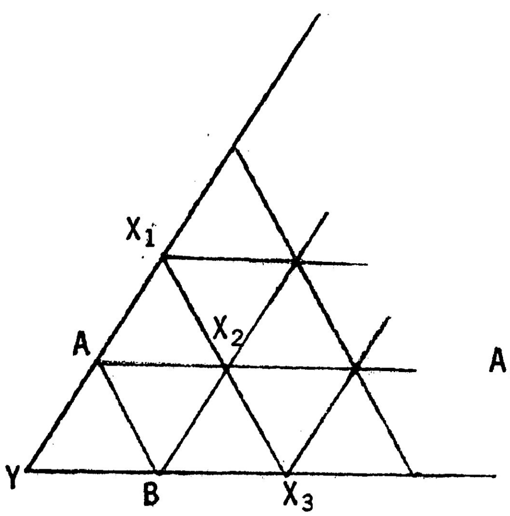


Figure 4.2.1

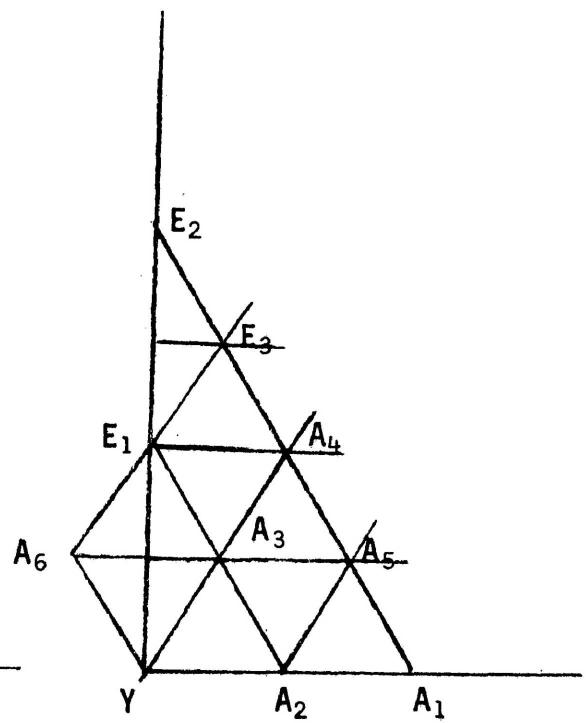


Figure 4.2.2

Y. For example, in Figure 4.2.2, the point Y is the center of the hexagon $Y+H$, but we may take $V_Y^3 = \{Y,A_1,A_2,A_3,A_4,A_5\}$ or $\{Y,E_1,E_2,E_3,A_3,A_4\}$; and the point A_6 is the center of a hexagon A_6+H, but $V_Y^3 = \{Y,E_1,E_2,E_3,A_3,A_4\}$ does not contain A_6.

Now, let us return to the above special case in which Y is the vertex of a 60° angle of Ω and $(Y+H)\cap\Omega = ABY = T$ as shown in Figure 4.2.1. Note that $\tau = \{ABY\}$. Thus

$$b(X,Y) = \sum_{T\varepsilon\tau} b^T(X,Y) = b^{ABY}(X,Y) = \int_{ABY} P_X\phi^Y, \tag{4.2.4}$$

for $X \varepsilon V_Y^m$, and zero otherwise.
Here $\phi^Y(X) = \phi(X-Y)$. To compute $\int_{ABY} P_X\phi^Y$, it is sufficient to consider this for $Y = C$, is the origin of the plane. Hence, it is convenient to define

$$\phi_{i,j} = \frac{2}{\sqrt{3}}\frac{1}{h^2}\int_{ABC}\phi\alpha^i\beta^j. \tag{4.2.5}$$

From Lemma 2.5.1 and a hexagonal k-partition ϕ, we can get the values of $\phi_{i,j}$, $0 \le i+j \le s \le k$. In particular, if $\phi = -\frac{1}{2} + \frac{5}{2}\gamma$ and $s = 2$, Table 4.2.1 shows these.

i,j	0,0	1,0	0,1	2,0	1,1	0,2
$\phi_{i,j}$	$\frac{1}{6}$	$\frac{1}{48}$	$\frac{1}{48}$	0	0	0

Table 4.2.1

Two further properties of ϕ from (4.1.1) to (4.1.4) and (4.2.5) are

$$(1+(-1)^{i+j})\phi_{i,j}+((-1)^{i}+(-1)^{j})\left(\sum_{u+v=i}\binom{i}{u,v}\phi_{u,v+j}+\sum_{u+v=j}\binom{j}{u,v}\phi_{u+i,v}\right) = 0 \tag{4.2.6}$$

for $0 < i+j \leq k,\ \ i,j \geq 0$;

and

$$\phi_{i,j}+\sum_{r+s+t=j}\binom{j}{r,s,t}(-1)^{s+t}\phi_{i+s,t}+\sum_{r+s+t=i}\binom{i}{r,s,t}(-1)^{s+t}\phi_{s,j+t} = \frac{i!j!}{(i+j+2)!}, \tag{4.2.7}$$

for $0 \leq i \leq i+j \leq k$.

Note that in Table 4.2.1 the first three values of $\phi_{i,j}$ follow directly from these two equations, and the last three do not, but they are related by

$$\phi_{1,1}+2\phi_{0,2} = \phi_{11}+2\phi_{2,0} = 0.$$

Now, let us compute the values of $b(X,Y)$ in (4.2.4) for Y, as shown in Figure 4.2.1, $T = ABY$ and $X \in V_Y^m$. When $m = 1$, $V_Y^1 = \{Y\}$, then $P_Y = 1$ and

$$\frac{2}{\sqrt{3}}\ \frac{1}{h^2}\times b(X,Y) = \frac{2}{\sqrt{3}}\frac{1}{h^2}\int_{ABC}\phi = \phi_{0,0} = \frac{1}{6}. \tag{4.2.8}$$

when $m = 2$, $V_Y^2 = \{Y, A_1, A_2\}$, then $P_Y = 1-\alpha-\beta$ $P_A = \alpha$ and $P_B = \beta$ and

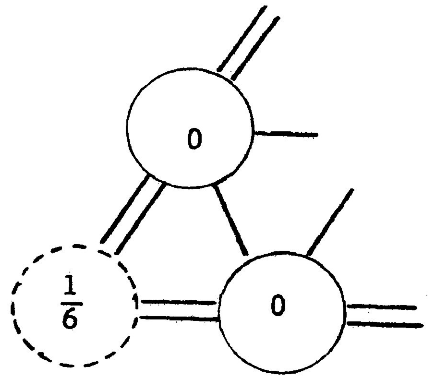
$$\frac{2}{\sqrt{3}}\frac{1}{h^2} \times b(X,Y) = \begin{cases} \frac{2}{\sqrt{3}}\frac{1}{h^2}\int_{ABC}\phi(1-\alpha-\beta) = \phi_{0,0}-2\phi_{0,1} = \frac{1}{8}, & \text{if } X = Y \\ \phi_{1,0} = \phi_{0,1} = \frac{1}{48}, & \text{if } X = A, \text{ or } B \end{cases}. \tag{4.2.9}$$

when $m = 3$, $V_Y^3 = \{Y, A_1, A_2, X_1, X_2, X_3\}$, then $P_Y = \frac{1}{2}(1-\alpha-\beta)(2-\alpha-\beta)$, $P_A = \alpha(2-\alpha-\beta)$, $P_B = \beta(2-\alpha-\beta)$, $P_{X_1} = -\frac{1}{2}\alpha(1-\alpha)$, $P_{X_2} = \alpha\beta$ and $P_{X_3} = -\frac{1}{2}\beta(1-\beta)$, and

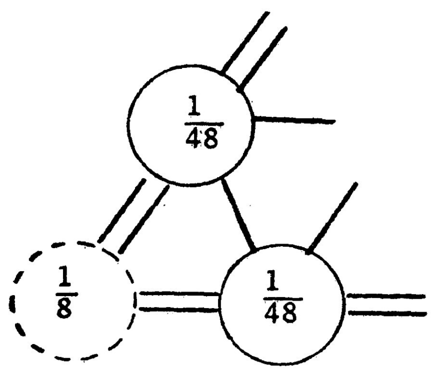
$$\frac{2}{\sqrt{3}}\frac{1}{h^2} \times b(X,Y) = \begin{cases} \frac{5}{48} & \text{if } X = Y \\ \frac{1}{24} & \text{if } X = A \text{ or } B \\ -\frac{1}{96} & \text{if } X = X_1 \text{ or } X_3 \\ 0 & \text{if } X = X_2 \end{cases}. \tag{4.2.10}$$

This formula is computed in the similar way as (4.2.9). For example, at the point $X = B$, $\frac{2}{\sqrt{3}}\frac{1}{h^2} \times b(X,Y) = \frac{2}{\sqrt{3}}\frac{1}{h^2}\int_{ABC}\phi\beta(2-\alpha-\beta)$ $= 2\phi_{0,1}-\phi_{1,1}-\phi_{0,2} = \frac{1}{24}$.

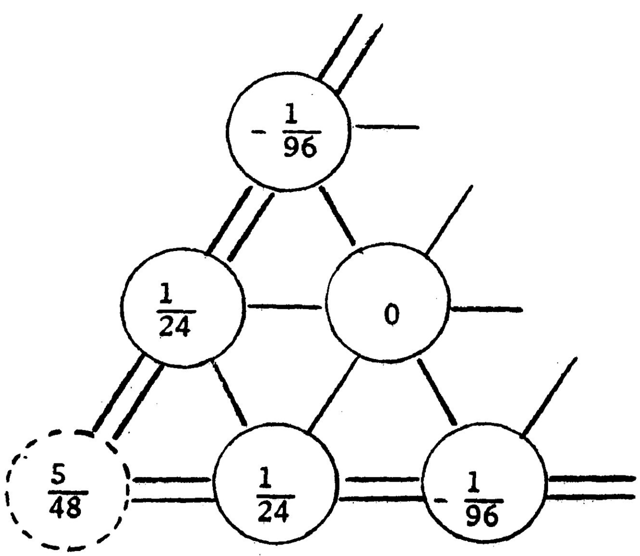
Note that the above three formulas can be represented symbolically in the following way,



(4.2.11)



(4.2.12)



(4.2.13)

Here, the double lines indicate the boundary of Ω, and the dashed circle indicates the center of the hexagon $Y+H$ we consider. (Sometimes, we also use "*" to indicate the center of $Y+H$.)

Now, consider $Y \varepsilon \Gamma$ is the vertex of a 120° angle of Ω such that $(Y+H) \cap \Omega = A_1A_5Y \cup A_2A_5Y$, where A_1A_5Y and A_2A_5Y are regular triangles of

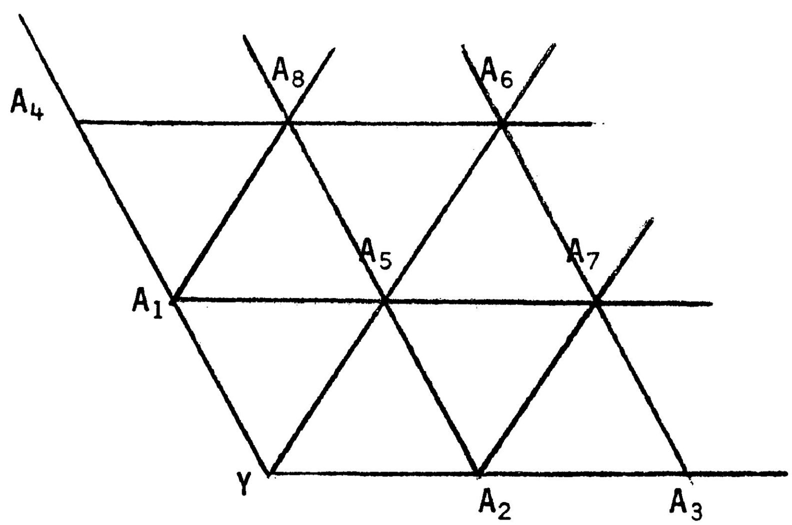
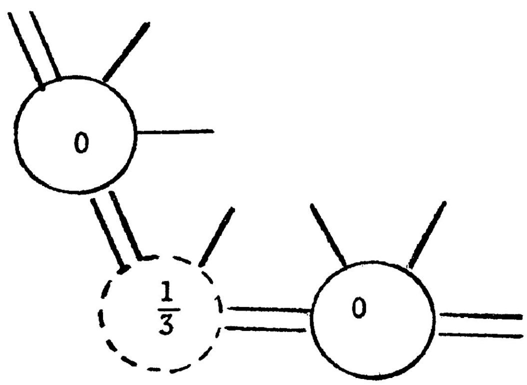


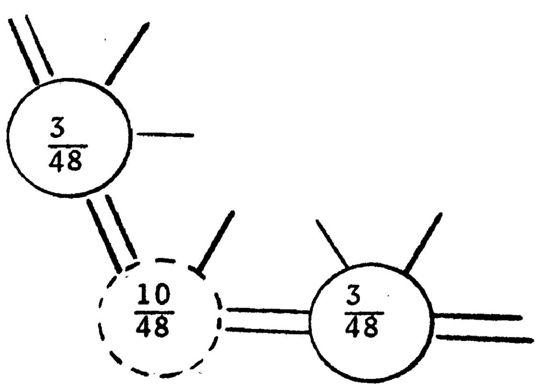
Figure 4.2.3

side h, as shown in Figure 4.2.3. In this case, we take $\tau_1 = \{A_1A_5Y, A_2A_5Y\}$ to be a triangular partition of $(Y+H) \cap \Omega$.

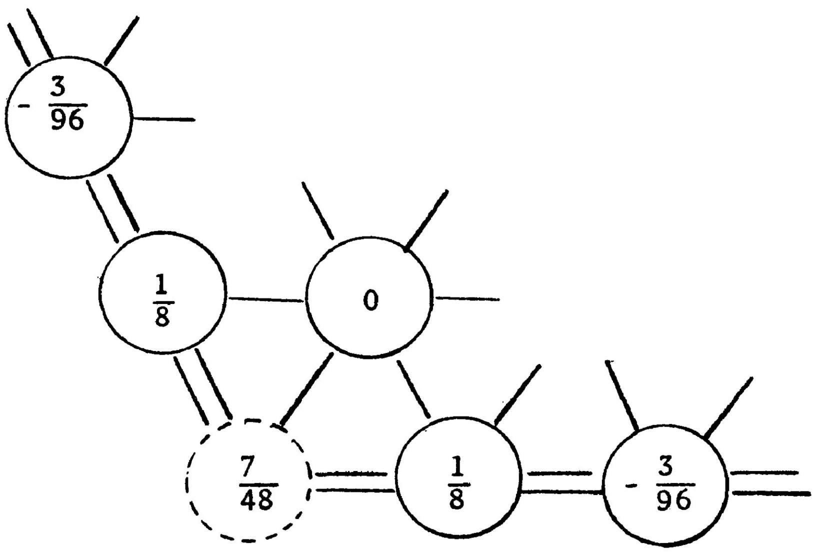
If $m = 1,2,3$ and $T \varepsilon \tau_1$, then we may take V_Y^m to be $\{Y\}$, $\{Y,A_1,A_2\}$ and $\{Y,A_1,A_2,A_3,A_4,A_5\}$ respectively. Then $\frac{2}{\sqrt{3}} \frac{1}{h^2} \times b(X,Y)$ for V_Y^m, $m = 1,2,3$ are



(4.2.14)



(4.2.15)

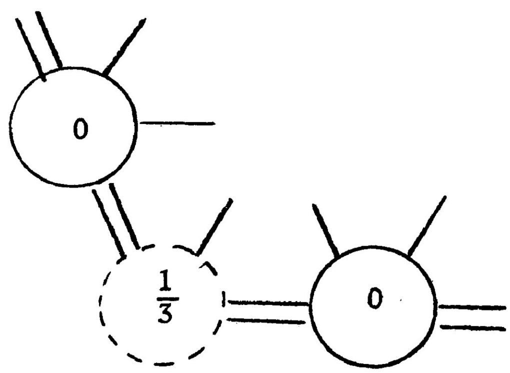


(4.2.16)

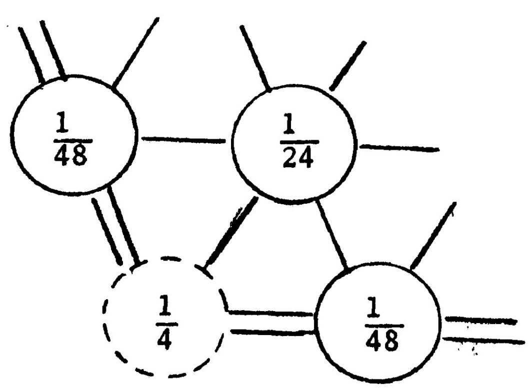
respectively.

On the other hand, we may consider a 120° angle to be two adjoining 60° angles with the same vertex Y. For example, in Figure 4.2.3, angle A_1YA_2 is equal to the sum of angles A_1YA_5 and A_2YA_5. Then, it is natural to consider two sets of V_Y^m for these two 60° angles repsectively, which have m points in common (as shown in figure 4.2.3, for $m = 3$), and the values of $b(X,Y)$ for X in either one of these V_Y^m are given in (4.2.4) except for those points X in both sets of V_Y^m, where the values of $b(X,Y)$ are double. For $m = 1,2$ and 3,

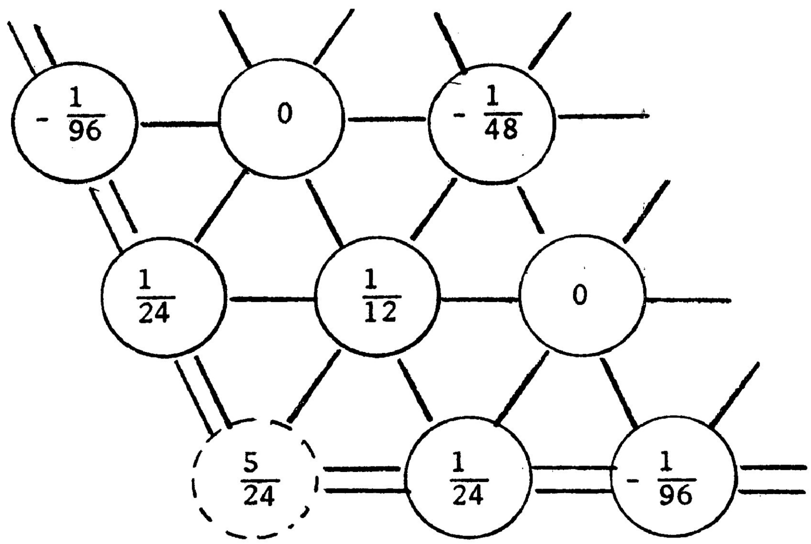
$\frac{2}{\sqrt{3}} \frac{1}{h^2} \times b(X,Y)$ are



(4.2.17)



(4.2.18)



(4.2.19)

respectively.

Generally, this procedure can be applied for any vertex Y of Ω (or any point $Y' \varepsilon V$ which is on the boundary of Ω, in which case we consider Y to be the vertex of a 180° angle of Ω) provided that the values of $b(X,Y)$ with respect to the sub-angles are known. For example, if we want to compute $b(X,Y)$ for Y as shown in Figure 4.2.4, then we may divide the angle A_1YA_4 into three 60° angles A_1YA_2, A_2YA_3 and A_3YA_4;

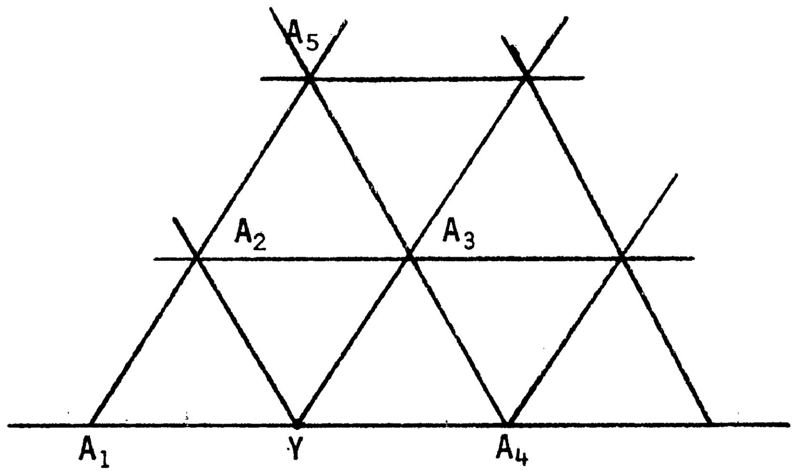
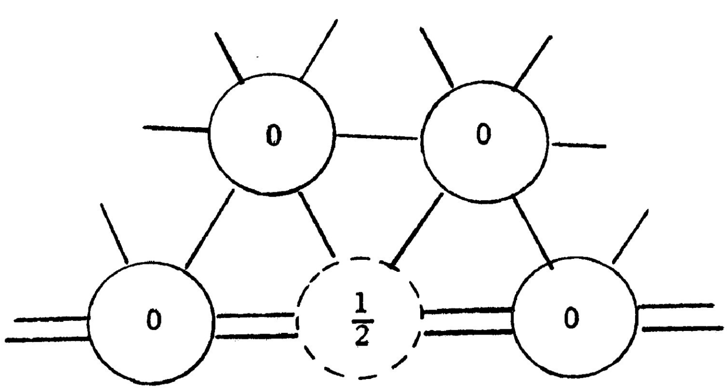


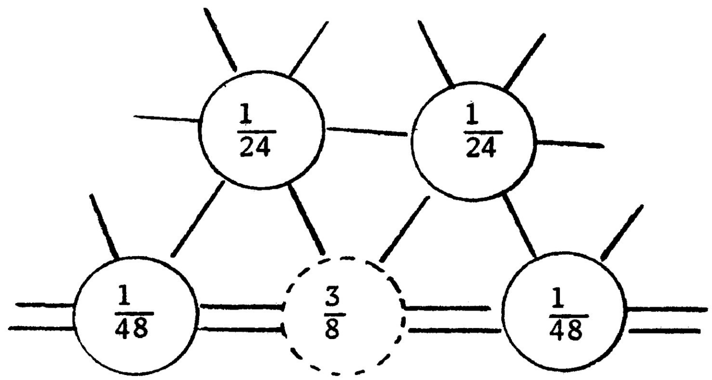
Figure 4.2.4

and V_Y^m and b(X,Y) for these angles are known, and hence b(X,Y) for the whole 180° angle are known. When $m = 1,2$,

$\frac{2}{\sqrt{3}}\frac{1}{h^2}\, b(X,Y)$ are



(4.2.20)



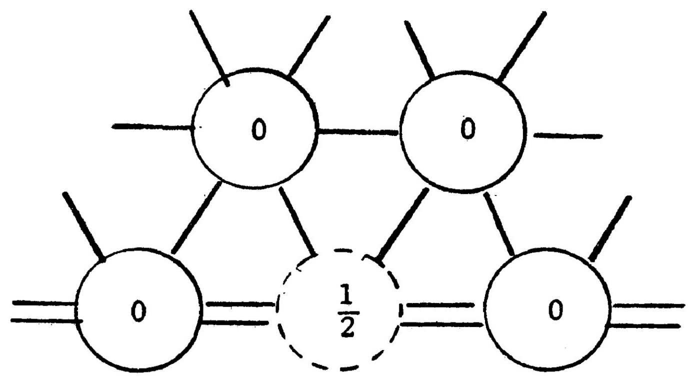
(4.2.21)

respectively.

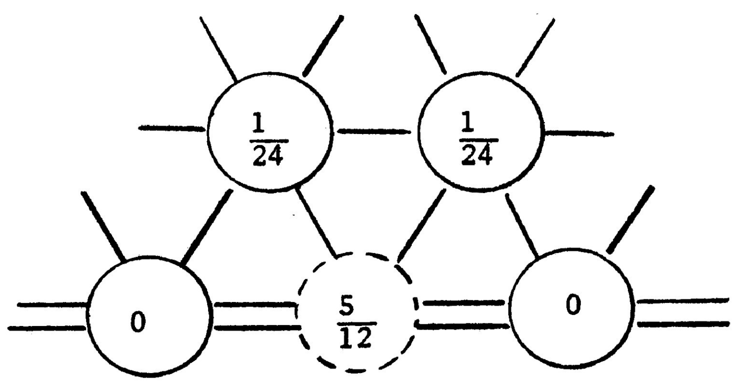
We observe that, to compute b(X,Y) at this Y for a mth order formula, we use $3 \times \binom{m+1}{2} - 2m$ points, which is a large number of points compared with $\binom{m+1}{2}$ points for $m \geq 3$. Thus, we do not like the higher order formulas at this Y obtained by the above procedure (by combining formulas of three angles).

Consider the point Y in Figure 4.2.4, we may take $\tau_2 = \{A_1A_2Y, A_2A_3Y, A_3A_4Y\}$ to be a triangular partition of $(Y+H) \cap \Omega$ and $T \in \tau_2$, and let V_Y^m be the set of points in V with the properties mentioned before. When $V_Y^1 = \{Y\}$,

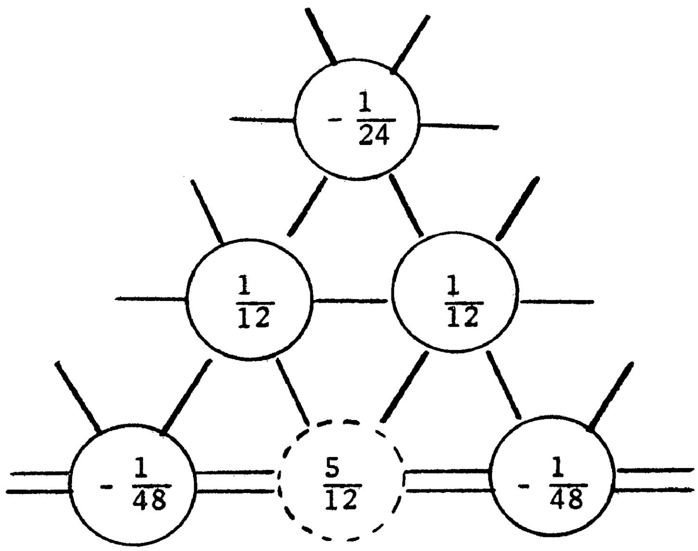
$V_Y^2 = \{A_2, A_3, Y\}$ and $V_Y^3 = \{A_1, A_2, A_3, A_4, A_5, Y\}$ then $\frac{2}{\sqrt{3}}\frac{1}{h^2} \times b(X,Y)$ are



(4.2.22)



(4.2.23)



(4.2.24)

respectively.

Let $\tau = \{T_1, T_2, \ldots, T_s\}$ be a triangular partition for $(Y+H) \cap \Omega$ for some given point Y in W. Sometimes, not all $T_i \in \tau$ are regular. For example, consider a plane region which contains right angles. The points in V around a right angle are distributed in the way shown in Figure 4.2.5.

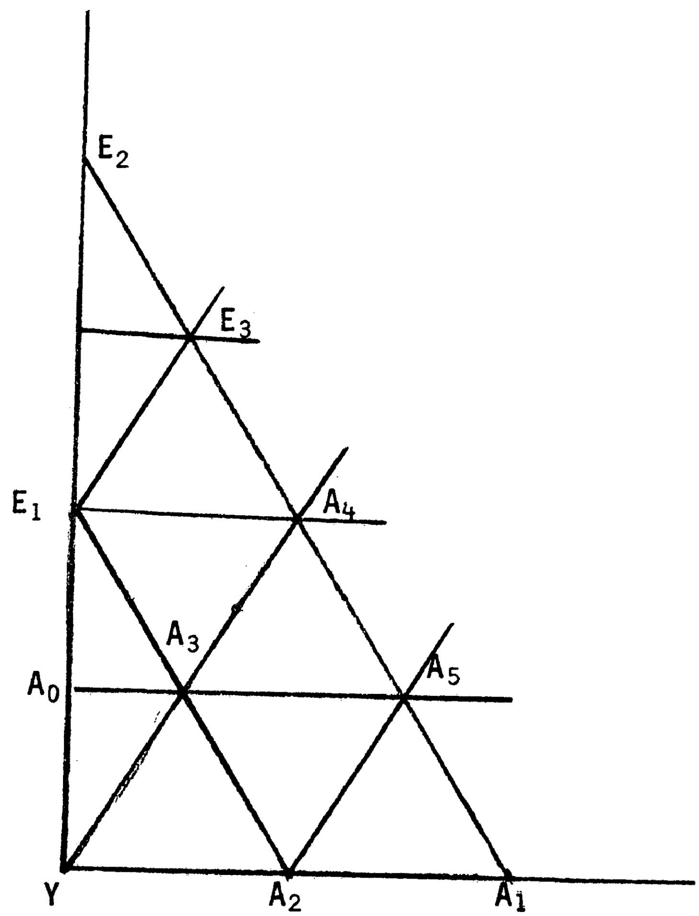


Figure 4.2.5

We observe that we may take $\tau_3 = \{A_2A_3Y, A_0A_3Y\}$ to be a triangular partition of $(Y+H) \cap \Omega$, but A_0A_3Y is not a regular triangle. In which case, we must compute the integral $\int_T \phi^Y \alpha^i \beta^j$ for

$T = A_0A_3Y$. As we mentioned before, it is sufficient to compute this for $Y = C$, the origin of the plane.

Let ABC and $\dot{A}\dot{B}\dot{C}$ be the two triangles shown in the following figure,

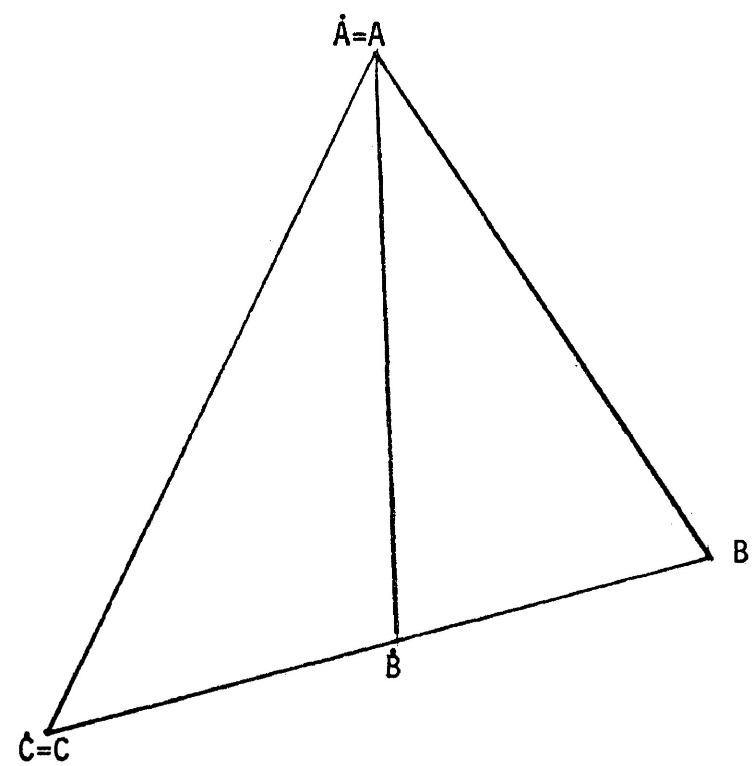


Figure 4.2.6

where $\dot{B}$ is the mid point of BC.

Let α,β and γ, and $\dot{\alpha},\dot{\beta}$ and $\dot{\gamma}$ be the barycentric coordinates with respect to these two triangles respectively. Let $\dot{\alpha}_1 = \alpha(A)$, $\dot{\alpha}_2 = \alpha(B)$ and $\dot{\alpha}_3 = \alpha(C)$, similarly for $\dot{\beta}_1,\dot{\beta}_2,\dot{\beta}_3$, $\dot{\gamma}_1,\dot{\gamma}_2$ and $\dot{\gamma}_3$. Then it is clear that

$$\begin{bmatrix} \dot{\alpha} \\ \dot{\beta} \\ \dot{\gamma} \end{bmatrix} = \begin{bmatrix} \dot{\alpha}_1 & \dot{\alpha}_2 & \dot{\alpha}_3 \\ \dot{\beta}_1 & \dot{\beta}_2 & \dot{\beta}_3 \\ \dot{\gamma}_1 & \dot{\gamma}_2 & \dot{\gamma}_3 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix} = J \begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix} \tag{4.3.25}$$

with

$$J = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 2 \end{bmatrix}$$

and

$$J^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} \end{bmatrix}.$$

Let T be a given sub-triangle of the regular triangle ABC of side h. Then we may define

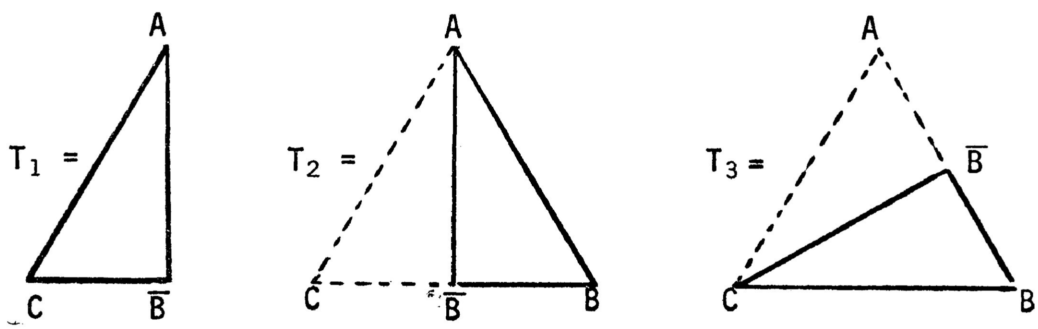
$$\phi^T_{i,j} = \frac{2}{\sqrt{3}}\frac{1}{h^2}\int_T \phi\alpha^i\beta^j. \tag{4.2.5'}$$

In particular, if $T = ABC$, then it is the case of (4.2.5). Here, we only consider T to be half triangle of ABC. We are interested in three types of half triangles. The values of $\phi^T_{i,j}$, $0 \le i \le i+j \le 2$ for these half triangles are shown in the following table:

T_ℓ \ $\phi^{T_\ell}_{i,j}$ \ i,j	0,0	1,0	0,1	2,0	1,1	0,2
T_1	$\frac{9}{8}\times\frac{1}{6}$	$\frac{7}{4}\times\frac{1}{48}$	$\frac{6}{4}\times\frac{1}{48}$	$\frac{1}{96}$	$\frac{1}{192}$	$\frac{1}{128}$
T_2	$-\frac{1}{8}\times\frac{1}{6}$	$-\frac{3}{4}\times\frac{1}{48}$	$-\frac{2}{4}\times\frac{1}{48}$	$-\frac{1}{96}$	$-\frac{1}{192}$	$-\frac{1}{128}$
T_3	$\frac{1}{2}\times\frac{1}{6}$	$\frac{1}{4}\times\frac{1}{48}$	$\frac{3}{4}\times\frac{1}{48}$	0	0	0

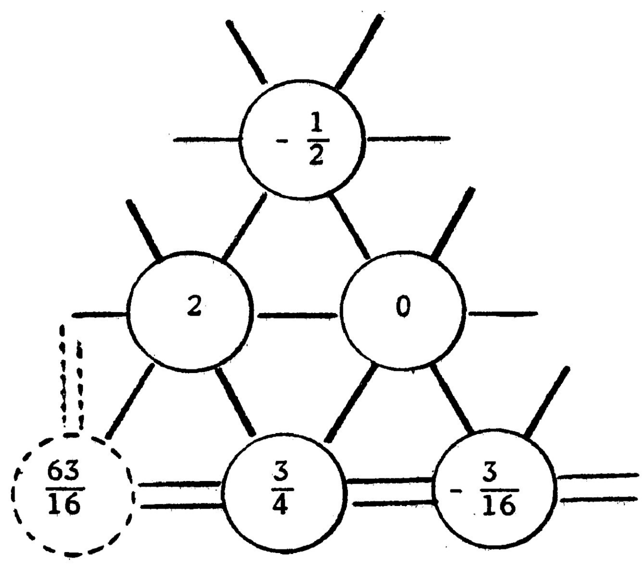
Table 4.2.2

where



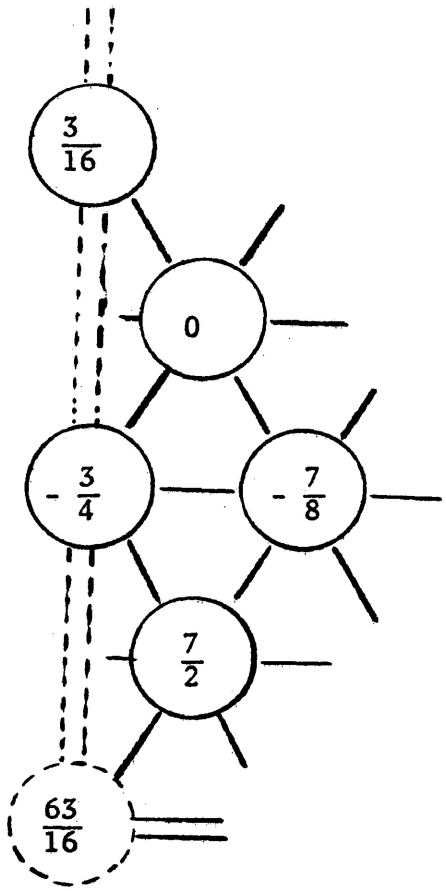
These formulas are obtained by using the transformation formula (4.3.25) and the matrices J and J^{-1}; and the value of $\phi_{i,j}$. Additionally, $\phi^{T_1}_{i,j}+\phi^{T_2}_{i,j} = \phi_{i,j}$ and $\phi^{T_3}_{i,j}+\phi^{T_3}_{j,i} = \phi_{i,j}$.

Now, return to the above example in which Y is the vertex of a 90° angle of Ω and $(Y+H)\cap\Omega = A_2A_3Y \cup A_0A_3Y$ as shown in Figure 4.2.5. For a third order formula, there are two sets of V_Y^3 we may use when computing $b(X,Y)$, they are $\{A_1, A_2, Y, A_3, A_4, A_5\}$ and $\{Y, E_1, E_2, E_3, A_4, A_3\}$. When we use the first set of V_Y^3, then $24 \times \frac{2}{\sqrt{3}} \frac{1}{h^2} \times b(X,Y)$ are



(4.2.26)

and $24 \times \frac{2}{\sqrt{3}} \frac{1}{h^2} b(X,Y)$ are



(4.2.27)

if we use the second one.

Another place we must use $\phi^T_{i,j}$ in Table 4.2.2 is when computing the formula of $b(X,Y)$ along one edge of a 90° angle of Ω. For example, in Figure 4.2.7 – 4.2.9, $(Y+H)\cap\Omega$ contains three types of half triangles and hence three different sets of $\phi^T_{i,j}$ will be used.

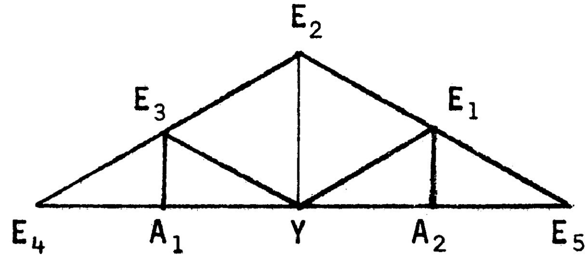


Figure 4.2.7

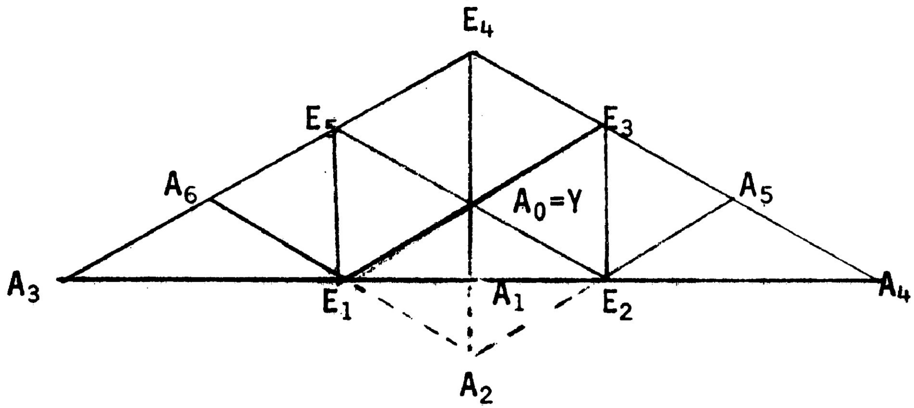


Figure 4.2.8

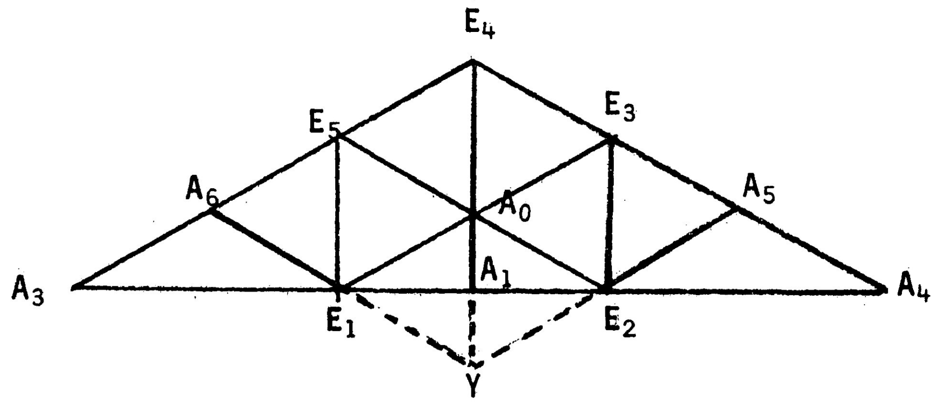
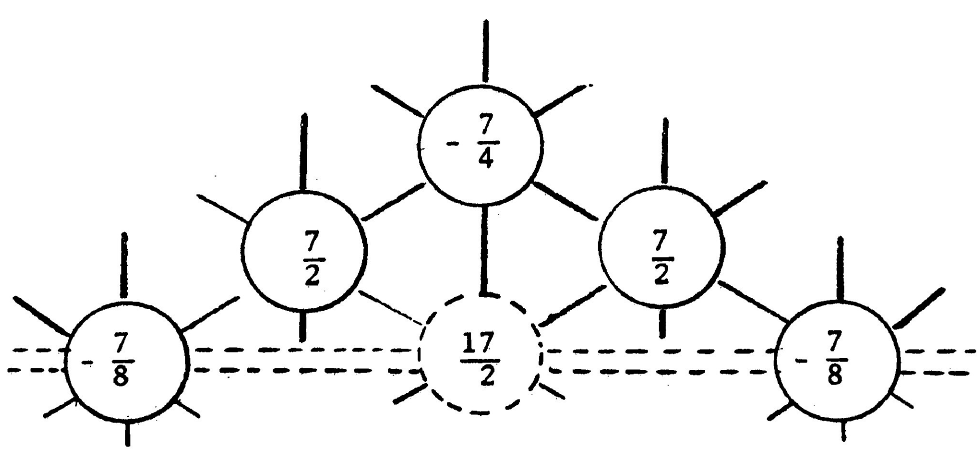


Figure 4.2.9

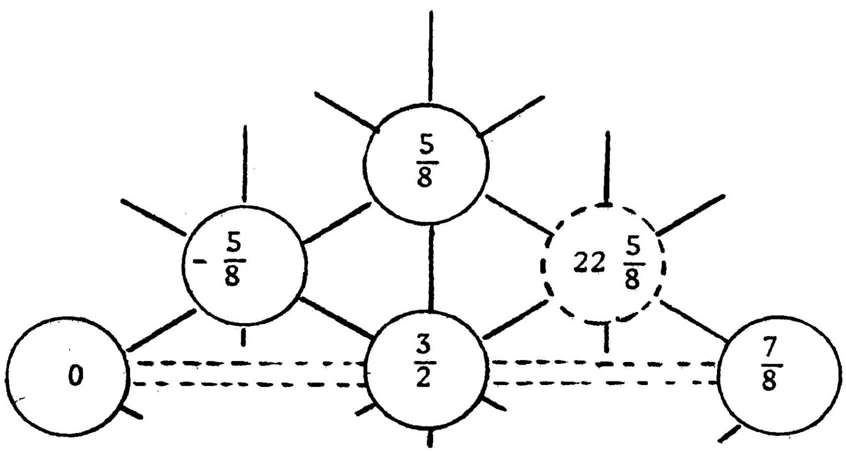
Consider $(Y+H)\cap\Omega$ in Figure 4.2.7, we may take $\tau_4 = \{A_1E_3Y, A_2E_1Y, E_2E_1Y, E_3E_2Y\}$ to be a triangular partition of $(Y+H)\cap\Omega$ and $V_Y^3 = \{Y, E_1, E_2, E_3, E_4, E_5\}$. Then we can compute $24 \times \frac{2}{\sqrt{3}}\frac{1}{h^2}\, b(X,Y)$ for $X \in V_Y^3$ and they are



(4.2.28)

In Figure 4.2.8, we may take $\tau_5 = \{A_1E_1Y, A_1E_2Y, E_2E_3Y, E_3E_4Y, E_4E_5Y, E_5E_1Y\}$, to be a triangular partition of $(Y+H) \cap \Omega$ and $V_Y^3 = \{A_3, E_1, E_2, A_0, E_5, A_6\}$ or $\{E_1, E_2, A_4, A_5, E_3, A_0\}$.

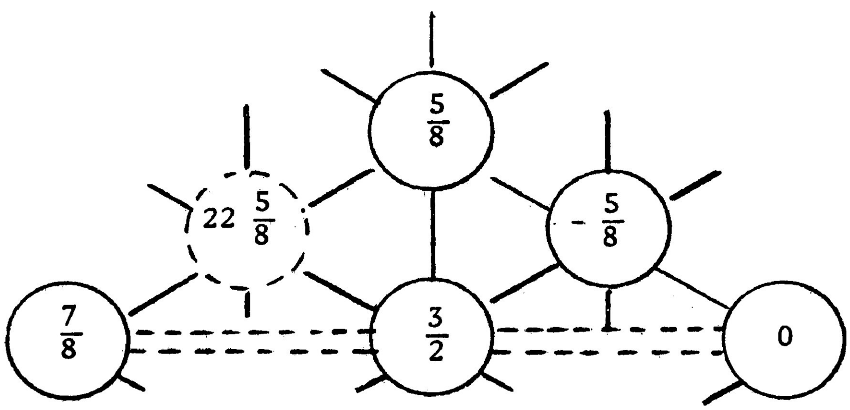
If we use the first set of V_Y^3, then $24 \times \frac{2}{\sqrt{3}} \frac{1}{h^2} b(X,Y)$ are



(4.2.29)

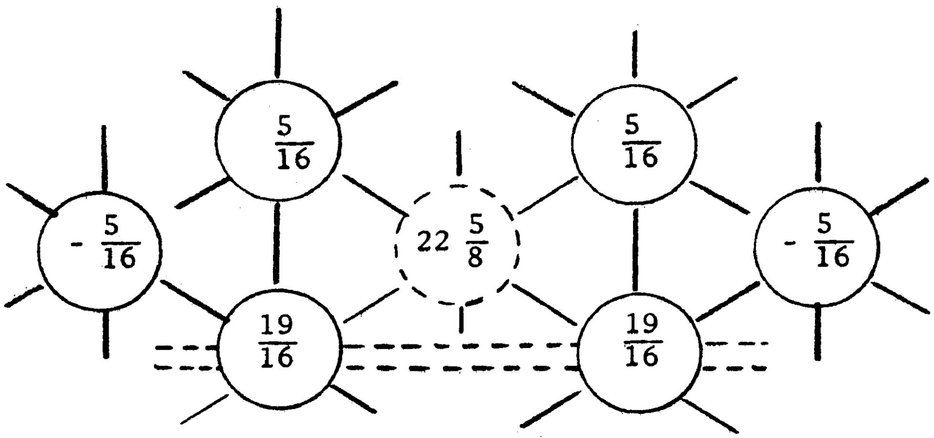
If we use the second set of V_Y^3 instead of the first one, then

$24 \times \frac{2}{\sqrt{3}} \frac{1}{h^2} \times b(X,Y)$ are



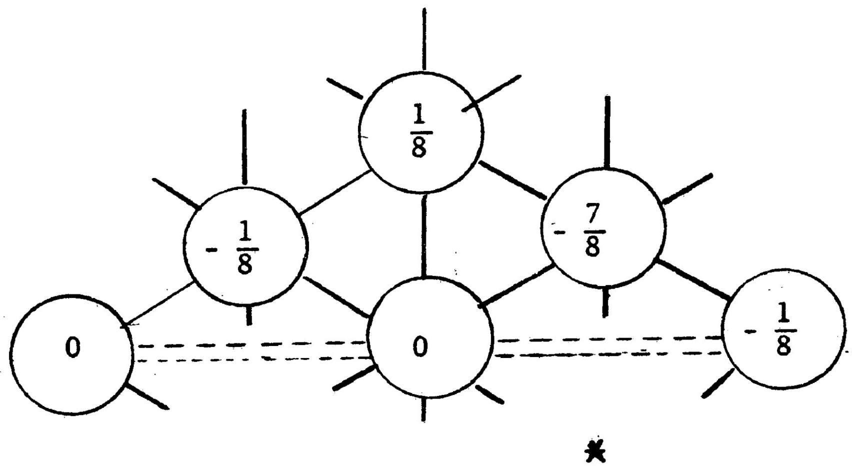
(4.2.30)

We also like the formula of $24 \times \frac{2}{\sqrt{3}} \frac{1}{h^2} \times b(X,Y)$ which is computed by taking the average of (4.2.29) and (4.2.30), and it is

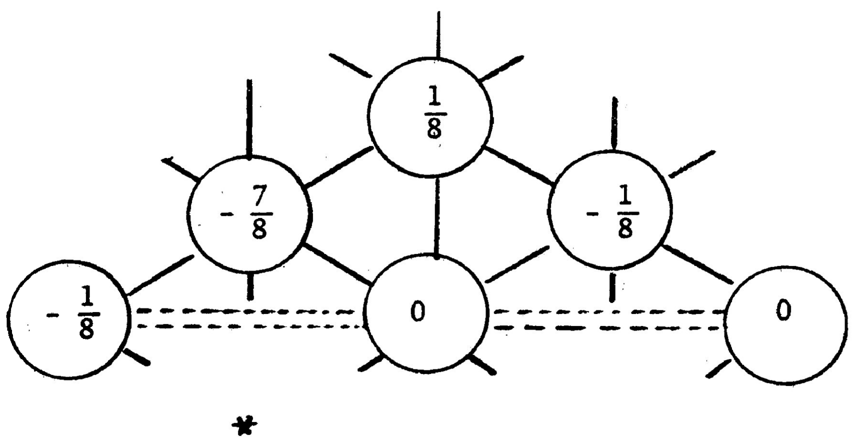


(4.2.31)

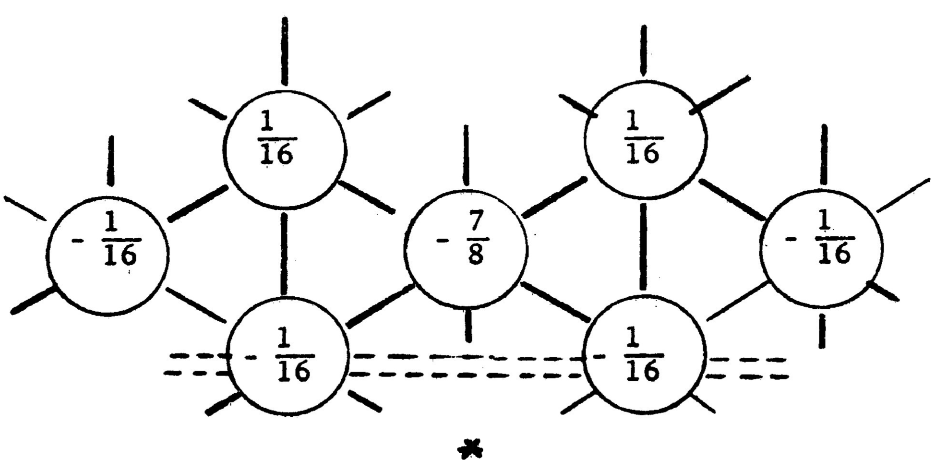
Now, let us consider Figure 4.2.9, we may take $\tau_6 = \{A_0A_1E_1, A_0A_1E_2\}$ to be a triangular partition of $(Y+H)\cap\Omega$ and two set of V_Y^3 are the same as those for Figure 4.2.8. Thus we have three similar sets of $24 \times \frac{2}{\sqrt{3}}\frac{1}{h^2} \times b(X,Y)$ (as those of Figure 4.2.8), and they are



(4.2.32)



(4.2.33)



(4.2.34)

Finally, sum all possible non-trivial $b(X,Y)$ for $X \in V$ and $Y \in W$, and get the coefficients $a(X)$. The resulting formula is a mth order Gregory type quadrature formula for Ω. In the next three sections, we will give some examples for two particular types of plane regions.

4.3 FORMULAS OVER TRIANGLES

In the previous section, the general procedures of the derivation of Gregory type quadrature of order m had been treated, for the general plane region with piece-wise linear boundary. Particularly, two kinds of such plane regions are interesting. One of them is a plane region that can be partitioned completely into a regular triangular grid of side h (and its vertices are in Γ). Some examples are an equilateral triangle, a regular hexagon, and a parallelogram with angles 60° and 120°. The most general type region we consider is the polygon with its vertices in Ω. We will discuss the parallelogram region and the rectangular region in the next two sections. In this section, we will show some Gregory type quadrature formulas on an equilateral triangle, and hence on an arbitrary triangle.

Let $\Omega = ABC$ be a given triangle of side nh with the property mentioned above. Initially, we assume that $n \geq 1$ for $m = 1$ and $n \geq 3m-3$ for $m \geq 2$. Note that the set $V = \Omega \cap \Gamma$ is a nth degree Newton-Cotes lattice. For a mth order Gregory type

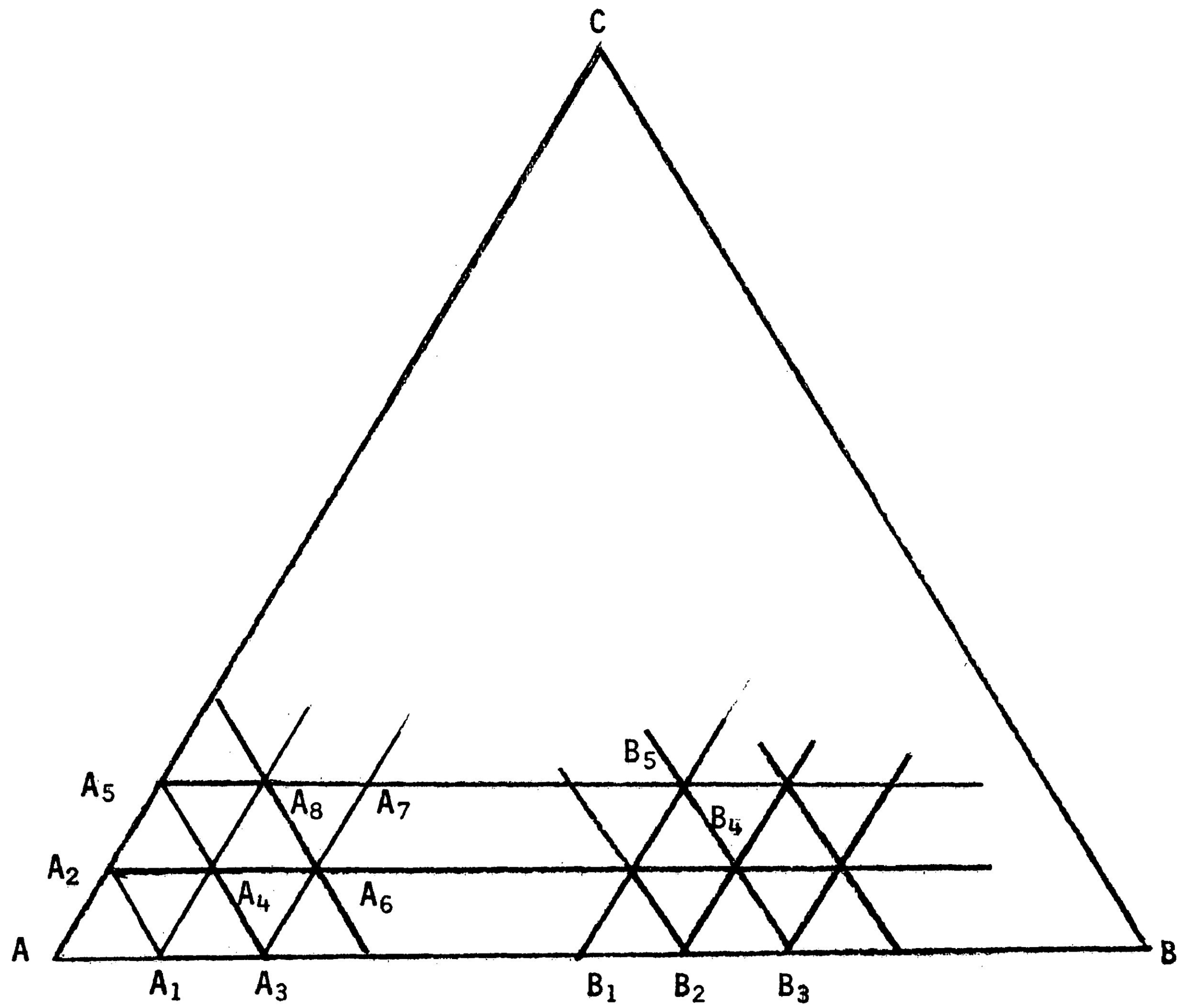


Figure 4.3.1

quadrature, we only need to compute $a(X)$ for X are the m^2 points around each 60° angle of Ω and m points along the edges such that $X+iH \subseteq \Omega$ but $X+(i+1)H \not\subseteq \Omega$, $i = 0,1,2,\ldots,m-1$, since for all other $X \in V$, $a(X) = \frac{\sqrt{3}}{2} h^2$. For example, when

$m = 3$, the nine points around a 60° angle of Ω are $A, A_1, A_2, A_3, A_4, A_5, A_6, A_7$ and A_8, and the three points along the edge of Ω are like B_2 (or B_1 or B_3), B_4 and B_5 as shown in Figure 4.3.1.

When $m = 1$, then $a(X) = 1 \times \frac{\sqrt{3}}{2} h^2$ if $X+H \subseteq \Omega$. If $X \in V^b$ but not a vertex of Ω, then $a(X) = \frac{1}{2} \times \frac{\sqrt{3}}{2} h^2$, by formula (4.2.22). If X is a vertex of Ω, then $a(X) = \frac{1}{6} \times \frac{\sqrt{3}}{2} h^2$ by formula (4.2.11). Hence the first order Gregory quadrature formula over Ω is

$$
\text{(GT1)} \qquad
\begin{array}{c}
1 \\
3 \quad 3 \\
3 \quad 6 \quad 3 \\
3 \quad 6 \quad 6 \quad 3 \\
\cdot^{\cdot^{\cdot}} \quad \cdot^{\cdot^{\cdot}} \qquad\qquad \cdot^{\cdot^{\cdot}} \quad \cdot^{\cdot^{\cdot}} \\
3 \qquad\qquad\qquad\qquad 3 \\
3 \quad 6 \qquad\qquad\qquad\qquad 6 \quad 3 \\
3 \quad 6 \quad 6 \quad \ldots \quad 6 \quad 6 \quad 3 \\
1 \quad 3 \quad 3 \quad 3 \quad \ldots \quad 3 \quad 3 \quad 3 \quad 1
\end{array}
$$

with a common factor $\frac{1}{6} \times \frac{\sqrt{3}}{2} h^2$.

When $m = 2$, then we must compute $a(X)$ for $X = B_2, B_4$ and A, A_1, A_2 and A_4. If we use formulas (4.2.2), (4.2.21), we have

$$a(B_2) = b(B_2,B_2)+b\,(B_2,B_1)+b(B_2,B_3) = \left(\frac{3}{8} + \frac{1}{48} + \frac{1}{48}\right) \frac{\sqrt{3}}{2} h^2 = \frac{10}{24} \times \frac{\sqrt{3}}{2} h^2,$$

$$a(B_4) = b(B_4,B_4)+b(B_4,B_2)+b(B_4,B_3) = \left(1 + \frac{1}{24} + \frac{1}{24}\right) \frac{\sqrt{3}}{2} h^2 = \frac{26}{24} \times \frac{\sqrt{3}}{2} h^2.$$

Thus, the formula of $24 \times \frac{2}{\sqrt{3}}\frac{1}{h^2} \times a(X)$ for X along the edge of Ω is

$$\begin{array}{lccccl} & \cdot^{\cdot^{\cdot}} & & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \\ \cdots & 24 & & 24 & 24 & \cdots \\ \cdots & 24 & & 24 & 24 & \cdots \\ \cdots & 26 & & 26 & 24 & \cdots \\ \cdots & 10 & & 10 & 10 & \cdots \end{array} \qquad (4.3.1)$$

If we use formula (4.2.23) instead of (4.2.21), then we get the same formula as (4.3.1). If we use formulas (4.2.2), (4.2.21), (4.2.12), then

$$a(A) = b(A,A)+b(A,A_1)+b(A,A_2) = \left(\frac{1}{8} + \frac{1}{48} + \frac{1}{48}\right) \times \frac{\sqrt{3}}{2} h^2 = \frac{1}{6} \times \frac{\sqrt{3}}{2} h^2,$$

$$a(A_4) = b(A_4,A_4)+b(A_4,A)+b(A_4,A_1)+b(A_4,A_2)+b(A_4,A_3)+b(A_4,A_5)$$

$$= \left(1 + \frac{1}{24} + \frac{1}{24} + \frac{1}{24} + \frac{1}{24}\right) \times \frac{\sqrt{3}}{2} h^2 = \frac{28}{24} \times \frac{\sqrt{3}}{2} h^2,$$

$$a(A_1) = b(A_1,A_1)+b(A_1,A)+b(A_1,A_3)+b(A_1,A_2)$$

$$= \left(\frac{3}{8} + \frac{1}{48} + \frac{1}{48} + \frac{1}{24}\right) \times \frac{\sqrt{3}}{2} h^2 = \frac{11}{24} \times \frac{\sqrt{3}}{2} h^2,$$

and $a(A_2) = a(A_1) = \frac{11}{24} \times \frac{\sqrt{3}}{2} h^2$.

Thus the formula of $24 \times \frac{2}{\sqrt{3}}\frac{1}{h^2} \times a(X)$ for X around a $60°$ angle of Ω is

$$\begin{array}{lllll} \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \\ 10 & 26 & 24 & 24 & \ldots \\ 10 & 26 & 24 & 24 & \ldots \\ 11 & 28 & 26 & 26 & \ldots \\ 4 & 11 & 10 & 10 & \ldots \end{array} \qquad (4.3.2)$$

If we use formula (4.2.23) instead of (4.2.21), we have another formula of $48 \times \frac{2}{\sqrt{3}} \frac{1}{h^2} \times a(X)$ for X around a $60°$ angle of Ω, and it is

$$\begin{array}{lllll} \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \\ 20 & 52 & 48 & 48 & \ldots \\ 20 & 52 & 48 & 48 & \ldots \\ 23 & 56 & 52 & 52 & \ldots \\ 6 & 23 & 20 & 20 & \ldots \end{array} \qquad (4.3.3)$$

This formula is computed in the same way as (4.3.2), for example

$$a(A_1) = \left(\frac{5}{12} + \frac{1}{48} + 0 + \frac{1}{24}\right) \times \frac{\sqrt{3}}{2} h^2 = \frac{23}{48} \times \frac{\sqrt{3}}{2} h^2 .$$

Hence, the two second order Gregory type quadrature formulas are $(GT2_1)$ and $(GT2_2)$ where $(GT2_1)$ is obtained by using formula (4.3.2) for each angle of Ω and formula (4.3.1) for the edges of Ω, while $(GT2_2)$ is obtained by using formula (4.3.3) instead of (4.3.2). Note that other second order formulas can also be obtained by taking the combinations of these two formulas.

When $m = 3$, then using formulas (4.2.2) and (4.2.24), we have

$$a(B_2) = b(B_2,B_2)+b(B_2,B_1)+b(B_2,B_3) = \left(\frac{5}{12} - \frac{1}{48} - \frac{1}{48}\right) \frac{\sqrt{3}}{2} h^2 = \frac{9}{24} \times \frac{\sqrt{3}}{2} h^2,$$

$$a(B_4) = b(B_4,B_4)+b(B_4,B_2)+b(B_4,B_3) = \left(1 + \frac{1}{12} + \frac{1}{12}\right) \frac{\sqrt{3}}{2} h^2 = \frac{28}{24} \times \frac{\sqrt{3}}{2} h^2,$$

$$a(B_5) = b(B_5,B_5)+b(B_5,B_2) = \left(1 - \frac{1}{24}\right) \frac{\sqrt{3}}{2} h^2 = \frac{23}{24} \times \frac{\sqrt{3}}{2} h^2.$$

Thus, the formula of $24 \times \frac{2}{\sqrt{3}} \frac{1}{h^2} \times a(X)$ for X along the edge of Ω is

$$\begin{array}{cccccc} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \\ \cdots & 24 & 24 & 24 & \cdots \\ \cdots & 24 & 24 & 24 & \cdots \\ \cdots & 23 & 23 & 23 & \cdots \\ \cdots & 28 & 28 & 28 & \cdots \\ \cdots & 9 & 9 & 9 & \cdots \end{array} \qquad (4.3.4)$$

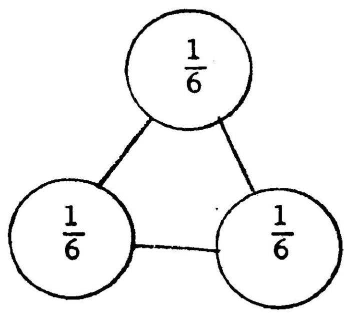
The formula of $96 \times \frac{2}{\sqrt{3}} \frac{1}{h^2} \times a(X)$ for X around a $60°$ angle of Ω is

$$\begin{array}{cccccc} \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \\ 36 & 112 & 92 & 96 & 96 & \cdots \\ 36 & 112 & 92 & 96 & 96 & \cdots \\ 31 & 108 & 88 & 92 & 92 & \cdots \\ 50 & 128 & 108 & 112 & 112 & \cdots \\ 6 & 50 & 31 & 36 & 36 & \cdots \end{array} \qquad (4.3.5)$$

if we use formulas (4.2.2), (4.2.24) and (4.2.13).

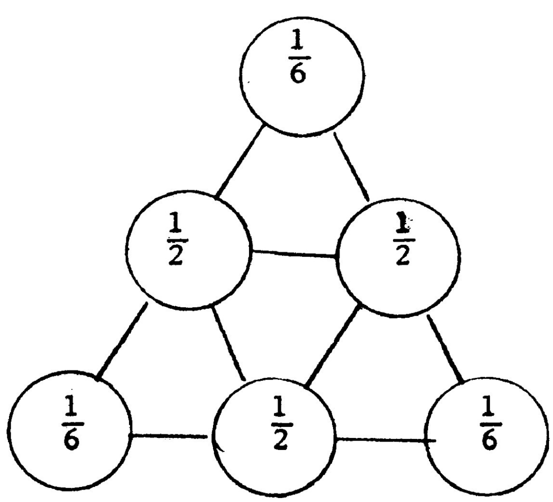
Hence, a third order Gregory type quadrature over Ω can be obtained by fixing each angle of Ω by formula (4.3.4) and each edge of Ω by formula (4.3.5).

Now, consider n is a small integer, say n = 1,2 or 3. When n = 1, then the first order Gregory type quadrature is simply



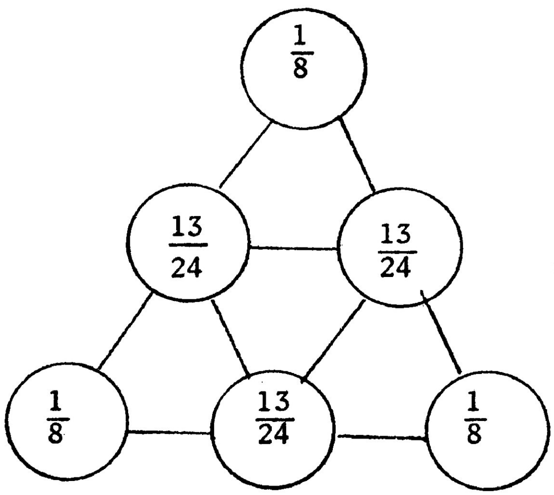
$$\times \frac{\sqrt{3}}{2} h^2 \qquad (4.3.6)$$

from (GT1). Observe that it is also a second order Gregory type quadrature, since it also can be computed by formulas (4.2.2) and (4.2.12); and a second order Newton-Cotes type quadrature. (See Chapter 3 and Sylvester [29].) When n = 2, the another first order Gregory type quadrature is



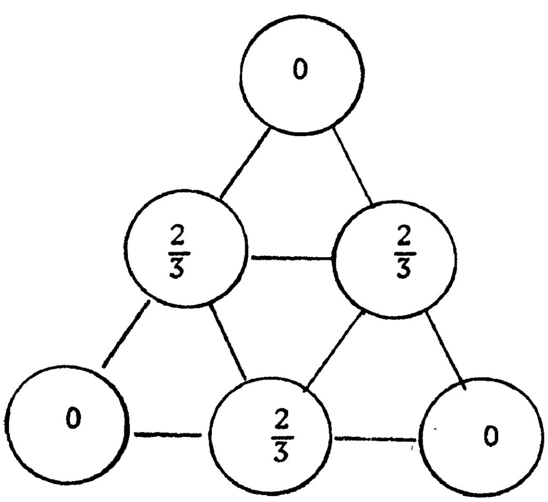
$$\times \frac{\sqrt{3}}{2} h^2 \qquad (4.3.7)$$

if we use formulas (4.2.2), (4.2.11) and (4.2.22). On the other hand, if we use formulas (4.2.2), (4.2.12) and (4.4.21), then we get the same formula as (4.3.7), but is a second order formula. Moreover, if we use (4.2.23), instead of (4.2.21), we get another second order Gregory type formula,



$$\times \frac{\sqrt{3}}{2} h^2 \qquad (4.3.8)$$

Note that, (4.3.7) and (4.3.8) are not the Newton-Cotes type formulas. When n = 3, we can easily get a third order Gregory type formula (and it is also a third order Newton-Cotes type formula) if we use formulas (4.2.2), (4.2.24) and (4.2.13), and it is



$$\times \frac{\sqrt{3}}{2} h^2 \qquad (4.3.9)$$

We observe that the above formulas also can be used for an arbitrary triangle ABC, but simply mulitplying by a constant, the area of ABC times $\frac{4}{\sqrt{3}n^2h^2}$.

4.4 FORMULAS OVER PARALLELOGRAMS

Let Ω be the parallelogram, with angles 60° and 120°, we will discuss, which is shown in Figure 4.4.1. Gregory type quadrature of the first three orders over Ω will follow from the formulas given in Section 4.2. We show them below.

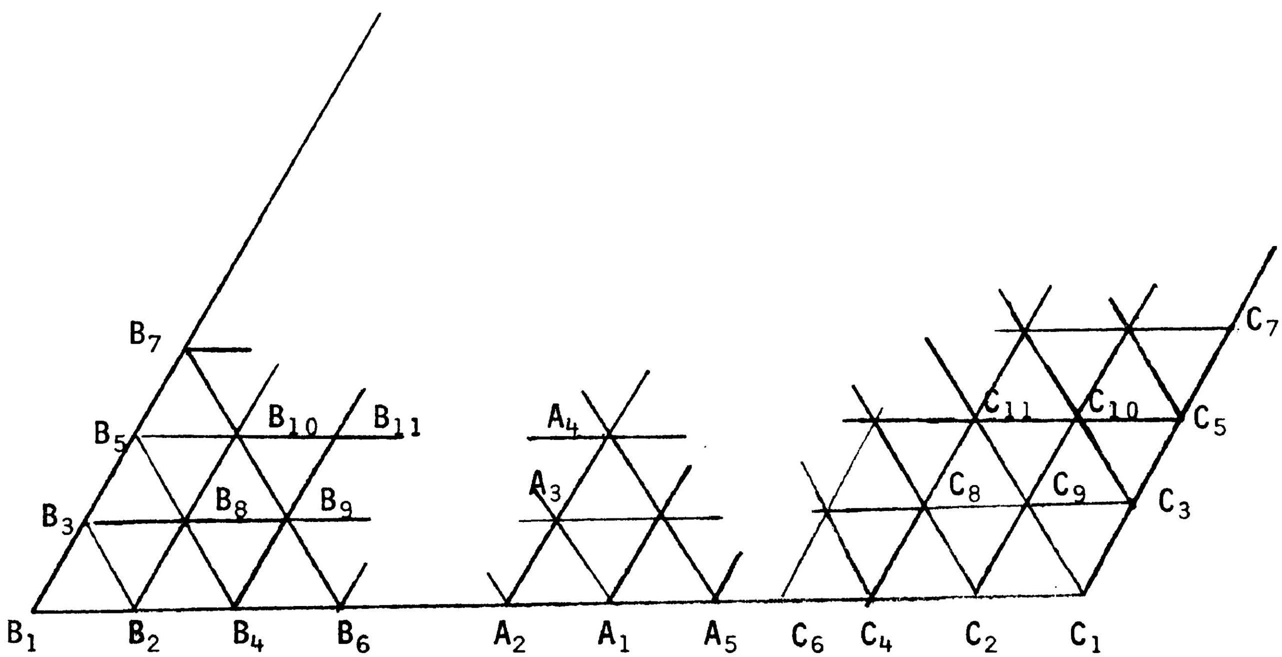


Figure 4.4.1

Note that the formulas of $a(X)$ for X along the edges and the 60° angles of Ω are the same as those of an equilateral triangles, which are given in Section 4.2 for $m = 1,2$ and 3.

(I) First order formula

In this case, the formula is simple, since the regular boundary layer of Ω is the set of points in V^b, and $a(X) = b(X,X)$ for all $X \in V$. As we mentioned before in section 4.2 that for any $X,Y \in V^i$, $b(X,Y) = 1 \times \frac{\sqrt{3}}{2} \times h^2$, if $X = Y$ and zero otherwise. If Y is the vertex of a 60° angle of Ω, then $b(X,Y) = \frac{1}{6} \times \frac{\sqrt{3}}{2} \times h^2$ if $X = Y$ and zero otherwise, from (4.2.11). If Y is the vertex of a 120° angle of Ω, then $b(X,Y) = \frac{1}{3} \times \frac{\sqrt{3}}{2} \times h^2$ if $X = Y$ and zero otherwise, from (4.2.14). In the case of $X \in V^b$ but not a vertex of Ω and $Y \in V^b$, then $b(X,Y) = \frac{1}{2} \times \frac{\sqrt{3}}{2} \times h^2$ if $X = Y$ and zero otherwise, from (4.2.22). Now, put these $b(X,X)$ (and hence $a(X)$) together, we have the first order Gregory type quadrature formula over Ω and it is,

(GG1)

```
  .  .  .    .  .  .    .  .  .
 .  .       .  .       .  .
  3   6 ...  6   6 ...  6   3
1   3  ... 3   3  ... 3   2
```

with a common factor $\frac{1}{6} \times \frac{\sqrt{3}}{2} \times h^2$.

(II) Second order formula

We only need to compute $a(X)$ for X are the four points which around a 120° angle of Ω, like C_1, C_2, C_3 and C_9 as shown in Figure 4.4.1. We may use formula (4.2.2), (4.2.15) and (4.2.21) when computing $a(X)$ for $X = C_1, C_2, C_3$ and C_9, and they are

$$a(C_1) = \left(\frac{10}{48} + \frac{1}{48} + \frac{1}{48}\right) \times \frac{\sqrt{3}}{2} h^2 = \frac{1}{4} \times \frac{\sqrt{3}}{2} h^2,$$

$$a(C_3) = a(C_2) = \left(\frac{3}{8} + \frac{1}{48} + \frac{3}{48}\right) \times \frac{\sqrt{3}}{2} h^2 = \frac{11}{24} \times \frac{\sqrt{3}}{2} h^2$$

and $$a(C_9) = \left(1 + \frac{1}{24} + \frac{1}{24}\right) \times \frac{\sqrt{3}}{2} h^2 = \frac{26}{24} \times \frac{\sqrt{3}}{2} h^2.$$

Thus, the formula of $48 \times \frac{2}{\sqrt{3}} \frac{1}{h^2} \times a(X)$ for X around a 120° angle of Ω is

$$\begin{array}{lcccc} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} \\ \cdots & 48 & 48 & 52 & 20 \\ \cdots & 48 & 48 & 52 & 20 \\ \cdots & 52 & 52 & 52 & 22 \\ \cdots & 20 & 20 & 22 & 12 \end{array} \qquad (4.4.1)$$

If we use formula (4.2.23) instead of (4.2.21), we have another formula of $48 \times \frac{2}{\sqrt{3}} \frac{1}{h^2} \times a(X)$ for X around a 120° angle of Ω and it is

$$\begin{matrix} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} \\ \cdots & 48 & 48 & 52 & 20 \\ \cdots & 48 & 48 & 52 & 20 \\ \cdots & 52 & 52 & 52 & 23 \\ \cdots & 20 & 20 & 23 & 10 \end{matrix} \qquad (4.4.2)$$

Similarly, if we use (4.2.18) instead of (4.2.15), we have another two formulas of $48 \times \frac{2}{\sqrt{3}} \frac{1}{h^2} \times a(X)$ for X around a 120° angle of Ω and they are

$$\begin{matrix} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} \\ \cdots & 48 & 48 & 52 & 20 \\ \cdots & 48 & 48 & 52 & 20 \\ \cdots & 52 & 52 & 54 & 20 \\ \cdots & 20 & 20 & 20 & 14 \end{matrix} \qquad (4.4.3)$$

and

$$\begin{matrix} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} \\ \cdots & 48 & 48 & 52 & 20 \\ \cdots & 48 & 48 & 52 & 20 \\ \cdots & 52 & 52 & 54 & 21 \\ \cdots & 20 & 20 & 21 & 12 \end{matrix} \qquad (4.4.4)$$

if we use (4.2.21) and (4.2.23) respectively.

Hence, we have four Gregory type formulas of second order, $GG2_1$, $GG2_2$, $GG2_3$, $GG2_4$, if we use formulas ((4.3.1), (4.3.2), (4.4.1)), ((4.3.1), (4.3.3), (4.4.2)), ((4.3.1), (4.3.2), (4.4.3)) and ((4.3.1), (4.3.3), (4.4.4)) respectively.

$(GG2_1)$

$$\begin{array}{ccccccccc} \iddots & \iddots & \iddots & & \iddots & & \iddots & \iddots & \iddots \\ 20 & 52 & 48 & \cdots & 48 & \cdots & 48 & 52 & 20 \\ 20 & 52 & 48 & \cdots & 48 & \cdots & 48 & 52 & 20 \\ 22 & 56 & 52 & \cdots & 52 & \cdots & 52 & 52 & 22 \\ 8 & 22 & 20 & \cdots & 20 & \cdots & 20 & 22 & 12 \end{array} \times \frac{1}{48} \times \frac{\sqrt{3}}{2} h^2$$

$(GG2_2)$

$$\begin{array}{ccccccccc} \iddots & \iddots & \iddots & & \iddots & & \iddots & \iddots & \iddots \\ 20 & 52 & 48 & \cdots & 48 & \cdots & 48 & 52 & 20 \\ 20 & 52 & 48 & \cdots & 48 & \cdots & 48 & 52 & 20 \\ 23 & 56 & 52 & \cdots & 52 & \cdots & 52 & 52 & 23 \\ 6 & 23 & 20 & \cdots & 20 & \cdots & 20 & 23 & 10 \end{array} \times \frac{1}{48} \times \frac{\sqrt{3}}{2} h^2$$

$(GG2_3)$

$$\begin{array}{ccccccccc} \iddots & \iddots & \iddots & & \iddots & & \iddots & \iddots & \iddots \\ 20 & 52 & 48 & \cdots & 48 & \cdots & 48 & 52 & 20 \\ 20 & 52 & 48 & \cdots & 48 & \cdots & 48 & 52 & 20 \\ 22 & 56 & 52 & \cdots & 52 & \cdots & 52 & 54 & 20 \\ 8 & 22 & 20 & \cdots & 20 & \cdots & 20 & 20 & 14 \end{array} \times \frac{1}{48} \times \frac{\sqrt{3}}{2} h^2$$

$(GG2_4)$

$$\begin{array}{ccccccccc} \iddots & \iddots & \iddots & & \iddots & & \iddots & \iddots & \iddots \\ 20 & 52 & 48 & \cdots & 48 & \cdots & 48 & 52 & 20 \\ 20 & 52 & 48 & \cdots & 48 & \cdots & 48 & 52 & 20 \\ 23 & 56 & 52 & \cdots & 52 & \cdots & 52 & 54 & 21 \\ 6 & 23 & 20 & \cdots & 20 & \cdots & 20 & 21 & 12 \end{array} \times \frac{1}{48} \times \frac{\sqrt{3}}{2} h^2$$

(III) Third order formula

In this case, we want to compute $a(X)$ for the nine points around a 120° angle of Ω, like $C_1,C_2,C_3,C_4,C_5,C_8,C_9,C_{10},C_{11}$ as shown in Figure (4.4.1). We may use formulas (4.2.2), (4.2.24), and (4.2.16) or (4.2.19), and $96 \times \frac{2}{\sqrt{3}}\frac{1}{h^2} \times a(X)$ are

$$\begin{array}{ccccc} & \iddots & \iddots & \iddots & \iddots \\ \cdots & 96 & 92 & 112 & 36 \\ \cdots & 92 & 88 & 112 & 33 \\ \cdots & 112 & 112 & 112 & 50 \\ \cdots & 36 & 33 & 50 & 10 \end{array} \qquad (4.4.5)$$

or

$$\begin{array}{ccccc} & \iddots & \iddots & \iddots & \iddots \\ \cdots & 96 & 92 & 112 & 36 \\ \cdots & 92 & 86 & 112 & 35 \\ \cdots & 112 & 112 & 120 & 42 \\ \cdots & 36 & 35 & 42 & 16 \end{array} \qquad (4.4.6)$$

these two formulas are computed in the same way as formulas (4.2.4). For example

$$a(C_4) = b(C_4,C_1)+b(C_4,C_4)+b(C_4,C_6)+b(C_4,C_2)$$

$$= \left(-\frac{3}{96}+\frac{5}{12}-\frac{1}{48}-\frac{1}{48}\right) \times \frac{\sqrt{3}}{2}h^2 = \frac{33}{96} \times \frac{\sqrt{3}}{2}h^2,$$

in formula (4.4.5).

Hence, we have the following two third order Gregory quadrature formulas ($GG3_1$) and ($GG3_2$),

($GG3_1$)

⋰	⋰	⋰	⋰			⋰	⋰	⋰	⋰
36	112	92	96	...	...	96	92	112	36
31	108	88	92	...	...	92	86	112	35
50	128	108	112	...	...	112	112	120	42
6	50	31	36	...	...	36	35	42	16

($GG3_2$)

⋰	⋰	⋰	⋰			⋰	⋰	⋰	⋰
36	112	92	96	...	...	96	92	112	36
31	108	88	92	...	...	92	88	112	33
50	128	108	112	...	...	112	112	112	50
6	50	31	36	...	...	36	33	50	10

where ($GG3_1$) and ($GG3_2$) are obtained by using formulas ((4.3.4), (4.3.5), (4.4.6)) and ((4.3.4), (4.3.5), (4.4.5)) respectively.

4.5 FORMULAS OVER RECTANGLES

In Section 4.4, we had computed some formulas for Gregory type quadrature of the first three orders on the parallelogram. In this section, the rectangle with its vertices in Γ, will be treated, but we only compute third order formula; first, second and higher order formulas will follow similarly.

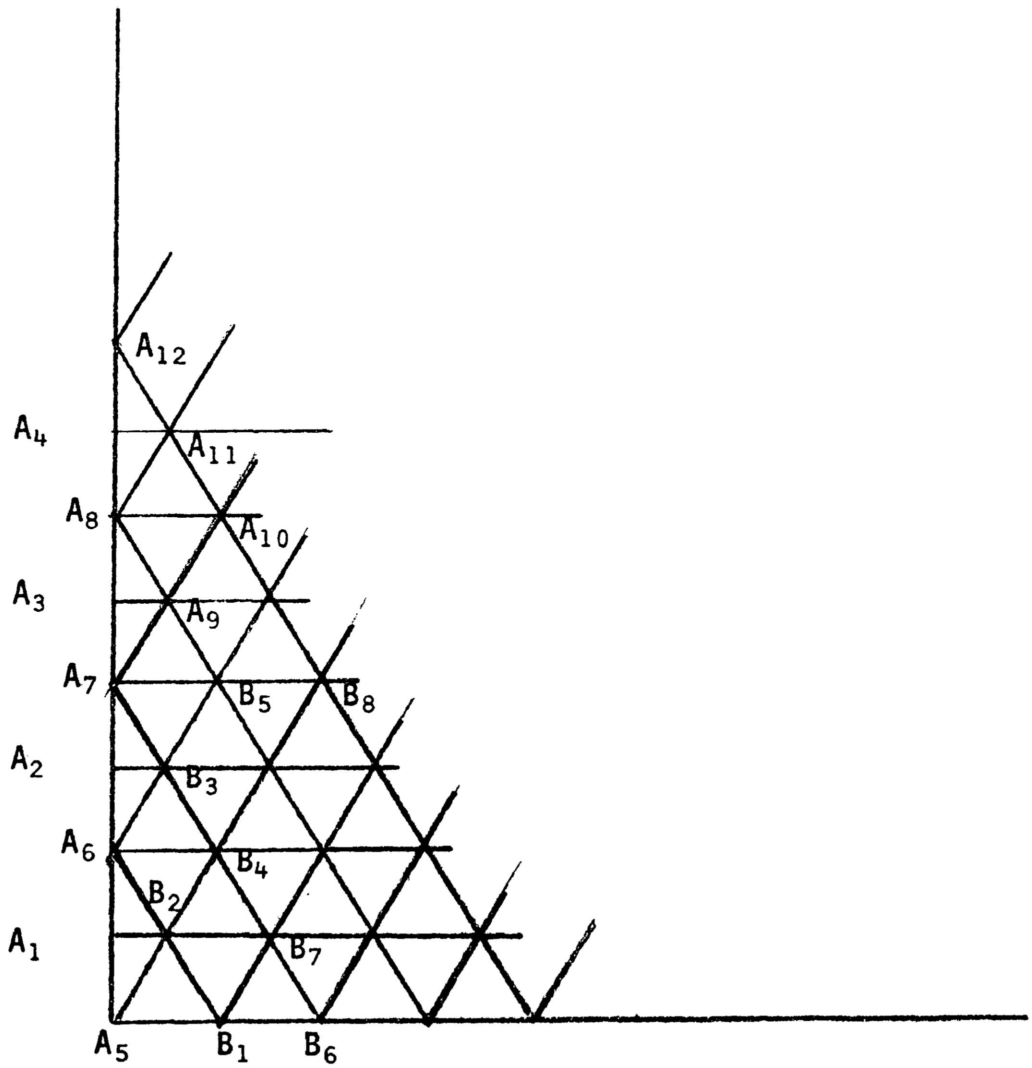


Figure 4.5.1

Consider the rectangle Ω as shown in Figure 4.5.1. We observe that along the horizontal edge of Ω, the formula of $a(X)$ should be the same as those of the triangle and is given in formula (4.3.4). We can expect the formula of $a(X)$ along the vertical edge of Ω will be the same as formula (4.3.4). In this case, we use formulas (4.2.2), (4.2.28), (4.2.31) and (4.2.34); and $a(X)$ are

$$a(A_8) = 24 \times \frac{\sqrt{3}}{2} h^2 \, [b(A_8,A_8)+b(A_8,A_4)+b(A_8,A_3)+b(A_8,A_9)+b(A_8,A_{11})$$

$$+b(A_8,A_7)+b(A_8,A_{12})]$$

$$= 24 \times \frac{\sqrt{3}}{2} h^2 \left(\frac{17}{2} - \frac{1}{16} - \frac{1}{16} + \frac{19}{16} + \frac{19}{16} - \frac{7}{8} - \frac{7}{8}\right. = \frac{9}{24} \times \frac{\sqrt{3}}{2} h^2,$$

$$a(A_9) = 24 \times \frac{\sqrt{3}}{2} h^2 [b(A_9,A_9)+b(A_9,A_{11})+b(A_9,B_3)+b(A_9,A_3)+b(A_9,A_4)$$

$$+b(A_9,A_2)+b(A_9,A_7)+b(A_9,A_8)]$$

$$= 24 \times \frac{\sqrt{3}}{2} h^2 \left[22\,\frac{5}{8} - \frac{5}{16} - \frac{5}{16} - \frac{7}{8} - \frac{1}{16} - \frac{1}{16} + \frac{7}{2} + \frac{7}{2}\right]$$

$$= \frac{28}{24} \times \frac{\sqrt{3}}{2} h^2,$$

and
$$a(A_{10}) = 24 \times \frac{\sqrt{3}}{2} h^2 \, [b(A_{10},A_{10})+b(A_{10},A_3)+b(A_{10},A_4)+b(A_{10},A_9)$$

$$+b(A_{10},A_{11})+b(A_{10},A_8)]$$

$$= 24 \times \frac{\sqrt{3}}{2} h^2 \left[24 + \frac{1}{16} + \frac{1}{16} + \frac{5}{16} + \frac{5}{16} - \frac{7}{4}\right] = \frac{23}{24} \times \frac{\sqrt{3}}{2} h^2.$$

Note that $(A_9+H)\ \Omega \neq A_9+H$, and hence $b(A_9,A_9) \neq 1 \times \frac{\sqrt{3}}{2} h^2$.

Now, let us compute the coefficients $a(X)$ for X around a right angle of Ω, which is shown in Figure 4.5.1. If we use formulas (4.2.24), (4.2.28) — (4.2.34) and (4.2.26), we get a third order Gregory type quadrature ($GR3_1$). If we use (4.2.27) instead of (4.2.26), we get another formula ($GR3_2$). The formula ($GR3_3$) is computed by using average of (4.2.26) and (4.2.27) instead of (4.2.26) or (4.2.27).

($GR3_1$) :

144	⋮								
	448	⋮							
144		368	⋮						
	448		384						
144		368		384	⋯				
	442		384		384	⋯			
164		350		368		368	⋯		
	462		448		448		448	⋯	
53		164		141		144		144	⋯

$(GR3_2)$

⋮								
144	⋮							
	448	⋮						
144		368	⋮					
	448		384					
147		368		384 ...				
	442		384		384 ...			
152		344		368		368 ...		
	486		448		448		448 ...	
53		152		144		144		144 ...

$(GR3_3)$

⋮								
288	⋮							
	896	⋮						
288		736	⋮					
	896		768					
291		736		768 ...				
	884		768		768 ...			
316		694		736		736 ...		
	948		896		896		896 ...	
106		316		285		288		288 ...

Note that these formulas are computed in the similar way as above (when we compute the formula along the edge). For example,

$$a(B_1) = b(B_2,B_2)+b(B_2,A_1)+b(B_2,B_3)+b(B_2,A_2)+b(B_2,B_1)+b(B_1,A_6)$$

$$+b(B_2,A_5)$$

$$= \left(22\,\frac{5}{8} - \frac{7}{8} - \frac{5}{16} - \frac{1}{16} + 2 + \frac{7}{2} + 2\right) \times \frac{16}{16\times 24}\,\frac{\sqrt{3}}{2}\,h^2 =$$

$$462 \times \frac{1}{384} \times \frac{\sqrt{3}}{2}\,h^2,$$

$$a(A_7) = b(A_7,A_7)+b(A_7,A_2)+b(A_7,B_3)+b(A_7,A_8)+b(A_7,A_6)+b(A_7,A_3)$$

$$+b(A_7,A_9)+b(A_7,A_5)$$

$$= \left(\frac{17}{2} - \frac{1}{16} + \frac{19}{16} - \frac{7}{8} - \frac{7}{8} - \frac{1}{16} + \frac{19}{16} + 0\right) \times \frac{16}{384} \times \frac{\sqrt{3}}{2}\,h^2 =$$

$$144 \times \frac{1}{384} \times \frac{\sqrt{3}}{2}\,h^2,$$

for ($GR3_1$) and

$$a(B_2) = \left(22\,\frac{5}{8} - \frac{7}{8} - \frac{5}{16} - \frac{1}{16} + 2 + \frac{7}{2} + \frac{7}{2}\right) \times \frac{16}{384} \times \frac{\sqrt{3}}{2}\,h^2 =$$

$$486 \times \frac{1}{384} \times \frac{\sqrt{3}}{2}\,h^2,$$

and $a(A_7) = \left(\frac{17}{2} - \frac{1}{16} + \frac{19}{16} - \frac{7}{8} - \frac{7}{8} - \frac{1}{16} + \frac{19}{16} + \frac{3}{16}\right) \times \frac{16}{384} \times \frac{\sqrt{3}}{2}\,h^2$

$$= 147 \times \frac{1}{384} \times \frac{\sqrt{3}}{2}\,h^2,$$

for ($GR3_2$).

APPENDIX

In this appendix, we list some working APL functions for computing the two dimensional Newton-Cotes coefficients $a_{\mathbf{i}}$. (See (3.1.4).) The function COD is the main function. If we type COD N, where N is a positive integer, then the output will be a $m \times 5$ matrix, $m \geq N$, of which the first three columns represent the index vectors $\mathbf{i}$, the fourth column represents $d \times a_{\mathbf{i}}$, and the last column represents d, as shown in Table 3.1.1. Note that all functions in the list, except ST and PROD1 (which are of)ORIGIN 1), are of)ORIGIN 0 (see Pakin [16, P.141]), and the matrix SN of Stirling numbers (which is computed by typing SN ← ST N) must be present in the active workspace before we use the main function COD.

```
    ∇ C←COD N;S;J
[1]    C←ρS←0
[2]    I←COC N
[3]   L1:C←C,J,CO J←I[S;]
[4]    →(((ρI)[0])>S←S+1)/L1
[5]    C←(((ρC)÷5),5)ρ⌊C
    ∇
```

```
    ∇ I←COC N;N1;L;M;K;S;T
[1]    I←ιS←0
[2]    K←,K←COB N
[3]   L1:→(K[S]<N1←N-K[S])/L3
[4]    →L5
[5]   L3:→(K[S]<N1←N1-1)/L3
[6]   L5:L←,L←COB N1
[7]    T←0
[8]   L2:→(L[T]<M←N-L[T]+K[S])/L4
[9]    I←I,,K[S],L[T],M
[10]  L4:→((ρL)>T←T+1)/L2
[11]   →((ρK)>S←S+1)/L1
[12]   I←(((ρ,I)÷3),3)ρI
    ∇
```

```
    ∇ C←CO I;L;M;K;S;T;U;E;D
[1]    N←+/I
[2]    C←ρK←L←M←0
[3]    U←I[1+ρ,T←I[ρ,S←I[0]]]
[4]   L1:KLM←(N*L+K+M)×(!K)×(!L)×(!M)
[5]    C←C,SN[S;K]×SN[T;L]×SN[U;M]×KLM××/(L+K+M+2)↓1+ιN+2
[6]    →(S≥K←K+1)/L1
[7]    K←0
[8]    →(T≥L←L+1)/L1
[9]    L←0
[10]   →(U≥M←M+1)/L1
[11]   C←2×+/C
[12]   D←C GD!N+2
[13]   E←D[0] GD(!S)×(!T)×(!U)
[14]   C←E[0],D[1]×E[1]
    ∇
```

```
      ∇ K←COB N
[1]     →(N>0)/L1
[2]     K←0
[3]     →0
[4]   L1:K←⌽(¯1+⌈N÷3)↓1+⍳N
      ∇
```

```
      ∇ D←A GD B;A1;B1
[1]     A1←A
[2]     B1←B
[3]     G←A GCD B
[4]     D←(A1÷G),B1÷G
      ∇
```

```
      ∇ G←X GCD Y;B
[1]     →((X←|X)≥(Y←|Y))/L1
[2]   L2:B←X
[3]     X←Y
[4]     Y←B
[5]   L1:X←Y|X
[6]     →(X>0)/L2
[7]     G←Y
      ∇
```

```
      ∇ S←ST N;P;I;II
[1]     S←((N+1),N+1)⍴0
[2]     S[1;]←S[;1]←1,N⍴0
[3]     S[2;2]←1
[4]     P← 0 1
[5]     II←-¯2+I←3
[6]   L1:S[I;]←(P←(II,1) PROD1 P),(N+II-1)⍴0
[7]     II←II-1
[8]     →((N+1)≥I←I+1)/L1
      ∇
```

```
      ∇ P←P1 PROD1 P2
[1]     P←+/[1]((⍴P2),¯1+⍴P1)⍴,P2∘.×(P1←P1,(⍴P2)⍴0)
      ∇
```

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