Boundary type quadrature formulas over axially symmetric regions

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Abstract

A boundary type quadrature formula (BTQF) is an approximate integration formula with all its of evaluation points lying on the boundary of the integration domain. This type formulas are particularly useful for the cases when the values of the integrand functions and their derivatives inside the domain are not given or are not easily determined. In this paper, we will establish the BTQFs over some axially symmetric regions. We will discuss the following three questions in the construction of BTQFs: (i) What is the highest possible degree of algebraic precision of the BTQF if it exists? (ii) What is the fewest number of the evaluation points needed to construct a BTQF with the highest possible degree of algebraic precision? (iii) How to construct the BTQF with the fewest evaluation points and the highest possible degree of algebraic precision?

1 Introduction

Although numerical multivariate integration is an old subject, it has never been applied as widely as it is now. We can find its applications everywhere in math, science, and economics. A good example might be the collateralized mortgage obligation (CMO), which can be formulated as a multivariate integral over the 180-dimensional unit cube ([2]). A boundary quadrature formula is an approximate integration formula with all its evaluation points lying on the boundary of the domain of integration. Such a formula may be particularly useful for the cases when the values of the integrand function and its derivatives inside the domain are not given or are not easily determined.

Indeed, boundary quadrature formulas are not really new. From the viewpoint of numerical analysis, the classical Euler-Maclaurin summation formula and the Hermite two-end multiple nodes quadrature formulas may be regarded as one-dimensional boundary quadrature formulas since they make use of only the integrand function values and their derivatives at the limits of integration. The earliest example of a boundary quadrature formula with some algebraic precision for multivariate integration is possibly the formula of algebraic precision (or degree) 5 for a triple integral over a cube given by Sadowsky [30] in 1940. He used 42 points

on the surface of a cube to construct the quadrature, which has been modified by the author with a quadrature of 32 points, the fewest possible boundary points (see [9] and [10]). Some 20 years later after Sadowsky's work, Levin [26] and [27], Federenko [6], and Ionescu [21] investigated individually certain optimal boundary quadrature formulas for double integration over a square using partial derivatives at some boundary points of the region. Despite these advances, however, both the general principle and the general technique for construction remained lacking for many years.

During 1978-87, based on the ideas of the dimension-reducing expansions (DRE) of multivariate integration shown in Hsu 1962 and 1963, Hsu, Wang, Zhou, Yang, and the author developed a general process for the construction of BTQFs in [17]-[20] and [9]-[15].

The analytic approach for constructing BTQFs is based on the dimension-reducing expansions (DRE), which reduces a higher dimensional integral to lower dimensional integrals with or without a remainder. Hence, a type of boundary quadratures can be constructed by using the expansions.

The DRE without remainder is also called an exact DRE. Obviously, a DRE can be used to reduce the computation load of many very high dimensional numerical integration's, such as the CMO problem mentioned above. Most DRE's are based on Green's Theorem in real or complex field. In 1963, using the theorem, Hsu [17] devised a way to construct a DRE with algebraic precision (degree of accuracy) for multivariate integrations. From 1978 to 1986, Hsu, Zhou, and the author (see [18], [19], [20], and [**?**]) developed a more general method to construct a DRE with algebraic precision and estimate its remainder. In 1972, with the aid of Green's Theorem and the Schwarz function, P.J. Davis [4] gave an exact DRE for a double integral over a complex field. In 1979, also by using Green's Theorem, Kratz [24] constructed an exact DRE for a function that satisfied a type of partial differential equations. Lastly, if we want this introduction to be complete, we must not overlook Burrows' DRE for measurable functions. His DRE can reduce a multivariate integration into an one dimensional integral. Some important applications of DRE include the construction of BTQFs and asymptotic formulas for oscillatory integrals, for instance, the integrals on spheres, $S^d = \{x \in R^d : |x| = 1\}$ and balls, $B^d = \{x \in R^d : |x| \leq 1\}$, presented by Kalnins, Miller, Jr., and Tratnik [22], Lebedev and Skorokhodov [25], Mhaskar, Narcowich, and Ward [28], Xu [35], etc.

In this paper, we will discuss the algebraic approach to constructing BTQFs for a multiple integral over a bounded closed region Ω in $\mathbb{R}^n$, which is of the form

$$\int_\Omega w(X)f(X)dX.$$

In this expression, $w(X)$ and $f(X)$ are continuous on Ω, and $w(X)$ is the weight function. ($w(X)$ can be 1 particularly.) We are seeking the BTQF of the integral with the form

$$\int_\Omega w(X)f(X)dX \approx \sum_{0\leq m_1+\cdots+m_n\leq m} \sum_{i\in I} a_i^{m_1,\cdots,m_n} D^{m_1,\cdots,m_n} f(X_i), \qquad (1)$$

where dX is the volume measure; $a_i^{m_1,\cdots,m_n}$ ($i \in I$ and $0 \leq m_1 + \cdots + m_n \leq m$) are real or complex quadrature coefficients; $D^{m_1,\cdots,m_n} = \partial^{m_1+\cdots+m_n} / \partial x_1^{m_1} \cdots x_n^{m_n}$;

and $X_i = (x_{i,1}, x_{i,2}, \cdots, x_{i,n})$ $(i \in I)$ are evaluation points (or nodes) of f on $\partial\Omega$, the boundary of Ω. In particular, when $m = 0$ we write $a_i^{m_1,\cdots,m_n} = a_i$ and formula (1) can be rewritten as

$$\int_\Omega w(X)f(X)dX \approx \sum_{i\in I} a_i f(X_i). \tag{2}$$

(2) is called a *BTQF without derivative terms*. When $m \neq 0$, (1) is called a *BTQF with derivative terms*. The corresponding error functionals of approximations (1) and (2) are defined respectively by

$$\begin{aligned} E(f) \equiv E(f;\Omega) &= \int_\Omega w(X)f(X)dX \\ &- \sum_{0\le m_1+\cdots+m_n\le m} \sum_{i\in I} a_i^{m_1,\cdots,m_n} D^{m_1,\cdots,m_n} f(X_i) \end{aligned} \tag{3}$$

and

$$E(f) \equiv E(f;\Omega) = \int_\Omega w(X)f(X)dX - \sum_{i\in I} a_i f(X_i). \tag{4}$$

Suppose that $\partial\Omega$ can be described by a system of parametric equations. In particular, the points $X = (x_1, \cdots, x_n)$ on $\partial\Omega$ satisfy the equation

$$\Phi(X) = 0, \tag{5}$$

where Φ has continuous partial derivatives. In addition, $\Phi(X) \le 0$ for all points in Ω.

Let S be another region in $\mathbb{R}^n$, and let $J : Y = JX$, $X \in \Omega$, be a transform from Ω to S with positive Jacobian

$$|J| = \left|\frac{\partial(Y)}{\partial(X)}\right| > 0,$$

$X \in \Omega$. J is one-to-one and has the inverse $J^{-1} : X = J^{-1}Y$, $Y \in S$. Denote $w_1(Y) = w_1(JX) = w(X)$. Then for any continuous function $g(X)$

$$\int_S w_1(Y)g(Y)dY = \int_\Omega w_1(Y)g(Y)|J|dX.$$

Denoting $Y_i = JX_i$ $(i \in I)$, $|J_i| = |J|_{X=X_i}$, and taking $f(X) = |J|g(Y) = |J|g(JX)$ in equation (4), we obtain

$$E(|J|g;\Omega) = \int_\Omega w(X)|J|g(Y)dX - \sum_{i\in I} a_i|J_i|g(Y_i) = \int_S w_1(Y)g(Y)dY - \sum_{i\in I} b_i g(Y_i),$$

where $b_i = a_i|J_i|$ $(i \in I)$. Obviously, if Y, the boundary points of S, satisfy $\Phi_1(Y) = \Phi_1(JX) = \Phi(X) = 0$, then J maps the boundary evaluation points X_i $(i \in I)$ on Ω onto the boundary evaluation points $Y_i = JX_i$ on S. Consequently, we have the following result.

Theorem 1 *Let the error functional of the quadrature formula*

$$\int_S w_1(Y)g(Y)dY \approx \sum_{i\in I} b_i g(Y_i) \tag{6}$$

be $E(g;S) = \int_S w_1(Y)g(Y)dY - \sum_{i\in I} b_i g(Y_i)$. *Then* $E(g;S) = E(|J|g;\Omega)$. *In particular, if* $|J|$ *is a constant, then* $E(g;S) = |J|E(g;\Omega)$. *In this case,* $E(g;\Omega) = 0$ *implies* $E(g;S) = 0$.

In addition, if the boundary of S *is defined by* $\Phi_1(Y) = \Phi_1(JX) = \Phi(X) = 0$ *and* $\Phi(X) = 0$ *defines the boundary of* Ω, *then quadrature formula (6) is also a BTQF.*

In this paper, we will establish the BTQFs over some axially symmetric regions or fully symmetric regions (see the definitions below). Theorem 1 tells us that we can construct the BTQFs over many more regions from the obtained BTQFs over the special regions by using certain transforms. In addition, if the transform is linear, then the new BTQF is of the same algebraic precision degree as the old BTQF.

2 BTQFs without derivatives

Three questions arise during the construction of BTQFs (1):

(i) What is the highest possible degree of algebraic precision of the BTQF if it exists?

(ii) What is the fewest number of the evaluation points needed to construct a BTQF with the highest possible degree of algebraic precision?

(iii) How to construct the BTQF with the fewest evaluation points with the fewest evaluation points and the highest possible degree of algebraic precision?

We now answer the first question. In most cases, BTQF (1) has an inherent highest degree of algebraic precision. For instance, if $\Phi(X)$ is a polynomial of degree m, then the highest possible degree of algebraic precision of the BTQF without derivative terms (i.e., formula (2)) cannot exceed $m-1$ because the summation on the right-hand side of (2) becomes zero and the integral value on the left-hand side is negative when $f = \Phi$. Hence, when the boundary function Φ is a polynomial of a low degree, to raise the degrees of algebraic precision of the quadrature formulas, we must construct BTQFs with derivative terms (i.e., formula (1) with $m \neq 0$).

In the following, we are going to find the solutions to questions (ii) and (iii). To simplify our discussion, we limit the region in question, Ω, to be axially symmetric or fully symmetric. An *axially symmetric region* is a region that for any point $X = (x_1, \cdots, x_n)$ in it, must contain all points with the form $(\pm x_1, \cdots, \pm x_n)$. The set of axially symmetric points associated with X forms a reflection group. If a region containing a point $X = (x_1, \cdots, x_n)$ also contains all points $(\pm a_1, \cdots, \pm a_n)$, where $(a_1, \cdots, a_n)$ is a permutation of $(x_1, \cdots, x_n)$, then the region is called a *fully symmetric region*. Throughout, we will denote all fully symmetric points, $(\pm a_1, \cdots, \pm a_n)$, associated with X by X_{FS} and call X the generator of the fully symmetric point set. The cardinal number of the set of fully symmetric points

associated with a generator $X \in \mathbb{R}^n$ is $2^n(n!)$. Obviously, a fully symmetric region is an axially symmetric region, but the converse is not true.

A quadrature formula is called a *fully symmetric quadrature formula* if the quadrature sum can be divided into several subsums such that in each of the subsums, the evaluation points are fully symmetric and the corresponding quadrature coefficients are the same. In addition, if the fully symmetric evaluation points are on the boundary of the integral region, then the corresponding quadrature formula is called a *fully symmetric BTQF.*

Denote a monomial in terms of X by X^α ($\alpha \in \mathbb{Z}_0^n$), which can be written in the form $X^\alpha = x_1^{\alpha_1}, \cdots, x_n^{\alpha_n}$, where $(\alpha_1, \cdots, \alpha_n)$ is called the exponent of X^α.

From the definition of the fully symmetric region, we immediately have the following results.

Theorem 2 *The value of a multiple integral of a monomial X^α over an axially symmetric region is zero if α contains an odd component. The value of a multiple integral of X^α over a fully symmetric region depends on α, but is independent of the order of α_i ($i = 1, \cdots, n$).*

Theorem 3 *Denote by $\pi_r^n(X)$ the set of all polynomials of degree no greater than r. Let Ω be a fully symmetric region,*

$$\int_\Omega f(X)dX \approx \sum_{i \in I} a_i f(X_i) \tag{7}$$

be a fully symmetric BTQF, and $E : f \to \mathbb{R}$ be the error operator defined by

$$E(f) \equiv E(f; \Omega) = \int_\Omega f(X)dX - \sum_{i \in I} a_i f(X_i).$$

(The above expression is a special form of (4) with $w(X) = 1$.) Then $\pi_{2k+1}^n \subset N(E)$, the null space of E, if and only if

$$x_1^{2k_1} \cdots x_n^{2k_n} \in N(E) \quad 0 \le k_1 \le \cdots \le k_n,\ k_1 + \cdots + k_n \le k. \tag{8}$$

Theorem 3 can be considered as the general principle for constructing fully symmetric BTQFs. First, we set one or more sets of fully symmetric evaluation points, with possibly some unknown points $\{X_i\}$, on the boundary $\partial\Omega$ and assume the quadrature coefficients a_i corresponding to each set to be the same. Then substituting all $f(X) = x_1^{2k_1} \cdots x_n^{2k_n}$ ($0 \le k_1 \le \cdots \le k_n$ and $k_1 + \cdots + k_n \le k$) into $E(f) = 0$, we obtain a system about X_i and a_i. Finally, we solve the system for X_i and a_i and a quadrature formula is constructed. However, a fully symmetric quadrature formula usually has too many evaluation points. (Remember that for a point $X \in \mathbb{R}^n$ there are, in general, $2^n(n!)$ fully symmetric points.) In order to reduce the number of evaluation points in the quadrature formula, we can use an alternative form of Theorem 3 to construct a different type of symmetric quadrature formulas. We will use the following example to illustrate the idea.

Example 1. Consider a triple integral over the region $C_3 = [-1, 1]^3$. Obviously, the inherent highest degree of algebraic precision of the BTQF

is 5. To construct a fully symmetric BTQF, we make use of the following fully symmetric evaluation points.

$$(1,0,0)_{FS}, \quad (1,1,0)_{FS}, \quad \text{and} (1,x_0,x_0)_{FS},$$

where x_0 $(0 < x_0 < 1)$ is undetermined. The three sets of fully symmetric points contain a total of 42 points (6, 12, and 24 points for the first, second, and third set respectively). Let the respective quadrature coefficients for each set of fully symmetric points be L, M, and N, all of which can be found using the general principle for constructing fully symmetric BTQFs. Substitute $f = 1$, x^2, x^4, and x^2y^2 into

$$\int_{C_3} f(x,y,z)dxdydz = a_1 \sum f_6 + a_2 \sum f_{12} + a_3 \sum f_{24},$$

where $\sum f_6$, $\sum f_{12}$, and $\sum f_{24}$ are the sums of the function values of f over the first, second, and third set of symmetric points, respectively. Solving the above system yields

$$x_0 = \sqrt{\frac{5}{8}}, \ a_1 = \frac{364}{225}, \ a_2 = -\frac{160}{225}, \ a_3 = \frac{64}{225},$$

giving the following BTQF of algebraic precision order 5.

$$\int_{C_3} f(x,y,z)dxdydz \approx \frac{4}{225}\left[91\sum f_6 - 40\sum f_{12} + 16\sum f_{24}\right]. \tag{9}$$

Quadrature formula (9), given by Sadowsky [30], uses too many evaluation points. Carefully considering Theorem 3, we find that the principle of constructing fully symmetric BTQFs shown in the theorem can be used to construct some "partial" symmetric BTQFs with fewer evaluation points.

A set of points $X_i \in \mathbb{R}^n$ $(i \in I)$ is called a *symmetric point set of degree k* if it possesses the following two properties.

(a) $\sum_{i\in I} f(X_i) = 0$ for all $f(X) = X^\alpha$, where α contains an odd component.

(b) $\sum_{i\in I} f(X_i)$ are the same for all $f(X) = x_1^{2k_1}\cdots x_n^{2k_n}$, $2(k_1 + \cdots + k_n) = r$. Here, $r \le k$.

Obviously, a set of fully symmetric points must be a set of symmetric points of any degree, but the converse is not true. For instance, a symmetric point set of degree 5 may not be a fully symmetric point set. We now list all symmetric point sets of degree 5 on the boundary of C_3 as follows. $I = \{(\pm1, \pm x_0, 0), (\pm x_0, 0, \pm1), (0, \pm1, \pm x_0), 0 < x_0 < 1\}$, $II = \{(\pm y_0, \pm1, 0), (\pm1, 0, \pm y_0), (0, \pm y_0, \pm1), 0 < y_0 < 1\}$, $III = \{(\pm1, \pm1, 0), (\pm1, 0, \pm1), (0, \pm1, \pm1)\}$, $IV = \{(\pm1, \pm1, \pm1)\}$, $V = \{(1,0,0)_{FS}\}$, $VI = \{(1, x_1, x_2)_{FS}, 0 < x_1, x_2 < 1\}$, $VII = \{(1,1,x_3)_{FS}, 0 < x_3 < 1\}$, where sets V, VI, and VII are fully symmetric, but others are not.

If a BTQF constructed by using symmetric point set of degree k satisfies condition (8), then it is called a *symmetric BTQF of degree k*.

Example 2. As an example, we now use the sets I, III, and IV to construct a symmetric BTQF of degree 5 with 32 evaluation points over C_3. Denote the quadrature coefficients corresponding to I, III, and IV as a_1, a_2, and a_3 respectively.

Following the procedure shown in Example 1, we obtain a symmetric BTQF of degree 5 as follows

$$\begin{aligned}&\int_{C_3} f(x,y,z)dxdydz\\ \approx\ &\frac{1}{63}\left[80\sum f_{12}(I)-52\sum f_{12}(III)+21\sum f_8(IV)\right],\end{aligned}\tag{10}$$

$\sum f_{12}(I)$, $\sum f_{12}(III)$, and $\sum f_8(IV)$ are the sums of the function values of f over the symmetric point sets I, III, and IV, respectively; the numbers in the sub-indices are the cardinal numbers of the corresponding set.

Similarly, we can use sets II, III, and IV to construct another symmetric BTQF of degree 5.

$$\begin{aligned}&\int_{C_3} f(x,y,z)dxdydz\\ \approx\ &\frac{1}{63}\left[80\sum f_{12}(II)-52\sum f_{12}(III)+21\sum f_8(IV)\right],\end{aligned}\tag{11}$$

where $y_0=\sqrt{\frac{3}{10}}$ in set II.

Quadratures (10) and (11) can be considered as two special cases of the following symmetric BTQF of degree 5, which is constructed by using I, II, and IV.

$$\begin{aligned}&\int_{C_3} f(x,y,z)dxdydz\approx\frac{4(1+y_0^2)}{9(y_0^2-x_0^2)}\sum f_{12}(I)\\ &+\frac{4(1+x_0^2)}{9(x_0^2-y_0^2)}\sum f_{12}(II)+\frac{1}{3}\sum f_8(IV),\end{aligned}\tag{12}$$

where

$$\sqrt{\frac{3}{10}}\le y\le 1,\ y_0\neq\sqrt{\sqrt{\frac{13}{5}}-1},\ \text{and}\ x_0=\sqrt{\frac{8-5y_0^2}{5(1+y_0^2)}}.$$

When $y_0=1$ and $y_0=\sqrt{\frac{3}{10}}$ we obtain formulas (10) and (11), respectively.

It can be proved that the minimum number of evaluation points of symmetric BTQFs is 32. Since the quadrature formula is symmetric, on each boundary plane we must have the same number of evaluation points. Let the number of evaluation points on each boundary plane be $k=2$ (Obviously, k cannot be 1). The symmetric point set has to be I or II. It is easy to check that the sets cannot yield a symmetric BTQF of degree 5. Similarly, for the cases of $k=3,\cdots,9$, no matter which symmetric point sets are chosen from $\{I,\cdots,VII\}$, we find that there does not exist any symmetric BTQFs of degree 5 with evaluation points less than 32. For $k\ge 10$, every symmetric BTQF of degree 5, if it exists, must have more than 32 evaluation points. Thus, we obtain the following proposition.

Proposition 4 *There exist infinitely many symmetric BTQFs of degree* 5 *with* 32 *evaluation points. In addition, the number of evaluation points of a symmetric BTQFs of degree* 5 *can not be less than* 32.

For BTQFS of degree 3, the minimum number of the evaluation points is reduced to 6. As an example, we give the following formula.

$$\int_{C_3} f(x,y,z)dxdydz \approx \frac{4}{3}\left[f(1,0,0)+f(-1,0,0)\right.$$
$$\left.+f(0,1,0)+f(0,-1,0)+f(0,0,1)+f(0,0,-1)\right].$$

Example 3. We will use a double layered spherical shell as an example to demonstrate the techniques of regrouping evaluation points to obtain the symmetric BTQF with the fewest evaluation points. A double layered spherical shell in $\mathbb{R}^n$, denoted by Sh_n, is defined by

$$Sh_n = \{X \in \mathbb{R}^n : a^2 \le |X| \le b^2\}.$$

It is easy to find that the largest degree of algebraic precision of BTQFs over Sh_n without derivatives is 3. We choose the following point sets as evaluation points: $VIII = \{(\pm b, 0, \cdots, 0), (0, \pm b, 0, \cdots, 0), \cdots, (0, \cdots, 0, \pm b, 0)\}$, $IX = \{(0, \cdots, 0, \pm b)\}$, $X = \{(0, \cdots, 0, \pm a)\}$.

Obviously, these sets are neither fully symmetric point sets nor symmetric point sets of degree 3, but by using these sets, we can construct a BTQF of degree 3 over Sh_n with the fewest evaluation points. Denote the quadrature coefficients corresponding to VIII, IX, and X by a_1, a_2, and a_3, respectively. The BTQF generated,

$$\int_{Sh_n} f(X)dX \approx a_1 \sum f_{2(n-1)}(VIII) + a_2 \sum f_2(IX) + a_3 \sum f_2(X), \qquad (13)$$

is of algebraic precision of degree 3 if it holds exactly for $f = 1$, x_1^2, and x_n^2; i.e., coefficients a_i $(i = 1, 2, 3)$ have to be

$$\begin{aligned} a_1 &= \alpha(b^2 - a^2)\left(b^{n+2} - a^{n+2}\right) \\ a_2 &= \alpha\left(b^{n+4} + (n+1)a^{n+2}b^2 - 3b^{n+2}a^2 - (n-1)a^{n+4}\right) \\ a_3 &= \alpha b^2\left(2b^{n+2} - (n+2)a^n b^2 + na^{n+2}\right), \end{aligned}$$

where

$$\alpha = \frac{\pi^{n/2}}{2b^2\Gamma\left(\frac{n}{2}+1\right)(n+2)(b^2-a^2)}.$$

When $n = 2$ and 3, formula (13) gives BTQFs over a ring domain and a 3-dimensional double layered spherical shell respectively as follows.

$$\begin{aligned} &\int_{Sh_2} f(x,y)dxdy \\ \approx\ &\frac{\pi(b^2-a^2)}{8b^2}\left\{(b^2+a^2)[f(b,0)+f(-b,0)] + 2b^2[f(0,a)+f(0,-a)]\right. \\ &\left.+(b^2-a^2)[f(0,b)+f(0,-b)]\right\} \end{aligned}$$

$$\begin{aligned}
&\int_{Sh_3} f(x,y,z)dxdydz \\
\approx\ & \frac{2\pi}{15b^2(b^2-a^2)}\left\{(b^2-a^2)(b^5-a^5)[f(b,0,0)+f(-b,0,0)+f(0,b,0)\right. \\
&+f(0,-b,0)]+b^2(2b^5-5a^3b^2+3a^5)[f(0,0,a)+f(0,0,-a)] \\
&\left.+(b^7-3a^2b^5+4a^5b^2-2a^7)[f(0,0,b)+f(0,0,-b)]\right\}.
\end{aligned}$$

Taking the limit $a \to 0$, from quadrature formula (13) we obtain the following quadrature formula over the sphere S_3, which has the algebraic precision of degree 3.

$$\begin{aligned}
\int_{S_3} f(x,y,z)dxdydz &\approx \frac{\pi^{n/2}b^n}{2(n+2)\Gamma\left(\frac{n}{2}+1\right)} \\
&\times\left(\sum f_{2(n-1)}(VIII)+\sum f_2(IX)+4f(0,\cdots,0)\right).
\end{aligned}$$

We now prove that BTQF (13) is a formula with the fewest evaluation points.

Theorem 5 *The minimum number of evaluation points of BTQFs over an n-dimensional double layered spherical shell Sh_n is $2(n+1)$. In particular, the minimum number of evaluation points for BTQFs over a ring domain and a 3-dimensional double layered spherical shell are respectively 6 and 8.*

Proof. For a BTQF over Sh_n with precision degree 3, we will first prove that the minimum number of evaluation points on the outside layer of Sh_n cannot be less than $2n$. Without a loss of generality, we assume that the number of evaluation points on the outside layer is $2n-1$. (The cases when the minimums are less than $2n-1$ can be proved similarly.) We will see that a contradiction from this assumption. If the assumption is valid, we take the limit $a \to 0$ to the BTQF and obtain a quadrature formula over an n-dimensional sphere with $2n-1$ evaluation points as follows.

$$\int_{S_n} f(X)dX \approx a_0 f(0,\cdots,0)+\sum_{i=1}^{2n-1} a_i f(X_i), \tag{14}$$

where X_i $(i=1,\cdots,2n-1)$ lie on the sphere surface and $a_i \neq 0$ $(i=1,\cdots,n)$. We will prove it cannot be of algebraic precision degree 3.

Let us consider the following $2n$ complex vectors

$$AX_1,\cdots,AX_n,Ax_1^2,AX_2^2,\cdots,AX_n^2, \tag{15}$$

where

$$AX_i=(\sqrt{a_1}x_{1,i},\sqrt{a_2}x_{2,i},\cdots,\sqrt{a_{2n-1}}x_{2n-1,i})$$

and

$$AX_i^2=(\sqrt{a_1}x_{1,i}^2,\sqrt{a_2}x_{2,i}^2,\cdots,\sqrt{a_{2n-1}}x_{2n-1,i}^2).$$

Assume that there exist constants b_i $(i=1,\cdots,2n)$ such that

$$\begin{aligned}
&b_1AX_1+\cdots+b_nAX_n \\
&+b_{n+1}Ax_1^2+b_{n+2}AX_2^2+\cdots+b_{2n}AX_n^2=0.
\end{aligned} \tag{16}$$

Taking dot product with AX_i $(i = 1, \cdots, n)$ on both sides of (16) and noting that the quadrature sums in (14) are vanishing for all $f = X^\alpha$ if α has an odd component and $|\alpha| \leq 3$, we obtain

$$b_i AX_i \cdot AX_i = b_i \sum_{i=1}^{2n-1} a_i x_i^2 = 0, \ i = 1, \cdots, n.$$

Since the sums in the above equation are the quadrature sums of BTQF (14) for $f(X) = X^\alpha$ with $\alpha = 2\mathbf{e}_i$ ($\{\mathbf{e}_1, \mathbf{e}_2, \cdots, \mathbf{e}_n\}$ being the standard basis of $\mathbb{R}^n$), which are not be zero, we obtain $b_i = 0$ for all $i = 1, \cdots, n$. Consequently, equation (16) is reduced to

$$b_{n+1} Ax_1^2 + b_{n+2} AX_2^2 + \cdots + b_{2n} AX_n^2 = 0. \tag{17}$$

Taking the dot product with $A = (\sqrt{a_1}, \cdots, \sqrt{a_{2n-1}})$ on both sides of equation (17) and noting that the quadrature sums in (14) are vanishing for all $f = X^\alpha$ if $\alpha = 3$, we obtain

$$\| \sum_{i=1}^{n} \sqrt{b_{n+i}} AX_i \|_{\ell_2}^2 = 0.$$

Hence,

$$\sqrt{b_{n+1}} AX_1 + \cdots + \sqrt{b_{2n}} AX_n = 0.$$

Similarly, we have $b_{n+i} = 0$ for all $n = 1, \cdots, n$. Thus, vectors (15) are linearly independent, but this is impossible because all of them have $2n - 1$ components. This contradiction means that the number of evaluation points on the outside layer for any BTQFs over Sh_n with algebraic precision degree 3 must be more than $2n-1$.

We now prove that the number of evaluation points on the inside layer for any BTQFs over Sh_n with precision degree 3 cannot be less than 2. Otherwise, if there is none or there is only one evaluation point, $X_0 = (x_{0,1}, x_{0,2}, \cdots, x_{0,n})$, on the inside layer of Sh_n, then a BTQF over Sh_n with algebraic precision degree 3 is not exact for quadratic polynomial $f(X) = \sum_{i=1}^{n} x_i^2 - b^2$ or for a cubic polynomial

$$f(X) = \left(\sum_{i=1}^{n} x_i^2 - b^2 \right) (x_j - x_{0,j}),$$

where $x_{0,j} \neq 0$. This completes the proof of theorem. □

A similar argument of the proof of Theorem 5 can be applied to solve other minimum evaluation point problem. For instance, we have the following result.

Theorem 6 *The minimum number of the evaluation points needed for constructing a quadrature formula over an axially symmetric region in $\mathbb{R}^n$ with algebraic precision degree 3 is $2n$.*

The construction of a quadrature formula of this type can be found in Section 3.9 of Stroud [33].

The minimum number of the evaluation points needed for constructing a quadrature formula over an axially symmetric region in $\mathbb{R}^n$ with certain algebraic precision degree is topologically invariant under a reflection group action.

3 BTQFs with derivatives

To improve the algebraic precision degrees of BTQR's, we use the derivatives of the integrands. As examples, we will construct symmetric quadrature formulas over the surfaces of the regions $C_2 = [-1,1]^2$, $C_3 = [-1,1]^3$, and the n-dimensional sphere S_n.

Example 4. Denote the sets of fully symmetric points $XI = \{(1,1)_{FS}\}$ and $XII = \{(1,0)_{FS}\}$. We construct a symmetric BTQF with precision degree 5 over $C_2 = [-1,1]$ as follows.

$$\begin{aligned}\int_{C_2} f(x,y)dxdy \approx a_1 \sum f_4(XI) + a_2 \sum f_4(XII)\\ +a_3[f'_x(1,1) - f'_x(-1,-1) + f'_x(1,-1) - f'_x(-1,1)\\ +f'_y(1,1) - f'_y(-1,-1) + f'_y(-1,1) - f'_y(1,-1)]\\ +a_4[f'_x(1,0) - f'_x(-1,0) + f'_y(0,1) - f'_y(0,-1)].\end{aligned}$$

Obviously, the above quadrature formula is of precision degree 5 if it is exact for $f(x,y) = 1$, x^2, x^4, and x^2y^2. Therefore, we obtain

$$a_1 = -\frac{1}{15},\ a_2 = \frac{16}{15},\ a_3 = \frac{2}{45},\ a_4 = -\frac{2}{9}.$$

We use the following numerical example to show the good accuracy of the above BTQF. Considering function $f(x,y) = e^{-x^2-y^2}$ and applying the last quadrature to the integral of $f(x,y)$ over $[0,2]^2$, we obtain

$$\begin{aligned}\int_{[0,2]^2} f(x,y)dxdy &= \frac{1}{4}\int_{C_2} e^{-((x+1)^2+(y+1)^2)/4}dxdy\\ &\approx -\frac{1}{60}\left(e^{-2}+2e^{-1}+1\right) + \frac{4}{15}\left(2e^{-5/4}+2e^{-1/4}\right)\\ &\quad -\frac{1}{90}\left(2e^{-2}+2e^{-1}\right) + \frac{1}{9}e^{-5/4} = 0.5576,\end{aligned}$$

while the actual integral value is 0.5577.

Similarly, we can construct a BTQF over $C_3 = [-1,1]^3$ with precision degree 7 and 50 fully symmetric evaluation points $XIII = \{(1,1,1)_{FS}\}$, $XIV = \{(1,0,0)_{FS}\}$, $XV = \{(1,\frac{1}{2},0)_{FS}\}$, and $XVI = \{(1,1,0)_{FS}\}$ as follows.

$$\begin{aligned}\int_{C_3} f(x,y,z)dxdydz \approx a_1 \sum f_8(XIII) + a_2 \sum f_6(XIV)\\ +a_3 \sum f_{24}(XV) + a_4 \sum f_{12}(XVI) + a_5 M_1 + a_6 M_2 + a_7 M_3,\end{aligned}$$

where $a_1 = \frac{1}{5}$, $a_2 = -\frac{16}{105}$, $a_3 = \frac{512}{945}$, $a_4 = -\frac{64}{135}$, $a_5 = -\frac{11}{405}$, $a_6 = -\frac{16}{81}$, $a_7 = \frac{172}{2835}$,

$$\begin{aligned}M_1 = {} & f'_x(1,1,1) - f'_x(-1,-1,-1) + f'_x(1,1,-1) - f'_x(-1,-1,1)\\ & +f'_x(1,-1,-1) - f'_x(-1,1,1) + f'_x(1,-1,1) - f'_x(-1,1,-1)\\ & +f'_y(-1,1,-1) - f'_y(1,-1,1) + f'_y(-1,1,1) - f'_y(1,-1,-1)\\ & +f'_y(1,1,-1) - f'_y(-1,-1,1) + f'_y(1,1,1) - f'_y(-1,-1,-1)\\ & +f'_z(-1,1,1) - f'_z(1,-1,-1) + f'_z(1,-1,1) - f'_z(-1,1,-1)\\ & +f'_z(1,1,1) - f'_z(-1,-1,-1) + f'_z(-1,-1,1) - f'_z(1,1,-1),\end{aligned}$$

$$M_2 = f'_x(1,0,0) - f'_x(-1,0,0) + f'_y(0,1,0) - f'_y(0,-1,0) + f'_z(0,0,1) - f'_z(0,0,-1),$$

and

$$\begin{aligned} M_3 = {} & f'_x(1,1,0) - f'_x(-1,-1,0) + f'_x(1,-1,0) - f'_x(-1,1,0) \\ & + f'_x(1,0,1) - f'_x(-1,0,-1) + f'_x(1,0,-1) - f'_x(-1,0,1) \\ & + f'_y(0,1,1) - f'_y(0,-1,-1) + f'_y(0,1,-1) - f'_y(0,-1,1) \\ & + f'_y(1,1,0) - f'_y(-1,-1,0) + f'_y(-1,1,0) - f'_y(1,-1,0) \\ & + f'_z(1,0,1) - f'_z(-1,0,-1) + f'_z(-1,0,1) - f'_z(1,0,-1) \\ & + f'_z(0,1,1) - f'_z(0,-1,-1) + f'_z(0,-1,1) - f'_z(0,1,-1). \end{aligned}$$

Example 5. Choose $2n$ fully symmetric evaluation points $XVII = \{(r,0,\cdots,0)_{FS}\}$. We can obtain a BTQF over $S_n(\sum_{i=1}^n x_i^2 \le r^2)$ with the precision degree 3 as follows.

$$\begin{aligned} & \int_{S_n} f(X)dX \approx \frac{\pi^{n/2} r^{n+1}}{2n(n+2)\Gamma\left(\frac{n}{2}+1\right)} \left[\frac{n+2}{r} \sum f_{2n}(XVII) \right. \\ & \left. -f'_{x_1}(r,0,\cdots,0) + f'_{x_1}(-r,0,\cdots,0) - \cdots - f'_{x_n}(0,\cdots,0,r) + f'_{x_n}(0,\cdots,0,-r) \right]. \end{aligned}$$

At the end of this section, we discuss the construction of the numerical quadrature formulas over $\bar{S}_n = \{X \in \mathbb{R}^n | |X| = 1\}$ using some recent results in [35], where $\bar{S}_n$ is the surface of the unit sphere $B_n = B_n(1) = \{X \in \mathbb{R}^n | |X| \le 1\}$ in $\mathbb{R}^n$. Let H be a function defined on $\mathbb{R}^n$ that is symmetric with respect to x_n; i.e., $H(X,x_n) = H(X,-x_n)$, $X \in \mathbb{R}^{n-1}$. Then for any continuous function f defined on $\bar{S}_n$,

$$\begin{aligned} & \int_{\bar{S}_n} f(Y)H(Y)d\mu_n \\ = {} & \int_{B_{n-1}} \left[f\left(X, \sqrt{1-|X|^2}\right) + f\left(X, -\sqrt{1-|X|^2}\right) \right] \\ & \times H(X, \sqrt{1-|X|^2}) \frac{dX}{\sqrt{1-|X|^2}}, \end{aligned} \tag{18}$$

where $Y \in \bar{S}_n$, $X \in \mathbb{R}^{n-1}$, $-1 \le t \le 1$, and $d\omega_n$ is the surface measure on $\bar{S}_n$. The volume of $\bar{S}_n$ is $\omega_n = \int_{\bar{S}_n} d\mu_n = 2\pi^{n/2}/\Gamma\left(\frac{n}{2}\right)$. Formula (18), shown in Xu [35], can be proved straightforwardly by substituting $d\mu_n = (1-t^2)^{(n-3)/2} dt d\mu_{n-1}$ and $Y = (\sqrt{1-t^2}X, t)$ into the left-hand integral of the equation.

(18) changes a boundary integral into an integral over the interior of the boundary. Hence it can be used to derive a BTQF over B_n from a quadrature formula of an integral over B_{n-1}. Following [35], suppose that there is a quadrature formula of precision degree m on B_{n-1}

$$\int_{B_{n-1}} g(X) H\left(X, \sqrt{1-|X|^2}\right) \frac{dX}{\sqrt{1-|X|^2}} \approx \sum_{i=1}^N a_i g(X_i);$$

that is, the quadrature formula is exact for all polynomials in π_m^{n-1}, which denotes the set of all polynomials defined in $\mathbb{R}^{n-1}$ with a total degree not more than m.

Then there is a quadrature formula of homogeneous precision degree m on $\bar{S}_n$:

$$\begin{aligned} & \int_{\bar{S}_n} f(Y)H(Y)d\mu_n \\ \approx & \sum_{i=1}^{N} a_i \left[f\left(X_i, \sqrt{1-|X_i|^2}\right) + f\left(X_i, -\sqrt{1-|X_i|^2}\right)\right]. \end{aligned} \tag{19}$$

Recently, Mhaskar, Narcowich, and Ward (see[28]) developed a new method for obtaining quadrature formulas on $\bar{S}_n$, which can be applied to the right-hand integrals of equation (20) in the following theorem, so that the BTQFs over B_n can be constructed.

Theorem 7 *Suppose that $F(X)$ is a continuous function defined on the sphere $B_n(x_1^2 + \cdots + x_n^2 \leq 1)$ that has $2m$ order continuous partial derivative with respect to x_n. Then there exists the following expansion that has m terms and possesses degree $2m-1$ of algebraic precision.*

$$\int_{B_n} F(X)dV = \sum_{k=0}^{m-1} \frac{(-1)^k}{m!} \int_{S_{n-1}} L_k\left(F(X), U_m(X)\right) dS + \rho_m, \tag{20}$$

where $L_k(\cdot,\cdot)$ is defined by

$$L_k(F,G) \equiv \left(\frac{\partial^k F}{\partial x_n^k}\right)\left(\frac{\partial^{m-k-1} G}{\partial x_n^{m-k-1}}\right)\left(\frac{\partial x_n}{\partial \nu}\right)$$

and ρ_m has estimate

$$|\rho_m| \leq \frac{\pi^{\frac{n}{2}} \cdot m!}{\Gamma\left(m+\frac{n}{2}+1\right)(2m)!} \left\| \frac{\partial^{2m} F}{\partial x_n^{2m}} \right\|_C \tag{21}$$

or

$$|\rho_m| \leq \left(\frac{\pi^{\frac{n}{2}} \cdot m!}{\Gamma\left(m+\frac{n}{2}+1\right)(2m)!}\right)^{\frac{1}{2}} \left\| \frac{\partial^{2m} F}{\partial x_n^{2m}} \right\|_{L_2}. \tag{22}$$

Formula (20) can be proved using the Green's formula successively, and it is omitted here.

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