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Numerical integration formulas of degree two

Dongbin Xiu

Department of Mathematics, Purdue University, West Lafayette, IN 47907, USA

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Abstract

Numerical integration formulas in n-dimensional nonsymmetric Euclidean space of degree two, consisting of $n+1$ equally weighted points, are discussed, for a class of integrals often encountered in statistics. This is an extension of Stroud's theory [A.H. Stroud, Remarks on the disposition of points in numerical integration formulas, Math. Comput. 11 (60) (1957) 257–261; A.H. Stroud, Numerical integration formulas of degree two, Math. Comput. 14 (69) (1960) 21–26]. Explicit formulas are given for integrals with nonsymmetric weights. These appear to be new results and include the Stroud's degree two formula as a special case.

Keywords: Numerical integration; Cubature formulas

1. Introduction

Here we discuss numerical integration formulas of the form

$$\int_D f(x)W(x)\,dx \approx \sum_k a_k f\left(u^{(k)}\right), \tag{1}$$

where $D \subset \mathbb{R}^n$ is a region in an n-dimensional, real, Euclidean space; $x = (x_1, x_2, \ldots, x_n)$ is the coordinates, a_k are constants; and $u^{(k)}$ are points in the space. The formulas are called degree of N if they are exact for integrations of any polynomials of x of degree at most N but not $N+1$. This is a subject that has been undergoing extensive research, with more efforts devoted to symmetric integration regions, particularly n-cube. See, for example, books and review articles in [2–5,8,11,7]. For n-dimensional symmetric integrals, Stroud analyzed the disposition of the points and gave sets of points for degree 2 and 3 formulas, consisting of $n+1$ and $2n$ equally weighted points, respectively [9]. He further presented theory for general integration weights and proved that $n+1$ is the minimum number of points for equally weighted degree 2 formulas [10].

Here we extend Stroud's results and present formulas of degree 2 of $n+1$ equally weighted points for integrals with nonsymmetric integration weights. In particular we consider integrals with non-negative weights of identical and independent components, i.e.,

$$W(x) = w(x_1)\cdots w(x_n), \qquad w(x_i) \geqslant 0, \quad i = 1, \ldots, n. \tag{2}$$

E-mail address: dxiu@math.purdue.edu.
URL: http://www.math.purdue.edu/~dxiu.

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Such integrals often arise in statistical analysis where one is required to evaluate expectations of multivariate distributions, where $W(x)$ represents a probability density function with identical and independent components. The specific cases considered in this article include, for $i = 1, \dots, n$,

- Gaussian weights in $\mathbb{R}^n$.

$$w(x_i) = \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-x_i^2}{2}\right), \quad -\infty < x_i < \infty. \tag{3}$$

- *beta* weights in n-cube.

$$w(x_i) \sim (1 - x_i)^\alpha (1 + x_i)^\beta, \quad \alpha, \beta \geqslant 0, \; x_i \in [-1, 1]. \tag{4}$$

  Note this is slightly different from the traditional notation in statistics, where *beta* distribution is usually defined in $x_i \in (0, 1)$.
- *gamma* weights in $[0, \infty)^n$.

$$w(x_i) \sim e^{-x_i} x_i^\alpha, \quad \alpha \geqslant 0, \; x_i \geqslant 0. \tag{5}$$

Note integral (1) with the Gaussian weights (3), and *beta* weights (4) with $\alpha = \beta$, fall into the cases of symmetric regions. And when $\alpha = \beta = 0$ in (4), it is the traditional n-cube integration with constant weights. Here we present an approach via the theory of orthogonal polynomials and derive *explicitly* the points of degree 2 formulas for these integrals with nonsymmetric integration weights. It should be clear now that even though the integration weights can be nonsymmetric, the integration domain always takes the form of a Cartesian product of identical one-dimensional domains — bounded interval, half real line, or the entire real line.

2. Points disposition of degree 2 formulas

For the integration weights (2) considered here, one can construct orthogonal polynomial systems such that

$$\int p_m(x_i) p_n(x_i) w(x_i)\, dx_i = h_m^2 \delta_{mn}, \quad m, n = 0, 1, 2, \dots, \tag{6}$$

where δ_{mn} is the Kronecker delta function and h_m^2 are the normalization constants. The orthogonal systems satisfy a three-term recurrence relation

$$x_i p_n(x_i) = a_n p_{n+1}(x_i) + b_n p_n(x_i) + c_n p_{n-1}(x_i), \quad n > 0, \tag{7}$$

along with $p_0 = 1$ and $p_{-1} = 0$. General properties of orthogonal polynomials and the conditions on weights under which an orthogonal system exists have been studied extensively. See, for example, [12,1].

Let us denote the first order polynomial as $p_1(x_i) = \gamma x_i + \delta$, where γ, δ are real and $\gamma \neq 0$. The following result characterizes the point disposition for degree 2 formulas with $n + 1$ equally weighted points.

Theorem 1 *(Formulas of degree 2). A necessary and sufficient condition that $n + 1$ equally weighted points $u^{(k)}$, $k = 0, 1, \dots, n$, form a numerical integration formula of degree 2 for* (1) *is that an affine transformation of the points $p_1(u^{(k)}) = \gamma u^{(k)} + \delta$ form the vertices of a regular n-simplex with centroid at the origin and lie on the surface of an n-sphere of radius $r = \sqrt{n\gamma c_1}$, where $p_1(x_i) = \gamma x_i + \delta$ is the first-order polynomial from the orthogonal system* (6) *and c_1 is the coefficient in its recurrence relation* (7).

Proof. Let

$$I_0 = \int_D W(x)\, dx, \qquad I_2 = \int_D p_1^2(x_1) W(x)\, dx = \cdots = \int_D p_1^2(x_n) W(x)\, dx.$$

To enforce polynomial exactness of degree 2, it suffices to require (1) to be exact for the orthogonality conditions (6) for up to second order polynomials.

$$\int_D p_1(x_i)W(x)\,dx = 0, \quad i = 1,\dots,n, \tag{8}$$

$$\int_D p_2(x_i)W(x)\,dx = 0, \quad i = 1,\dots,n, \tag{9}$$

$$\int_D p_1(x_i)p_1(x_j)W(x)\,dx = I_2\delta_{ij}, \quad i,j = 1,\dots,n. \tag{10}$$

By using the recurrence relation (7) and orthogonality (8) and (9), we have

$$I_2 = \int_D p_1^2(x_i)W(x)\,dx = \int_D (\gamma x_i + \delta)p_1(x_i)W(x)\,dx = \gamma c_1 I_0.$$

That is,

$$I_2/I_0 = \gamma c_1. \tag{11}$$

Therefore, in order to satisfy the conditions (8), (9), and (10), it suffices to satisfy (8), (10), and (11). Let

$$u^{(k)} = (u_{k1}, u_{k2}, \dots, u_{kn}), \quad k = 0,1,\dots,n,$$

be the $n+1$ points of an integration formula of degree 2 with equal weights of $I_0/(n+1)$. Then conditions (8) and (10) require, respectively,

$$p_1(u_{0i}) + p_1(u_{1i}) + \cdots + p_1(u_{ni}) = 0, \quad i = 1,\dots,n, \tag{12}$$

$$p_1(u_{0i})p_1(u_{0j}) + \cdots + p_1(u_{ni})p_1(u_{nj}) = \frac{n+1}{I_0}I_2\delta_{ij}, \quad i,j = 1,\dots,n. \tag{13}$$

Let $v^{(k)} = p_1(u^{(k)}) = \gamma u^{(k)} + \delta$ be the affine transformation of points $u^{(k)}$, i.e.,

$$v^{(k)} = (v_{k1}, \dots, v_{kn}) = \big(p_1(u_{k1}), \dots, p_1(u_{kn})\big), \quad k = 0,1,\dots,n.$$

Eqs. (12) and (13) can be written as

$$v_{0i} + v_{1i} + \cdots + v_{ni} = 0, \quad i = 1,\dots,n, \tag{14}$$

$$v_{0i}v_{0j} + v_{1i}v_{1j} + \cdots + v_{ni}v_{nj} = \frac{n+1}{I_0}I_2\delta_{ij}, \quad i,j = 1,\dots,n. \tag{15}$$

From this point on, the procedure by Stroud [9] for symmetric integrals can be applied to the transformed points $v^{(i)}$. For self-completeness, we carry out the rest of the proof here.

By defining a matrix

$$A = \begin{bmatrix} v_{01} & v_{11} & v_{21} & \cdots & v_{n1} \\ v_{02} & v_{12} & v_{22} & \cdots & v_{n2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ v_{0n} & v_{1n} & v_{2n} & \cdots & v_{nn} \\ \sqrt{I_2/I_0} & \sqrt{I_2/I_0} & \sqrt{I_2/I_0} & \cdots & \sqrt{I_2/I_0} \end{bmatrix},$$

we can rewrite (14) and (15) as

$$AA^{\mathrm{T}} = \frac{(n+1)I_2}{I_0}I,$$

where I is the identity matrix. Hence

$$A^{\mathrm{T}}A = \frac{(n+1)I_2}{I_0}I$$

is equivalent to the following equations

$$v_{i1}v_{j1} + \cdots + v_{in}v_{jn} + \frac{I_2}{I_0} = \frac{(n+1)I_2}{I_0}\delta_{ij}, \quad i,j = 0,\dots,n. \tag{16}$$

Therefore the points $v^{(k)}$ lie on a sphere of radius $r = \sqrt{nI_2/I_0} = \sqrt{n\gamma c_1}$ with centroid at the origin. It is also straightforward to show that they are equidistant, i.e., from (16) we have

$$d^2(v^{(k)}, v^{(j)}) = v_{k1}^2 + \cdots + v_{kn}^2 + v_{j1}^2 + \cdots + v_{jn}^2 - 2(v_{k1}v_{j1} + \cdots + v_{kn}v_{jn}) = \frac{2(n+1)I_2}{I_0}.$$

Therefore $v^{(k)}$ are the vertices of a regular n-simplex. Reversal of the above argument proves the conditions of the theorem are sufficient. This completes the proof.

3. Formulas of degree two

We have shown that by using orthogonal polynomials defined by the integration weights $W(x)$, the analysis by Stroud for symmetric integrals can be extended to integrals with nonsymmetric weights. Here we present explicit points locations for formulas of degree 2 with $n+1$ equally weighted points, for the three kinds of integrals listed in Section 1. The polynomial exactness of the formulas have been verified numerically.

3.1. *Integrals with Gaussian weights*

The orthogonal polynomials corresponding to the Gaussian weights (3) are the Hermite polynomials and $\gamma c_1 = 1$ in (11). Let us define $n+1$ points

$$x^{(k)} = (x_{k,1}, x_{k,2}, \ldots, x_{k,n}), \quad k = 0, 1, \ldots, n$$

as

$$x_{k,2r-1} = \sqrt{2}\cos\frac{2rk\pi}{n+1}, \qquad x_{k,2r} = \sqrt{2}\sin\frac{2rk\pi}{n+1}, \quad r = 1, 2, \ldots, [n/2], \tag{17}$$

where $[n/2]$ is the greatest integer not exceeding $n/2$, and if n is odd $x_{k,n} = (-1)^k$. Then $x^{(k)}$ form an integration formula of degree 2 for integral (1) with Gaussian weights (3). These points lie on the surface of an n-sphere of radius $r = \sqrt{n}$.

3.2. *Integrals with* beta *weights*

For *beta* integration weights (4), the corresponding orthogonal polynomials are the Jacobi polynomials and $\gamma c_1 = (\alpha+1)(\beta+1)/(\alpha+\beta+3)$ in (11). A set of points for the degree 2 formulas are

$$y^{(k)} = \frac{1}{\alpha+\beta+2}\left[2\sqrt{\frac{(\alpha+1)(\beta+1)}{\alpha+\beta+3}}x^{(k)} - (\alpha-\beta)\right], \quad \alpha, \beta \geqslant 0, \tag{18}$$

where the points $x^{(k)}$ are defined in (17). Note the Stroud formula of degree 2 from [9] is a special case of (18) with $\alpha = \beta = 0$, in which case the points lie on the surface of an n-sphere of radius $r = \sqrt{n\gamma c_1} = \sqrt{n/3}$. (See Theorem 3.8-5 in [11].) For general symmetric weights $\alpha = \beta$, the points lie on the surface of an n-sphere of radius $r = (\alpha+1)\sqrt{n/(2\alpha+3)}$.

3.3. *Integrals with* gamma *weights*

For *gamma* integration weights (5), the corresponding orthogonal polynomials are the (associated) Laguerre polynomials and $\gamma c_1 = \alpha + 1$ in (11). A set of integration points for the degree 2 formulas are

$$z^{(k)} = -\sqrt{\alpha+1}\cdot x^{(k)} + (\alpha+1), \quad \alpha \geqslant 0, \tag{19}$$

where again the points $x^{(k)}$ are defined in (17).

3.4. Integrals with more general weights

For more general integration weights (2) satisfying certain conditions, one can uniquely determine, numerically if needed, the coefficients in the three-term recurrence relation (7) (cf. [6]). One can then construct the polynomial system (6) and identify the specific form of its first order polynomial $p_1(x_i) = \gamma x_i + \delta$. Degree 2 formulas can be readily obtained as follows

$$t^{(k)} = \frac{1}{\gamma}\left[\sqrt{\gamma c_1}x^{(k)} - \delta\right], \quad k = 0, 1, \ldots, n, \tag{20}$$

where c_1 is the coefficient in the recurrence relation (7) and the points $x^{(k)}$ are defined in (17).

4. Discussion on formulas of degree three

The key ingredient in the derivation of the degree 2 formulas for nonsymmetric region is the introduction of the affine transformation via the first order orthogonal polynomials defined by the integration weights. Such a transformation effectively makes the polynomial exactness requirements for up to second order (8) and (10) "symmetric". The same procedure, however, cannot be applied to Stroud's formulas of degree 3, whose construction hinges on the fact that integrals of odd polynomials are automatically zeros in symmetric regions. Although the affine transformation can automatically satisfy

$$\int_D p_1(x_i)p_1(x_j)p_1(x_k)W(x)\,dx = 0, \quad i, j, k = 1, \ldots, n,$$

it cannot satisfy

$$\int_D p_3(x_i)W(x)\,dx = 0, \quad i = 1, \ldots, n,$$

unless the integration region is symmetric. Nevertheless, here we list the integration formulas of degree 3 with $2n$ equally weighted points, for integrals (1) with Gaussian weights in $\mathbb{R}^n$ and symmetric *beta* weights. These are straightforward generalizations of the Stroud formulas of degree 3. They are presented here because of the practical importance of such kinds of integrals. We remark other constructions of $2n$ points formulas are also available in the literature [11,3].

For Gaussian integration weights (3), a set of $2n$ equally weighted points for integration of degree 3 are

$$q^{(k)} = (q_{k,1}, q_{k,2}, \ldots, q_{k,n}), \quad k = 1, \ldots, 2n,$$

with

$$q_{k,2r-1} = \sqrt{2}\cos\frac{(2r-1)k\pi}{n}, \qquad q_{k,2r} = \sqrt{2}\sin\frac{(2r-1)k\pi}{n}, \quad r = 1, 2, \ldots, [n/2], \tag{21}$$

and if n is odd $q_{k,n} = (-1)^k$.

For symmetric *beta* integration weights (4) with $\alpha = \beta$, a set of integration points for degree 3 formulas are

$$s^{(k)} = \frac{1}{\sqrt{2\alpha + 3}}q^{(k)}, \tag{22}$$

where the points $q^{(k)}$ are defined in (21). Again the Stroud formula of degree 3 from [9] is a special case with $\alpha = 0$.

5. Summary

The analysis by Stroud for integration formulas of degree 2 in symmetric n-dimensional space involving $n + 1$ equally weighted points is extended to a class of integrals in nonsymmetric regions, which often arise in statistical analysis. We also present explicit sets of points for such integrals with Gaussian, *beta*, and *gamma* integration weights. The formulas can be useful in statistical analysis as they employ the minimum number of equally weighted points, $n + 1$, for degree 2 polynomial exactness. Similar extensions cannot, however, be obtained to degree 3 formulas for integrals with nonsymmetric integration weights.

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