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HIGHER-DIMENSIONAL INTEGRATION WITH GAUSSIAN WEIGHT FOR APPLICATIONS IN PROBABILISTIC DESIGN*

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Abstract. Higher-dimensional Gaussian weighted integration is of interest in probabilistic simulations. Motivated by the need for variance calculations with functions being at least quadratic, the family of degree 5 formulae is considered. Using an existing formula for the integration over the surface of an n-sphere, an efficient, new formula for Gaussian weighted integration is obtained. Several other formulae that have appeared in the numerical integration literature are also given. The number of function evaluations required by the formulae is compared to a minimal bound result. The degree 5 formulae are applied to simple test problems and the relative errors are compared.

Key words. numerical integration, Gaussian weight, probabilistic design

AMS subject classifications. 65D32, 60H35

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1. Introduction.

In probabilistic studies, random inputs are often modeled to have Gaussian distributions. The calculation of mean or variance of certain outputs under random inputs requires the evaluation of certain integrals. After an affine change of variables of the form $\tilde{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{c}$, this amounts to performing an integral of the form

$$I[f] = \int_{\mathbb{R}^n} e^{-\mathbf{x}^T\mathbf{x}} f(\mathbf{x}) d\mathbf{x}. \tag{1.1}$$

Typically, the integrand $f(\mathbf{x})$ in (1.1) is usually not an analytical expression but an output from some computational simulation. Hence, approximation methods for (1.1) are needed, using the values of integrand at a certain number of points. Efficient procedures for approximating Gaussian weighted integrals are also of interest for implementations of stochastic finite element methods [11].

Presently, the prevalent methods for approximating integral (1.1) include the Monte Carlo and response surface methods. Although these methods may give good accuracy, they are typically not the most efficient. In this paper, we consider numerical cubature schemes,

$$Q[f] = \sum_{j=1}^{N} w_j f(\mathbf{x}^{(j)}), \tag{1.2}$$

with certain choices of weights w_j and points $\mathbf{x}^{(j)}$, dependent on the method but not on $f(\mathbf{x})$. In the context of probabilistic design, the integration problem is characterized by high dimensionality and expensive function evaluations. Hence, our focus is on formulae that give reasonable accuracy, requiring a small number of evaluation points and capable of generalization to arbitrarily high dimensions.

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There are several ways of specifying the accuracy of cubature formulae [2]. Perhaps the most widely used criterion is the algebraic degree. Let us denote $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_n) \in \mathbb{N}_0^n$, $\mathbf{x}^{\boldsymbol{\alpha}} = \prod_{i=1}^n x_i^{\alpha_i}$. A nonzero polynomial in n variables,

$$p(\mathbf{x}) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}_0^n} a_{\boldsymbol{\alpha}} \mathbf{x}^{\boldsymbol{\alpha}}, \tag{1.3}$$

is said to be of algebraic degree d if

$$d = \max \left\{ \sum_{j=1}^n |\alpha_j| : a_{\boldsymbol{\alpha}} \neq 0 \right\}. \tag{1.4}$$

For variance calculations, the integrand in (1.1) is of the form $f(\mathbf{x}) = [g(\mathbf{x}) - \mu_M]^2$, where $g(\mathbf{x})$ is the function whose variance is desired and μ_M is the mean of $g(\mathbf{x})$.

Many common approaches to estimate the impact of variability on an output assume that $f(\mathbf{x})$ is at most quadratic. Seeking cubature formulae which are exact for mean and variance of quadratic functions, this translates to examining those of algebraic degree at least 4. As it happens, many of the degree 4 formulae are also automatically exact for all odd degree polynomials. Hence, our attention is focused on 5th algebraic degree formulae. The numerical integration literature is vast, containing a large variety of formulae for several regions and weight functions. Much of work pre-1970s is largely contained in Stroud's book [20]. Recent compilations of cubature formulae have also been carried out [5, 1]. Tight bounds on the minimal number of cubature points necessary have also been derived for some of the integration problems. However, since traditionally the integrands are analytical expressions that are easily computable, there has been more emphasis on formulae having desirable numerical accuracy qualities (such as weights having the same sign) rather than on the efficiency. For probabilistic design applications, the focus is different, with efficiency being the prominent concern. The purpose of this paper is to present a new, asymptotically optimal (in the sense of efficiency) degree 5 formula for (1.1) that is valid for all higher dimensions and to review previous work on cubature formulae for the same integration problem (1.1). In particular, the view is on efficient, higher-dimensional rules.

In section 2, the question of the strongest known theoretical bound on the minimal number of cubature points necessary for 5th degree rules is addressed. This result aids in gauging the closeness to minimality for the various formulae and gives an indication of the extent for possible efficiency improvements. In section 3, some approaches to formula construction are mentioned, together with references for further information. Of the most interest is the method based on invariant theory, from which nearly all the formulae given here are derived. In section 4, we give a new 5th degree formula, derived from a formula due to Mysovskikh [16], that is valid for all higher dimensions and is asymptotically optimal. Also, several others that have appeared in the numerical integration literature are also collected. We have not included every 5th degree cubature formulae for Gaussian weighted integration. In particular, formulae that require that the number of evaluations grow exponentially with the problem dimension are ruled out on the grounds of practical infeasibility. As an example, the formula given by Dobrodeev [6] is not listed here as for dimension 13; the formula already requires in excess of 50,000 function evaluations. In section 5, we mention in passing other cubature formulae that are potentially useful in the context of probabilistic design. Degrees 7, 9, and 11 formulae are considered, showing what the theoretical minimum number of functional evaluations are, and what the presently available formulae require. Also considered is the family of embedded formulae, being the most efficient formulae known for $d \geq 13$. In section 6, the cubature formulae given in section 4 are tested on simple test problems. It is observed that whether the location of the cubature points scales with the problem dimension or not may have consequences for the accuracy of the cubature formulae.

2. Minimal bound. Minimal bound results are obtained from theoretical arguments which show that, for a general cubature formula of the form (1.2) of a certain algebraic degree accuracy for approximating integrals of certain forms, the number of function evaluations must exceed a certain number. As such, the existence of formulae attaining the bounds is not assured. However, using the special symmetry structure of the integration region and weight function, tight bounds have been obtained. For the Gaussian weighted integration (1.1), which may be viewed as a linear functional evaluated with $\mathbf{f}(\mathbf{x})$, the tightest bound is still that by Möller [14], also given in [24].

DEFINITION 2.1. *A linear functional $I[\cdot]$ is centrally symmetric if*

$$I[\mathbf{x}^{\boldsymbol{\alpha}}] = 0 \quad \forall \boldsymbol{\alpha} \in \mathbb{N}_0^n,\ \sum_{j=1}^{n} \alpha_j \text{ odd.} \tag{2.1}$$

THEOREM 2.2 (Möller's second lower bound). *Let $I[\cdot]$ be centrally symmetric. Then the number of nodes N of a cubature formula of degree $d = 2s-1$ satisfies*

$$N \geq N_{min} = 2\dim \mathcal{P}_{s-1}^{n} - \begin{cases} 1 & \text{if } s \text{ odd}, \\ 0 & \text{if } s \text{ even}, \end{cases} \tag{2.2}$$

where $\mathcal{P}_{2k}^n$ is the subspace generated by even polynomials of algebraic degree $2k$ and $\mathcal{P}_{2k+1}^n$ is the subspace generated by odd polynomials of algebraic degree $2k+1$.

Written more explicitly, N_{min} in (2.2) is

$$N_{min} = \begin{cases} \binom{n+s-1}{n} + \sum_{k=1}^{n-1} 2^{k-n} \binom{k+s-1}{k} & s \text{ even}, \\ \\ \binom{n+s-1}{n} + \sum_{k=1}^{n-1} (1-2^{k-n}) \binom{k+s-2}{k} & s \text{ odd}. \end{cases} \tag{2.3}$$

The integral (1.1) is certainly a centrally symmetric functional on $f(\mathbf{x})$. Applying Theorem 2.2 for degree 5 formulae, we obtain

$$N_{min} = n^2 + n + 1. \tag{2.4}$$

3. Methods of formula construction. Consider the one-dimensional version of (1.1), the integral

$$\int_{-\infty}^{\infty} e^{-x^2} f(x) dx. \tag{3.1}$$

With the quadrature formulae of the form (1.2), exactness of degree d implies that the weights w_j and quadrature points $x^{(j)}$ satisfy the following nonlinear system of moment equations:

$$\sum_{j=1}^{N} w_j (x^{(j)})^{\alpha} = \int_{-\infty}^{\infty} e^{-x^2} x^{\alpha} dx, \ \ 0 \leq \alpha \leq d. \tag{3.2}$$

Hence, an obvious but algebraically difficult way of obtaining quadrature formulae is to seek solutions to the above nonlinear system. An alternative is to take the quadrature points $x^{(j)}$ to be some appropriately chosen values and solve only the above system for the weights w_j. For example, by taking $x^{(j)}$ to be the zeros of Hermite polynomials, the resulting quadrature formula is optimal for (3.1) in the sense of requiring the least number of quadrature points.

For higher dimensions, the technique of orthogonal polynomials could similarly be used. However, the problem of finding common zeros of orthogonal polynomials is much more complex in higher dimensions, and many questions have not been settled yet. Some of the ideas and further references are given in section 3.1.

The approach of seeking solutions to the nonlinear moment equations also becomes more difficult in higher dimensions. To reduce the algebraic problem, some postulates are made regarding the cubature points. One method is to choose the quadrature points to be of certain simple forms [22]. For example, the quadrature points may be taken to have many of the coordinates taking identical values (see Formula IV of section 4.4) or set to zero so as to significantly decrease the resulting degrees of freedom. A more attractive way of solving the nonlinear moment equations is to require that, as linear functionals, the cubature rules satisfy some of the symmetry properties of the integral functional. This greatly simplifies the algebra and is the approach from which most higher-dimensional cubature formulae are obtained. This is discussed in section 3.2.

3.1. Multidimensional orthogonal polynomials. It is known that a Gaussian cubature formula of degree $d = 2s - 1$ in n variables with

$$N_{GS} = \binom{s-1+n}{n} \tag{3.3}$$

points exists if and only if the orthogonal polynomials of degree $2s - 1$ have N_{GS} distinct real zeros. However, the properties of orthogonal polynomials are not known for higher dimensions; much of the result and formulae are known only for $n = 2$ [7]. In [4], an extensive survey of the connection between orthogonal polynomials and cubature formulae is given, showing some of the approaches and difficulties in higher dimensions. In [24], a characterization of quasi-orthogonal polynomials is given. Cubature formulae may be found by solving a nonlinear system of equations. For higher dimensions, this remains a difficult problem.

3.2. Invariance theory. Let G be a finite subgroup of the group of all orthogonal transformations of $\mathbb{R}^n$ onto itself, leaving the origin fixed. Then G is a transformation group of a regular polyhedron centered at the origin, onto itself.

DEFINITION 3.1. *A function $p(\mathbf{x})$ defined on $\mathbb{R}^n$ is said to be invariant with respect to the group G if $p(g \cdot \mathbf{x}) = p(\mathbf{x})$ for all $g \in G$.*

DEFINITION 3.2. *A linear functional $I[\cdot]$ is said to be G-invariant if the domain of integration and the weight function are both invariant with respect to G.*

Let $a \in G$. Then the set obtained by taking the group composition of g with a, $g \cdot a$, as g runs through all elements of G, is called the G-orbit containing the point a.

DEFINITION 3.3. *A cubature formula (1.2) for a G-invariant functional $I[\cdot]$ is G-invariant if the set of points $\{\mathbf{x}^{(j)}\}$ is a union of G-orbits, with all points belonging to the same orbit having the same coefficient w_j.*

Formula construction based on invariance theory places the reasonable requirement that the cubature formulae be linear functionals having some of the same symmetries as that for the functional $I[\cdot]$ that is to be approximated. Observe that the algebraic degree of a polynomial is preserved under G. Application of a result due to Sobolev [18] (also in [12, 16]) shows how the invariance requirement simplifies the cubature formula construction, as follows.

THEOREM 3.4. *In order for a G-invariant cubature formula $Q[\cdot]$ of a G-invariant functional $I[\cdot]$ to be exact for all functions of algebraic degree d, it is necessary and sufficient that $Q[\cdot]$ be exact for the subspace of algebraic degree d functions which are invariant with respect to G.*

4. Efficient degree 5 cubature formulae. In this section, the most efficient known degree 5 formulae for the integral (1.1) are shown. Formulae valid only for isolated low dimensions (e.g., 2 or 3) are not shown. For all the formulae listed here, the number of function evaluations grows quadratically with the problem dimension.

4.1. Formula I: $4 \leq n$, $n^2 + 3n + 3$ points. Here, we give a new cubature formulae for the integration (1.1), derived from a formulae due to Mysovskikh. In [16], Mysovskikh derives a cubature formulae for the surface of the sphere, $U_n \equiv \{\mathbf{x} \in \mathbb{R}^n : x_1^2 + x_2^2 + \cdots + x_n^2 = 1\}$, based on the transformation group of the regular simplex, with vertices

$$\mathbf{a}^{(r)} = (a_1^{(r)}, a_2^{(r)}, \ldots, a_n^{(r)}), \quad r = 1, 2, \ldots, n+1, \tag{4.1}$$

where

$$a_i^{(r)} \equiv \begin{cases} -\sqrt{\frac{n+1}{n(n-i+2)(n-i+1)}}, & i < r, \\ \sqrt{\frac{(n+1)(n-r+1)}{d(n-r+2)}}, & i = r, \\ 0, & i > r. \end{cases} \tag{4.2}$$

The set of midpoints of the vertices projected onto the surface of the sphere U_n is

$$\left\{\mathbf{b}^{(j)}\right\} \equiv \left\{\sqrt{\frac{n}{2(n-1)}}(\mathbf{a}^{(k)} + \mathbf{a}^{(l)}) : k < l, \;\; l = 1, 2, \ldots, n+1\right\}. \tag{4.3}$$

Taking as cubature points the sets $\{\mathbf{a}^{(j)}\}$ and $\{\mathbf{b}^{(j)}\}$ and further requiring central symmetry of the cubature formula, Mysovskikh shows how a 5th degree formula requiring $n^2 + 3n + 2$ points may be constructed of the form

$$\int_{U_n} f(\mathbf{x}) d\mathbf{x} \approx Q[f] = A \sum_{j=1}^{n+1} \left[f(\mathbf{a}^{(j)}) + f(-\mathbf{a}^{(j)}) \right] + B \sum_{j=1}^{n(n+1)/2} \left[f(\mathbf{b}^{(j)}) + f(-\mathbf{b}^{(j)}) \right]. \tag{4.4}$$

The above cubature formula over the spherical surface may be used to derive an efficient cubature formula for (1.1) if the Gaussian weighted integral is written as

$$\int_{\mathbb{R}^n} e^{-\mathbf{x}^T\mathbf{x}} f(\mathbf{x}) d\mathbf{x} = \int_0^\infty e^{-r^2} r^{n-1} \left(\frac{1}{r^{n-1}} \int_{\|\mathbf{x}\|=r} f(\mathbf{x}) d\mathbf{x} \right) dr. \tag{4.5}$$

Now, if $f(\mathbf{x})$ is of algebraic degree d in $\mathbf{x}$, then as a function of r,

$$g(r) \equiv \frac{1}{r^{n-1}} \int_{\|\mathbf{x}\|=r} f(\mathbf{x}) d\mathbf{x} \tag{4.6}$$

is of degree d as well. Since a degree 5 quadrature formula for the integral

$$\int_0^\infty e^{-r^2} r^{n-1} g(r) dr \tag{4.7}$$

is of the form

$$c_0 g(0) + c_1 g(\sqrt{n/2+1}), \tag{4.8}$$

then, using Mysovskikh's degree 5 formula [16] for integration over the $r = \sqrt{n/2+1}$ spherical surface, we obtain

$$\begin{aligned} Q[f] &= \frac{2\pi^{n/2}}{n+2} f(\mathbf{0}) \\ &+ \frac{n^2(7-n)\pi^{n/2}}{2(n+1)^2(n+2)^2} \sum_{j=1}^{n+1} \left[f(\sqrt{n/2+1} \times \mathbf{a}^{(j)}) + f(-\sqrt{n/2+1} \times \mathbf{a}^{(j)}) \right] \\ &+ \frac{2(n-1)^2\pi^{n/2}}{(n+1)^2(n+2)^2} \sum_{j=1}^{n(n+1)/2} \left[f(\sqrt{n/2+1} \times \mathbf{b}^{(j)}) + f(-\sqrt{n/2+1} \times \mathbf{b}^{(j)}) \right], \end{aligned} \tag{4.9}$$

where the point sets $\{\mathbf{a}^{(j)}\}$ and $\{\mathbf{b}^{(j)}\}$ are defined in (4.1) and (4.3), respectively.

4.2. Formula II: $2n^2+1$ points. This formula is shown in Stroud and Secrest [23] and also in [20]:

$$\begin{aligned} Q[f] &= \frac{2}{n+2} \pi^{n/2} f(\mathbf{0}) \\ &+ \frac{4-n}{2(n+2)^2} \pi^{n/2} \sum_{\text{full sym.}} f(\sqrt{n/2+1}, 0, \ldots, 0) \\ &+ \frac{1}{(n+2)^2} \pi^{n/2} \sum_{\text{full sym.}} f(\sqrt{n/4+1/2}, \sqrt{n/4+1/2}, 0, \ldots, 0), \end{aligned} \tag{4.10}$$

where the summation is performed over all distinct reflections and permutations of the input variables. As shown in p. 294 of Stroud's book [20], this formula is derived from the formula for integration over the surface of the unit n-sphere. Comparison with Formula I shows that, applied to radially symmetric functions $f(|\mathbf{x}|)$, Formulae I and II obtain exactly the same values.

4.3. Formula III: $2n^2+1$ points. A class of formulae based on invariant theory is constructed by McNamee and Stenger in [15] and also by Phillips [17] for general fully symmetric regions, which are invariant under reflections and index permutations. Specifically, the following degree 5 formula for (1.1) is given in [17]:

$$\begin{aligned} Q[f] &= \frac{n^2-7n+18}{18} \pi^{n/2} f(\mathbf{0}) \\ &+ \frac{4-n}{18} \pi^{n/2} \sum_{\text{full sym.}} f(\sqrt{3/2}, 0, \ldots, 0) \\ &+ \frac{1}{36} \pi^{n/2} \sum_{\text{full sym.}} f(\sqrt{3/2}, \sqrt{3/2}, 0, \ldots, 0), \end{aligned} \tag{4.11}$$

where the summation is performed over all distinct reflections and permutations of the input variables. As noted in [17], for $n = 2$, this formula is identical to the product-Gauss rule.

The main difference between Formulae II and III is that whereas the cubature points of III lie on the surface of a sphere with fixed radius (independent of the problem dimension n), those of Formula II lie on a surface that grows with n (as do those of Formula I). As is demonstrated in section 6, this appears to bring about significant differences in the accuracy.

4.4. Formula IV: $2 \leq n \leq 7$, $n^2 + n + 2$ points. This is a formula valid for $2 \leq n \leq 7$ given by Stroud [20, pp. 92–96]. While this formula is valid only for a limited range of dimensions, it is perhaps the most efficient possible since it requires only one point more than the number given by the theoretical lower bound of section 2. The formula is of the form

$$
\begin{aligned}
Q[f] = {} & A\left[f(\eta,\eta,\ldots,\eta) + f(-\eta,-\eta,\ldots,-\eta)\right] \\
& + B\left[\sum_{\text{Perm.}} f(\lambda,\xi,\xi,\ldots,\xi) + f(-\lambda,-\xi,-\xi,\ldots,-\xi)\right] \\
& + C\left[\sum_{\text{Perm.}} f(\mu,\mu,\gamma,\ldots,\gamma) + f(-\mu,-\mu,-\gamma,\ldots,-\gamma)\right],
\end{aligned}
\tag{4.12}
$$

where the summations are taken over all distinct permutations of the input variables. The constants are obtained, where there may be multiple real solutions. For instance, the constants μ, γ, η are obtained from the expressions [20, p. 96]

$$
\begin{aligned}
\mu &= \left(-3 \pm \sqrt{16 - 2n}\right)\gamma, \\
\gamma^2 &= \frac{3 \pm \sqrt{7 - n}}{2(16 - n \pm 4\sqrt{16 - 2n})}, \\
\eta^2 &= \frac{n(n-7) \mp (n^2 - 3n - 16)\sqrt{7 - n}}{2(2n^3 - 7n^2 - 16n + 128)}.
\end{aligned}
\tag{4.13}
$$

For completeness, the table of values of coefficients μ, γ, η, A, B, C on pp. 316–317 of [20] is reproduced in Table 1. As can be seen from (4.13), for $n > 7$, some of the cubature points take on complex values.

4.5. Efficiency comparison. From Figure 1, it may be seen that together, Formulae I and IV provide near optimally efficient degree 5 rules over all dimensions.

5. Further possibilities.

5.1. Higher degree formulae. For cubature formulae of accuracy degrees 7, 9, and 11, Table 2 gives the minimal bound result (2.2) and references to some presently known formulae for these degrees. Again, formulae requiring the number of functional evaluations growing exponentially with the problem dimension are not listed here. In [19], Stoyanova gives an efficient new 7th degree formula for integration over the n-sphere, using the simplex symmetry similar to that shown in section 4.1. It might be possible to use a similar approach to derive a degree 7 rule for the case of Gaussian weighted integration.

TABLE 1

Coefficients and constants for (4.12). *Taken from A. H. Stroud,* Approximate Calculation of Multiple Integrals*, 1st ed.,* 1971. *Reprinted by permission of Pearson Education, Inc., Upper Saddle River, NJ.*

n		Values I	Values II
2	η	0.44610 31830 94540	
	λ	0.13660 25403 78444 $\times 10^1$	
	ζ	−0.36602 54037 84439	
	μ	0.19816 78829 45871 $\times 10^1$	
	γ		
	A	0.32877 40197 78636 $\pi^{n/2}$	
	B	0.83333 33333 33333 $\pi^{n/2} \times 10^{-1}$	
	C	0.45593 13554 69736 $\pi^{n/2} \times 10^{-2}$	
3	η	0.47673 12946 22796	0.47673 12946 22796
	λ	0.93542 90188 79534	0.12867 93203 34269 $\times 10^1$
	ζ	−0.73123 76477 87132	−0.37987 34633 23979
	μ	0.43315 53094 77649	−0.19238 67294 47751 $\times 10^1$
	γ	0.26692 23286 97744 $\times 10^1$	0.31330 06830 22281
	A	0.24200 00000 00000 $\pi^{n/2}$	0.24200 00000 00000 $\pi^{n/2}$
	B	0.81000 00000 00000 $\pi^{n/2} \times 10^{-1}$	0.81000 00000 00000 $\pi^{n/2} \times 10^{-1}$
	C	0.50000 00000 00000 $\pi^{n/2} \times 10^{-2}$	0.50000 00000 00000 $\pi^{n/2} \times 10^{-2}$
4	η	0.52394 56582 87507	
	λ	0.11943 37825 52719 $\times 10^1$	
	ζ	−0.39811 26085 09063	
	μ	−0.31856 93729 20112	
	γ	0.18567 58374 24096 $\times 10^1$	
	A	0.15550 21169 82037 $\pi^{n/2}$	
	B	0.77751 05849 10183 $\pi^{n/2} \times 10^{-1}$	
	C	0.55822 74842 31506 $\pi^{n/2} \times 10^{-2}$	
5	η	0.21497 25643 78798 $\times 10^1$	0.61536 95283 65158
	λ	0.46425 29860 16289 $\times 10^1$	0.13289 46983 87445 $\times 10^1$
	ζ	−0.62320 10540 93728	−0.17839 43638 77324
	μ	−0.44710 87006 73434	−0.74596 32665 07289
	γ	0.81217 14260 76331	0.13550 39723 10817 $\times 10^1$
	A	0.48774 92591 89752 $\pi^{n/2} \times 10^{-3}$	0.72641 50244 14905 $\pi^{n/2} \times 10^{-1}$
	B	0.48774 92591 89752 $\pi^{n/2} \times 10^{-3}$	0.72641 50244 14905 $\pi^{n/2} \times 10^{-1}$
	C	0.49707 35044 44862 $\pi^{n/2} \times 10^{-1}$	0.64150 98535 10569 $\pi^{n/2} \times 10^{-2}$
6	η	0.10000 00000 00000 $\times 10^1$	0.10000 00000 00000 $\times 10^1$
	λ	0.14142 13562 37309 $\times 10^1$	0.94280 90415 82063
	ζ	0.00000 00000 00000	−0.47140 45207 91032
	μ	−0.10000 00000 00000 $\times 10^1$	−0.16666 66666 66667 $\times 10^1$
	γ	0.10000 00000 00000 $\times 10^1$	0.33333 33333 33333
	A	0.78125 00000 00000 $\pi^{n/2} \times 10^{-2}$	0.78125 00000 00000 $\pi^{n/2} \times 10^{-2}$
	B	0.62500 00000 00000 $\pi^{n/2} \times 10^{-1}$	0.62500 00000 00000 $\pi^{n/2} \times 10^{-1}$
	C	0.78125 00000 00000 $\pi^{n/2} \times 10^{-2}$	0.78125 00000 00000 $\pi^{n/2} \times 10^{-2}$
7	η	0.00000 00000 00000	
	λ	0.95972 43187 48357	
	ζ	−0.77232 64888 20521	
	μ	−0.14121 42701 31942 $\times 10^1$	
	γ	0.31990 81062 49452	
	A	0.11111 11111 11111 $\pi^{n/2}$	
	B	0.13888 88888 88889 $\pi^{n/2} \times 10^{-1}$	
	C	0.13888 88888 88889 $\pi^{n/2} \times 10^{-1}$	

5.2. Embedded cubature schemes. In [10], Genz and Malik consider cubature formulae of degree $d = 2s + 1$ over fully symmetric regions based on taking full symmetry sums of the $s + 1$ generators, which are the set of distinct real numbers

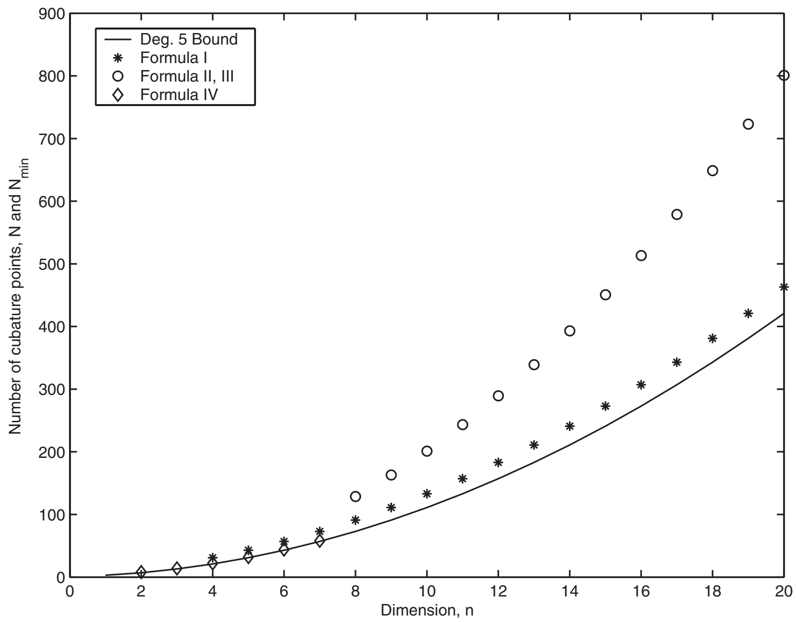

Fig. 1. *Comparison of the number of cubature points needed for Formulae* I–IV *with the degree* 5 *minimal bound* (2.4).

Table 2
Presently known higher degree Gaussian weighted cubature formulae.

Form.	Minimal bound	Points required	Ref.
7-I	$\frac{1}{3}n(n^2+3n+8)$	$\frac{1}{3}\left(4n^3+8n+3\right)$	[20]
II		$\frac{1}{3}\left(4n^3+12n^2-4n+3\right)$	[13, 5]
9-I	$\frac{1}{12}\left(n^4+6n^3+23n^2+18n+12\right)$	$\frac{1}{3}\left(2n^4-4n^3+22n^2-8n+3\right)$	[20]
II		$\frac{1}{3}\left(2n^4+20n^3-50n^2+40n+3\right)$	[13]
11-I	$\frac{1}{60}n\left(n^4+10n^3+55n^2+110n+184\right)$	$\frac{1}{15}\left(4n^5-20n^4+140n^3-130n^2+96n+15\right)$	[20]
II		$\frac{1}{15}\left(4n^5+770n^4-4180n^3+7360n^2-3864n+15\right)$	[13]

from which the coordinate components of the cubature points are selected. The sets of generators are chosen to have a certain nested structure so that for each degree, the cubature points include all those of lower degrees. This has the advantage of allowing the computation of a conservative error estimate and of reusing the previously obtained function values if a higher degree accuracy is needed. However, the number of cubature points required is larger than 2^n, and hence grows exponentially with the problem dimension. In [3], the Genz and Malik family of embedded cubature formu-

TABLE 3
Estimates of mean and variance (exact values $\approx 0.32, 0.089$*, respectively) for function* (6.1).

Form.	Points required	Relative error for mean	Relative error for variance
I	73	1.076%	14.132%
II	99	72.705%	40.707%
III	99	54.029%	5.147%
VI	58	2.221%	16.922%

lae is applied to the integral with Gaussian weight function (1.1). For this problem, explicit expressions for the weights are given in [3] for degrees ≤ 9.

Attempts have been made to decrease the number of cubature points necessary for embedded cubature schemes that are fully symmetric interpolatory. In [8], a Lagrange interpolation technique is considered to explicitly calculate cubature weights in terms of the generators. By placing a simple condition on the generators, some of the weights may be made to be zero, thereby eliminating some of the terms in the summation. There, the general theory is applied to the problem of unweighted integration over the hypercube. In [9], application to the problem of Gaussian weighted integral (1.1) is carried out. For degrees higher than 13, the two family of formulae given in [9] are the most efficient known.

6. Test results.

6.1. Mean and variance estimates. We consider the mean and variance calculation for the function

$$g(x_1, x_2, x_3, x_4, x_5, x_6, x_7) = \frac{|x_1|^{\frac{8}{7}} |x_2|^{\frac{2}{7}}}{(1 + x_3^2 + x_4^2 + x_5^2 + x_6^2 + x_7^2)^{\frac{1}{4}}}. \tag{6.1}$$

The relative error in the mean estimate obtained from a cubature formula $Q[g]$ is defined to be

$$\text{Rel. error} \equiv \left| \frac{\mu_M - Q[g]}{\mu_M} \right|, \quad \mu_M \equiv \frac{1}{\pi^{7/2}} \int_{\mathbb{R}^7} e^{-\mathbf{x}^T \mathbf{x}} g(\mathbf{x}) d\mathbf{x}. \tag{6.2}$$

Using the same quadrature points as that used for the mean calculation, we similarly obtain the variance estimate by approximating the integral

$$\frac{1}{\pi^{7/2}} \int_{\mathbb{R}^7} e^{-\mathbf{x}^T \mathbf{x}} [g(\mathbf{x})^2 - \mu_M^2] d\mathbf{x}, \tag{6.3}$$

where μ_M is the true mean. Again, the variance relative error is defined by normalizing the error in the variance estimate by the true variance. The relative errors in the mean and variance estimates are shown in Table 3. It is seen that whereas Formulae I and IV provide good mean estimates and satisfactory variance estimates, Formulae II and III are far less accurate.

Using Monte Carlo to achieve the accuracy of mean estimate obtained from Formula I would take $N \approx 78000$ function evaluations (with 99% confidence). For the variance calculation, a simple estimate using chi-squared distribution gives $N \approx 700$. This shows that the use of quadrature rules can result in orders-of-magnitude computational saving.

Table 4
Scaling of relative error with dimension for (6.4).

Dim. n	Relative error Formulae I, II	Relative error Formula III
10	12.041%	121.06%
15	13.231%	434.02%
20	13.571%	1029.05%
25	13.562%	1966.74%
30	13.399%	3298.41%

6.2. Dimensionality study. For higher-dimensional applications, it is of interest to determine how the relative errors for the cubature rules scale with the problem dimension. Here, Formulae I–III are applied to a function whose general form is dimension independent. In particular, we consider the following radially symmetric function:

$$f(\mathbf{x}) = \frac{1}{\sqrt{1+\mathbf{x}^T\mathbf{x}}}. \tag{6.4}$$

In this test case, Formulae I and II obtain exactly the same values, $f(\mathbf{x})$ being radially symmetric. The results are shown in Table 4. Here, the relative errors for Formulae I and II appear to be relatively constant with respect to the dimension. However, the error in Formula III grows steadily with the dimension. This suggests that there is an advantage in having cubature points located at a radius scaling with the square root of the problem dimension. An intuitive explanation may be provided by the following argument. Consider the integration (1.1) of the function $f(\mathbf{x}) = r^q$, $r \equiv \sqrt{\mathbf{x}^T\mathbf{x}}$. This may be written as an integration over the radial variable

$$\int_0^\infty \left(e^{-r^2} \frac{2\pi^{n/2}}{\Gamma(n/2)} r^{n+q-1} \right) dr. \tag{6.5}$$

The integrand

$$e^{-r^2} \frac{2\pi^{n/2}}{\Gamma(n/2)} r^{n+q-1}, \tag{6.6}$$

as a function of r, has the peak occurring at

$$r^* = \sqrt{\frac{n+q-1}{2}}, \tag{6.7}$$

showing a scaling with the square root of n.

7. Conclusion. Numerical integration methods were considered for probabilistic design applications, which are characterized by high dimensionality and possibly high computational costs required for function evaluations. An asymptotically optimal formulae was given that is able to capture the variance of quadratic functions. On simple test problems, some of the formulae were shown to give reasonable accuracy. For better accuracies, higher degree formulae may be used. However, significantly many more function evaluations may be necessary, as shown by the minimal bound result.

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