

CUBATURE FORMULAE FOR THE GAUSSIAN WEIGHT. SOME OLD AND NEW RULES.*

RAMÓN ORIVE[†], JUAN C. SANTOS-LEÓN[†], AND MIODRAG M. SPALEVIĆ[‡]

Abstract. In this paper we review some of the main known facts about cubature rules to approximate integrals over domains in \mathbb{R}^n , in particular with respect to the Gaussian weight $w(\mathbf{x}) = e^{-\mathbf{x}^T \mathbf{x}}$, where $\mathbf{x} = (x_1, \dots, x_n) \in \mathbb{R}^n$. Some new rules are also presented. Taking into account the well-known issue of the “curse of dimensionality”, our aim is at providing rules with a certain degree of algebraic precision and a reasonably small number of nodes as well as an acceptable stability. We think that the methods used to construct these new rules are of further applicability in the field of cubature formulas. The efficiency of new and old rules are compared by means of several numerical experiments.

Key words. cubature formulas, Gaussian weight

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1. Introduction. The problem of providing suitable estimates for integrals of functions of several variables has received growing interest, especially during the last sixty years, connected with the rise of the computational age and the subsequent possibility of implementing increasingly powerful algorithms. One of the main reasons for this boom is rooted in the growing field of applications in engineering, automatic and control theory, financial mathematics (in particular, the evaluation of risks), econometric models (see, e.g., the references [6, 15], among many others), and other fields. In particular, our motivation lies partially in some recent contributions in control theory, more precisely, in the filter design for dynamical systems; see, e.g., [1, 12].

To be a bit more precise, the subject of this paper is the approximation of integrals of the form

$$(1.1) \quad I(f) := \int_{\mathbb{R}^n} f(\mathbf{x}) w(\mathbf{x}) d\mathbf{x},$$

where $\mathbf{x} = (x_1, \dots, x_n) \in \mathbb{R}^n$ and $w(\mathbf{x}) > 0$ in \mathbb{R}^n by means of linear cubature formulas

$$(1.2) \quad Q(f) := \sum_{j=1}^N w_j f(\mathbf{x}^{(j)}),$$

where $w_j \in \mathbb{R}$ are the weights or coefficients and $\mathbf{x}^{(j)} = (x_1^{(j)}, \dots, x_n^{(j)}) \in \mathbb{R}^n$ are called the nodes of the cubature formula.

The choice of nodes and weights to construct suitable cubature formulas is far away from being as clear as in the univariate case. Indeed, especially in the case of high dimensions, we have to be careful in taking a reasonably small number of nodes to avoid the well-known “curse of dimensionality”. Roughly speaking, the methods for numerical integration in several variables developed so far may be split into two big groups, namely

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[†]Departamento de Análisis Matemático, Universidad de La Laguna, 38200 La Laguna, Spain ({rorive, jcsantos}@ull.es).

[‡]Department of Mathematics, Faculty of Mechanical Engineering, University of Beograd, Kraljice Marije 16, 11120 Belgrade 35, Serbia (mspalevic@mas.bg.ac.rs).

- polynomial-based cubature formulas:
 These kinds of rules follow the idea of the well-known Gaussian quadrature formulas in the univariate case, that is, they are formulas with the number of nodes as small as possible, and they exactly integrate polynomials up to a certain degree. This idea is also applicable to trigonometric polynomials. Nevertheless, the problem is considerably more difficult in the multivariate case and strongly depends both on the domain of integration and the weight function.
- Monte Carlo- or quasi Monte Carlo-type cubature formulas:
 For this kind of methods, the weight function is interpreted as a probability density and the integral as the average of the integrand. In this way, the nodes are chosen as random variables distributed according to the weight function. In general, although so far this kind of methods have been the last resort in case of very high dimensions, their convergence is relatively slow, and they only provide probabilistic estimates of the error.

In this note we are concerned with the first of the above mentioned types of cubature formulas. It is not our purpose here to provide an exhaustive introduction to the topic of cubature formulas; for more details, the reader can consult some of the papers by R. Cools, such as [3, 4].

Our aim is to deal with linear cubature rules of the form (1.2) to approximate integrals (1.1), where w stands for the Gaussian weight

$$(1.3) \quad w(\mathbf{x}) = \exp(-\mathbf{x}^T \mathbf{x}) = \exp\left(-\sum_{j=1}^n x_j^2\right), \quad \mathbf{x} \in \mathbb{R}^n.$$

As mentioned above, we consider so-called polynomial-based formulas, that is, those built by imposing the condition that they exactly integrate polynomials up to a certain degree (commonly called the degree of precision or degree of exactness). Namely, we say that the cubature rule $Q(\cdot)$ has degree of precision $\geq d$ if

$$(1.4) \quad Q(f) = I(f), \quad f \in P_d^n,$$

where P_d^n denotes the space of polynomials in n variables with total degree less than or equal to d . The degree of precision is said to be exactly d if there exists some polynomial p of degree $d + 1$ for which $Q(p) \neq I(p)$.

Our main concern is to construct formulas with an acceptable degree of precision that have as few nodes as possible. In the univariate case, the Gauss quadrature formula provides a solution to this problem. Indeed, if we need to construct a quadrature formula with k nodes with the prescribed (odd) degree of precision $2k - 1$ to estimate the integral (1.1), then for a certain nonnegative weight function w , it is necessary and sufficient to take the nodes $x^{(j)}$, $j = 1, \dots, k$, as the k real and simple zeros of the k -th orthogonal polynomial q_k with respect to the weight w . However, the answer to this problem is far from being solved in the multivariate case. Indeed, the use of orthogonal polynomials to select the appropriate nodes is considerably more difficult in the multidimensional case since their properties (in particular, the existence of common zeros of the vector of orthogonal polynomials of the same total degree) are not well known. In this sense, it is often necessary to solve the nonlinear moment system derived from (1.4). Therefore, the problem of providing cubature rules with a prescribed degree of precision with the minimal number of nodes is not solved in general and strongly depends on the particularities of the domain of integration and the weight function. *Invariant theory* tries to exploit the possible symmetries of the domain and the weight function to simplify the choice of nodes and weights. In this way, H. M. Möller [9] provided the best

lower bound for the case where the linear operator $I(f)$ is *centrally symmetric*, which means that $I(f) = 0$ when f is any monomial of odd degree (obviously, (1.1) with the Gaussian weight (1.3) satisfies this requirement), and we look for an odd degree of precision. Next, we state the precise result of Möller.

THEOREM 1.1. *The number of nodes N of a cubature of degree $d = 2s - 1$ satisfies $N \geq N_{min}$ with*

$$(1.5) \quad N_{min} = \begin{cases} \binom{n+s-1}{n} + \sum_{k=1}^{n-1} 2^{k-n} \binom{k+s-1}{k}, & s \text{ even,} \\ \binom{n+s-1}{n} + \sum_{k=1}^{n-1} (1 - 2^{k-n}) \binom{k+s-2}{k}, & s \text{ odd.} \end{cases}$$

It is easy to verify that for $d = 3$, $N_{min} = 2n$, while for $d = 5$ the theorem yields $N_{min} = n^2 + n + 1$. But in general, no cubature rule with the minimal number of nodes given by the lower bound (1.5) is known; nevertheless, a noticeable exception takes place when the degree of precision $d = 3$ is considered. Section 2 is mainly devoted to a formula for which this minimal number of nodes occurs and which has several nice properties and allows us to introduce and motivate the subsequent sections of the paper; also, some extensions known in the literature are considered. Then, Section 3 deals with our findings about cubature formulas of higher degree of precision with a reasonable number of nodes. Finally, the different cubature rules considered are compared by means of several illustrative examples in Section 4.

2. A spherical-radial cubature formula of degree 3 and some extensions. In [14] the following rule was introduced:

$$(2.1) \quad Q(f) = \frac{\sqrt{\pi^n}}{2n} \sum_{\text{FS}} f(\sqrt{n/2}, 0, \dots, 0).$$

Here and in the sequel the symbol FS stands for fully symmetric, which means that the summation is over all the nodes obtained by permutations and changes of signs of the coordinates. Thus, in this case, the formula uses $2n$ nodes. This formula has degree $d = 3$ and is collected in ([13, $E_n^2 : 3 - 1$, p. 315]).

On the other hand, formula (2.1) can be obtained by writing the integral $I(f)$ in (1.1) in the form of a spherical-radial integral

$$(2.2) \quad \int_{\mathbb{R}^n} f(\mathbf{x}) e^{-\mathbf{x}^T \mathbf{x}} d\mathbf{x} = \int_0^\infty \int_{U_n} f(r\mathbf{y}) r^{n-1} e^{-r^2} d\sigma dr,$$

where $U_n = \{\mathbf{y} \in \mathbb{R}^n : \mathbf{y}^T \mathbf{y} = 1\}$ is the unit n -sphere, and then approximating the integral on the sphere by the cubature formula [13, $U_n : 3 - 1$, p. 294] and the radial integral with a generalized Gauss-Laguerre formula with a single node; see, e.g., [1].

Formula (2.1) uses $2n$ nodes, which, according to Möller’s Theorem 1.1, is the minimum number of nodes for degree $d = 3$. In addition, note that all cubature weights are equal and positive, which implies nice stability properties. Indeed, the maximum degree of stability is achieved when all the weights have the same sign; when this is not the case, the following stability coefficient is commonly used (provided that the cubature exactly integrates the constant function):

$$(2.3) \quad \rho := \frac{\sum_{j=0}^N |w_j|}{\sum_{j=0}^N w_j} = \frac{\sum_{j=0}^N |w_j|}{I(1)} \geq 1,$$

in such a way that the minimum value $\rho = 1$ is only attained when all the weights are positive, as it occurs for (2.1).

In addition we point out other nice properties of the nodes of the rule (2.1). Indeed, the nodes are placed on a sphere of radius $\sqrt{n/2}$, that is, at a distance of $\sqrt{n/2}$ from the origin, which increases with the dimension but not too much. In this sense, taking into account that the Gaussian weight function has an absolute maximum at the origin (whose importance increases with the dimension), the underlying ideas in the Laplace and the subsequent steepest descent methods seem to show that the nodes should not be too far away from the origin. Thus, the location of the nodes in (2.1) seems to be suitable.

The cubature formula (2.1) is optimal for degree $d = 3$ and may be considered a multivariate counterpart of Simpson's rule. In the area of nonlinear filtering problems, the nonlinear filter based on this cubature formula is referred to as *Cubature Kalman Filter*, hereafter CKF; see [1]. However, it is worth noting that because of its low degree and though it provides quite good results for integrals of the form $f(\mathbf{x}) = g(\mathbf{x}^T \mathbf{x})$ (see Table 4.1 in Section 4), it may suffer from low accuracy for many integrands (see other numerical examples in Section 4).

Therefore, it seems convenient to consider an increase in the degree of precision. Next, we review some of the existing cubature rules with degree of precision $d = 5$. Taking into account the well-known problem of the dimensionality, we restrict ourselves to those with $O(n^2)$ nodes. McNamee and Stenger in [8] (see also [11]) constructed a fully symmetric cubature formula of degree $d = 5$ with $2n^2 + 1$ nodes of the form

$$(2.4) \quad Q(f) = w_0 f(\mathbf{0}) + w_1 \sum_{\text{FS}} f(\nu, 0, \dots, 0) + w_2 \sum_{\text{FS}} f(\nu, \nu, 0, \dots, 0),$$

where the weights w_0, w_1, w_2 and the parameter ν are determined by requiring that the cubature formula has degree of precision $d = 5$. Here and in the sequel, we denote the zero vector by $\mathbf{0} = (0, \dots, 0) \in \mathbb{R}^n$. Due to the full symmetric character of both the integral operator and the cubature formula, the latter has degree $d = 5$ if it is exact for $f = 1, x_1^2, x_1^2 x_2^2, x_1^4$. Solving this nonlinear system yields

$$\begin{aligned} \nu &= \sqrt{3/2}, \\ w_0 &= (n^2 - 7n + 18)\sqrt{\pi^n}/18, \quad w_1 = (4 - n)\sqrt{\pi^n}/18, \quad w_2 = \sqrt{\pi^n}/36. \end{aligned}$$

The stability coefficient of this cubature formula is given by $\rho_n = (2n^2 - 8n + 9)/9$, $n \geq 4$, and thus, it is numerically very unstable with respect to the dimension n . Observe that the distances of the cubature nodes to the origin are independent of the dimension n .

Better stability is provided by a formula given by Lu and Darmofal [7]. They also considered the factorization (2.2) of the Gaussian integral as the product of a spherical and a radial integral, but now the integral on the surface of the sphere is approximated by the Mysovskikh cubature formula [10], and the radial integral is approximated (after the change of variable $r^2 = t$) by a generalized Laguerre quadrature formula with a preassigned node at $r = 0$. Combining these spherical and radial rules, they obtain the product cubature formula with degree of precision $d = 5$ given by

$$(2.5) \quad \begin{aligned} Q(f) &= W_1 f(\mathbf{0}) + W_2 \sum_{j=1}^{n+1} \left(f(r\mathbf{a}^{(j)}) + f(-r\mathbf{a}^{(j)}) \right) \\ &\quad + W_3 \sum_{j=1}^{n(n+1)/2} \left(f(r\mathbf{b}^{(j)}) + f(-r\mathbf{b}^{(j)}) \right), \end{aligned}$$

where

$$W_1 = \frac{2\pi^{n/2}}{n+2}, \quad W_2 = \frac{n^2(7-n)\pi^{n/2}}{2(n+1)^2(n+2)^2}, \quad W_3 = \frac{2(n-1)^2\pi^{n/2}}{(n+1)^2(n+2)^2},$$

$$r = \sqrt{n/2+1},$$

and

$$\mathbf{a}^{(j)} = (a_1^{(j)}, a_2^{(j)}, \dots, a_n^{(j)}), \quad j = 1, 2, \dots, n+1,$$

with

$$a_i^{(j)} = \begin{cases} -\sqrt{\frac{n+1}{n(n-i+2)(n-i+1)}}, & i < j, \\ \sqrt{\frac{(n+1)(n-j+1)}{n(n-j+2)}}, & i = j, \\ 0, & i > j, \end{cases}$$

and

$$\mathbf{b}^{(j)} = \sqrt{\frac{n}{2(n-1)}}(\mathbf{a}^{(k)} + \mathbf{a}^{(\ell)}), \quad k < \ell, \ell = 1, \dots, n+1.$$

This cubature formula has, so far, the least number of nodes among all the cubature rules of degree $d = 5$ for an arbitrary dimension n . However, its number of nodes, $N = N(n) = n^2 + 3n + 3$, exceeds the theoretical lower bound by $2(n+1)$ nodes. As for the stability, we have that, in terms of the dimension n ,

$$\rho_n = \frac{1}{I(1)} \sum |w_j| = \frac{3n^3 - 9n^2 + 8n + 4}{(n+2)^2(n+1)} \approx 3, \quad n \text{ large},$$

and thus, it is quite stable.

To end this short section, let us include another cubature rule, also based on a spherical-radial decomposition, due to Stroud and Secrest [14], which is collected in [13, p. 317], namely

$$(2.6) \quad Q(f) = Af(\mathbf{0}) + B \sum_{\text{FS}} f(r, \mathbf{0}) + C \sum_{\text{FS}} f(s, s, \mathbf{0}),$$

where

$$r = \sqrt{n/2+1}, \quad s = \sqrt{n/4+1/2},$$

$$A = \frac{2\pi^{n/2}}{n+2}, \quad B = \frac{(4-n)\pi^{n/2}}{2(n+2)^2}, \quad C = \frac{\pi^{n/2}}{(n+2)^2}.$$

It is known that this cubature formula is also of the spherical-radial type. It is obtained when the integral on the unit n -sphere is approximated by the cubature formula for U_n given in [13, $U_n : 5 - 1$, p. 294], while the radial part is approximated by means of the same Laguerre quadrature used to arrive at (2.5). Then, because of their construction, formulas (2.5) and (2.6) give the same estimate for radially symmetric integrands.

In the next section, some new ways to obtain cubature formulas with an acceptable degree of precision ($d = 5$) will be given, maintaining some of the nice properties of (2.1), that is, a small number of nodes, stability, and even positivity or almost-positivity of the weights (this concept will be specified below).

3. Some new ways to build stable rules of degree $d = 5$. We would like to determine cubature rules with a higher degree of precision than (2.1) that possess many of the nice properties of the rule (2.1). First, we remind that, as it was observed in Theorem 1.1, the minimal number N_{min} of nodes of a cubature formula of degree of precision $d = 5$ for the Gaussian weight is $N_{min} = n^2 + n + 1$. Next, we list, for different dimensions n , the cubature formulas known in the literature so far with degree of precision $d = 5$ and with the least number of nodes for integrals with Gaussian weights.

- For $n = 2$, 7 nodes ($= N_{min}$). See [14], [13, p. 324].
- For $n = 3$, 13 nodes ($= N_{min}$). See [14], [13, p. 326].
- For $n = 4$, 22 nodes ($= N_{min} + 1$), formula $E_4^{r^2} : 5 - 1$. See [13, Section 3.10 and p. 316].
- For $n = 5$, 32 nodes ($= N_{min} + 1$), formulas $E_5^{r^2} : 5 - 1$. See [13, Section 3.10 and p. 316].
- For $n = 6$, 44 nodes ($= N_{min} + 1$), formula $E_6^{r^2} : 5 - 1$. See [13, Section 3.10 and p. 317].
- For $n = 7$, 57 nodes ($= N_{min}$), formula $E_7^{r^2} : 5 - 1$. See [13, Section 3.10 and p. 317].
- For $n \geq 8$, $n^2 + 3n + 3$ nodes ($= N_{min} + 2(n + 1)$). This is (2.5) (see [7]).

3.1. The use of higher-order divided differences. Our first proposal to increase the degree of precision consists in the use of higher-order divided differences (as discretizations of higher-order partial derivatives) to modify an initial cubature rule. Namely, suppose that we take formula (2.1) as the starting point, and consider a modification of it given by

$$(3.1) \quad T(f) = Q(f) + A \sum_{i=1}^n \frac{\partial^4 f(\mathbf{0})}{\partial x_i^4} + B \sum_{i < j} \frac{\partial^4 f(\mathbf{0})}{\partial x_i^2 \partial x_j^2}$$

in order to get a degree of precision $d = 5$ for the modified rule $T(\cdot)$. Observe that the full symmetry implies the exactness of $T(\cdot)$ for monomials of odd degree, and we only have to take into account monomials of the type x_i^4 and $x_i^2 x_j^2$. Indeed, imposing the condition that (3.1) exactly integrates monomials of the type x_i^4 easily yields $A = (3 - n)\sqrt{\pi^n}/96$. Since (3.1) is not written in the form of a linear cubature formula, we need to rewrite the terms involving partial derivatives as a linear combination of function values. To do this, we can consider the following (central) divided difference for a univariate function g at an arbitrary real point a ,

$$g^{(4)}(a) \approx \frac{g(a - 2h) - 4g(a - h) + 6g(a) - 4g(a + h) + g(a + 2h)}{h^4},$$

to approximate the terms $\frac{\partial^4 f(\mathbf{0})}{\partial x_i^4}$. Since the atom of the original formula (2.1) is given by $\sqrt{n/2}$, we can take $h = \sqrt{n/2}$ in order to reduce the number of nodes of the rule. Next, proceeding analogously with the second term of the modification (3.1), if the condition $T(x_i^2 x_j^2) = I(x_i^2 x_j^2)$ is required, we immediately obtain that $B = \sqrt{\pi^n}/16$. Finally, as above, we need to discretize the partial derivatives of the type $\frac{\partial^4 f(\mathbf{0})}{\partial x_i^2 \partial x_j^2}$, now using the divided difference

$$g^{(2)}(a) \approx \frac{g(a - h) - 2g(a) + g(a + h)}{h^2}, \quad h > 0.$$

Summarizing all the preceding computations defines the rule

$$\begin{aligned}
 (3.2) \quad T(f) = & w_0 f(\mathbf{0}) + w_1 \sum_{\text{FS}} f(\sqrt{n/2}, 0, \dots, 0) \\
 & + w_2 \sum_{\text{FS}} f(2\sqrt{n/2}, 0, \dots, 0) + w_3 \sum_{\text{FS}} f(\sqrt{n/2}, \sqrt{n/2}, 0, \dots, 0),
 \end{aligned}$$

where the weights are given by

$$w_0 = \frac{(n+1)\sqrt{\pi^n}}{4n}, \quad w_1 = \frac{\sqrt{\pi^n}}{6n}, \quad w_2 = \frac{(3-n)\sqrt{\pi^n}}{24n^2}, \quad w_3 = \frac{\sqrt{\pi^n}}{4n^2}.$$

By construction, this rule has degree $d \geq 5$, but it is easy to verify that it is exactly $d = 5$. It has $2n^2 + 2n + 1$ nodes. Observe that the weight w_2 is negative for $n > 3$. The stability coefficient of the rule, defined in (2.3), is given by ($n \geq 3$)

$$\rho_n = \frac{7n-3}{6n} \approx \frac{7}{6} = 1.1666\dots, \quad n \text{ large,}$$

and thus is smaller than the coefficient for (2.5) and (2.6). The number of nodes exceeds by $n^2 + n$ the theoretical lower bound given by Theorem 1.1. This cubature rule is, as far as we know, new.

3.2. Optimization of cubature rules with a prescribed structure. Suppose that we are given a parametric family of cubature rules of degree $d = 5$ of the same structure. We propose different ways to choose the parameter (or parameters) in order to optimize certain important properties, such as decreasing the number of nodes or assuring the positivity of the weights. For the sake of simplicity, we restrict ourselves to the degree $d = 5$, but the method below is applicable for any d . Due to the ‘‘curse of the dimensionality’’ it is not convenient to deal with much larger values of d .

First, take the previous formula (3.2) as a model. It has the structure

$$Q(f) = w_0 f(\mathbf{0}) + w_1 \sum_{\text{FS}} f(u, \mathbf{0}) + w_2 \sum_{\text{FS}} f(2u, \mathbf{0}) + w_3 \sum_{\text{FS}} f(u, u, \mathbf{0}),$$

where u is the generating atom of the rule (in (3.2), $u = \sqrt{n/2}$). Suppose now that this atom can be varied in order to decrease the number of nodes. Then, if we solve the system of nonlinear equations to guarantee $d = 4$ (and, by symmetry, $d = 5$), we get the solution

$$\begin{aligned}
 w_0 = \frac{(16u^4 - 10nu^2 + 2n^2 + n)\sqrt{\pi^n}}{16u^4}, & \quad w_1 = \frac{(8u^2 - 3n)\sqrt{\pi^n}}{24u^4}, \\
 w_2 = \frac{(-2u^2 + 3)\sqrt{\pi^n}}{96u^4}, & \quad w_3 = \frac{\sqrt{\pi^n}}{16u^4},
 \end{aligned}$$

with $u > 0$. We observe that for $u = \sqrt{3/2}$, for which the weight w_2 vanishes, we obtain (2.4) (let us remind the reader that it is an unstable rule). Another natural choice is $u = \sqrt{3n/8}$, which cancels the weight w_1 . One then gets the cubature formula

$$(3.3) \quad Q(f) = w_0 f(\mathbf{0}) + w_2 \sum_{\text{FS}} f(2u, 0, \dots, 0) + w_3 \sum_{\text{FS}} f(u, u, 0, \dots, 0),$$

where

$$w_0 = \frac{2(n+2)\sqrt{\pi^n}}{9n}, \quad w_2 = \frac{(4-n)\sqrt{\pi^n}}{18n^2}, \quad w_3 = \frac{4\sqrt{\pi^n}}{9n^2}.$$

This cubature formula has $2n^2 + 1$ nodes, $2n$ fewer than the cubature formula (3.2), and its stability coefficient is given by (for $n \geq 4$)

$$\rho_n = \frac{11n - 8}{9n} \approx \frac{11}{9} = 1.222\dots, \quad n \text{ large,}$$

which is just a little bit larger than in the case of (3.2). This rule is, as far as we know, a new cubature formula.

Therefore, (3.2) and, especially, (3.3) reach in part the goals of having both a reasonably small number of nodes and a quasi-optimal asymptotic stability coefficient. But now we are still concerned with improving this last aspect. To do this and having in mind the structure of (3.3), consider a family of cubature rules with the general structure

$$(3.4) \quad Q(f) = w_0 f(\mathbf{0}) + w_2 \sum_{FS} f(r, 0, \dots, 0) + w_3 \sum_{FS} f(s, s, 0, \dots, 0),$$

where $r = 2s$ in (3.3). From the viewpoint of invariant theory, one has five unknowns, w_0, w_2, w_3, r, s , to be determined. For a fully symmetric cubature formula of degree of precision $d = 5$, it is necessary and sufficient that the four equations $Q(f) = I(f)$, for $f = 1, x_1^2, x_1^4, x_1^2 x_2^2$, are satisfied. So, one has one degree of freedom. Thus, it seems reasonable to consider $r = \lambda s$ and choose the parameter λ to optimize some property of the family (3.4). Let us consider cubature formulas of the form

$$Q(f) = Af(0, 0, \dots, 0) + B \sum_{FS} f(r, 0, \dots, 0) + C \sum_{FS} f(\lambda r, \lambda r, \dots, 0)$$

of degree of precision $d = 5$, where A, B, C , and r are unknowns and λ is a parameter at our disposal. We determine the unknowns by solving the algebraic and nonlinear system $Q(f) = I(f)$ for $f = 1, x_1^2, x_1^4, x_1^2 x_2^2$. The dimension n is going to play an important role, and we consider different values of n .

Case $n = 2$. In this case, we have

$$A = \frac{4\lambda^2\pi}{(1 + 2\lambda^2)^2}, \quad B = \frac{\lambda^4\pi}{(1 + 2\lambda^2)^2}, \quad C = \frac{\pi}{4(1 + 2\lambda^2)^2}, \quad r^2 = \frac{1 + 2\lambda^2}{2\lambda^2}, \quad \lambda > 0,$$

which provides a family of one-parameter cubature formulas of degree of precision $d = 5$ with 9 nodes (that is, just 2 over the theoretical lower bound given in Theorem 1.1) and positive cubature weights for any $\lambda > 0$. For $\lambda = 1$, the formula $E_2^{n^2} : 5 - 2$ given in [13, p. 324] is recovered. Furthermore, one can compute the parameter λ such that the cubature formula has additionally trigonometric degree of precision 1 by requiring that $Q(f) = I(f)$ for $f(x, y) = e^{ix}$, $i = \sqrt{-1}$. This kind of integrands arise in many applications. Doing so, one obtains $\lambda \doteq 0.4592$, and then

$$A \doteq 0.4173\pi, \quad B \doteq 0.02199\pi, \quad C \doteq 0.1237\pi, \quad r \doteq 1.836, \quad \lambda r \doteq 0.8431.$$

Case $n = 3$. Similarly, one obtains the one-parameter family of rules with degree of precision $d = 5$ and 19 nodes (5 over the lower bound) given by

$$A = -\frac{(2\lambda^4 - 4\lambda^2 - 1)\pi^{3/2}}{(2 + \lambda^2)^2}, \quad B = \frac{\lambda^4\pi^{3/2}}{2(2 + \lambda^2)^2}, \quad C = \frac{\pi^{3/2}}{4(2 + \lambda^2)^2},$$

$$r^2 = \frac{2 + \lambda^2}{2\lambda^2}, \quad \lambda > 0.$$

All cubature weights are positive for $0 < \lambda < \sqrt{4 + 2\sqrt{6}}/2$. In particular, the choice $\lambda = \sqrt{2}/2$ provides the cubature formula (2.6) corresponding to $n = 3$. As above, we have that for $\lambda \doteq 2.178$, the cubature has additionally trigonometric degree of precision 1, although in this case the weight A becomes negative and is of fairly large magnitude:

$$A \doteq -3.064, \quad B \doteq 1.378, \quad C \doteq 0.03062, \quad r \doteq 0.8431, \quad \lambda r \doteq 1.836.$$

Case $n = 4$. It is easy to verify that one gets the cubature formula given by

$$A = \frac{\pi^2}{3}, \quad B = 0, \quad C = \frac{\pi^2}{36}, \quad s^2 = 3/2,$$

corresponding to a cubature formula of degree of precision $d = 5$ with 25 nodes (that is, it exceeds the lower bound by 4) and positive cubature weights. It is the cubature formula $E_4^{r^2} : 5 - 1$ given in [13, p. 329].

Case $n \geq 5$. The situation is different in this case. First, the nonlinear system of equations yields, for $0 < \lambda < \sqrt{\frac{n-1}{n-4}}$,

$$\begin{aligned} A &= \frac{n^2(4\lambda^4 - 4\lambda^2 + 1) + n(-24\lambda^4 + 20\lambda^2 - 3) + 32\lambda^4 - 16\lambda^2 + 2}{2(-n + 1 + \lambda^2n - 4\lambda^2)^2} V, \\ B &= -\frac{(n-4)\lambda^4}{2(-n + 1 + \lambda^2n - 4\lambda^2)^2} V, \\ C &= \frac{1}{4(-n + 1 + \lambda^2n - 4\lambda^2)^2} V, \\ r^2 &= \frac{\lambda^2(4-n) + n-1}{2\lambda^2}, \end{aligned}$$

where hereafter $V = \pi^{n/2}$, which yields a one-parameter family of cubature formulas of degree of precision $d = 5$ with $2n^2 + 1$ nodes. Observe that for $\lambda = \sqrt{2}/2$, the formula (2.6) it is reproduced, while for $\lambda = 1$, the cubature formula (2.4) obtained by McNamee and Stenger in [8] is recovered, and (3.3) is obtained for $\lambda = \sqrt{3n}/8$.

It is easy to observe that in this case the cubature weight B is negative for any λ . However, it is possible to choose the parameter λ in order to make the negative weight B as small in magnitude as one desires with the consequent positive effect for the stability of the rule. Indeed, if for a given dimension n we consider, for instance, $\lambda = 1/n^k$ with an appropriate value of k , one obtains

$$\begin{aligned} A &= \frac{(4n^2 - 24n + 32 - 4n^{2+2k} + 20n^{1+2k} - 16n^{2k} + n^{2+4k} - 3n^{1+4k} + 2n^{4k})\pi^{n/2}}{2(n^{4k} + n^{2+4k} - 2n^{1+4k} - 2n^{2+2k} + 10n^{1+2k} - 8n^{2k} + n^2 - 8n + 16)}, \\ B &= -\frac{(n-4)\pi^{n/2}}{2(-n^{1+2k} + n^{2k} + n - 4)^2}, \\ C &= \frac{n^{4k}\pi^{n/2}}{4(n^{4k} + n^{2+4k} - 2n^{1+4k} - 2n^{2+2k} + 10n^{1+2k} - 8n^{2k} + n^2 - 8n + 16)}, \\ r^2 &= (n^{2k+1} - n^{2k} - n + 4)/2. \end{aligned}$$

In Table 3.1, some illustrative computations of the cubature weights and generators of the nodes corresponding to $\lambda = 1/n$ ($k = 1$) are displayed.

This suggests the following definition:

TABLE 3.1
Illustrative computations corresponding to $\lambda = 1/n$.

n	A	B	C	r	$s = \lambda r$
5	0.3628V	$-0.5102 \cdot 10^{-4}V$	$0.1594 \cdot 10^{-1}V$	7.036	1.407
10	0.4370V	$-0.3754 \cdot 10^{-5}V$	$0.3128 \cdot 10^{-2}V$	21.14	2.114
15	0.4605V	$-0.5582 \cdot 10^{-6}V$	$0.1284 \cdot 10^{-2}V$	39.62	2.641

DEFINITION 3.1. *We say that a one parametric family of cubature formulas $Q_{n,\lambda}$ has quasi-positive cubature weights if for any n and any given tolerance $\epsilon > 0$ there exist a λ_0 such that the stability coefficient $\rho_n(Q_{n,\lambda_0})$ of the corresponding cubature rule satisfy $|1 - \rho_n(Q_{n,\lambda_0})| < \epsilon$.*

In the sense of this definition, we can say that it is possible to construct cubature rules of degree $d = 5$ for $n \geq 5$ with quasi-positive cubature weights.

4. Numerical examples. As it was pointed out in the introduction, the use of stable cubature rules with a reasonably small number of nodes is of great importance when iterative numerical integration is required such as in the area of dynamical systems; see, e.g., [1, 2]. Next, some numerical results are presented, which are obtained when applying some of the old and new rules discussed in the previous sections to different examples. In the following tables, we denote by FI the cubature formula (2.1), by FII the formula (2.4), FIII and FIV will denote the rules (2.5) and (2.6), respectively, and the cubature formulas (3.2) and (3.3) will be called, respectively, FV and FVI. Finally, cubature rules of the one-parameter family corresponding to other values of the parameter λ will be denoted by simply indicating the value of this parameter.

4.1. Radially symmetric integrands. For radially symmetric functions, $f(\mathbf{x}) = g(|\mathbf{x}|)$, one can rewrite after some calculations the n -dimensional integral (1.1) for the weight (1.3) as an integral over the radial dimension

$$(4.1) \quad I(f) = \frac{\pi^{n/2}}{\Gamma(n/2)} \int_0^\infty g(\sqrt{r}) e^{-r} r^{n/2-1} dr, \quad r = \sqrt{\mathbf{x}^T \mathbf{x}}.$$

On the other hand, the cubature rule (2.1) for radially symmetric integrands reduces to

$$Q(f) = \pi^{n/2} g(\sqrt{n/2}),$$

which, as expected, agrees with a Laguerre formula with a single node (for $\alpha = n/2 - 1$) for approximating the integral (4.1) ([5, p. 222]).

In addition, as observed in [7], formulas (2.5) and (2.6) give the same integral estimate for radially symmetric functions. We observe after some calculations that this common value is given by

$$Q(f) = \frac{\pi^{n/2}}{n+2} \left(n g(\sqrt{n/2+1}) + 2g(0) \right),$$

which, as expected, agrees with the Radau-Laguerre formula for $\alpha = n/2 - 1$ ([5, p. 223]),

$$\int_0^\infty g(x) x^\alpha e^{-x} dx \doteq w_0 g(0) + w_1 g(x_1),$$

$$w_0 = \frac{2\Gamma(\frac{n}{2})}{n+2}, \quad w_1 = \frac{2\Gamma(\frac{n}{2}+1)}{n+2}, \quad x_1 = \frac{n}{2} + 1,$$

where $w_0 = \frac{2\Gamma(\frac{n}{2})}{n+2}$, $w_1 = \frac{2\Gamma(\frac{n}{2}+1)}{n+2}$, $x_1 = \frac{n}{2} + 1$, for the integral (4.1) with a preassigned node $x_0 = 0$.

In Table 4.1 some numerical computations for radially symmetric functions are displayed. The relative errors are shown (in percentage). We can see that for the considered integrals formula I exhibits the best performance.

TABLE 4.1
 Relative errors for $n = 5$ and $f_1(\mathbf{x}) = (1 + \mathbf{x}^T \mathbf{x})^{-1/2}$, $f_2(\mathbf{x}) = \exp(-\mathbf{x}^T \mathbf{x})$, $f_3(\mathbf{x}) = \sin(\mathbf{x}^T \mathbf{x})$.

f	FI	FV	FII ($\lambda = 1$)	FIII-FIV ($\lambda = \sqrt{2}/2$)	FVI ($\lambda = 0.5$)
f_1	6.8%	10.2%	13.2%	8.6%	9.9%
f_2	53.6%	86.7%	112.6%	73.8%	85.4%
f_3	54.1%	142.7%	202.3%	164.5%	210.0%

4.2. Integrands depending only on a few variables. First, consider integrands of the form $f(x_1, x_2, \dots, x_n) = g(x_i)$, for some $i = 1, \dots, n$. In this case, formula II becomes (after some calculations)

$$Q(f) = \pi^{\frac{n-1}{2}} \left(\frac{2}{3} \pi^{1/2} g(0) + \frac{1}{6} \pi^{1/2} g(\nu) + \frac{1}{6} \pi^{1/2} g(-\nu) \right),$$

with $\nu = \sqrt{3/2}$, which agrees, up to a multiplicative constant, with the Gauss-Hermite quadrature formula with three nodes for approximating the integral $\int_{-\infty}^{\infty} g(x_i) e^{-x_i^2} dx_i$.

In the same way, when integrands $f(x_1, x_2, \dots, x_n) = g(x_i, x_j)$, $i \neq j$, are handled, the same rule agrees with

$$Q(f) = \pi^{\frac{n-2}{2}} \left(\frac{4}{9} \pi g(0, 0) + \frac{1}{9} \pi \sum_1^4 (g(\pm\nu, 0) + g(0, \pm\nu)) + \frac{1}{36} \pi \sum_1^4 g(\pm\nu, \pm\nu) \right),$$

with $\nu = \sqrt{\frac{3}{2}}$, which is, up to a multiplicative constant, the Cartesian product formula of two Gauss-Hermite quadrature formulas with three nodes for approximating the integral $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(x_i, x_j) e^{-x_i^2 - x_j^2} dx_i dx_j$.

Due to these simplifications, it is easy to verify in Table 4.2 that both for functions of a single variable or two separate variables, the cubature formula FII, that is, the one corresponding to $\lambda = 1$, gives better results than the others.

TABLE 4.2
 Relative errors for $n = 10$, $f_1 = \frac{1}{1 + x_3^2}$, $f_2 = \sin^2(x_4)$, $f_3 = e^{x_5} x_7^2$.

f	FI	FIII	FV	FVI ($\lambda = 0.5$)	FIV ($\lambda = \sqrt{2}/2$)	FII ($\lambda = 1$)	$\lambda = 1.1$
f_1	21.0%	4.1%	19.1%	16.1%	11.9%	5.6%	9.6%
f_2	80.4%	11.3%	77.6%	56.8%	28.3%	6.7%	9.4%
f_3	22.1%	0.2%	6.9%	4.2%	2.7%	0.091%	1.2%

For functions of three variables, the cubature formula FIII and the one corresponding to $\lambda = 0.93$ seem to give, in general, the best results in the examples, as we can see in Table 4.3.

TABLE 4.3

Relative errors for $n = 10$, $f_1 = x_3^4 x_2^2 e^{x_5}$, $f_2 = e^{x_2 + x_5 + x_9}$, $f_3 = \cos(x_1 + x_2 + x_3 + x_4)$.

f	FI	FIII	FV	FVI ($\lambda = 0.5$)	FIV ($\lambda = \sqrt{2}/2$)	$\lambda = 0.93$	FII ($\lambda = 1$)	$\lambda = 1.1$
f_1	100%	3.3%	159.6%	94.7%	55.8%	1.1%	22.1%	54.8%
f_2	0.1%	0.09%	3.2%	0.7%	0.9%	0.6%	1.3%	2.5%
f_3	4.0%	3.6%	5.5%	1.7%	2.4%	6.3%	11.5%	20.8%

4.3. Additional examples. Table 4.4 displays results obtained for some additional examples, where the number of independent variables of the integrand is comparable to the dimension. In particular, the following examples correspond to integrands of the form $f(x_1, x_2, \dots, x_n) = g(x_1 + x_2 + \dots + x_n)$. Among all considered parameters, the cubature formula corresponding to $\lambda = 0.5$, that is, our formula VI (given by (3.3)) gives the minimum relative errors although the cubature formula FIII gives even better results. In this sense, take into account that for this kind of integrands, the rule (3.3) yields

$$Q(f) = \pi^{\frac{n-1}{2}} \left(\frac{2}{3} \pi^{1/2} g(0) + \frac{1}{6} \pi^{1/2} g(t) + \frac{1}{6} \pi^{1/2} g(-t) \right), \quad t = \sqrt{3n/2},$$

which, after some computations, agrees, up to a multiplicative constant, with the Gauss-Hermite quadrature formula with three nodes for the approximation of the integral

$$\frac{1}{\sqrt{n}} \int_{-\infty}^{\infty} g(x) e^{-x^2/n} dx.$$

TABLE 4.4

Relative errors for $n = 5$, $f_1 = \cos(\sum_{i=1}^5 x_i)$, $f_2 = e^{-\sum_{i=1}^5 x_i}$.

f	FI	FIII	FV	$\lambda = 0.2$	FVI ($\lambda = 0.5$)	FIV ($\lambda = \sqrt{2}/2$)	FII ($\lambda = 1$)	$\lambda = 1.1$
f_1	103.6%	9.8%	15.2%	32.4%	25.7%	27.4%	34.0%	37.1%
f_2	27.4%	3.7%	5.0%	12.3%	6.7%	7.0%	7.9%	8.3%

5. Conclusions and further remarks. In many applications in engineering (automatic and control theory (see, e.g., [1, 2, 12]), financial mathematics, economy, and many others (see, e.g., [6, 15]), it is necessary to estimate multiple integrals (usually related to means and covariances of random variables) with a Gaussian weight. In general, it is desirable to use stable cubature rules with an acceptable degree of precision, and with a reasonably small number of nodes. We review some of the rules of degree 3 and 5 known in the literature and introduce some rules of degree 5 that satisfy optimal or quasi-optimal properties with respect to the number of nodes and the stability. We believe that the methods we propose to derive these new rules, namely the use of higher-order divided differences and the optimization of families of cubature formulas with a prescribed structure, are applicable in a more general context.

The performance of both available and new rules is verified by means of several examples, many of them of the types that arise in applications. The results show that our new rules are competitive.

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