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Journal of Computational and Applied Mathematics 188 (2006) 190–204
JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS
www.elsevier.com/locate/cam

Improved cubature formulae of high degrees of exactness for the square

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Received 16 July 2004; received in revised form 5 April 2005

Abstract

The method of constructing minimal cubature rules with high algebraic degrees of exactness is developed by adapting a powerful algorithm for solving the system of nonlinear equations. As a result, new cubature formulae of degrees 15, 17, 19, 21, and 23 are derived for the square. They lead to lower numbers of knots and/or to better quality with respect to those known previously. The formulae obtained should be considered as the most efficient for the calculation of two-dimensional integrals with a high precision.

Keywords: Cubature; Multivariate integration; Nonlinear solver

1. Introduction

The necessity of performing two-dimensional integration appears in many mathematical and physical applications. Only in rare cases this integration allows an analytical representation. The approximation of integrals is one of the corner stones of numerical analysis. It is also an important step in methods on solutions of integral equations. Despite intensive previous studies [2–4,10,11,17–19], the construction of high-quality integration rules still remains a current problem.

Functions are usually approximated by weighted sums of simpler functions, such as monomials or splines. Similarly, an integral is typically approximated by a weighted sum of integrand evaluations. In the case of one dimension this approximation is called a quadrature formula. The most notorious example

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0377-0427/$ - see front matter © 2005 Elsevier B.V. All rights reserved.
doi:10.1016/j.cam.2005.04.005

is the famous Gaussian quadratures [1,20]. The Gaussian approach is the basic tool to carry out one-variable integration with a high precision and minimal computational costs. In two or more dimensions we come to so-called cubature formulae.

There exists no unique best criterion for the choice of weights and points in the integral approximation. The generally accepted rule is that this choice should provide the exact integration for a class of integrands in the form of polynomials of a certain algebraic degree. In particular, the N_G-point Gaussian quadrature is exact for all one-dimensional polynomials of degree at most $P = 2N_G - 1$. Analogously, in the case of two variables it is necessary to construct an N-point cubature scheme which would be perfect for all two-dimensional polynomials with the maximal total degree P. In order that cubature rule is efficient, the number N of points should be as small as possible for each given value P.

Up to now, the lowest possible number $N_{\min}$ of points (knots) is unknown, in general. For example, for orders $P > 11$, there is a gap between the highest known lower theoretical bound $\mathscr{N}_{\min}$ and the lowest number $\mathscr{N}$ of knots in known cubature formulae [4,12]. Moreover, only for low orders $P < 11$, the positions of knots at $\mathscr{N} \sim \mathscr{N}_{\min}$ can be presented analytically or expressed in terms of common zeros for sets of orthogonal polynomials in two dimensions [17,19]. This is in a sharp contrast to the one-dimensional case, where the nodes of the Gaussian quadrature can be associated for any P with zeros of orthogonal Legendre polynomials [1,20]. In two dimensions, the nonlinear equations, which appear when constructing the cubature rule of a high degree, become too complicated to be analyzed theoretically, and the only way is to solve them numerically using one or the other algorithm.

Note that the straightforward scheme, based on the product of two Gaussian quadratures to yield a cubature formula, is very inefficient for large P as the resulting number $N_G^2 = (P + 1)^2/4$ of knots will significantly exceed the minimal value $\mathscr{N}_{\min}$. Among other theoretical approaches it is necessary to mention the method of reproducing kernel [24]. This method gives a relatively simple presentation of knots in terms of zeros of polynomials for, in principle, arbitrary values of P. However, only for small degrees $P \lesssim 9$ the number of nodes will be close to the lower bound. With increasing P this number quickly tends to the Gaussian product limit N_G^2.

It should be emphasized that the knots of a cubature formula must lie inside the domain (which always can be reduced to a square) of the integration in order to be useful in practical applications. Unfortunately, beginning from relatively small degree $P = 15$, all the known cubature rules over the square with the lowest number $\mathscr{N}$ of knots do not meet this requirement [5,6]. Moreover, for $P \geqslant 15$ there is a considerable gap between $\mathscr{N}$ and $\mathscr{N}_{\min}$.

The main aim of the present investigation is to remedy such a situation. Developing a powerful algorithm for solving the nonlinear equations allows us to obtain new efficient cubature formulae of high algebraic degrees of exactness. These formulae contain smaller numbers of knots and lead to a better precision in comparison with those known earlier.

2. Theory

According to the cubature formalism, the integral of a function is approximated by the sum of its functional values at a set of points, multiplied by weighting coefficients. In the case of two dimensions, the region of integration can always be reduced by an appropriate replacement of variables to the square

with boundaries -1 and 1. Then the N-point cubature formula reads

$$\int_{-1}^{1}\int_{-1}^{1} f(x, y)\,\mathrm{d}x\,\mathrm{d}y = \sum_{i=1}^{N} w_i f(x_i, y_i) + \mathscr{R}_N, \tag{1}$$

where w_i and (x_i, y_i) are the weights and positions of knots, respectively. In general, the truncation errors $\mathscr{R}_N$ cannot be reduced to zero at any finite numbers N. Because of this, it is quite natural to choose the knots and weights in such a way to make the cubature formula (1) exact ($\mathscr{R}_N = 0$) for a class of integrands composed of all algebraic monomials $x^k y^l$ with degrees $k + l \leqslant P$. This is justified by the fact that an arbitrary differentiable function of two variables can be expanded in these monomials as

$$f(x, y) = \sum_{k,l=0}^{k+l\leqslant P} a_{kl} x^k y^l + \mathscr{R}_P, \tag{2}$$

where $a_{kl} = (1/k!l!)\partial^k\partial^l f/\partial x^k \partial y^l|_{(0,0)}$ are the constants, and the remainder $\mathscr{R}_P$ decreases with increasing the order P of the polynomial.

Therefore, we are concerned with cubature formulae that are exact for a vector space of all two-dimensional algebraic polynomials with the total degree at most P. This leads to the necessity of numerically solving the following system of nonlinear equations:

$$\sum_{i=1}^{N} w_i x_i^k y_i^l = g_{kl}, \quad k + l \leqslant P, \tag{3}$$

where

$$g_{kl} = \int_{-1}^{1}\int_{-1}^{1} x^k y^l \mathrm{d}x\mathrm{d}y = \begin{cases} \dfrac{2}{k+1}\dfrac{2}{l+1}, & \text{for even } k \text{ and } l, \\ 0, & \text{otherwise.} \end{cases}$$

For each given order P, there exists some minimal value $N_{\min}$ beginning from which ($N \geqslant N_{\min}$) the system (3) can have (real) solutions. Despite intensive studies, the lowest possible number $N_{\min}$ of knots is still unknown, in general. For example, for orders $P > 11$, there is a gap between the highest known [4,12] lower theoretical bound $\mathscr{N}_{\min} = (P+1)(P+3)/8 + [(P+1)/4]$ (where $[\ ]$ denotes the integer part) and the lowest number $\mathscr{N}$ of knots in known cubature formulae (see below, Table 1). Another difficulty is that the total number $L = P(P+3)/2 + 1$ of equations in (3) increases too rapidly with raising P and the system can be actually solved only at relatively small orders $P \lesssim 11$. Note that the solution of the system of nonlinear equations presents a very complicated task. When the number of equations becomes too large we come to unresolvable numerical problems.

A way to reduce the number of equations consists in imposing a symmetry on the knot positions (x_i, y_i). This should reflect the symmetry of basic equations (3) following from the properties $g_{kl} = g_{lk}$ and $g_{kl} = 0$ if k or l or both are odd. Although, the fully symmetric schemes (with eight knots $(\pm x_i, \pm y_i)$ and $(\pm y_i, \pm x_i)$ for each i) will correspond to the smallest system of equations, they cannot be recommended (at least for orders $P \lesssim 23$) because the total number N of knots appears to be considerably larger than $N_{\min}$. It is worth emphasizing that we are interested in constructing the most efficient formulae of high degrees P with the lowest possible value of N. In this respect, the rotational symmetry approach [9] seems to be

Table 1
Properties of cubature rules for orders up to 23

P	L	L^*	$\hat{L}^*$	$\mathcal{N}_{\min}$	N_G^2	$\mathcal{N}$	Type	M^*	O^*	N^*
1	3	1	0	1	1	1 (PI) [19]	I	0	1	1
3	10	2	1	4	4	4 (PI) [19]	II	1	0	4
5	21	5	3	7	9	7 (PI) [19]	II	2	0	8
7	36	8	5	12	16	12 (PI) [19]	II	3	0	12
9	55	13	8	17	25	17 (PI) [17]	I	4	1	17
11	78	18	12	24	36	24 (PI) [8,23]	III	6	0	24
13	105	25	16	31	49	33 (PI) [8]	I	8	1	33
15	136	32	21	40	64	44 (NO) [19]	II	11	0	44
17	171	41	27	49	81	57 (NO) [7]	II	14	0	56
19	210	50	33	60	100	68 (NO) [21,22]	II	17	0	68
21	253	61	40	71	121	85 (NO) [16]	I	20	1	81
23	300	72	48	84	144	112 (NI) [21]	III	24	0	96

optimal among others (full, central, and axes symmetries, etc.). It involves four knots (x_i, y_i), $(-y_i, x_i)$, $(-x_i, -y_i)$ and $(y_i, -x_i)$ for each i with the same weight w_i. Then

$$\sum_{i=1}^{N} w_i f(x_i, y_i) \equiv \sum_{i=1}^{M} w_i [f(x_i, y_i) + f(-y_i, x_i) + f(-x_i, -y_i) + f(y_i, -x_i)] \tag{4}$$

where $(0 \leqslant x_i \leqslant 1,\ 0 \leqslant y_i \leqslant 1)$ are the generators, and $N = 4M$. The knots of the rotationally invariant cubature formula (4) lie, in fact, in N vertices of M different squares rotated with respect to the basic square region of integration. As a result, a significant part of equations in (3) will be satisfied automatically. In particular, the symmetrized expression (4) tends to zero when $f(x, y)$ is an arbitrary monomial $x^k y^l$ of odd order $p = k + l$. For this reason, the degree of rotationally invariant cubature formulae can accept only odd numbers. It is necessary to point out that no cubature formulae of even degree have been found for $P > 9$ within any symmetry. Moreover, the minimal number of knots $\mathcal{N}_{\min} = 12$, 17 and 24 for orders $P = 7$, 9 and 11, respectively, can be reproduced [8,17,19,23] within the rotationally invariant scheme.

In view of the rotational symmetry, system (3) of nonlinear equations transforms to the form

$$2 \sum_{i=1}^{M} w_i (x_i^k y_i^l + (-1)^k y_i^k x_i^l) = g_{kl}, \quad k + l \leqslant P - 1, \tag{5}$$

where P should be odd, $k + l$ should be even and $k \geqslant l$ (excluding the case $k = l$ for odd k). These restrictions reduce the number of equations significantly, namely, more than 4 times (for $P > 1$), from L to $L^* \lesssim L/4$ (see Table 1). Theoretical studies of system (5) at $N \sim N_{\min}$ is possible only for low orders $P \leqslant 9$. In particular, for $P = 1$, 3, and 5, the solutions can be presented analytically. For $P \leqslant 9$ the nodes (x_i, y_i) can be expressed in terms of common zeros for sets of orthogonal polynomials in two dimensions [17,19]. No analytical results are known at $N \sim N_{\min}$ for $P > 9$. Here, the nonlinear equations become too complicated and the only way is to solve them with the help of a numerical algorithm.

Our investigations have shown that the minimal number N^* of knots related to system (5) can be achieved if the number of unknowns Q^* is equal to the number of equations L^*. The number of unknowns is equal to $Q^* = 3M$ if, in general, $x_i \neq y_i \neq 0$ for all square generators $i = 1, 2, \ldots, M$. Then $L^* = 3M$ and such solutions will be referred to as type III. For $L^* = 3M - 1$, we should decrease the number of unknowns on one. This can be done by letting either $x_M \neq y_M = 0$ (type IIA), or $x_M = y_M \neq 0$ (type IIB). The number of knots corresponding to types IIA, IIB, and III is equal to $N^* = 4M \equiv 4M^*$. Finally, when $L^* = 3M - 2$, we should put $x_M = y_M = 0$ (type I). Here, all the four rotational symmetry knots collapse in the central point (0,0), and the corresponding four terms in the right-hand side of Eq. (4) at $i = M$ can be cast simply as $4w_M f(0,0) \equiv w_0 f(0,0)$. So the total number of nodes will be actually equal to $N^* = 4M^* + O^*$ with $M^* = M - O^*$ and $O^* = 1$. The numbers L^*, N^*, and M^* as well as the central point indicator O^* are collected together with L, $\mathscr{N}_{\min}$, and N_{G}^2 in Table 1 up to order $P_{\max} = 23$.

The best results for the lowest number $\mathscr{N}$ of knots in previously known cubature formulae and the corresponding references are also shown in the table. The quality of these formulae is presented too using an abbreviated notation with two letters. The first letter indicates that either all the weight coefficients are positive (P) or at least one of them is negative (N). The second letter points out that either all the knots are located inside (I) the integration region or at least one knot is outside (O) of that region. In this context, it should be emphasized that cubature formulae with outside knots are, rigorously speaking, unacceptable, because the function $f(x, y)$ can be undetermined outside the region of integration. Another disadvantage is that such formulae lead to a very poor precision in actual applications. Indeed, in view of Eqs. (1)–(3), the error of integral approximations within the cubature approach is

$$\mathscr{E}_P = \sum_{k+l=P+1}^{\infty} a_{kl} \left(\sum_{i=1}^{N} w_i x_i^k y_i^l - g_{kl} \right). \tag{6}$$

When $|x_i| > 1$ or $|y_i| > 1$, this error may be very large (or even the sum in Eq. (6) over k and l be divergent at all) because then $\lim_{k\to\infty} |x_i|^k = \lim_{l\to\infty} |y_i|^l = \infty$, whereas $\lim_{k,l\to\infty} g_{kl} = 0$. The outside schemes can thus be used only for sufficiently "flat" integrands for which the partial derivatives $a_{kl} = (1/k!l!)\partial^k \partial^l f/\partial x^k \partial y^l|_{(0,0)}$ tend to zero rapidly with increasing $p = k + l$. On the other hand, the inside ($|x_i| < 1$ and $|y_i| < 1$) cubature formulae are free of this restriction since then $\lim_{k\to\infty} x_i^k = \lim_{l\to\infty} y_i^l = 0$ like $\lim_{k,l\to\infty} g_{kl} = 0$. They lead to a much more precise integration with a negligible small remainder $\mathscr{E}_P$. Further, the cubature rules with all positive coefficients are more accurate with respect to those where some weights are negative. The negativeness usually indicates that the cubature formula is overloaded, i.e., its number of knots exceeds the possible minimum. From the aforesaid, the NO and PO schemes should be treated as the worst, the NI as acceptable, and the PI formulae as the best.

As can be seen from Table 1, beginning from a relatively small order $P = 15$, all the known cubature rules with the lowest number $\mathscr{N}$ of knots do not meet the high (PI) quality standard. Most of them ($P = 15, 17, 19, 21$) are of the worst (NO) quality. The NI scheme with $P = 23$ is unsatisfactory as well in view of the too high value $\mathscr{N} = 112$ which exceeds considerably the lowest possible number $N^* = 96$ of knots corresponding to the rotational symmetry approach. For orders $P = 17$ and $P = 21$ there is also a gap between $\mathscr{N}$ and N^*. Therefore, significant improvements in the two-dimensional integration may be achieved by finding actual (inside) solutions to Eq. (5).

3. Algorithm

As has been demonstrated above, up to now there are no satisfactory cubature formulae for degrees $P > 13$. Moreover, in spite of the fact that the speed of computers has increased in several orders, no new achievements on the cubature rules for the square have been reported during the last 10 years. Our previous intensive attack on the system of polynomial equations using standard methods (see below) also resulted in no improvements. We then came to a conclusion that the development of more efficient algorithms plays a much more important role in solving the problem considered than the growing speed of modern computers.

Many algorithms and computational strategies have been used over the years to handle nonlinear equations. Almost all of them are reduced to the application of conjugate-gradient type schemes and the well-known Newton method. The latter method exhibits a fast convergence of the iterations, but requires a very good initial approximation to the solution. With increasing the number of equations and their nonlinearity, the region of convergence decreases dramatically. The conjugate-gradient schemes are more stable, but the convergence of the iterations becomes very slow when the number of equations increases. Moreover, both approaches require the knowledge of derivatives of the equations with respect to unknowns.

Quite recently, a method of modified direct inversion in the iterative subspace (MDIIS) has been proposed [14] to solve complicated systems of nonlinear constraints appearing in the integral equation theory of liquids. It has been shown that the convergence of the iterations can be accelerated drastically with respect to other known algorithms. This convergence was observed almost for arbitrary initial guesses and was not so sensitive to increasing the number of equations. For this reason, it is very enticing to try to develop the MDIIS method in the context of the cubature theory.

The first step consists in reducing the system (5) of L^* polynomial equations to an equivalent system with the smallest possible number $\hat{L}^*$ of nonlinear constraints. This indeed can be realized, because the weights w_i ($i = 1, 2, \ldots, M^* + O^*$) enter into the polynomial equations (5) linearly. Then the first $M^* + O^*$ equations can be treated as a linear system with the knots $(x_i, y_i)|_{i=1,\ldots,M} \equiv s_i|_{i=1,\ldots,2M^*+O^*}$ being at the moment as parameters of that system. Whenever it is necessary, this system can readily be solved with respect to w_i using a linear solver, for instance, the well-recognized Gaussian elimination (that gives exact solutions in of order $(M^* + O^*)^3$ elementary steps without applying any iterations). The obtained values of w_i are further substituted into the rest polynomial equations. As a result, we come to the system

$$R_\alpha(s_1, s_2, \ldots s_{\hat{L}^*}) = 0, \quad \alpha = 1, 2, \ldots, \hat{L}^* \tag{7}$$

of $\hat{L}^* = L^* - M^* - O^* \equiv 2M^* + O^*$ nonlinear equations with the same number of unknowns s_i ($i = 1, 2, \ldots, \hat{L}^*$).

Let $s_i^{(\gamma)}$ be an approximation to the solution s_i obtained after the γth iteration in the course of the iterative process. The MDIIS approach claims that a much better approximation can be achieved by using the linear combination

$$\hat{s}_i^{(\gamma)} = \sum_{\beta=1}^{m} c_\beta s_i^{(\gamma-\beta+1)} \tag{8}$$

of vectors $s_i^{(\gamma-\beta+1)}$ corresponding to the m last iterations ($\beta=1, 2, \ldots, m$). The coefficients c_β are defined by requiring the corresponding linear combination of the residuals,

$$\hat{R}_\alpha^{(\gamma)} = \sum_{\beta=1}^{m} c_\beta R_\alpha \left(s_1^{(\gamma-\beta+1)}, \ldots, s_{\hat{L}^*}^{(\gamma-\beta+1)} \right) \equiv \sum_{\beta=1}^{m} c_\beta R_\alpha^{(\gamma-\beta+1)}, \tag{9}$$

provides a (local) minimum for the vector norm

$$\lambda = \min \sqrt{\sum_{\alpha=1}^{\hat{L}^*} (\hat{R}_\alpha^{(\gamma)})^2} \tag{10}$$

and are subject to the additional constraint $\sum_{\beta=1}^{m} c_\beta = 1$. This leads to the system of $m+1$ linear equations for the expansion coefficients,

$$\begin{pmatrix} S_{11} & \ldots & S_{1m} & -1 \\ \vdots & \vdots & \vdots & \vdots \\ S_{m1} & \ldots & S_{mm} & -1 \\ -1 & \ldots & -1 & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_m \\ \lambda^2 \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ -1 \end{pmatrix}, \tag{11}$$

where

$$S_{\beta v} = \sum_{\alpha} R_\alpha^{(\gamma-\beta+1)} R_\alpha^{(\gamma-v+1)} \tag{12}$$

is a scalar product of the residual vectors, and λ^2 is a Lagrangian multiplier yielding the squared norm of the minimized residual components (9). The next idea is based on the fact that the extrapolated residual vector $\hat{R}_\alpha$ is perpendicular to the $(m-1)$-dimensional plane passing through the points specifying the basic residuals R_α. Thus this vector can be a reasonable approximation of the direction to the global (zero) minimum ($\sum_{\alpha=1}^{\hat{L}^*} R_\alpha^2 = 0$), i.e., to the $\hat{L}^*$-dimensional point $(s_1, \ldots, s_{\hat{L}^*})$ of solution to system (7). Then the next MDIIS iteration will read

$$s_i^{\gamma+1} = \hat{s}_i^{\gamma} + \eta \hat{R}_\alpha^{(\gamma)}, \tag{13}$$

where $\eta \neq 0$ is the relaxation parameter to be adjusted for the best convergence. The iterative procedure starts with one set of the residuals, sequentially incrementing the MDIIS matrix size up to $m \times m$, and thereafter discarding the earlier predictions.

The quantity m should be of order of the number $\hat{L}^*$ of equations to properly generate the direction to the global minimum. For instance, in the case of $\hat{L}^*$ pure linear equations, the MDIIS procedure exactly converges to the solution in $\hat{L}^* + 1$ iterations independently of $\eta \neq 0$, provided $m = \hat{L}^* + 1$. For smaller $m < \hat{L}^* + 1$, the number of iterations will increase. In the case of a large number $\hat{L}^* \gg 1$ of nonlinear equations, the situation is different. On the initial stage of the iteration process, where the current approximations are far from the solution, we should decrease m to $\sim \hat{L}^*/2$ to extend the region of convergence. Here the precision of determining the current direction to a minimum is not so important,

but the computational time per iteration will decrease significantly (note that this time is proportional to m^3 due to the inversion of matrix $S_{\beta\gamma}$ needed to evaluate the expansion coefficients c_β). On approaching the solution (where the nonlinear equations allow more and more linearization), the value m can be consecutively increased first to $2/3\hat{L}^*$, say, and further up to $\hat{L}^*$ in order to minimize the number of iterations.

From the mathematical point of view, the relaxation parameter η should be chosen in a way to minimize the one-variable function $\Psi^{(\gamma+1)}(\eta)=\sum_{\alpha=1}^{\hat{L}^*} R_\alpha^2(\hat{s}_1^\gamma+\eta\hat{R}_\alpha^{(\gamma)},\ldots,\hat{s}_{\hat{L}^*}^\gamma+\eta\hat{R}_\alpha^{(\gamma)})$. This requires, however, significant extra computational costs at each iteration. Moreover, the location of a minimum of $\Psi^{(\gamma+1)}(\eta)$ may have nothing to do with the point of solution if the current approximation is far from it. A similar situation arises in conjugate-gradient-type schemes. In this respect, the MDIIS method is close to them but should be considered as more preferable because of the acceleration of iterations by the additional minimization of the linearized construction of the residuals. Moreover, unlike the gradient and Newton approaches, the MDIIS method does not require the calculation of derivatives. This reduces the computational efforts.

In practice, the optimal value of η is determined for a given system by a particular ratio between the scales of the residual functions R_α and their arguments s_i. To better linearize the residuals in the region of the next $(\gamma+1)$th iteration, it is desirable to provide the updating term $\eta\hat{R}_\alpha^{(\gamma)}$ in Eq. (13) such that the corresponding change $R_\alpha^{(\gamma+1)}-\hat{R}_\alpha^{(\gamma)}$ is close in magnitude to the minimized residual $\hat{R}_\alpha^{(\gamma)}$. In the region of quadratic convergence (when the iterated predictions are close to the solution and the nonlinearity allows a linearization) the effect of varying η vanishes like in the pure linear case. In the case of nonlinear system (7) it has been established that the above criterion is reached when $\eta\sim 1$ for any $\hat{L}^*$. We used the value $\eta=1$ in all our calculations.

It should be stressed that outside a quadratic region of the convergence, the root mean square value of the current residual

$$\overline{R}^{(\gamma)}=\sqrt{\frac{1}{\hat{L}^*}\sum_{\alpha=1}^{\hat{L}^*}(R_\alpha^{(\gamma)})^2} \tag{14}$$

does not necessarily decrease monotonically with iterations. The residual at the new prediction, which is even somewhat larger than the previous one, updates and improves the representation of the residual functions by the MDIIS vectors. Such a rise is usually followed by a substantial drop of the residual magnitude at the next steps. However, if the root mean square residual calculated at the next point appears to be essentially larger (three orders of magnitude, say) than the smallest value of those for the last m MDIIS vectors, i.e., $\overline{R}^{(\gamma+1)}>K_R\min(\overline{R}^{(\gamma)},\overline{R}^{(\gamma-1)},\ldots,\overline{R}^{(\gamma-m+1)})$ with $K_R\sim 10^3$, it is worthwhile to restart the MDIIS procedure from the point of the smallest residual because the old MDIIS vectors no longer model the behavior of the residual function properly. The procedure should also be restarted if the MDIIS predictions do converge to the solution to within a given precision after a significantly large number of iterations. This usually means that initial guesses where chosen outside the region of convergence and they should be regenerated.

In our case, the initial guesses for s_i were generated at random within the interval $[-1, 1]$ in each of the $\hat{L}^*$ dimensions. In such a way, after several days of continuous attacking the system of nonlinear equations (7) (for each given degree P) on a Silicon Graphics Origin 3800 workstation, the desired

solutions have been found. We have used a high-speed Intel Fortran compiler within the double precision (sixteen significant digits) and limited the initial accuracy of the calculations to $\overline{R}\lesssim 10^{-12}$. A few additional Newton's iterations have been performed in each case to reduce the residual to a negligible small level of $\overline{R}\lesssim 10^{-200}$. For this we have employed the Maple 9 package with up to 200 digits for internal computations, taking the solutions obtained already in Fortran as initial guesses. All the numerical results will be shown with 32 significant digits.

4. Results

We have successfully reproduced the known rotation invariant cubature rules for degrees $P = 1$, 3, 5, 7, 9, 11, and 13. Such rules can be found in Refs. [6,8,17,19,23] (see also Table 1) and they will not be shown in this paper to save space. Only new cubature formulae of higher degrees $P = 15$, 17, 19, 21, and 23 will be presented and compared with previous schemes. For some values of P, the system (5) of nonlinear equations can have two or more solutions. In particular, the cubature rule related to type II (see Table 1) can provide us with solutions of subtypes IIA and IIB (they will be marked below simply as A and B). We will try to mention about all possible ones (PI, NI, PO, and NO). In such a situation, the preference will be given to an optimal (PI) cubature formula which leads to the smallest norm

$$E_P = \sqrt{\sum_{k,l}^{k+l=P+1} \left(\sum_{i=1}^{N} w_i x_i^k y_i^l - g_{kl} \right)^2} \tag{15}$$

of the main term of uncertainty (6) (the quantity E_P presents in fact the norm of residuals corresponding to the next degree $P + 1$). The total number of PI solutions found will be indicated as well.

Due to the rotational symmetry (4) of cubature formulae derived, we will present only basic coordinates $0 \leqslant x_i \leqslant 1$ and $0 \leqslant y_i \leqslant 1$ of each knot square i in the order of increasing its weight w_i. The rest three coordinate pairs can readily be generated as $(-y_i, x_i)$, $(-x_i, -y_i)$, and $(y_i, -x_i)$. So that writing the solution in the form $(w_i; x_i, y_i)$ we will have in mind all the four coordinate pairs for each i with the same weight w_i. From the symmetrical properties it follows that if $(w_i; x_i, y_i)$ is a solution to the nonlinear system (5), then $(w_i; y_i, x_i)$ (where x_i and y_i are interchanged for all i) is also a solution to that system. In other words, each rotationally symmetric cubature formula may have its symmetrical counterpart. The number of counterparts can increase from one to three for solutions of type A, where $x_{i^*} \neq 0$ and $y_{i^*} = 0$ for some number i^*. This follows from the fact that replacing $(w_{i^*}; x_{i^*}, 0)$ by $(w_{i^*}; 0, x_{i^*})$ and do not changing all the rest ($i \neq i^*$) knot square generators $(w_i; x_i, y_i)$ also lead to a solution, because the system of nonlinear equations (5) is invariant to the above transformation. All the counterparts are completely equivalent and thus indistinguishable within the cubature formalism.

A. Order $P = 15$

For $P = 15$ the best cubature rule known before our investigations was the PI formula with 48 points [19] (the NO formulae with 44 points [19] should be ignored because of outside solutions).

Table 2
New formula of degree 15 with 44 points

w_i	x_i	y_i
0.20881470204497523521771058289754E–1	0.98798456650771809034922121236542	0.77126821223875533899886933446485
0.25545901574497276542640153395248E–1	0.90815949600657000212015099547736	0.95703183434690690872237176442598
0.31203866624933300871149690867662E–1	0.67928365833453330499132539100332 5	0.88260197593087253601344445274335
0.38010761595074827467645518285610E–1	0.50911373411758353514778637359508	0.97120312974183699854692313856226
0.41449061852426148002787373214871E–1	0.97675332466910190352385200798077	0.83559862608781647288448365846813E–1
0.79320407004083334044710201039891E–1	0.75619936719149244012005066365912	0.75619936719149244012005066365912
0.88901265758751523303980720079987E–1	0.89778569328633877480008574782677	0.46676265923796434848237353795400
0.12016982158206027507823569713056	0.20599307074252141729418963873618	0.84079448454078540426562160968883
0.16882043410639799754153511014621	0.45144312511299139017533875886564	0.56245686233219940637540066298377
0.16987162497336185160489786440053	0.66683824538360873834071399129626	0.19046630243571720761679616635243
0.21582538472391594202064661314968	0.74295704755765822553432311307323E–1	0.32397702249753019818251854432752

Table 3
New formula of degree 17 with 56 points

w_i	x_i	y_i
0.10693483986974526468925667171638E–1	0.83395914422050762595707520328329	0.99690134998258294114169765276688
0.16771622989325482379964908559201E–1	0.96701240760377864958940778776159	0.92101565015369642619085740576658
0.21520834803173017585623196363995E–1	0.98651441086033068583570701960810	0.56251780244667252352153081833715
0.24893201532665059892584476318209E–1	0.17035060808995408160378979789427E–1	0.98204914256843033449712481990261
0.42463258472030940473501779894230E–1	0.42523896522453030941022314252505	0.95796453236865195741899809390262
0.53711265037645010830029221647514E–1	0.88194109089215356624316729768736	0.74117688569732509081061208741447
0.54579479693382460849318673206721E–1	0.69978907719058600912388980227382	0.88728024293255774907349992409998
0.67375653622461385504403959336007E–1	0.90858412958838344797723547617253	0.25843122151820770173022364732347
0.98025282885102299426881768287454E–1	0.73933759205292015806620475085721	0.47295583257297618882242532468520
0.98325651584666601742691443856667E–1	0.21246155837885419289305793553062	0
0.10576898319665727200249259468733	0.15644172095846342514322716437912	0.81259212523912311994061744159953
0.10593453574575401283483020818374	0.50398563819427997044830482422504	0.68201093297792530795370853308359
0.14990405484916921950315250394890	0.58243895074467257078462336257058	0.11846544560647891209927499369579
0.15003269160099271050559959853839	0.28970323065541272212557470108155	0.40876985953794338411643329876836

Instead, we have found 5 PI solutions of type A and 11 PI solutions of type B with 44 points each (it seems that no other PI solutions exist). Some NI, PO, and NO have also been identified. The optimal PI solution, that minimizes the error norm E_P, appears to be of type B. It has the form as shown in Table 2.

The CPU time spent per solution was $t = 40$ s.

The new formula reduces the number of knots within the inside solutions from 48 to 44 and improves the quality from the worst NO to the best PI within 44 knots.

B. Order $P = 17$

For $P = 17$ the best cubature rules known earlier were the PI formula with 60 points [13] and the NO formula with 57 points [7] (the latter should be ignored because of outside solutions).

Instead, we have found 4 PI solutions of type A and 5 PI solutions of type B (some NI, PO, and NO have also been identified). The optimal PI cubature that minimizes the error norm E_P appears to be of type A. It is presented in Table 3.

The CPU time spent per solution was $t = 15$ min.

The new formula reduces the number of knots within the inside solutions from 60 to 56, improves the quality from the worst NO at 57 points to the best PI with 56 knots, and updates the lower boundary limit to $\mathcal{N} = 56$.

Note that beginning from this order, one cannot guarantee that all possible solutions have been recognized. This is because of the rapid increase in the CPU time, t, (up to $t = 15$ min for $P = 17$) spent to figure out at least one solution. However, on attacking the system on a computer during significantly long time ($T = 7$ days in our case), one can say with a great probability (because $T \gg t$) that we have found almost all solutions and chosen among them the nearly optimal set.

C. Order $P = 19$

For $P = 19$ the best cubature rules known previously were the NO and PO formulae with 68 [21,22] and 72 [13] points, respectively. However, they both contain outside knots and should be considered as unapplicable.

Instead, we have found the PI solution with 68 points (Table 4).

This solution has been obtained in $t = 5$ hours (and no others were found during the whole run of $T = 7$ days).

The new formula improves the quality from the worst NO to the best PI within 68 points.

D. Order $P = 21$

For $P = 21$ the best previous cubature rules were the NO [16] and PO [13] formulae with 85 and 88 points, respectively. Again, they contain outside knots and should be considered as useless.

Instead, we have found the PI solution with 81 points (Table 5).

This solution has been obtained in $t = 5$ days.

Table 4
New formula of degree 19 with 68 points

w_i	x_i	y_i
0.42157189312457273371400997162954E–2	0.93790944060174636724164305692148	0.99998546072852907260205380652647
0.99237601014741223600089798896376E–2	0.59787966519157168521483636741590	0.98732847941781540087026300838966
0.15078678879581549295330034135223E–1	0.96865781747798834472115427804246	0.89837495163532572964949889543009
0.15121496864822956266676863866018E–1	0.98871713276447330663578670732177	0.62259634389530287767136776393609
0.23821621047339582724750103846036E–1	0.98398534132338386681313796251589	0.81109463487824943619725131193050E–1
0.28746437252189671047629194361029E–1	0.36585775934555586089438861852973	0.96462400422891970516096923553526
0.31348715503861464721826917341708E–1	0.78392149176096602345110934186655	0.93756444544378175318295617860873
0.49762852666717116332578404045926E–1	0.86937144898957875204792277623522	0.74380866034597101765279618918913
0.55534775159604041101829554407116E–1	0.91889377777573801032232199904313	0.38410875822737883260638757649426
0.65013710432173970207381031565964E–1	0.14078396804456848628363687508206	0.87987957307981017658529064786666
0.73819068900731731823980126564345E–1	0.56379666815446526573028097449771	0.81879210607636015929368719928237
0.90385825968150641564727715959435E–1	0.76200274293070327698230061865243	0.15749920122732269808023356410127
0.91881833336425013923433485117405E–1	0.69745388342191267884442122044750	0.54657527460177776847334916572487
0.94967142638856099564605740671378E–1	0.52310392339404494392757182766006	0
0.10498174724102843457467466433826	0.30566836903929191370033838487568	0.65017670270687960549278395428873
0.11871336850928058424347422704556	0.44898642628288082765338494532756	0.34240465380680230945939322837053
0.12668324656651729290995285712867	0.98253418759835132805054567507033E–1	0.23509621629115532325303789785547

Table 5
New formula of degree 21 with 81 points

w_i	x_i	y_i
0.59245289910274777823163684444026E–2	0.99742844318071465788852153329446	0.52349333540342268677302187698119
0.63181879993530976749052313712955E–2	0.90092205722857715090631770295789	0.99213624611198765984022577926158
0.77654356771885822575525989789117E–2	0.98137581661152322617866583081353	0.93577766500519228442627576803182
0.13313236524649387539261801099149E–1	0.47562398846061921636952360049609	0.98806503981406364167006543205075
0.18028023632000303112294832251383E–1	0.68396217875524370909034162562144E–1	0.98289142121346795894575007552095
0.20759211084811453614957408545828E–1	0.96445171170290974019893928634261	0.73079564192792033198229729840349
0.24345594686962939048122829629801E–1	0.96789534067760540982739074113386	0.28416943704022564251542547384397
0.27291829813157459363923440908365E–1	0.71204626183902144323409345553631	0.95001737577395264422880843244573
0.31313724489320677669626239379042E–1	0.86686503563504933746419509606443	0.85754514904426211818642071770359
0.43028684463625497581941353350492E–1	0.29388895765490255861532312924984	0.91478375374420147743639913929870
0.47435107497760585342967184111271E–1	0.88245289720509646533706783064117	0.78310571319347967606817150072422E–1
0.49535232791099913534195616930148E–1	0.88356465549777630296872390851348	0.50650027819745540446699219481203
0.59086609737522776429493659734483E–1	0.53714330328796591598235477256257	0.82111662321535962574448188332070
0.61598898755573131953283218720393E–1	0.73297737278688849035966507531475	0.67811474157990352881988795983159
0.68662882737105569078247834904061E–1	0.74340815897994389367005251095709	0.25891212405917942502949658613377
0.77511025760449779132628565445376E–1	0.14352379867257862891820869134808	0.73714284444878233387764988974016
0.77655900861398148704502327066780E–1	0.57716374806487034338151001622839	0.42605137832252378501649531823938
0.84165159143253389201574044182295E–1	0.38010653105519745774291045326124	0.59190980196005469388929534014808
0.11664395742356559711226466539621	0.49380304750704567296572150088764	0.46968438389915362845722235027390E–1
0.12587077966701428595400393561138	0.23300694276964919884562248755586	0.27854054992870057594151995625227
0.13498395305263979164774737575571	0	0

The new formula improves the quality from the NO/PO to PI, and shifts the lower boundary limit from 85 to $\mathcal{N} = 81$ points.

E. Order $P = 23$

For $P = 23$ the best cubature rule known previously was the NI formula with 112 points [21]. Instead, we have found the NI solution with 100 points (see Table 6 below). The new formula shifts significantly the lower boundary limit up to 12 points, namely, from 112 to $\mathcal{N} = 100$.

Note that according to Table 1, we should obtain a solution at $P = 23$ with even less number $N^* = 96$ of knots. However, hard attacking the corresponding system of nonlinear equations during $T = 10$ days did not lead to any result. In such a case we were enforced to increase the number of points from $N^* = 96$ to 100 by adding one extra knot square of type A. This results in two extra unknowns, so that two additional nonlinear equations have been appended to the system to make the solution to be unique (otherwise we obtain the infinite number of solutions continuously covering a plane in the multidimensional space). We have attached the two equations corresponding to taking into account the higher order ($P = 24$) monomials $x^{15}y^9$ and $x^{22}y^2$.

Another trick consists in changing the strategy of generating initial guesses during the MDIIS iterative process. This is caused by the fact that within the usual strategy the CPU time t spent to find at least one solution increases approximately in a factor of 20 with rising P to $P + 2$. This follows from the previous values of t corresponding to the lower degrees $P = 21$, 19, 17 and 15 (see above). Extrapolating these values to degree $P = 23$ yields $t = 3$ months, i.e., the calculations become exclusively expensive. The change of the strategy at extremely high degrees $P \gtrsim 23$ is possible since then with rising P to $P + 2$ the incrementation $\Delta P = 2 \ll P$. Therefore, we should expect a slight modification in the positions of existing

Table 6
New formula of degree 23 with 100 points

w_i	x_i	y_i
–0.22499144590180737573666435988313E–1	0.22475776435269587875683347524503	0.29562926123440075779470457695520
0.56757797279709720956600059513997E–2	0.87420793087689680287386901266229	0.99164484170232374329954582252223
0.61294541632385752564605990154598E–2	0.97602267261364022197431910391898	0.96038644389988149213812916422733
0.77307399716921584473393426863691E–2	0.98901025758028347071424940975698	0.79476170695439095037125111357424
0.79851030689059360294239183531451E–2	0.99326920924031633712313940841625	0.45269906826670511998507618989211
0.10747724909071103372536638574027E–1	0.56499592316621278816917834165965	0.98963443963546680882582623594845
0.14073722901914630236333688287280E–1	0.12479933234667809522764885071235	0.98891634511573107523317221688555
0.22950166656215871772211451659864E–1	0.90240439932034384398117518141661	0.86681747165850322502643568236158
0.23104503668552704581666880144042E–1	0.96603416099961004557874518675109	0.22128837983587450545659391256077
0.24886583460620943481070103801115E–1	0.74327403381257373930317209035852	0.93739279789140167477396439558006
0.25495608710781325077549951029551E–1	0.94397158234337348119479988763974	0.62734373811214363563025812471848
0.35148791457392415926700843453924E–1	0.36473593323821554671165638117641	0.93654053553190687038241524198386
0.39967612471275640012053163262252E–1	0.90025309287443275420616285586643	0.25070990341427951813078348104539E–1
0.42210906199290840139296408236284E–1	0.48034665839500246850252725186282E–1	0.65304687691990057591624038872149
0.45629308917602135087674549832202E–1	0.54919116214309328871373834754894	0
0.47184931543983842485535616621711E–1	0.86487537690899969927500100353866	0.42021700731140387645536924573814
0.48004360511784007777329600464972E–1	0.78769621309348012773202186731599	0.71486137179637184939863361570348
0.51407132281965816724265717022986E–1	0.57671028420945643394316234476328	0.82649643106250383189783444260321
0.54210495031621259406088939636629E–1	0.20013408262762044788586320030931	0.80824267349292209367541999626505
0.63980226470850872129000560206633E–1	0.74602728783032388650354427676695	0.20581981165646397971556679713472
0.71999854713967554049756153858067E–1	0.64177280458672645848207064078009	0.51516637687706181290564290685967
0.74130368424485001536304396403399E–1	0.40236411309752397363192555539035	0.64890781819854093908140818020446
0.87075597857073455631778823034765E–1	0.46993983120051570507268178090848	0.27714799151429808758023024246803
0.10080008323810791275764368651352	0.22491749438123049571812018957130	0.40375503517268762210602535023913
0.11197008823181576355998539793872	0.22831753386455276245209947736815	0.56116790982355323182358196190726E–1

knots during the transform from P to $P+2$, whereas the extra knots should appear at smaller and smaller (with further increasing P) weights. In our case, the 81 knots of the cubature formula of degree $P=21$ were chosen as initial approximations to the solution of the cubature formula of degree $P=23$ with 100 points. The coordinates of the rest 19 knots were generated at random within the $[-1, 1]$ interval. In such a way, our cubature formula of degree 23 with 100 points has been obtained in $t=10$ days.

5. Conclusion

During the last decade, a stagnation of progress has been observed in the area of building cubature formulas exact for polynomials. In particular, for the case of two-dimensional integration over the square, almost no new theoretical results were obtained, and no new cubature formulas were constructed. This is despite the fact that beginning already from relatively small degree $P=15$, all the earlier known cubature rules with the lowest number of knots are useless in practical applications. The reason is that they either produce nodes lying outside the region of integration or/and have the number of knots $\mathcal{N}$ exceeding considerably the minimal theoretical limit $\mathcal{N}_{\min}$. Even for integrands determined outside of the integration domain, using the outside cubature rules leads to a very poor precision of the calculations.

In the present study we have developed the method of construction of minimal cubature rules with high degrees of exactness and adapted a powerful algorithm for solving the corresponding system of nonlinear polynomial equations. This has allowed us to reach the obvious achievements in two-dimensional integration. Namely, the whole set of new inside cubature formulae of degrees $P=15$, 17, 19, 21, and 23

Table 7
Achievements in two-dimensional cubature integration

Previous results					Our new results				
P	$\mathcal{N}$	Quality	References	Year	P	$\mathcal{N}$	Quality	References	Year
15	44	NO	[19]	1971	15	44	PI (16)[a]	this work	2003[b]
	48	PI	[19]	1971					
		NI	[15]	1989					
17	57	NO	[7]	1985	17	56	PI (9)[a]	this work	2003[c]
	60	PI	[13]	1985					
19	68	NO	[21,22]	1991	19	68	PI	this work	2003
	72	PO	[13]	1985					
21	85	NO	[16]	1978	21	81	PI	this work	2003
	88	PO	[13]	1985					
23	112	NI	[21]	1993	23	100	NI	this work	2003

[a]If more than one solution is found, the total number is pointed out in parentheses.
[b]Some PI solutions for $P = 15$ have been found by us in earlier 1988 and 2001. The whole set as well as the optimal solution have been obtained in 2004.
[c]The whole set of solutions has been obtained in 2004.

has been introduced. The new formulae exhibit the best quality and appear to be the most efficient for the evaluation of two-variable integrals with a high precision. In addition, for degrees $P = 17$, 21, and 23, we have improved the previous results (57, 85, and 112, respectively) for the lower known boundary limit $\mathcal{N}$. The new lower boundaries now read, correspondingly, $\mathcal{N} = 56$, 81, and 100. It seems that in the feature it will be impossible to shift the obtained values of $\mathcal{N}$ to lower levels at least for orders $P = 15$, 17, 19, and 21. The fact that these values are still greater than the highest known lower theoretical bounds $\mathcal{N}_{\min}$ indicates most likely that the existing theory underestimates $\mathcal{N}_{\min}$ at $P \geqslant 13$ (see Table 1). Our new achievements are summarized in Table 7.

The proposed approach can readily be extended to derive efficient cubature formulae for higher dimensions, orders, and other regions of integration. It can also be used for constructing cubature rules exact for a class of integrands in the form of polynomials multiplied on some known functions (the last ones being chosen to analytically remove possible integrable singularities from some integrals). These and related questions will be addressed in further investigations.

Acknowledgements

The authors thank Prof. R. Cools for giving us access to Encyclopedia of Cubature Formulas (see Ref. [6]).

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