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Modified product cubature formulae ☆

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ABSTRACT

In the univariate case, there is a well-developed theory on the error estimation of the quadrature formulae for integrands from the Sobolev classes of functions. It is based on the Peano kernel representation of linear functionals, which yields sharp error bounds for the quadrature remainder. The product cubature formulae are the usual tool for the approximation of a double integral over a rectangular domain. In this paper we suggest a modification of the product cubature formulae, based on blending interpolation of bivariate functions. Besides the usual point evaluations, the modified cubature formulae involve few line integrals. Our approach allows application of the Peano kernel theory for derivation of error bounds for both standard cubature formulae and their modifications. Sufficient conditions for the definiteness of the modified product cubature formulae are given, and some classes of integrands are specified, for which a product cubature formula is inferior to its modified version.

1. Requisites

1.1. Peano kernel theory for quadratures

Throughout this paper π_m will mean the class of univariate algebraic polynomials of degree not exceeding m. A quadrature formula for approximation of the definite integral

$$\ell[g] := \int_a^b g(t)\mathrm{d}t$$

is any linear functional of the form

$$Q[g] = \sum_{\nu=1}^{n} a_\nu g(x_\nu), \quad a \le x_1 < \cdots < x_n \le b. \tag{1}$$

The quadrature formula Q is said to have algebraic degree of precision m (in short, $ADP(Q) = m$), if the remainder functional

$$R[Q; g] := \ell[g] - Q[g]$$

satisfies

$$R[Q; g] = 0 \quad \text{if } g \in \pi_m, \text{ and } R[Q; g] \neq 0, \quad \text{if } g \in \pi_{m+1} \setminus \pi_m.$$

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For $r \in \mathbb{N}$, the truncated power function x_+^r is defined by $x_+^r = (\max\{x, 0\})^r$. According to a classical result of Peano (see, e.g., [2,11,9] or [3]), if $\mathcal{L}$ is a linear functional defined on $C[a, b]$, which vanishes on π_{r-1}, and $g^{(r-1)}$ is absolutely continuous on $[a, b]$, then $\mathcal{L}[g]$ admits the representation

$$\mathcal{L}[g] = \int_a^b K_r(t) g^{(r)}(t) \mathrm{d}t, \quad \text{where } K_r(t) = \mathcal{L}\left[\frac{(\cdot - t)_+^{r-1}}{(r-1)!}\right].$$

Applied to the remainder of a quadrature formula Q with $ADP(Q) = m$, where $m \geq r - 1$, the Peano result states that if $g^{(r-1)}$ is absolutely continuous on $[a, b]$, then

$$R[Q; g] = \int_a^b K_r(Q; t) g^{(r)}(t) \mathrm{d}t. \tag{2}$$

The function $K_r(Q; t)$ is called the rth *Peano kernel of the quadrature formula* Q, and, for $t \in [a, b]$, explicit representations of $K_r(Q; t)$ are

$$K_r(Q; t) = \frac{(b-t)^r}{r!} - \frac{1}{(r-1)!} \sum_{\nu=1}^{n} a_\nu (x_\nu - t)_+^{r-1}$$

and

$$K_r(Q; t) = (-1)^r \left[\frac{(t-a)^r}{r!} - \frac{1}{(r-1)!} \sum_{\nu=1}^{n} a_\nu (t - x_\nu)_+^{r-1}\right].$$

For $1 \leq p < \infty$, the $L_p[a, b]$-norm is defined by $\|g\|_{L_p[a,b]} := \left(\int_a^b |g(t)|^p \mathrm{d}t\right)^{1/p}$, and $\|g\|_{L_\infty[a,b]} = \operatorname{esssup}_{t\in[a,b]} |g(t)|$, for $p = \infty$. The Sobolev class of functions $W_p^r[a, b]$ is defined by

$$W_p^r[a, b] := \{g \in C^{r-1}[a, b] : g^{(r-1)} \text{ abs. cont.on } [a, b], \|g^{(r)}\|_{L_p[a,b]} < \infty\}.$$

For integrand $g \in W_p^r[a, b]$ and quadrature formula Q with $ADP(Q) \geq r - 1$, application of Hölder's inequality to (2) yields the sharp error estimate

$$|R[Q; g]| \leq c_{r,p}(Q) \|g^{(r)}\|_{L_p[a,b]}, \tag{3}$$

where

$$c_{r,p}(Q) = \|K_r(Q; \cdot)\|_{L_q[a,b]}, \qquad p^{-1} + q^{-1} = 1.$$

The most frequently used error constants $c_{r,p}(Q)$ are those with $p = 1, 2$ and ∞. $c_{r,\infty}(Q)$ is particularly easy for calculation when $K_r(Q; t)$ does not change its sign in (a, b). In such a case Q is said to be *definite quadrature formula of order r* (positive definite, if $K_r(Q; t) \geq 0$, and negative definite, if $K_r(Q; t) \leq 0$ in (a, b)). In the case when Q is a definite quadrature formula of order r, we have $c_{r,\infty}(Q) = |R[Q; (\cdot)^r/r!]|$. The definite quadrature formulae of order r provide one-sided approximation to $\ell[g]$ whenever $g^{(r)}$ has a permanent sign in (a, b). For such an integrand one can apply two definite (of opposite kinds) quadrature formulae to obtain an interval containing the true value of $\ell[g]$. Properties like definiteness and monotonicity in quadrature sequences are often used in numerical integration for derivation of a posteriori error estimates and rules for termination of calculations (the so-called stopping rules), see [5–7] and the references therein.

In [8] we initiated investigations on how the Peano kernel theory can be extended to the error estimation of some cubature formulae for double integrals on a rectangular region. In the present paper we give some further results in this direction.

1.2. Blending interpolation of bivariate functions

Let $\Delta = \{(x, y) \in \mathbb{R}^2 : a \leq x \leq b,\ c \leq y \leq d\}$. For $m, n \in \mathbb{N}$, the class of blending functions $B^{m,n}(\Delta)$ (see, e.g., [1]) is defined by

$$B^{m,n}(\Delta) := \{f \in C^{m,n}(\Delta) : D^{m,n}f = 0\},$$

where $D^{m,n}f := \frac{\partial^{m+n}f}{\partial x^m \partial y^n}$, and

$$C^{m,n}(\Delta) := \{f : \Delta \to \mathbb{R} : D^{i,j}f \text{ continuous},\ 0 \leq i \leq m,\ 0 \leq j \leq n\}.$$

Given two sets $\mathbf{X} = \{x_1, x_2, \ldots, x_m\}$ and $\mathbf{Y} = \{y_1, y_2, \ldots, y_n\}$, such that $a \leq x_1 < x_2 < \cdots < x_m \leq b$ and $c \leq y_1 < y_2 < \cdots < y_n \leq d$, we define a *blending grid* $G = G(\mathbf{X}, \mathbf{Y})$ by

$$G(\mathbf{X}, \mathbf{Y}) := \left\{(x, y) \in \Delta : \prod_{\mu=1}^{m}(x - x_\mu) \prod_{\nu=1}^{n}(y - y_\nu) = 0\right\}.$$

For any bivariate function f defined on Δ there exists a unique *Lagrange blending interpolant* $Bf = B_G f \in B^{m,n}(\Delta)$, which satisfies $Bf_{|G(X,Y)} = f_{|G(X,Y)}$. It is given explicitly by

$$Bf = \mathcal{L}_x f + \mathcal{L}_y f - \mathcal{L}_x \mathcal{L}_y f, \tag{4}$$

where $\mathcal{L}_x$ and $\mathcal{L}_y$ are the Lagrange interpolation operators with respect to variables x and y, defined by the interpolation points $\mathbf{X}$ and $\mathbf{Y}$, respectively. Let $\{l_\mu\}_{\mu=1}^m$ and $\{\bar{l}_\nu\}_{\nu=1}^n$ be the Lagrange fundamental polynomials, defined by $l_\mu(x_j) = \delta_{\mu j}$ ($j = 1, \ldots, m$) and $\bar{l}_\nu(y_k) = \delta_{\nu k}$ ($k = 1, \ldots, n$), respectively, with δ_{ij} being the Kronecker symbol. Then

$$Bf(x, y) = \sum_{\mu=1}^{m} l_\mu(x) f(x_\mu, y) + \sum_{\nu=1}^{n} \bar{l}_\nu(y) f(x, y_\nu) - \sum_{\mu=1}^{m} \sum_{\nu=1}^{n} l_\mu(x) \bar{l}_\nu(y) f(x_\mu, y_\nu).$$

For $r, s \in \mathbb{N}$ satisfying $r \le m$ and $s \le n$, and for $f \in C^{r,s}(\Delta)$, two iterated applications of the Peano formula to $f - Bf = (Id - \mathcal{L}_x)(Id - \mathcal{L}_y)f$ (with *Id* being the identity operator) yield, for $(x, y) \in \Delta$,

$$f(x, y) - Bf(x, y) = \iint_\Delta \mathcal{K}_r(x, t) \overline{\mathcal{K}}_s(y, \tau) D^{r,s} f(t, \tau) \mathrm{d}t \mathrm{d}\tau, \tag{5}$$

where

$$\mathcal{K}_r(x, t) = \frac{1}{(r-1)!} \left[(x - t)_+^{r-1} - \sum_{\mu=1}^{m} l_\mu(x)(x_\mu - t)_+^{r-1} \right]$$

and

$$\overline{\mathcal{K}}_s(y, \tau) = \frac{1}{(s-1)!} \left[(y - \tau)_+^{s-1} - \sum_{\nu=1}^{n} \bar{l}_\nu(y)(y_\nu - \tau)_+^{s-1} \right].$$

The described Lagrange blending interpolation scheme is extended in an obvious way to the case of blending grids $G(\mathbf{X}, \mathbf{Y})$ containing multiple gridlines, i.e., for $\mathbf{X}$'s and $\mathbf{Y}$'s whose components are not necessarily distinct. In such a situation, the Lagrange interpolation operators $\mathcal{L}_x$ and $\mathcal{L}_y$ are replaced by the corresponding Hermite interpolation operators, and Bf involves not only the traces of f over the gridlines, but also the traces of some partial derivatives of f.

2. Product cubature formulae and their blending counterparts

Consider the problem of calculation of a double integral over the rectangular region $\Delta = \{(x, y) \in \mathbb{R}^2 : a \le x \le b, c \le y \le d\}$,

$$I[f] := \iint_\Delta f(x, y) \mathrm{d}x \mathrm{d}y.$$

A standard way for approximation of $I[f]$ is by a cubature formula $C[f]$,

$$I[f] \approx C[f] = \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} a_{ij} f(t_i, \tau_j),$$

where the points $\{(t_i, \tau_j)\}$ are usually assumed to belong to the integration domain. The case of a rectangular region admits usage of cubature formulae of product type (cf. [12,4]),

$$C[f] = C(Q_1, Q_2)[f] := \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} c_i d_j f(t_i, \tau_j), \tag{6}$$

where $Q_1[g] = \sum_{i=1}^{n_1} c_i g(t_i)$ and $Q_2[g] = \sum_{j=1}^{n_2} d_j g(\tau_j)$ are quadrature formulae approximating $\ell_1[g] := \int_a^b g(x)\mathrm{d}x$ and $\ell_2[g] := \int_c^d g(x)\mathrm{d}x$, respectively.

Some natural questions arise about the magnitude of the error

$$E[C; f] := I[f] - C[f].$$

How small is $|E[C; f]|$? Is it possible, as in the univariate case, to estimate $|E[C; f]|$ by a certain norm of a single derivative of the integrand, say, $D^{r,s}f$? Can we build definite cubature formulae of order (r, s) ?

The answer to the second question is in the negative. Indeed, an estimate of the form $|E[C; f]| \le c_{r,s}(C)\|D^{r,s}f\|$ would mean that the cubature formula C is exact for all functions from $B^{r,s}(\Delta)$. Hence, while in the univariate case we deal with *algebraic degree of precision*, in the bivariate case we have to deal with the notion of *blending degree of precision*. However, in contrast to the univariate case, the linear space of blending functions $B^{r,s}(\Delta)$ is of infinite dimension, and no cubature formula exists, which uses only finite number of point evaluations and is exact for all $f \in B^{r,s}(\Delta)$.

We show that error estimation of the above mentioned type is still possible, if we allow our cubature formulae to involve, in addition to the standard data of point evaluations, some line integrals. The construction of such cubature formulae is realized through the following scheme (see [8]):

We approximate $I[f - Bf]$ by $C[f - Bf]$, where C is a cubature formula of the customary type, i.e., which involves only point evaluations of the integrand. This results in a cubature formula $S[f]$ for approximate calculation of $I[f]$,

$$I[f] \approx S[f], \qquad S[f] := C[f] + I[Bf] - C[Bf]. \tag{7}$$

Among the components of the new cubature formula S, $I[Bf]$ is the one that looks different from the conventional cubature formulae. Indeed, by the explicit form of $Bf(x, y)$ we obtain

$$I[Bf] = \sum_{\mu=1}^{m} b_\mu \ell_2[f(x_\mu, \cdot)] + \sum_{\nu=1}^{n} \overline{b}_\nu \ell_1[f(\cdot, y_\nu)] - \sum_{\mu=1}^{m}\sum_{\nu=1}^{n} b_\mu \overline{b}_\nu f(x_\mu, y_\nu) =: C_B[f]. \tag{8}$$

Here,

$$Q'[g] = \sum_{\mu=1}^{m} b_\mu g(x_\mu)$$

is the interpolatory quadrature formula for $\ell_1[g] = \int_a^b g(x)\mathrm{d}x$, generated by $\mathcal{L}_x$, and

$$Q''[g] = \sum_{\nu=1}^{n} \overline{b}_\nu g(y_\nu)$$

is the interpolatory quadrature formulae for $\ell_2[g] = \int_c^d g(y)\mathrm{d}y$, generated by $\mathcal{L}_y$. $C_B[f]$ is called *blending cubature formula*, and it involves $m+n$ univariate integrals over the gridlines of G. Of course, one can use solely the approximation $I[f] \approx C_B[f]$ instead of $I[f] \approx S[f]$. However, there is a good reason for preferring S to C_B, which will be explained below.

On using (5) one obtains

$$E[C_B; f] = I[f] - C_B[f] = \iint_\Delta K_r(Q'; t) K_s(Q''; \tau) D^{r,s} f(t, \tau)\mathrm{d}t\mathrm{d}\tau,$$

where $K_r(Q'; t) = \ell_1[\mathcal{K}(\cdot, t)]$ and $K_s(Q''; \tau) = \ell_2[\overline{\mathcal{K}}(\cdot, \tau)]$ are the rth Peano kernel of Q' and the sth Peano kernel of Q'', respectively. From the above formula and Hölder's inequality holds the sharp inequality

$$|E[C_B; f]| \le c_{(r,s),p}(C_B)\|D^{r,s} f\|_{L_p(\Delta)}.$$

Due to the separated variables, the error constant of the blending cubature formula C_B is simply the product of the error constants of Q' and Q'',

$$c_{(r,s),p}(C_B) = c_{r,p}(Q')c_{s,p}(Q'').$$

Thus, for the blending cubature formula C_B we have a sharp theoretical error bound in terms of the norm of a single derivative of the integrand. On the other hand, for practical implementation, we should be able to construct a sequence of cubature formulae of improved quality to make possible the calculation of $I[f]$ with any prescribed tolerance. This goal can be achieved by either increasing the number of gridlines or usage of compound blending cubature formulae. Both approaches lead to increase of the number of the univariate integrals involved. This, however, is an undesirable effect, as these integrals are not always possible to be exactly calculated.

For this reason we give preference to the approximation scheme (7). In this scheme the blending grid G is fixed, and m and n are relatively small numbers. Hence, the $m+n$ line integrals involved in S stay unchanged during the calculations. For getting better approximations to $I[f]$ one varies the cubature formula C (e.g., uses compound product cubature formulae with increasing number of nodes).

In what follows, C is assumed to be a product cubature formula for approximate calculation of I, i.e., C is of the form (6). For easy reference, every cubature formula S obtained from a product cubature formula C through (7) will be called henceforth *modified product cubature formula* (MPCF). Clearly, there are two pairs of quadrature formulae which determine uniquely a modified product cubature formula S: the pair (Q', Q''), which defines the blending interpolation operator B, and the pair (Q_1, Q_2), which generates the product cubature formula $C(Q_1, Q_2)$.

3. Peano kernels and error bounds for MPCF

The statements in this section are valid under some general assumptions, which we give below.

S is a MPCF of the form (7), where $C = C(Q_1, Q_2)$ is a product cubature formula generated through (6), and B is a given blending interpolation operator, defined by a blending grid $G(\mathbf{X}, \mathbf{Y})$ with $\#(\mathbf{X}) = m$ and $\#(\mathbf{Y}) = n$. Recall that associated with B are the interpolatory quadrature formulae Q' and Q''. Further, r and s are natural numbers, satisfying $r \le ADP(Q') + 1$ and $s \le ADP(Q'') + 1$. We denote the corresponding Peano kernels of Q' and Q'' by $K_r(Q'; t)$ and $K_s(Q''; \tau)$. (For the sake of simplicity, here and hereafter we use the same notation for the Peano kernels of quadrature formulae designed for definite integrals on different intervals! Recall that Q' and Q_1 approximate ℓ_1, while Q'' and Q_2 approximate ℓ_2. The same notational convention applies to the reminders and error constants of these quadrature formulae.) Finally, it is assumed that the integrand f is smooth enough so that $D^{r,s}f$ exists and is integrable on Δ.

Making use of (5), one easily deduces that the remainder $E[S; f]$ admits the following integral representation:

$$E[S; f] = \iint_{\Delta} K_{r,s}(S; t, \tau) D^{r,s} f(t, \tau) \mathrm{d}t \mathrm{d}\tau, \tag{9}$$

where the Peano kernel of S of order (r, s) is given by

$$\begin{aligned} K_{r,s}(S; t, \tau) &= K_r(Q', t) K_s(Q'', \tau) - \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} c_i d_j \mathcal{K}_r(t_i, t) \overline{\mathcal{K}}_s(\tau_j, \tau) \\ &= K_r(Q', t) K_s(Q'', \tau) - Q_1[\mathcal{K}_r(\cdot, t)] Q_2[\overline{\mathcal{K}}_s(\cdot, \tau)]. \end{aligned} \tag{10}$$

Further representations of $K_{r,s}(S; t, \tau)$ are given in the following theorem.

Theorem 1. *Let, in addition to the assumptions made in the beginning of this section, $ADP(Q_1) \ge m - 1$ and $ADP(Q_2) \ge n - 1$. Then, for $(t, \tau) \in \Delta$, the Peano kernel $K_{r,s}(S; t, \tau)$ possesses the following representations:*

$$K_{r,s}(S; t, \tau) = K_r(Q', t) K_s(Q_2; \tau) + K_r(Q_1; t) Q_2[\overline{\mathcal{K}}_s(\cdot, \tau)], \tag{11}$$

$$K_{r,s}(S; t, \tau) = K_s(Q'', \tau) K_r(Q_1; t) + K_s(Q_2; \tau) Q_1[\mathcal{K}_r(\cdot, t)], \tag{12}$$

$$K_{r,s}(S; t, \tau) = K_r(Q', t) K_s(Q_2; \tau) + K_r(Q_1; t) K_s(Q''; \tau) - K_r(Q_1; t) K_s(Q_2; \tau). \tag{13}$$

Proof. The proofs of (11) and (12) make use of formulae $K_r(Q', t) = \ell_1[\mathcal{K}_r(\cdot, t)]$ and $K_s(Q'', \tau) = \ell_2[\overline{\mathcal{K}}_s(\cdot, \tau)]$. By subtracting and adding $K_r(Q'; t) Q_2[\overline{\mathcal{K}}_s(\cdot, \tau)]$ to the right-hand side of (10), one obtains

$$\begin{aligned} K_{r,s}(S; t, \tau) &= K_r(Q'; t) \left[K_s(Q''; \tau) - Q_2[\overline{\mathcal{K}}_s(\cdot, \tau)] \right] + Q_2[\overline{\mathcal{K}}_s(\cdot, \tau)] \left[K_r(Q'; t) - Q_1[\mathcal{K}_r(\cdot; t)] \right] \\ &= K_r(Q'; t) \left[\ell_2[\overline{\mathcal{K}}_s(\cdot, \tau)] - Q_2[\overline{\mathcal{K}}_s(\cdot, \tau)] \right] + Q_2[\overline{\mathcal{K}}_s(\cdot, \tau)] \left[\ell_1[\mathcal{K}_r(\cdot; t)] - Q_1[\mathcal{K}_r(\cdot; t)] \right] \\ &= K_r(Q'; t) R[Q_2; \overline{\mathcal{K}}_s(\cdot, \tau)] + Q_2[\overline{\mathcal{K}}_s(\cdot, \tau)] R[Q_1; \mathcal{K}_r(\cdot, t)] \\ &= K_r(Q', t) K_s(Q_2; \tau) + K_r(Q_1; t) Q_2[\overline{\mathcal{K}}_s(\cdot, \tau)]. \end{aligned}$$

For the last equality we have used the fact that $R[Q_2; \overline{\mathcal{K}}_s(\cdot, \tau)] = K_s(Q_2; \tau)$ and $R[Q_1; \mathcal{K}_r(\cdot, t)] = K_r(Q_1; t)$. To verify, e.g., the last identity, one writes

$$\begin{aligned} R[Q_1; \mathcal{K}_r(\cdot, t)] &= R\left[Q_1; \frac{(\cdot - t)_+^{r-1}}{(r-1)!} \right] - \frac{1}{(r-1)!} \sum_{\mu=1}^{m} R[Q_1; l_\mu](x_\mu - t)_+^{r-1} \\ &= R\left[Q_1; \frac{(\cdot - t)_+^{r-1}}{(r-1)!} \right] = K_r(Q_1; t), \end{aligned}$$

as $R[Q_1; l_\mu] = 0$ for $\mu = 1, \ldots, m$, by virtue of the assumption $ADP(Q_1) \ge m - 1$. The proof of (12) goes along the same lines, this time one subtracts and adds to the right-hand side of (10) $K_s(Q''; \tau) Q_1[\mathcal{K}_r(\cdot, t)]$. We omit the details.

The proof of (13) follows by substituting $Q_2[\overline{\mathcal{K}}_s(\cdot, \tau)] = K_s(Q''; \tau) - K_s(Q_2; \tau)$ in (11). For the latter identity, we observe that

$$\begin{aligned} Q_2[\overline{\mathcal{K}}_s(\cdot, \tau)] &= Q_2\left[\frac{(\cdot - \tau)_+^{s-1}}{(s-1)!} \right] - \frac{1}{(s-1)!} \sum_{\nu=1}^{n} Q_2[\bar{l}_\nu](y_\nu - \tau)_+^{s-1} \\ &= Q_2\left[\frac{(\cdot - \tau)_+^{s-1}}{(s-1)!} \right] - \frac{1}{(s-1)!} \sum_{\nu=1}^{n} \bar{b}_\nu (y_\nu - \tau)_+^{s-1} \end{aligned}$$

$$
\begin{aligned}
&= Q_2\left[\frac{(\cdot-\tau)_+^{s-1}}{(s-1)!}\right] - Q''\left[\frac{(\cdot-\tau)_+^{s-1}}{(s-1)!}\right] \\
&= R\left[Q''; \frac{(\cdot-\tau)_+^{s-1}}{(s-1)!}\right] - R\left[Q_2; \frac{(\cdot-\tau)_+^{s-1}}{(s-1)!}\right] \\
&= K_s(Q''; \tau) - K_s(Q_2; \tau)
\end{aligned}
$$

(we have used the assumption $ADP(Q_2) \ge n-1$, yielding $Q_2[\bar{l}_\nu] = \ell_2[\bar{l}_\nu] = \bar{b}_\nu$ for $\nu = 1, \ldots, n$). The theorem is proved. $\square$

For $1 \le p \le \infty$, let $W_p^{r,s}(\Delta)$ be the Sobolev class of functions

$$W_p^{r,s}(\Delta) := \{f : \Delta \to \mathbb{R} : \|D^{r,s}f\|_{L_p(\Delta)} < \infty\}.$$

If the integrand f belongs to $W_p^{r,s}(\Delta)$, then (9) and Hölder's inequality imply a sharp error estimate for S:

$$|E[S; f]| \le c_{(r,s),p}(S)\|D^{r,s}f\|_{L_p(\Delta)}, \tag{14}$$

where

$$c_{(r,s),p}(S) = \|K_{r,s}(S; \cdot, \cdot)\|_{L_q(\Delta)}, \qquad p^{-1} + q^{-1} = 1.$$

If the calculation of the error constant $c_{(r,s),p}(S)$ turns out to be a difficult task (which is the typical case, especially for values of p different from 1, 2 and ∞), one can resort to some further estimates. The connection (13) between the Peano kernels of S and the related quadrature formulae Q', Q'', Q_1 and Q_2 furnishes an upper bound for $c_{(r,s),p}(S)$ in terms of the error constants of these quadrature formulae.

Corollary 2. *Under the assumptions of Theorem 1, for $1 \le p \le \infty$ there holds*

$$c_{(r,s),p}(S) \le c_{r,p}(Q')c_{s,p}(Q_2) + c_{r,p}(Q_1)c_{s,p}(Q'') + c_{r,p}(Q_1)c_{s,p}(Q_2). \tag{15}$$

Proof. From (13) and the triangle inequality, we have

$$
\begin{aligned}
c_{(r,s),p}(S) &= \|K_{r,s}(S; \cdot, \cdot)\|_{L_q(\Delta)} \\
&\le \|K_r(Q'; \cdot)\|_{L_q[a,b]} \cdot \|K_s(Q_2; \cdot)\|_{L_q[c,d]} + \|K_r(Q_1; \cdot)\|_{L_q[a,b]} \cdot \|K_s(Q''; \cdot)\|_{L_q[c,d]} \\
&\quad + \|K_r(Q_1; \cdot)\|_{L_q[a,b]} \cdot \|K_s(Q_2; \cdot)\|_{L_q[c,d]} \\
&= c_{r,p}(Q')c_{s,p}(Q_2) + c_{r,p}(Q_1)c_{s,p}(Q'') + c_{r,p}(Q_1)c_{s,p}(Q_2). \quad \square
\end{aligned}
$$

As was already mentioned, no error bound exists for a conventional cubature formula C, in terms of the norm of a single partial derivative of the integrand. We show below that three partial derivatives do this job. To this end, we derive an alternative representation of the modified product cubature formula S.

Theorem 3. *Under the assumptions of Theorem 1, the modified product cubature formula S admits the representation*

$$S[f] = C[f] + Q'\left[R[Q_2; f((\cdot)_{Q'}, (\cdot)_R)]\right] + Q''\left[R[Q_1; f((\cdot)_R, (\cdot)_{Q''})]\right]. \tag{16}$$

If the integrand f belongs to $W_p^{r,s}(\Delta)$, then the error of the product cubature formula C satisfies

$$|E[C; f]| \le c_{(r,s),p}(S) \cdot \|D^{r,s}f\|_{L_p(\Delta)} + c_{s,p}(Q_2) \cdot \|Q'\| \cdot \|D^{0,s}f\|_{L_p(\Delta)} + c_{r,p}(Q_1) \cdot \|Q''\| \cdot \|D^{r,0}f\|_{L_p(\Delta)}. \tag{17}$$

(Here, $\|Q'\| = \sum_{i=1}^{n_1} |c_i|$ and $\|Q''\| = \sum_{i=1}^{n_2} |d_i|$.)

Proof. Since $ADP(Q_1) \ge m-1$ and $ADP(Q_2) \ge n-1$, then $Q_1[l_\mu] = \ell_1[l_\mu] = b_\mu$ ($\mu = 1, \ldots, m$), and $Q_2[l_\nu] = \ell_2[\bar{l}_\nu] = \bar{b}_\nu$ ($\nu = 1, \ldots, n$). Therefore,

$$
\begin{aligned}
C[Bf] &= \sum_{\mu=1}^{m} Q_1[l_\mu]Q_2[f(x_\mu, \cdot)] + \sum_{\nu=1}^{n} Q_2[\bar{l}_\nu]Q_1[f(\cdot, y_\nu)] - \sum_{\mu=1}^{m}\sum_{\nu=1}^{n} Q_1[l_\mu]Q_2[\bar{l}_\nu]f(x_\mu, y_\nu) \\
&= \sum_{\mu=1}^{m} b_\mu Q_2[f(x_\mu, \cdot)] + \sum_{\nu=1}^{n} \bar{b}_\nu Q_1[f(\cdot, y_\nu)] - \sum_{\mu=1}^{m}\sum_{\nu=1}^{n} b_\mu \bar{b}_\nu f(x_\mu, y_\nu) \\
&= Q'\left[Q_2[f(x_\mu, \cdot)]\right] + Q''\left[Q_1[f(\cdot, y_\nu)]\right] - \sum_{\mu=1}^{m}\sum_{\nu=1}^{n} b_\mu \bar{b}_\nu f(x_\mu, y_\nu).
\end{aligned}
$$

On the other hand, according to (8),

$$\begin{aligned} I[Bf] &= \sum_{\mu=1}^{m} b_\mu \ell_2[f(x_\mu,\cdot)] + \sum_{\nu=1}^{n} \bar{b}_\nu \ell_1[f(\cdot,y_\nu)] - \sum_{\mu=1}^{m}\sum_{\nu=1}^{n} b_\mu \bar{b}_\nu f(x_\mu,y_\nu) \\ &= Q'\left[\ell_2[f(x_\mu,\cdot)]\right] + Q''\left[\ell_1[f(\cdot,y_\nu)]\right] - \sum_{\mu=1}^{m}\sum_{\nu=1}^{n} b_\mu \bar{b}_\nu f(x_\mu,y_\nu). \end{aligned}$$

Since $S[f] = C[f] + I[Bf] - C[Bf]$, we deduce (16) from the above formulae for $C[Bf]$ and $I[Bf]$:

$$\begin{aligned} S[f] &= C[f] + Q'\left[\ell_2[f(x_\mu,\cdot)] - Q_2[f(x_\mu,\cdot)]\right] + Q''\left[\ell_1[f(\cdot,y_\nu)] - Q_1[f(\cdot,y_\nu)]\right] \\ &= C[f] + Q'\left[R[Q_2; f((\cdot)_{Q'},(\cdot)_R)]\right] + Q''\left[R[Q_1; f((\cdot)_R,(\cdot)_{Q''})]\right]. \end{aligned}$$

Now (17) follows from (14) and (16):

$$\begin{aligned} |E[C;f]| &\le |E[S;f]| + \left|Q'\left[R[Q_2; f((\cdot)_{Q'},(\cdot)_R)]\right]\right| + \left|Q''\left[R[Q_1; f((\cdot)_R,(\cdot)_{Q''})]\right]\right| \\ &\le |E[S;f]| + \|Q'\| \max_{x\in[a,b]} |R[Q_2; f(x,\cdot)]| + \|Q''\| \max_{y\in[c,d]} |R[Q_1; f(\cdot,y)]| \\ &\le c_{(r,s),p}(S)\cdot \|D^{r,s}f\|_{L_p(\Delta)} + c_{s,p}(Q_2)\cdot\|Q'\|\cdot\|D^{0,s}f\|_{L_p(\Delta)} + c_{r,p}(Q_1)\cdot\|Q''\|\cdot\|D^{r,0}f\|_{L_p(\Delta)}. \end{aligned}$$

Theorem 3 is proved. □

Remark 4. In fact, the following more general error bound for $|E[C;f]|$ can be derived with the same proof:

$$|E[C;f]| \le c_{(r,s),p_1}(S)\cdot\|D^{r,s}f\|_{L_{p_1}(\Delta)} + c_{\mu,p_2}(Q_2)\|Q'\|\cdot\|D^{0,\mu}f\|_{L_{p_2}(\Delta)} + c_{\nu,p_3}(Q_1)\cdot\|Q''\|\cdot\|D^{\nu,0}f\|_{L_{p_3}(\Delta)},$$

provided that $1 \le p_i \le \infty$ $(i = 1, 2, 3)$, $\mu \le ADP(Q_2) - 1$, $\nu \le ADP(Q_1) - 1$, and the derivatives of the integrand appearing in the right-hand side exist along with their norms. It is worth mentioning that the derivation of error estimates for cubature formulae is a non-trivial task. Authors mainly concentrate on the construction of cubature formulae of a given algebraic degree of precision, which is another difficult problem (see e.g., [10]). For a different error estimate for cubature formulae (which however is expressed in terms of the norms of more derivatives of the integrand), see [12, Chapter 5].

4. Definite MPCF

A MPCF S is said to be *positive definite of order* (r,s), if $K_{r,s}(S;t,\tau) \ge 0$ (resp., *negative definite of order* (r,s), if $K_{(r,s)}(S;t,\tau) \le 0$) on Δ. In general, the verification of definiteness is a difficult task, but Theorem 1 provides some sufficient conditions. Recall that a quadrature formula Q is said to be *positive* if all the coefficients of Q are positive.

Theorem 5. *The following are sufficient conditions for a MPCF S to be positive definite of order (r,s):*
(i) *Q_1 and Q' are positive definite of order r, Q_2 is positive, and positive definite of order s, and $\overline{\mathcal{K}}_s \ge 0$ on Δ;*
(ii) *Q_1 and Q' are negative definite of order r, Q_2 is positive, and negative definite of order s, and $\overline{\mathcal{K}}_s \le 0$ on Δ;*
(iii) *Q_2 and Q'' are positive definite of order s, Q_1 is positive, and positive definite of order r, and $\mathcal{K}_r \ge 0$ on Δ;*
(iv) *Q_2 and Q'' are negative definite of order s, Q_1 is positive, and negative definite of order r, and $\mathcal{K}_r \le 0$ on Δ;*
(v) *Q_1 and Q' are definite of opposite type of order r, Q_2 and Q'' are definite of opposite type of order s, and Q_1 and Q_2 are definite of opposite type.*
The following are sufficient conditions for a MPCF S to be negative definite of order (r,s):
(i′) Q_1 and Q' are positive definite of order r, Q_2 is positive, and negative definite of order s, and $\overline{\mathcal{K}}_s \le 0$ on Δ;
(ii′) Q_1 and Q' are negative definite of order r, Q_2 is positive, and positive definite of order s, and $\overline{\mathcal{K}}_s \ge 0$ on Δ;
(iii′) Q_2 and Q'' are positive definite of order s, Q_1 is positive, and negative definite of order r, and $\mathcal{K}_r \le 0$ on Δ;
(iv′) Q_2 and Q'' are negative definite of order s, Q_1 is positive, and positive definite of order r, and $\mathcal{K}_r \ge 0$ on Δ;
(v′) Q_1 and Q' are definite of opposite type of order r, Q_2 and Q'' are definite of opposite type of order s, and Q_1 and Q_2 are definite of the same type.

Proof. The assumptions (i)–(v′) guarantee that all the summands appearing in the right-hand sides of formulae (11)–(13) have the same constant sign on Δ, which yields the sign consistency of $K_{r,s}(S;t,\tau)$ on Δ. Either of the assumptions (i) and (ii) ensures that the two summands in the right-hand side of (11) are positive on Δ, while the same summands are both negative on Δ under either of the assumptions (i′) and (ii′). Similarly, the two summands in the right-hand side of (12) are positive Δ if one of assumptions (iii) and (iv) is fulfilled. The same summands are both negative on Δ if either (iii′) or (iv′) holds true. Finally, all the summands in the right-hand side of (13) are positive or negative on Δ depending on whether (v) or (v′) is assumed. Theorem 5 is proved. □

Table 1
Sufficient conditions for $0 \le E[S; f] \le E[C; f]$

Q'	Q''	Q_1	Q_2	$D^{r,s}f$	$D^{r,0}f$	$D^{0,s}f$
$\mathcal{PPD}(r)$	$\mathcal{PPD}(s),\ \overline{\mathcal{K}}_s \ge 0$	$\mathcal{PD}(r)$	$\mathcal{PPD}(s)$	≥ 0	≥ 0	≥ 0
$\mathcal{PND}(r)$	$\mathcal{PND}(s),\ \overline{\mathcal{K}}_s \le 0$	$\mathcal{ND}(r)$	$\mathcal{PND}(s)$	≥ 0	≤ 0	≤ 0
$\mathcal{PPD}(r),\ \mathcal{K}_r \ge 0$	$\mathcal{PPD}(s)$	$\mathcal{PPD}(r)$	$\mathcal{PD}(s)$	≥ 0	≥ 0	≥ 0
$\mathcal{PND}(r),\ \mathcal{K}_r \le 0$	$\mathcal{PND}(s)$	$\mathcal{PND}(r)$	$\mathcal{ND}(s)$	≥ 0	≤ 0	≤ 0
$\mathcal{PPD}(r)$	$\mathcal{PND}(s)$	$\mathcal{ND}(r)$	$\mathcal{PD}(s)$	≥ 0	≤ 0	≥ 0
$\mathcal{PND}(r)$	$\mathcal{PPD}(s)$	$\mathcal{PD}(r)$	$\mathcal{ND}(s)$	≥ 0	≥ 0	≤ 0
$\mathcal{PPD}(r)$	$\mathcal{PND}(s),\ \overline{\mathcal{K}}_s \le 0$	$\mathcal{PD}(r)$	$\mathcal{PND}(s)$	≤ 0	≥ 0	≤ 0
$\mathcal{PND}(r)$	$\mathcal{PPD}(s),\ \overline{\mathcal{K}}_s \ge 0$	$\mathcal{ND}(r)$	$\mathcal{PPD}(s)$	≤ 0	≤ 0	≥ 0
$\mathcal{PND}(r),\ \mathcal{K}_r \le 0$	$\mathcal{PPD}(s)$	$\mathcal{PND}(r)$	$\mathcal{PD}(s)$	≤ 0	≤ 0	≥ 0
$\mathcal{PPD}(r),\ \mathcal{K}_r \ge 0$	$\mathcal{PND}(s)$	$\mathcal{PPD}(r)$	$\mathcal{ND}(s)$	≤ 0	≥ 0	≤ 0
$\mathcal{PPD}(r)$	$\mathcal{PPD}(s)$	$\mathcal{ND}(r)$	$\mathcal{ND}(s)$	≤ 0	≤ 0	≤ 0
$\mathcal{PND}(r)$	$\mathcal{PND}(s)$	$\mathcal{PD}(r)$	$\mathcal{PD}(s)$	≤ 0	≥ 0	≥ 0

Remark 6. Since $K_r(Q'; t) = \ell_1[\mathcal{K}_r(\cdot, t)]$, the assumption that $\mathcal{K}_r(x, t)$ does not change its sign on Δ implies that Q' is definite of order r. Similarly, the assumption that $\overline{\mathcal{K}}_s(y, \tau)$ does not change its sign on Δ implies that Q'' is definite of order s. On the other hand, the requirement that $\mathcal{K}_r(x, t)$ (resp. $\overline{\mathcal{K}}_s(y, \tau)$) does not change its sign inside Δ means that each of the distinct interior components of $\mathbf{X}$ (resp. of $\mathbf{Y}$) appears even times, which means that the blending interpolation operator is of Hermite type. In order that Bf (and, consequently, $S[f]$) does not involve derivatives of f, the interior gridlines of the blending grid $G(\mathbf{X}, \mathbf{Y})$ must be double and have to pass through the abscissae of certain Gauss-type quadrature formulae. That is to say, Q' and Q'' must be Gauss-type quadrature formulae.

In general, the influence of the "correction term" $I[Bf] - C[Bf]$, which we add to a product type cubature formula $C[f]$ to obtain its modified counterpart $S[f]$, is indeterminate: depending on B, C and f, it may reduce or increase the error magnitude. In some cases equation (16) can be used to compare the errors of S and C. To describe these cases, we observe that

$$E[S; f] = E[C; f] - Q'\left[R[Q_2; f((\cdot)_{Q'}, (\cdot)_R)]\right] - Q''\left[R[Q_1; f((\cdot)_R, (\cdot)_{Q''})]\right],$$

by virtue of (16). Assume that the sign of $E[S; f]$ is known, e.g., $E[S; f] \ge 0$. This is the case, for instance, when S is positive definite of order (r, s) and $D^{r,s}f \ge 0$ on Δ, or when S is negative definite of order (r, s) and $D^{r,s}f \le 0$ on Δ. If

$$Q'\left[R[Q_2; f((\cdot)_{Q'}, (\cdot)_R)]\right] \ge 0 \quad \text{and} \quad Q''\left[R[Q_1; f((\cdot)_R, (\cdot)_{Q''})]\right] \ge 0, \tag{18}$$

then

$$0 \le E[S; f] \le E[C; f],$$

i.e., S has smaller error than C.

The inequalities (18) are fulfilled, for instance, when Q' and Q'' are positive quadrature formulae, Q_1 and Q_2 are definite of order r and s, respectively, and $D^{r,0}f$ and $D^{0,s}f$ have appropriate constant signs on Δ (or at least on the gridlines of G). The latter requirements for Q', Q'', Q_1 and Q_2 are in close connection with the assumptions in Theorem 5 which guarantee the definiteness of S.

Our last statement summarizes the various conditions yielding superiority of a definite modified product cubature formula S to the associated with S product cubature formula C. For the sake of brevity, we shall denote that a quadrature formula Q is positive (negative) definite of order m by writing that Q is $\mathcal{PD}(m)$ ($\mathcal{ND}(m)$). If, in addition, Q is positive, i.e., all the coefficients of Q are positive, then we shall write that Q is $\mathcal{PPD}(m)$ ($\mathcal{PND}(m)$, respectively).

Proposition 7. *Let $C = C(Q_1, Q_2)$ be the product cubature formula generated by the quadrature formulae Q_1 and Q_2, and let the MPCF S be generated by Q', Q'', Q_1 and Q_2. Assume that the integrand f is in $C^{r,s}(\Delta)$, and its derivatives $D^{r,s}f$, $D^{r,0}f$ and $D^{0,s}f$ do not change their signs in Δ. Then the requirements in each row of Table 1 imply the inequalities $0 \le E[S; f] \le E[C; f]$: If we reverse the inequalities in the last three columns of Table 1, then the requirements in each row imply the reversed inequalities $0 \ge E[S; f] \ge E[C; f]$.*

5. Application

The implementation of MPCF requires the exact calculation of some line integrals, and this circumstance is perhaps the only objection against their usage. On the other hand, if the integrand admits exact calculation of the line integrals involved, it is worth applying MPCF as an alternative to the standard product cubature formulae. For instance, a class of such integrands is described by $f(x, y) = g(x \cdot y)$, where the univariate function $g(t)$ admits application of the Leibnitz–Newton rule.

To demonstrate how the theory developed in the preceding sections works, we construct below sequences of definite modified product cubature formulae for the square $\Delta = [0, 1] \times [0, 1]$. As was mentioned in Section 2, every such cubature formula is generated by four quadrature formulae Q', Q'', Q_1 and Q_2, all of them approximating the definite integrals over the interval $[0, 1]$.

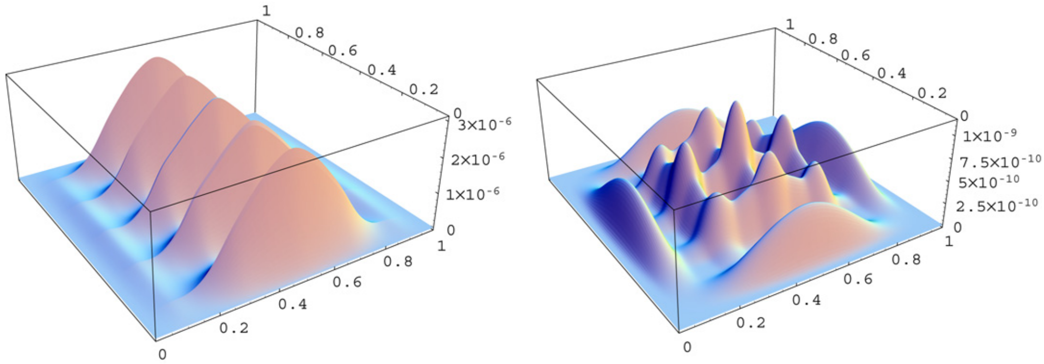

Fig. 1. The graphs of $K_{4,2}(S^{+}_{4,2,5}; t, \tau)$ (left) and $K_{4,4}(S^{+}_{4,4,5}; t, \tau)$ (right).

Positive definite MPCF of order (4, 2). The nth member of the sequence $\{S^{+}_{(4,2,n)}\}_{n=1}^{\infty}$ of positive definite MPCF of order (4, 2) is built by the quadrature formulae Q', Q'', Q_1 and Q_2, selected as follows (see Theorem 5,(v)):

- Q' is the (elementary) Simpson quadrature formula;
- Q'' is the (elementary) midpoint quadrature formula;
- Q_1 is the nth compound quadrature formula, based on the three-point open Newton–Cotes quadrature formula

$$Q[f] = \frac{1}{3}\left[2f(1/4) - f(1/2) + 2f(3/4)\right];$$

- Q_2 is the nth compound trapezium quadrature formula.

Negative definite MPCF of order (4, 2). The sequence $\{S^{-}_{(4,2,n)}\}_{n=1}^{\infty}$ consists of negative definite cubature formulae of order (4, 2), and the quadrature formulae Q', Q'', Q_1 and Q_2, which generate $S^{-}_{(4,2,n)}$ are chosen as follows (see Theorem 5, (ii$'$)):

- Q' is the (elementary) Simpson quadrature formula;
- Q'' is the (elementary) midpoint quadrature formula;
- Q_1 is the nth compound Simpson quadrature formula;
- Q_2 is the nth compound midpoint quadrature formula.

Positive definite MPCF of order (4, 4). The sequence $\{S^{+}_{(4,4,n)}\}_{n=1}^{\infty}$ consists of positive definite cubature formulae of order (4, 4), where in $S^{+}_{(4,4,n)} Q' \equiv Q''$ is the two-point Gaussian quadrature formula

$$Q'[f] = \frac{1}{2}f\left(\frac{3-\sqrt{3}}{6}\right) + \frac{1}{2}f\left(\frac{3+\sqrt{3}}{6}\right), \tag{19}$$

and $Q_1 \equiv Q_2$ is the nth compound quadrature formulae, based on (19). Here, the positive definiteness of $S^{+}_{(4,4,n)}$ is justified by Theorem 5(i).

Negative definite MPCF of order (4, 4). The sequence $\{S^{-}_{(4,4,n)}\}_{n=1}^{\infty}$ consists of negative definite cubature formulae of order (4, 4). Here, in $S^{-}_{(4,4,n)}$, $Q' \equiv Q''$ is the two-point Gaussian quadrature formula (19), and $Q_1 \equiv Q_2$ is the nth compound Simpson quadrature formula. The negative definiteness of $S^{-}_{(4,4,n)}$ is verified by Theorem 5(v$'$).

The Peano kernels of two positive definite MPCF are depicted in Fig. 1.

The above MPCF and the associated with them product cubature formulae have been tested with the following two integrands:

$$f_1(x, y) = e^{xy}, \qquad f_2(x, y) = \cos xy.$$

Notice that $D^{i,j} f_1(x, y) \geq 0$ for every i, j and $(x, y) \in \Delta$, while $D^{4,2} f_2(x, y)$ and $D^{4,4} f_2(x, y)$ change their signs in $[0, 1]^2$.

The double integrals of f_1 and f_2 over $[0, 1]^2$ can be reduced to univariate ones, namely, we have

$$I[f_1] = \int_0^1 \frac{e^u - 1}{u} du, \qquad I[f_2] = \int_0^1 \frac{\sin u}{u} du.$$

Making use of the MacLaurin expansion of the integrands and appropriate estimation of the truncation error, one finds for the true values of $I[f_1]$ and $I[f_2]$

$$I[f_1] = 1.317902151454403\ldots, \qquad I[f_2] = 0.946083070367183\ldots.$$

Table 2
The error of $S^{+}_{4,2,n}$ and the related product cubature formulae C_n

n	$E[C_n; f_1]$	$E[S^{+}_{4,2,n}; f_1]$	$E[C_n; f_2]$	$E[S^{+}_{4,2,n}; f_2]$
5	-1.666×10^{-3}	8.802×10^{-6}	1.005×10^{-3}	3.772×10^{-6}
10	-4.167×10^{-4}	2.188×10^{-6}	2.511×10^{-4}	9.324×10^{-7}
15	-1.852×10^{-4}	9.714×10^{-7}	1.116×10^{-4}	4.136×10^{-7}
20	-1.042×10^{-4}	5.462×10^{-7}	6.275×10^{-5}	2.325×10^{-7}
25	-6.667×10^{-5}	3.496×10^{-7}	4.016×10^{-5}	1.488×10^{-7}
30	-4.630×10^{-5}	2.428×10^{-7}	2.789×10^{-5}	1.033×10^{-7}

Table 3
The error of $S^{-}_{4,2,n}$ and the related product cubature formulae C_n

n	$E[C_n; f_1]$	$E[S^{-}_{4,2,n}; f_1]$	$E[C_n; f_2]$	$E[S^{-}_{4,2,n}; f_2]$
5	8.326×10^{-4}	-4.438×10^{-6}	-5.024×10^{-4}	-1.915×10^{-6}
10	2.083×10^{-4}	-1.097×10^{-6}	-1.256×10^{-4}	-4.683×10^{-7}
15	9.259×10^{-5}	-4.863×10^{-7}	-5.578×10^{-5}	-2.073×10^{-7}
20	5.209×10^{-5}	-2.733×10^{-7}	-3.138×10^{-5}	-1.164×10^{-7}
25	3.334×10^{-5}	-1.749×10^{-7}	-2.008×10^{-5}	-7.443×10^{-8}
30	2.315×10^{-5}	-1.214×10^{-7}	-1.395×10^{-5}	-5.167×10^{-8}

Table 4
The error of $S^{+}_{4,4,n}$ and the related product cubature formulae C_n

n	$E[C_n; f_1]$	$E[S^{+}_{4,4,n}; f_1]$	$E[C_n; f_2]$	$E[S^{+}_{4,4,n}; f_2]$
5	2.320×10^{-7}	1.319×10^{-8}	1.314×10^{-7}	1.572×10^{-9}
10	1.451×10^{-8}	8.267×10^{-10}	8.201×10^{-9}	9.753×10^{-11}
15	2.867×10^{-9}	1.634×10^{-10}	1.620×10^{-9}	1.924×10^{-11}
20	9.069×10^{-10}	5.170×10^{-11}	5.125×10^{-10}	6.085×10^{-12}
25	3.715×10^{-10}	2.118×10^{-11}	2.100×10^{-10}	2.492×10^{-12}
30	1.792×10^{-10}	1.022×10^{-11}	1.013×10^{-10}	1.202×10^{-12}

Table 5
The error of $S^{-}_{4,4,n}$ and the related product cubature formulae C_n

n	$E[C_n; f_1]$	$E[S^{-}_{4,4,n}; f_1]$	$E[C_n; f_2]$	$E[S^{-}_{4,4,n}; f_2]$
5	-3.480×10^{-7}	-1.983×10^{-8}	-1.970×10^{-7}	-2.360×10^{-9}
10	-2.177×10^{-8}	-1.241×10^{-9}	-1.231×10^{-8}	-1.463×10^{-10}
15	-4.300×10^{-9}	-2.451×10^{-10}	-2.430×10^{-9}	-2.886×10^{-11}
20	-1.361×10^{-9}	-7.756×10^{-11}	-7.687×10^{-10}	-9.126×10^{-12}
25	-5.573×10^{-10}	-3.177×10^{-11}	-3.149×10^{-10}	-3.738×10^{-12}
30	-2.688×10^{-10}	-1.533×10^{-11}	-1.519×10^{-10}	-1.803×10^{-12}

We used Wolfram's *Mathematica* to perform some numerical experiments with the above definite MPCF. The results are given in Tables 2–5.

In the cases $S = S^{+}_{4,2,n}$ and $S = S^{-}_{4,2,n}$ we cannot refer to Proposition 7 to claim that either $0 \le E[S; f_i] \le E[C_n; f_i]$ or $0 \ge E[S; f_i] \ge E[C_n; f_i]$, $(i = 1, 2)$. The reason for f_2 is that $D^{4,2}f_2$ does not have a permanent sign in $[0, 1]^2$. As to f_1, neither of the requirements in Proposition 7 for the quadrature formulae Q', Q'', Q_1 and Q_2, which generate S, matches the sign pattern of the derivatives $D^{4,2}f_1$, $D^{4,0}f_1$ and $D^{0,2}f_1$, as required in Table 1. Nevertheless, Tables 2 and 3 clearly indicate that the use of S instead of C_n reduces the error magnitude by factors approximately equal to 188 for f_1 and 270 for f_2. Notice that the cost of this reduction is the additional calculation of four line integrals.

Since in $[0, 1]^2$, $\operatorname{sign} D^{4,4}f_1 = \operatorname{sign} D^{4,0}f_1 = \operatorname{sign} D^{0,4}f_1 = 1$, we see that the assumptions of Proposition 7 are satisfied (specifically, in rows two and twelve of Table 1). Consequently, we have $0 < E[S; f_1] < E[C_n; f_1]$ in Table 4, and the reversed inequalities in Table 5. The same behavior is observed for $E[S; f_2]$ and $E[C_n; f_2]$, though $D^{4,4}f_2$ changes its sign in $[0, 1]^2$. The error reduction factor is approximately 17.5 for f_1, and 84 for f_2. This reduction is achieved at the expense of four (in the case $S^{+}_{4,4,n}$) or five (in the case of $S^{-}_{4,4,n}$) additionally calculated line integrals.

It is also observed that for all n, $E[S^{+}_{4,2,n}; f_1]$ and $E[S^{+}_{4,4,n}; f_1]$ are positive, while $E[S^{-}_{4,2,n}; f_1]$ and $E[S^{-}_{4,4,n}; f_1]$ are negative, in accordance with the theory.

If a MPCF S is shown to be definite of order (r, s) through Theorem 5, its error constant $c_{(r,s),\infty}(S)$ can be expressed in terms of the error constants of the four quadrature formulae Q', Q'', Q_1 and Q_2, generating S. Namely, integration of (13) over Δ yields

$$c_{(r,s),\infty}(S) = |\widetilde{c}_{r,\infty}(Q')\widetilde{c}_{s,\infty}(Q_2) + \widetilde{c}_{r,\infty}(Q_1)\widetilde{c}_{s,\infty}(Q'') - \widetilde{c}_{r,\infty}(Q_1)\widetilde{c}_{s,\infty}(Q_2)|,$$

where $\widetilde{c}_{m,\infty}(Q) := \ell_1[K_m(Q;\cdot)]$ or $\widetilde{c}_{m,\infty}(Q) := \ell_2[K_m(Q;\cdot)]$ depending on whether Q approximates ℓ_1 or ℓ_2. In the cases when Q is positive or negative definite of order m we have $\widetilde{c}_{m,\infty}(Q) = c_{m,\infty}(Q)$ or $\widetilde{c}_{m,\infty}(Q) = -c_{m,\infty}(Q)$, respectively. This observation together with the well-known error constants of the Newton–Cotes quadratures with one, two or three nodes, and the two-point Gaussian quadrature formula, yields

$$c_{(4,2),\infty}(S^+_{4,2,n}) = \frac{1}{34\,560n^2}\left(1 + \frac{7}{16n^2} + \frac{7}{8n^4}\right),$$

$$c_{(4,2),\infty}(S^-_{4,2,n}) = \frac{1}{69\,120n^2}\left(1 + \frac{1}{n^2} - \frac{1}{n^4}\right),$$

$$c_{(4,4),\infty}(S^+_{4,4,n}) = \frac{1}{9331\,200n^4}\left(1 - \frac{1}{2n^4}\right),$$

$$c_{(4,4),\infty}(S^-_{4,4,n}) = \frac{1}{6220\,800n^4}\left(1 + \frac{3}{4n^4}\right).$$

Using that $\|D^{4,2}f_1\|_{C(\Delta)} = 21e$, $\|D^{4,4}f_1\|_{C(\Delta)} = 209e$, $\|D^{4,2}f_2\|_{C(\Delta)} = 12$, $\|D^{4,4}f_2\|_{C(\Delta)} < 92.8$, and the above error constants, one can compare the actual error in Tables 2–5 (columns two and four) with the theoretical bounds, given by the Peano kernel theory through (14) with $p = \infty$. Although the latter bounds usually well overestimate the real error magnitude, in our case we observe a remarkably stable (with respect to n) and reasonably small error overestimation factor. Namely, for $S^\pm_{4,2,n}$ this factor varies between 7.56 and 7.74 for f_1, and between 3.73 and 3.77 for f_2. For $S^\pm_{4,4,n}$ (definite MPCF of order (4, 4)), the error overestimation factor ranges between 7.35 and 7.38 for f_1, and between 10.1 and 10.22 for f_2.

We can also derive upper bounds for $|E[C_n; f_i]|$, $i = 1, 2$, with C_n being the product cubature formulae appearing in $S^\pm_{4,2,n}$ and $S^\pm_{4,4,n}$. To this end we make use of Theorem 3 (estimate (17) with $p = \infty$), and the error constants $c_{(4,2),\infty}(S^\pm_{4,2,n})$ and $c_{(4,4),\infty}(S^\pm_{4,4,n})$ given above. Notice that $\|Q'\| = \|Q''\| = 1$ whenever Q' and Q'' are positive (which is always the case in the above definite MPCF). Observe that $\|D^{4,0}f_1\|_{C(\Delta)} = \|D^{0,2}f_1\|_{C(\Delta)} = \|D^{0,4}f_1\|_{C(\Delta)} = e$, and $\|D^{4,0}f_2\|_{C(\Delta)} = \|D^{0,2}f_2\|_{C(\Delta)} = \|D^{0,4}f_2\|_{C(\Delta)} = 1$. Comparison of the sharp error magnitude $|E[C_n; f_i]$ in Tables 2 and 3 (columns one and three) with the error bounds furnished by Theorem 3 reveals an error overestimation factor ranging between 5.47 and 5.49 for f_1, and an error overestimation factor approximately equal to 3.33 for f_2. Similarly, the actual error magnitude $|E[C_n; f_i]$, given in columns one and three in Tables 4 and 5, is overestimated in the bounds provided by Theorem 3 by a factor not exceeding 9.1 for f_1 and 5.77 for f_2.

Let us mention once again that, for other integrands, the numerical results could show better performance of a product cubature formula C than its modified counterpart S. Our main goal in this paper was to show how the Peano kernel theory can be adopted for error estimation of both S and C.

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