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ASYMPTOTICALLY OPTIMAL QUADRATURE FORMULAE IN CERTAIN SOBOLEV CLASSES

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We construct sequences of asymptotically optimal quadrature formulae in the Sobolev classes W_p^3 $(1 \le p \le \infty)$, and W_1^4. Sharp error bounds for these quadrature formulae are given.

Keywords: Quadrature formulae, Sobolev classes of functions, asymptotically optimal quadrature formulae, spline functions, Peano kernels, Euler-MacLaurin summation formulae

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1. INTRODUCTION

We study quadrature formulae of the type

$$Q[f] = \sum_{i=1}^{n} a_i\, f(x_i), \qquad 0 \le x_1 < x_2 < \cdots < x_n \le 1\,, \tag{1.1}$$

that serve as an estimate for the definite integral

$$I[f] := \int_0^1 f(x)\, dx. \tag{1.2}$$

Throughout this paper π_k will stand for the set of algebraic polynomials of degree not exceeding k.

The classical approach for construction of quadrature formulae is based on the concept of *algebraic degree of precision*. The quadrature formula (1.1) is said to have algebraic degree of precision m (in short, $ADP(Q) = m$), if its remainder

$$R[Q; f] := I[f] - Q[f]$$

vanishes whenever $f \in \pi_m$, and $R[Q; f] \neq 0$ when f is a polynomial of degree $m+1$.

The ADP-concept is justified by the Weierstrass theorem about the density of algebraic polynomials in spaces of continuous functions on compacts. The pursuit of quadrature formulae (1.1) with the highest possible ADP leads to the well-known quadrature formulae of Gauss, Radau and Lobatto. The latter are uniquely determined by having ADP equal to $2n-1$, $2n-2$ and $2n-3$, respectively, where, in addition, the Radau quadrature formula has one fixed node being an end-point of the integration interval, and the Lobatto quadrature formula has two fixed nodes at the ends of the integration interval.

An alternative concept for evaluation of the quality of quadrature formulae emerged in the forties of the 20-th century, namely, the concept of optimality in a given class of functions. Its founders are A. Kolmogorov, A. N. Sard and S. M. Nikolskii. Let us briefly describe the setting of optimal quadrature formulae in a given class of functions.

Let X be a normed linear space of functions defined in $[0, 1]$, with a norm $\|\cdot\|$. For a quadrature formula Q of the form (1.1), we denote by $\mathcal{E}(Q, X)$ the largest possible error of Q for functions from the unit ball of X, i.e.

$$\mathcal{E}(Q, X) := \sup_{\|f\|_X \leq 1} |R[Q; f]|.$$

We look for the best possible choice of the coefficients $\{a_i\}_{i=1}^n$ and the nodes $\{x_i\}_{i=1}^n$ of Q, and set

$$\mathcal{E}_n(X) := \inf_Q \mathcal{E}(Q, X).$$

If the infimum is attained for a quadrature formula Q^{opt} of the form (1.1), then Q^{opt} is said to be an *optimal quadrature formula* of the type (1.1) in the space X. Of particular interest is the case when X is some of the Sobolev classes of functions $\widetilde{W}_p^r$ and W_p^r, defined by

$$\widetilde{W}_p^r := \{f \in C^{r-1}[0, 1],\ f - \ 1\text{–periodic},\ f^{(r-1)}\ \text{ abs. cont.},\ \|f\|_p < \infty\},$$

$$W_p^r := \{f \in C^{r-1}[0, 1],\ f^{(r-1)}\ \text{ abs. cont.},\ \|f\|_p < \infty\},$$

where

$$\|f\|_p := \Big(\int_0^1 |f(t)|^p dt\Big)^{1/p}, \quad \text{if} \quad 1 \leq p < \infty, \quad \text{and} \quad \|f\|_\infty = \sup_{t\in(0,1)} \text{vrai}\, |f(t)|.$$

In the periodic Sobolev classes $\widetilde{W}_p^r$ there is an universal optimal quadrature formula (i.e. optimal for all $r \in \mathbb{N}$ and $p \geq 1$) of the form (1.1), namely, the n-point rectangles quadrature formula and its translates. This is a result due to Zhensykbaev [14], special cases have been obtained earlier by Motornii [10], and Ligun [9]. The existence and uniqueness of optimal quadrature formulae in the non-periodic Sobolev spaces W_p^r is equivalent to the existence and uniqueness of specific monosplines of degree r with a minimal L_q-deviation from zero, $(1/p + 1/q = 1)$. This was proved by Zhensykbaev [15], and Bojanov extended Zhensykbaev's result to more general classes of quadrature formulae involving derivatives of the integrand. Obviously, $\mathcal{E}_n(\widetilde{W}_p^r) \le \mathcal{E}_n(W_p^r)$, and it is known that (see Brass [6]) for $1 < p \le \infty$,

$$\lim_{n\to\infty} \frac{\mathcal{E}_n(\widetilde{W}_p^r)}{\mathcal{E}_n(W_p^r)} = 1.$$

A drawback of the optimality concept is that, in general, the explicit form of the optimal quadrature formulae is unknown, a fact that vitiates their importance from practical point of view. In particular, except for some special cases of $r = 1$ and $r = 2$, the optimal quadrature formulae in the non-periodic Sobolev spaces W_p^r are unknown.

The way out of this situation is to step back from the requirement for optimality, and to look for quadrature formulae which are nearly optimal. A sequence $\{Q_n\}$ of quadrature formulae is said to be asymptotically optimal in the function class X, if

$$\lim_{n\to\infty} \frac{\mathcal{E}(Q_n, X)}{\mathcal{E}_n(X)} = 1$$

(here, Q_n is supposed to be a quadrature formula with n nodes).

It has been shown in [8] that the Gauss-type quadrature formulae associated with the spaces of spline functions with equidistant knots are asymptotically optimal in the non-periodic Sobolev classes W_p^r. The existence and uniqueness of such Gauss-type quadrature formulae is equivalent to the fundamental theorem of algebra for monosplines satisfying zero boundary conditions, which was proved in [7]. This fact was a motivation for investigation of such quadratures. Algorithms for the construction along with sharp error estimates of the Gauss-type quadrature formulae associated with spaces of linear and parabolic spline functions were proposed in [11] and [13] (see also [12] for the case of cubic splines with double equidistant knots). Recently, an algorithm for the construction of Gaussian quadrature formulae associated with spaces of cubic splines with equidistant knots was proposed in [1].

It should be noted that the complexity of the algorithms for the construction of Gauss-type quadrature formulae associated with spaces of spline functions with equidistant knots increases with increasing of the degree (that is, of parameter r in W_p^r). For $r \ge 3$ such quadratures are constructed only numerically. This requires high accuracy computations, especially when the number of the nodes is large. An additional difficulty causes the fact that the mutual location of the spline knots and the quadratures nodes is unknown.

In [2] we proposed an alternative approach for generation of sequences of asymptotically optimal quadrature formulae. There we constructed sequences of asymptotically optimal quadrature formulae in the Sobolev classes W_p^4, for $p = 2$ and $p = \infty$. Our approach makes use of Euler–MacLaurin–type summation formulae, in which the derivatives are replaced by suitable formulae for numerical differentiation. An advantage of our quadrature formulae, besides their asymptotical optimality, is the explicit form of their weights and nodes. In fact, most of the nodes of our quadrature formulae are either those of the compound trapezium or of the compound midpoint quadratures, to which we add a few more nodes.

Here we continue our study on this subject. The paper is organized as follows. In Section 2 we provide some well-known facts, including the Peano kernel representation of linear functionals, the Bernoulli polynomials, monosplines and numbers, the Euler–MacLaurin–type expansion formulae, and the error representation of the compound trapezium and midpoint quadrature formulae in the periodic Sobolev classes $\widetilde{W}_p^r$. In Section 3 we construct some sequences of asymptotically optimal quadrature formulae in the non-periodic Sobolev classes W_1^3, $1 \le p \le \infty$, and evaluate their sharp error constants in the cases $p = 1, 2, \infty$. In Section 4 we construct two sequences of asymptotically optimal quadrature formulae in the Sobolev classes W_1^4. Section 5 contains some concluding remarks.

2. PRELIMINARIES

2.1. SPLINE FUNCTIONS AND PEANO KERNELS OF LINEAR FUNCTIONALS

A spline function of degree $r-1$ ($r \in \mathbb{N}$) with knots $x_1 < x_2 < \cdots < x_n$ is a function $s(t)$ satisfying the requirements

$$\begin{aligned} &1) \qquad s(t)_{|t\in(x_i,x_{i+1})} \in \pi_{r-1}, \quad i = 0, \ldots, n, \\ &2) \qquad s(t) \in C(\mathbb{R}), \end{aligned}$$

where $x_0 := -\infty$ and $x_{n+1} := \infty$. The set $S_{r-1}(x_1, \ldots, x_n)$ of spline functions of degree $r-1$ with knots $x_1 < x_2 < \cdots < x_n$ is a linear space of dimension $n + r$, and a basis of $S_{r-1}(x_1, \ldots, x_n)$ is given by the functions

$$\{1, t, \ldots, t^{r-1}, (t-x_1)_+^{r-1}, \ldots, (t-x_n)_+^{r-1}\},$$

where $u_+(t)$ is defined by

$$u_+(t) = \max\{t, 0\}, \quad t \in \mathbb{R}.$$

If $\mathcal{L}$ is a linear functional defined on $C[0,1]$ which vanishes on π_s, then by a classical result of Peano, for $r \in \mathbb{N}$, $1 \le r \le s+1$ and $f \in W_1^r$, $\mathcal{L}$ admits the integral representation

$$\mathcal{L}[f] = \int_0^1 K_r(t) f^{(r)}(t)\,dt, \qquad \text{where} \qquad K_r(t) = \mathcal{L}\Big[\frac{(\cdot - t)_+^{r-1}}{(r-1)!}\Big], \quad t \in [0,1].$$

In the case when $\mathcal{L}$ is the remainder $R[Q;\cdot]$ of a quadrature formula Q with algebraic degree of precision s, the function $K_r(t) = K_r(Q;t)$ is referred to as the r-th Peano kernel of Q. For Q as in (1.1), explicit representations for $K_r(Q;t)$, $t \in [0,1]$, are

$$K_r(Q;t) = \frac{(1-t)^r}{r!} - \frac{1}{(r-1)!}\sum_{i=1}^{n} a_i (x_i - t)_+^{r-1}, \tag{2.1}$$

$$K_r(Q;t) = (-1)^r \Big[\frac{t^r}{r!} - \frac{1}{(r-1)!}\sum_{i=1}^{n} a_i (t - x_i)_+^{r-1}\Big]. \tag{2.2}$$

If the integrand f belongs to the Sobolev class W_p^r, $(1 \le p \le \infty)$, then from

$$R[Q;f] = \int_0^1 K_r(Q;t) f^{(r)}(t)\, dt$$

and from Hölder's inequality one obtains the sharp error estimate

$$|R[Q;f]| \le c_{r,p}(Q)\|f^{(r)}\|_p, \quad \text{where} \quad c_{r,p}(Q) = \|K_r(Q;\cdot)\|_q, \quad p^{-1} + q^{-1} = 1. \tag{2.3}$$

In other words, we have $\mathcal{E}(Q, W_p^r) = c_{r,p}(Q)$. Throughout, $c_{r,p}(Q)$ will be referred to as *the error constant of* Q *in the Sobolev class* W_p^r.

$K_r(Q;t)$ is also called a monospline of degree r with knots $\{x_i \;:\; x_i \in (0,1)\}$. From $K_r(Q;x) = R[Q;(\cdot - x)_+^{r-1}/(r-1)!]$ we deduce that $K_r(Q;x) = 0$ for some $x \in (0,1)$ if and only if Q evaluates to the exact value the integral of the spline function $f(t) = (t-x)_+^{r-1}$. Thus, in order that a quadrature formula Q has *maximal spline degree of precision*, i.e., Q is exact for a space of spline functions of degree $r-1$ with a maximal dimension, it is necessary and sufficient that the corresponding monospline $K_r(Q;\cdot)$ has maximal number of zeros in $(0,1)$. Quadrature formulae of the form (1.1) with maximal spline degree of precision are called, analogously to the classical algebraic case, as Gauss, Radau, and Lobatto quadrature formulae, associated with the corresponding spaces of spline functions. Similarly to the classical Gauss–type quadrature formulae, all the nodes of the Gauss-type quadratures associated with spaces of spline functions lie in the integration interval, and all their weights are positive [7, Theorem 7.1].

2.2. BERNOULLI POLYNOMIALS AND MONOSPLINES. EULER–MACLAURIN TYPE SUMMATION FORMULAE

Recall that the Bernoulli polynomials B_ν are defined recursively by

$$B_0(x) = 1, \quad B_\nu'(x) = B_{\nu-1}(x), \quad \text{and} \quad \int_0^1 B_\nu(t)\, dt = 0, \quad \nu \in \mathbb{N}.$$

In particular, $B_1(x) = x - \dfrac{1}{2}$, $B_2(x) = \dfrac{x^2}{2} - \dfrac{x}{2} + \dfrac{1}{12}$, $B_3(x) = \dfrac{x^3}{6} - \dfrac{x^2}{4} + \dfrac{x}{12}$,

$$B_4(x) = \frac{x^2(1-x)^2}{24} - \frac{1}{720}.$$

The Bernoulli numbers $\mathcal{B}_\nu$ are defined by $\mathcal{B}_\nu = \dfrac{B_\nu(0)}{\nu!}$.

The notation $\widetilde{B}_\nu(x)$ stands for the 1-periodic extension of the Bernoulli polynomial $B_\nu(x)$ on $\mathbb{R}$. The functions $\widetilde{B}_\nu(x)$, $\nu = 0, 1, \dots$, are called Bernoulli monosplines.

Throughout this paper, $n \in \mathbb{N}$ will be fixed, and $\{x_{k,n}\}_{k=0}^n$ and $\{y_{\ell,n}\}_{\ell=1}^n$ are given by

$$x_{k,n} = \frac{k}{n}, \quad k = 0, \dots, n; \qquad y_{\ell,n} = \frac{2\ell - 1}{2n}, \quad \ell = 1, \dots, n\,. \tag{2.4}$$

The points $\{x_{k,n}\}_{k=0}^n$ and $\{y_{\ell,n}\}_{\ell=1}^n$ are the nodes of the n-th compound trapezium and midpoint quadrature formulae Q_{n+1}^{Tr} and Q_n^{Mi}, given by

$$Q_{n+1}^{Tr}[f] = \frac{1}{2n}\big(f(x_{0,n}) + f(x_{n,n})\big) + \frac{1}{n}\sum_{k=1}^{n-1} f(x_{k,n})\,, \tag{2.5}$$

$$Q_n^{Mi}[f] = \frac{1}{n}\sum_{k=1}^{n-1} f(y_{k,n})\,. \tag{2.6}$$

Our asymptotically optimal quadrature formulae are obtained as appropriate modifications of Q_{n+1}^{Tr} and Q_n^{Mi}.

The following summation formulae of Euler–MacLaurin type (adopted for the interval $[0,1]$) are well-known, see, e.g., [6, Satz 98, 99]:

Lemma 1. *Assume that $f \in W_1^s$. Then*

$$\begin{aligned} \int_0^1 f(x)\,dx =& Q_{n+1}^{Tr}[f] - \sum_{\nu=1}^{[\frac{s}{2}]} \frac{\mathcal{B}_{2\nu}}{(2\nu)!}\,\frac{f^{(2\nu-1)}(1) - f^{(2\nu-1)}(0)}{n^{2\nu}} \\ &+ \frac{(-1)^s}{n^s}\int_0^1 \widetilde{B}_s(nx) f^{(s)}(x)\,dx \end{aligned} \tag{2.7}$$

and

$$\begin{aligned} \int_0^1 f(x)\,dx =& Q_n^{Mi}[f] + \sum_{\nu=1}^{[\frac{s}{2}]} \left(1 - 2^{1-2\nu}\right) \frac{\mathcal{B}_{2\nu}}{(2\nu)!}\,\frac{f^{(2\nu-1)}(1) - f^{(2\nu-1)}(0)}{n^{2\nu}} \\ &+ \frac{(-1)^s}{n^s}\int_0^1 \widetilde{B}_s\Big(nx - \frac{1}{2}\Big) f^{(s)}(x)\,dx\,. \end{aligned} \tag{2.8}$$

Here, $[t]$ denotes the integer part of t.

As was already mentioned, the midpoint quadrature formulae $\{Q_n^{Mi}\}_{n=1}^{\infty}$ and their translates are the unique optimal quadrature formulae in the periodic Sobolev classes $\widetilde{W}_p^r$. The trapezium quadrature formulae $\{Q_{n+1}^{Tr}\}_{n=1}^{\infty}$ also can be considered as translates of $\{Q_n^{Mi}\}_{n=1}^{\infty}$, as the values of the integrand at the endpoints are equal. For $f \in \widetilde{W}_p^s$, $1 \le p \le \infty$, the sums in the right-hand sides of (2.7) and (2.8) disappear, due to the periodicity of the integrand. Hence we obtain

$$R[Q_{n+1}^{Tr}; f] = \frac{(-1)^s}{n^s} \int_0^1 \Big[\widetilde{B}_s(nx) - d\Big]\, f^{(s)}(x)\, dx \tag{2.9}$$

and

$$R[Q_n^{Mi}; f] = \frac{(-1)^s}{n^s} \int_0^1 \Big[\widetilde{B}_s\Big(nx - \frac{1}{2}\Big) - d\Big]\, f^{(s)}(x)\, dx\,, \tag{2.10}$$

where d is an arbitrary constant. Applying Hölder's inequality to (2.9) and (2.10), and taking into account that Q_{n+1}^{Tr} and Q_n^{Mi} are optimal quadrature formulae in $\widetilde{W}_p^s$, we obtain

$$|R[Q_{n+1}^{Tr}; f[| \le \mathcal{E}_n(\widetilde{W}_p^s)\, \|f^{(s)}\|_p\,, \quad |R[Q_n^{Mi}; f[| \le \mathcal{E}_n(\widetilde{W}_p^s)\, \|f^{(s)}\|_p\,,$$

where

$$\mathcal{E}_n(\widetilde{W}_p^s) = \frac{1}{n^s} \inf_d \|B_s - d\|_q =: \|B_s - d_{s,p}\|_q\,, \qquad \frac{1}{p} + \frac{1}{q} = 1\,. \tag{2.11}$$

Some known values of the constant $d_{s,p}$ are (see, e.g., [14])

$$d_{s,p} = 0 \quad \text{for odd} \quad s \in \mathbb{N} \quad \text{and} \quad 1 \le p \le \infty, \tag{2.12}$$

$$d_{s,p} = \begin{cases} 2^{-s} B_s(0) & \text{for even } \ s \in \mathbb{N} \ \text{ and } \ p = 1, \\ 0 & \text{for all } \ s \in \mathbb{N} \ \text{ and } \ p = 2, \\ B_s\big(\frac{1}{4}\big) & \text{for even } \ s \in \mathbb{N} \ \text{ and } \ p = \infty\,. \end{cases} \tag{2.13}$$

We shall need constants $\mathcal{E}_n(\widetilde{W}_p^s)$ for $s = 3$, 4 and $p = 1$, 2 and ∞. In the case $s = 3$, these constants are

$$\mathcal{E}_n(\widetilde{W}_\infty^3) = \frac{1}{n^3}\, \|B_3\|_1 = \frac{1}{192\, n^3}\,, \tag{2.14}$$

$$\mathcal{E}_n(\widetilde{W}_2^3) = \frac{1}{n^3}\, \|B_3\|_2 = \frac{1}{12\sqrt{210}\, n^3}\,, \tag{2.15}$$

$$\mathcal{E}_n(\widetilde{W}_1^3) = \frac{1}{n^3}\, \|B_3\|_\infty = \frac{1}{72\sqrt{3}\, n^3}\,. \tag{2.16}$$

In the case $s = 4$, the corresponding constants are

$$\mathcal{E}_n(\widetilde{W}^4_\infty) = \frac{1}{n^4}\,\|B_4(\cdot) - B_4(1/4)\|_1 = \frac{5}{6144\,n^4}\,, \tag{2.17}$$

$$\mathcal{E}_n(\widetilde{W}^4_2) = \frac{1}{n^4}\,\|B_4\|_2 = \frac{1}{240\sqrt{21}\,n^4}\,, \tag{2.18}$$

$$\mathcal{E}_n(\widetilde{W}^4_1) = \frac{1}{n^4}\,\|B_4(\cdot) - 2^{-4}B_4(0)\|_\infty = \frac{1}{768\,n^4}\,. \tag{2.19}$$

3. ASYMPTOTICALLY OPTIMAL QUADRATURE FORMULAE IN W^3_p

Let us start with a brief outline of our method for the construction of asymptotically optimal quadrature formulae in the Sobolev classes W^3_p.

The Euler–MacLaurin summation formulae in Lemma 1 in the case $s = 3$ reduce to

$$\int_0^1 f(x)\,dx = Q^{Tr}_{n+1}[f] - \frac{1}{12\,n^2}\big[f'(1) - f'(0)\big] + \frac{1}{n^3}\int_0^1 \widetilde{B}_3(nx)\,f^{(3)}(x)\,dx \tag{3.1}$$

and

$$\int_0^1 f(x)\,dx = Q^{Mi}_n[f] + \frac{1}{24\,n^2}\big[f'(1) - f'(0)\big] + \frac{1}{n^3}\int_0^1 \widetilde{B}_3\Big(nx - \frac{1}{2}\Big)\,f^{(3)}(x)\,dx\,. \tag{3.2}$$

The derivatives $f'(0)$ and $f'(1)$ appearing in the right-hand side of (3.1) and (3.2) will be replaced by suitable formulae for numerical differentiation. For the sake of brevity, we give the following definition.

Definition 1. Given $0 \le t_1 < t_2 < t_3 < 1$, we denote by $D_1(t_1, t_2, t_3)[f]$ the interpolatory formula for numerical differentiation with nodes $\{t_i\}_{i=1}^3$, which approximates $f'(0)$, i.e.

$$D_1[f] = D_1(t_1, t_2, t_3)[f] = \sum_{i=1}^{3} c_i\, f(t_i) \approx f'(0)\,.$$

We shall use formulae for numerical differentiation with $t_3 = O(n^{-1})$. For instance, such a formula is

$$D_1(x_{0,n}, y_{1,n}, x_{2,n})[f] = \frac{n}{6}\big[-15f(x_{0,n}) + 16f(y_{1,n}) - f(x_{2,n})\big]\,.$$

For the sake of simplicity, $f'(1)$ is approximated by a numerical differentiation formula, obtained from $D_1(t_1,t_2,t_3)[f]$ by a reflection, i.e.,

$$f'(1) \approx \widetilde{D}_1[f] := D_1(t_1,t_2,t_3)[g]\,, \qquad g(t) = -f(1-t)\,.$$

The linear functionals $L[f] := f'(0) - D_1[f]$ and $\widetilde{L}[f] := f'(1) - \widetilde{D}_1[f]$ vanish on π_2, and by Peano's theorem, for $f \in W_1^3$ they are representable in the form

$$L[f] = \int_0^1 K_3(L;t) f'''(t)\,dt\,, \qquad \widetilde{L}[f] = \int_0^1 K_3(\widetilde{L};t) f'''(t)\,dt$$

with $K_3(L;t) = L\big[(\cdot - t)_+^2/2\big]$ and $K_3(\widetilde{L};t) = \widetilde{L}\big[(\cdot - t)_+^2/2\big]$. This representation also implies

$$\begin{aligned} K_3(L;t) &\equiv 0 \quad \text{for } t \in (t_3,1]\,,\\ K_3(\widetilde{L};t) &\equiv 0 \quad \text{for } t \in [0,1-t_3)\,. \end{aligned}$$

Replacement in (3.1) of $f'(0)$ and $f'(1)$ by $D_1[f]$ and $\widetilde{D}_1[f]$, respectively, results in a new quadrature formula Q,

$$Q[f] = Q_{n+1}^{Tr}[f] + \frac{1}{12\,n^2} \sum_{i=1}^{3} c_i \left[f(t_i) + f(1-t_i)\right] \tag{3.3}$$

with at most $n+7$ nodes (including $\{x_{k,n}\}_{k=0}^{n}$), and a Peano kernel $K_3(Q;t)$ given by

$$K_3(Q;t) = \frac{1}{n^3}\,\widetilde{B}_3(n\,t) + \frac{1}{12\,n^2}\big[K_3(L;t) - K_3(\widetilde{L};t)\big]\,, \quad t \in [0,1]\,.$$

Analogously, replacement in (3.1) of $f'(0)$ and $f'(1)$ by $D_1[f]$ and $\widetilde{D}_1[f]$, respectively, yields a quadrature formula Q,

$$Q[f] = Q_{n}^{Mi}[f] - \frac{1}{24\,n^2} \sum_{i=1}^{3} c_i \left[f(t_i) + f(1-t_i)\right] \tag{3.4}$$

with at most $n+6$ nodes (including $\{y_{\ell,n}\}_{\ell=1}^{n}$), and a Peano kernel $K_3(Q;t)$ given by

$$K_3(Q;t) = \frac{1}{n^3}\,\widetilde{B}_3\Big(nx - \frac{1}{2}\Big) - \frac{1}{24\,n^2}\big[K_3(L;t) - K_3(\widetilde{L};t)\big]\,, \quad t \in [0,1]\,.$$

An important observation for quadrature formulae (3.3) and (3.4) is that their third Peano kernels coincide in the interval $t \in (t_3, 1-t_3)$ with $n^{-3}\widetilde{B}_3(n\,t)$ and $n^{-3}\widetilde{B}_3(n\,t - 1/2)$, respectively. That is to say, except for some small neighborhoods of the endpoints, their third Peano kernels coincide with the third Peano kernels of Q^{Tr}_{n+1} and Q^{Mi}_n in the periodic case. Consequently, for the error constants of quadrature formulae (3.3) and (3.4) we have

$$c_{3,p}(Q) = \|K_3(Q;\cdot)\|_q = \mathcal{E}_n(\widetilde{W}^3_p)(1+o(1)) \quad \text{as } n \to \infty\,, \tag{3.5}$$

which implies their asymptotical optimality in W^3_p, $1 < p \le \infty$.

3.1. ASYMPTOTICALLY OPTIMAL QUADRATURE FORMULAE BASED ON Q^{Tr}_{n+1}

Here, we present quadrature formulae of the form (3.3) generated by some formulae for numerical differentiation.

1. A quadrature formula generated by $D_1(x_{0,n}, x_{1,n}, x_{2,n})[f]$.

Since

$$D_1(x_{0,n}, x_{1,n}, x_{2,n})[f] = \frac{n}{2}\big(-3f(x_{0,n}) + 4f(x_{1,n}) - f(x_{2,n})\big)\,,$$

the resulting quadrature formula (it is assumed that $n \ge 6$) is

$$Q_{n+1}[f] = \sum_{k=1}^{n+1} A_{k,n+1}\, f(x_{k-1,n}) \tag{3.6}$$

with

$$\begin{aligned} &A_{1,n+1} = A_{n+1,n+1} = \frac{3}{8\,n}\,, \quad A_{2,n+1} = A_{n,n+1} = \frac{7}{6\,n}\,,\\ &A_{3,n+1} = A_{n-1,n+1} = \frac{23}{24\,n}\,, \quad A_{k,n+1} = \frac{1}{n}\,, \quad 4 \le k \le n-2\,. \end{aligned} \tag{3.7}$$

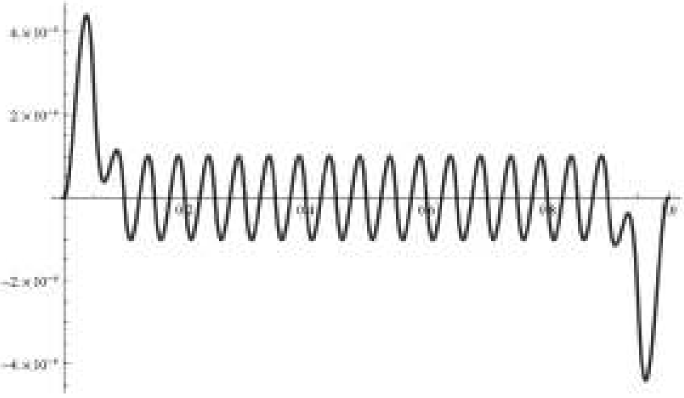

Figure. 1. The third Peano kernel $K_3(Q_{n+1};t)$ of quadrature formula (3.6), $n = 20$.

The graph of the third Peano kernel of quadrature formula (3.6) for $n = 20$ is shown on Figure 1. Since (3.6) is a symmetrical quadrature formula, $K_3(Q_{n+1};t)$

is an odd function with respect to $t = 1/2$. We proceed with evaluating the error constant $c_{3,p}(Q_{n+1})$, $p = \infty$ and $p = 2$. By symmetry, we have

$$c_{3,\infty}(Q_{n+1}) = \|K_3(Q_{n+1};\cdot)\|_1 = 2\int_0^{x_{2,n}} |K_3(Q_{n+1};t)|\,dt + \int_{x_{2,n}}^{x_{n-2,n}} |K_3(Q_{n+1};t)|\,dt\,.$$

For $t \in (x_{2,n}, x_{n-2,n})$ we have $K_3(Q_{n+1};t) = n^{-3}\widetilde{B}_3(n\,t)$, therefore for the second summand we have

$$\int_{x_{2,n}}^{x_{n-2,n}} |K_3(Q_{n+1};t)|\,dt = \frac{1}{n^3}\int_{\frac{2}{n}}^{\frac{n-2}{n}} |\widetilde{B}_3(n\,t)|\,dt = \frac{n-4}{n^3}\,\|B_3\|_1 = \frac{n-4}{192\,n^4}\,.$$

Before evaluating the first summand, we show that $K_3(Q_{n+1};t) > 0$ for $t \in (0, x_{2,n})$. Performing a change of the variable $t = u/n$, $u \in (0,2)$, we obtain, for $t \in (0, x_{2,n})$,

$$K_3(Q_{n+1};t) = -\frac{t^3}{6} + \frac{3}{16\,n}\,t^2 + \frac{7}{12\,n}(t - x_{1,n})_+^2 = \frac{1}{n^3}\Big[-\frac{u^3}{6} + \frac{3u^2}{16} + \frac{7(u-1)_+^2}{12}\Big]\,.$$

The term in the brackets is positive for $u \in (0,2)$. Indeed, if $0 < u \le 1$, then

$$-\frac{u^3}{6} + \frac{3u^2}{16} + \frac{7(u-1)_+^2}{12} = \frac{3u^2}{16}\Big(1 - \frac{8u}{9}\Big) > 0\,,$$

while, if $1 < u < 2$, then

$$-\frac{u^3}{6} + \frac{3u^2}{16} + \frac{7(u-1)_+^2}{12} = -\frac{u^3}{6} + \frac{37u^2}{48} - \frac{7u}{6} + \frac{7}{12} = (2-u)\Big(\frac{u^2}{6} - \frac{7u}{16} + \frac{7}{24}\Big) > 0\,.$$

Therefore,

$$\begin{aligned}2\int_0^{x_{2,n}} |K_3(Q_{n+1};t)|\,dt &= 2\int_0^{\frac{2}{n}} \Big[-\frac{t^3}{6} + \frac{3}{16\,n}\,t^2 + \frac{7}{12\,n}\Big(t - \frac{1}{n}\Big)_+^2\Big]\,dt \\ &= \frac{2}{n^4}\int_0^2 \Big[-\frac{u^3}{6} + \frac{3u^2}{16} + \frac{7(u-1)_+^2}{12}\Big]\,du = \frac{1}{18\,n^4}\,.\end{aligned}$$

Hence,

$$c_{3,\infty}(Q_{n+1}) = \frac{n-4}{192\,n^4} + \frac{1}{18\,n^4} = \frac{1}{192\,n^3}\left(1 + \frac{20}{3\,n}\right).$$

In a similar manner we evaluate the error constant $c_{3,2}(Q_{n+1})$. We have

$$[c_{3,2}(Q_{n+1})]^2 = \int_0^1 [K_3(Q_{n+1};t]^2\,dt = 2\int_0^{x_{2,n}} [K_3(Q_{n+1};t)]^2\,dt + \int_{x_{2,n}}^{x_{n-2,n}} [K_3(Q_{n+1};t)]^2\,dt\,.$$

The second summand is

$$\int\limits_{x_{2,n}}^{x_{n-2,n}} [K_3(Q_{n+1};t)]^2\,dt = \frac{1}{n^6}\int\limits_{\frac{2}{n}}^{\frac{n-2}{n}} [\widetilde{B}_3(n\,t)]^2\,dt = \frac{n-4}{n^7}\,\|B_3\|_2^2\,,$$

and for the first one after some algebra we find

$$\begin{aligned} 2\int\limits_0^{x_{2,n}} [K_3(Q_{n+1};t)]^2\,dt &= \frac{2}{n^7}\int\limits_0^2 \Big[-\frac{u^3}{6}+\frac{3u^2}{16}+\frac{7(u-1)_+^2}{12}\Big]^2\,du \\ &= \frac{2}{n^7}\bigg(\int\limits_0^1 \Big[-\frac{u^3}{6}+\frac{3u^2}{16}\Big]^2\,du + \int\limits_1^2 \Big[-\frac{u^3}{6}+\frac{3u^2}{16}+\frac{7(u-1)^2}{12}\Big]^2\,du\bigg) \\ &= \frac{13}{10080\,n^7} = \frac{39}{n^7}\,\|B_3\|_2^2\,. \end{aligned}$$

After summing the two expressions and taking square root we obtain

$$c_{3,2}(Q_{n+1}) = \frac{1}{n^3}\,\|B_3\|_2\left(1+\frac{35}{n}\right)^{1/2} = \frac{1}{12\sqrt{210}\,n^3}\left(1+\frac{35}{n}\right)^{1/2}.$$

Comparison of the error constants $c_{3,\infty}(Q_{n+1})$ and $c_{3,2}(Q_{n+1})$ of quadrature formula (3.6) with the best possible constant (2.14) and (2.15) in the corresponding 1-periodic Sobolev classes shows the asymptotical optimality of $\{Q_{n+1}\}_{n=6}^{\infty}$ in the Sobolev classes W_∞^3 and W_2^3. Certainly, this sequence is not asymptotically optimal in W_1^3, as is seen also on Figure 1. In fact, $\|K_3(Q_{n+1};\cdot)\|_\infty$ is attained at the point $t_n^* = \frac{3}{4n}$, and

$$c_{3,1}(Q_{n+1}) = K_3(Q_{n+1};t_n^*) = \frac{9}{256\,n^3} = \frac{81\sqrt{3}}{32}\,\mathcal{E}_n(\widetilde{W}_1^3) \approx 4.384\;\mathcal{E}_n(\widetilde{W}_1^3)\,,$$

i.e., the error constant is more than four times greater than the best possible. We shall however construct sequences of quadrature formulae, which are asymptotically optimal in W_1^3, too, see quadrature formulae (3.9) and (3.13) below.

The next quadrature formulae are obtained in the same way as quadrature formula (3.6), and the evaluation of their coefficient and error constants follows the same lines as above. That is why we only give the results.

2. A quadrature formula generated by $\boldsymbol{D_1(x_{0,n}, y_{1,n}, x_{1,n})[f]}$.

Here, $D_1(x_{0,n}, y_{1,n}, x_{1,n})[f] = n\big(-3f(x_{0,n}) + 4f(y_{1,n}) - f(x_{1,n})\big)$, and the resulting quadrature formula (3.3) involves $n+3$ nodes,

$$Q_{n+3}[f] = \sum_{k=1}^{n+3} A_{k,n+3}\,f(\tau_{k,n+3})\,. \tag{3.8}$$

Table 1. The coefficients, nodes and error constants of quadrature formula (3.8).

$A_{1,n+3},\ A_{n+3,n+3}$	$A_{2,n+3},\ A_{n+2,n+3}$	$A_{3,n+3},\ A_{n+1,n+3}$	$A_{k,n+3},\ 4 \le k \le n$
$\frac{1}{4n}$	$\frac{1}{3n}$	$\frac{11}{12n}$	$\frac{1}{n}$

$\tau_{1,n+3}$	$\tau_{2,n+3}$	$\tau_{k,n+3},\ 3 \le k \le n+1$	$\tau_{n+2,n+3}$	$\tau_{n+3,n+3}$
$x_{0,n}$	$y_{1,n}$	$x_{k-2,n}$	$y_{n,n}$	$x_{n,n}$

$c_{3,\infty}(Q_{n+3})$	$c_{3,2}(Q_{n+3})$
$\frac{1}{192\,n^3}\left(1+\frac{2}{3\,n}\right)$	$\frac{1}{12\sqrt{210}\,n^3}\left(1+\frac{7}{4\,n}\right)^{1/2}$

The coefficients, nodes and error constants of this quadrature formula are given in Table 1.

3. A quadrature formula generated by $D_1(x_{0,n}, x_{1,3n}, x_{2,3n})[f]$. Here, $D_1(x_{0,n}, x_{1,3n}, x_{2,3n})[f] = \frac{3n}{2}\big(-3f(x_{0,n}) + 4f(x_{1,3n}) - f(x_{2,3n})\big)$, and by (3.3) we obtain the $(n+5)$-point quadrature formula

$$Q_{n+5}[f] = \sum_{k=1}^{n+5} A_{k,n+5} f(\tau_{k,n+5}) \tag{3.9}$$

with coefficients, nodes and error constants given in Table 2.

Table 2. The coefficients, nodes and error constants of quadrature formula (3.9).

$A_{1,n+5},\ A_{n+5,n+5}$	$A_{2,n+5},\ A_{n+4,n+5}$	$A_{3,n+5},\ A_{n+3,n+5}$	$A_{k,n+5},\ 5 \le k \le n+1$
$\frac{1}{8n}$	$\frac{1}{2n}$	$-\frac{1}{8n}$	$\frac{1}{n}$

$\tau_{1,n+5}$	$\tau_{2,n+5}$	$\tau_{3,n+5}$	$\tau_{k,n+5},\ 4 \le k \le n+2$	$\tau_{n+3,n+5}$	$\tau_{n+4,n+5}$	$\tau_{n+5,n+5}$
$x_{0,n}$	$x_{1,3n}$	$x_{2,3n}$	$x_{k-3,n}$	$x_{3n-2,3n}$	$x_{3n-1,3n}$	$x_{n,n}$

$c_{3,\infty}(Q_{n+5})$	$c_{3,2}(Q_{n+5})$	$c_{3,1}(Q_{n+5})$
$\frac{1}{192\,n^3}\left(1-\frac{22}{27\,n}\right)$	$\frac{1}{12\sqrt{210}\,n^3}\left(1+\frac{8}{81\,n}\right)^{1/2}$	$\frac{1}{72\sqrt{3}\,n^3}$

Here we would like to point out that, unlike the situation with quadrature formulae (3.6) and (3.8), here the third Peano kernel of quadrature formula (3.9) attains its $C[0,1]$-norm away from the boundary intervals affected by the numerical differentiation formulae, and therefore we have

$$c_{3,1}(Q_{n+5}) = \|K_3(Q_{n+5};\cdot)\|_\infty = n^{-3}\|B_3\|_\infty = \frac{1}{72\sqrt{3}\,n^3}\,,$$

showing that $\{Q_{n+5}\}$ is a sequence of asymptotically optimal quadrature formulae in the Sobolev class W_1^3. Figure 2 depicts $K_3(Q_{n+5};t)$ for $n = 20$.

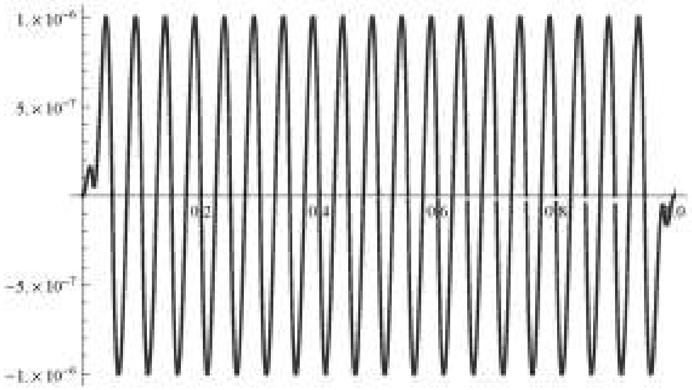

Figure. 2. The third Peano kernel $K_3(Q_{n+5};t)$ of quadrature formula (3.9), $n = 20$.

3.2. ASYMPTOTICALLY OPTIMAL QUADRATURE FORMULAE BASED ON Q_n^{Mi}

Here, we present quadrature formulae generated by various formulae for numerical differentiation through (3.4). Again, we only present in a table form the coefficients, nodes and error constants of these quadrature formulae, skipping the straightforward but sometimes tedious calculations. Occasionally, we have used Wolfram Mathematica for the evaluation of the L_1-norm of the third Peano kernels; in such cases the corresponding error constants $c_{3,\infty}$ are given with approximate numbers.

1. A quadrature formula generated by $D_1(y_{1,n}, y_{2,n}, y_{3,n})[f]$.

This choice is motivated by the aim of not introducing nodes other than $\{y_{\ell,n}\}_{\ell=1}^n$. We have

$$D_1(y_{1,n}, y_{2,n}, y_{3,n})[f] = n\big(-2f(y_{1,n}) + 3f(y_{2,n}) - f(y_{3,n})\big)\,,$$

and by (3.4) we obtain (assuming that $n > 6$) an n-point quadrature formula

$$Q_n[f] = \sum_{k=1}^{n} A_{k,n}\, f(y_{k,n}) \tag{3.10}$$

with weights $\{A_{k,n}\}$ and error constants $c_{3,\infty}(Q_n)$, $c_{3,2}(Q_n)$ as given in Table 3.

Table 3. The coefficients and error constants of quadrature formula (3.10).

$A_{1,n},\ A_{n,n}$	$A_{2,n},\ A_{n-1,n}$	$A_{3,n},\ A_{n-2,n}$	$A_{k,n},\ 3 \le k \le n-3$
$\dfrac{13}{12n}$	$\dfrac{7}{8n}$	$\dfrac{25}{24n}$	$\dfrac{1}{n}$

$c_{3,\infty}(Q_n)$	$c_{3,2}(Q_n)$
$\dfrac{1}{192\,n^3}\Big(1+\dfrac{10.83836617}{n}\Big)$	$\dfrac{1}{12\sqrt{210}\,n^3}\Big(1+\dfrac{475}{4\,n}\Big)^{1/2}$

2. A quadrature formula generated by $D_1(x_{0,n}, y_{1,n}, x_{1,n})[f]$.

We already applied this formula for numerical differentiation in the preceding section, this time we get through (3.4) an $(n+4)$-point quadrature formula

$$Q_{n+4}[f] = \sum_{k=1}^{n+4} A_{k,n+4}\, f(\tau_{k,n+1}) \qquad (3.11)$$

with coefficients, nodes and error constants given in Table 4.

Table 4. The coefficients, nodes and error constants of quadrature formula (3.11).

$A_{1,n+4},\ A_{n+4,n+4}$	$A_{2,n+4},\ A_{n+3,n+4}$	$A_{3,n+4},\ A_{n+2,n+4}$	$A_{k,n+4},\ 4 \le k \le n+1$
$\dfrac{1}{8n}$	$\dfrac{5}{6n}$	$\dfrac{1}{24n}$	$\dfrac{1}{n}$

$\tau_{1,n+4}$	$\tau_{2,n+4}$	$\tau_{3,n+4}$	$\tau_{k,n+4},\ 4 \le k \le n+1$	$\tau_{n+2,n+4}$	$\tau_{n+3,n+4}$	$\tau_{n+3,n+4}$
$x_{0,n}$	$y_{1,n}$	$x_{1,n}$	$y_{k-2,n}$	$x_{n-1,n}$	$y_{n-1,n}$	$x_{n,n}$

$c_{3,\infty}(Q_{n+4})$	$c_{3,2}(Q_{n+4})$
$\dfrac{1}{192\,n^3}\Big(1-\dfrac{175}{384\,n}\Big)$	$\dfrac{1}{12\sqrt{210}\,n^3}\Big(1+\dfrac{25}{16\,n}\Big)^{1/2}$

3. A quadrature formula generated by $D_1(x_{0,n}, y_{1,n}, y_{2,n})[f]$.

In this case, $D_1(x_{0,n}, y_{1,n}, y_{2,n})[f] = \frac{n}{3}\big(-8f(x_{0,n}) + 9f(y_{1,n}) - f(y_{2,n})\big)$, and by (3.4) we obtain an $(n+2)$-point quadrature formula

$$Q_{n+2}[f] = \sum_{k=1}^{n+2} A_{k,n+2}\, f(\tau_{k,n+2}) \qquad (3.12)$$

with coefficients, nodes and error constants given in Table 5.

Table 5. The coefficients, nodes and error constants of quadrature formula (3.12).

$A_{1,n+2},\ A_{n+2,n+2}$	$A_{2,n+2},\ A_{n+1,n+2}$	$A_{3,n+2},\ A_{n,n+2}$	$A_{k,n+2},\ 4\le k\le n-1$
$\dfrac{1}{9\,n}$	$\dfrac{7}{8\,n}$	$\dfrac{73}{72\,n}$	$\dfrac{1}{n}$

$\tau_{1,n+2}$	$\tau_{k,n+2},\ 2\le k\le n+1$	$\tau_{n+2,n+2}$
$x_{0,n}$	$y_{k-1,n}$	$x_{n,n}$

$c_{3,\infty}(Q_{n+2})$	$c_{3,2}(Q_{n+2})$
$\dfrac{1}{192\,n^3}\Big(1-\dfrac{0.06659022}{n}\Big)$	$\dfrac{1}{12\sqrt{210}\,n^3}\Big(1+\dfrac{19}{4\,n}\Big)^{1/2}$

4. A quadrature formula generated by $D_1(x_{0,n}, x_{1,6n}, x_{1,3n})[f]$.

We showed that (3.10), (3.11) and (3.12) generate sequences of asymptotically optimal quadrature formulae in the Sobolev classes W^3_∞ and W^3_2, however, the asymptotical optimality does not hold in W^3_1. With $D_1(x_{0,n}, x_{1,6n}, x_{1,3n})[f]$ we obtain through (3.4) an $(n+6)$-point quadrature formula

$$Q_{n+6}[f] = \sum_{k=1}^{n+6} A_{k,n+6}\, f(\tau_{k,n+6})\,, \tag{3.13}$$

which generates a sequence of asymptotically optimal quadrature formulae in all Sobolev classes W^3_p, $1\le p\le\infty$. The coefficients, nodes and error constants of (3.13) are given in Table 6.

Table 6. The coefficients, nodes and error constants of quadrature formula (3.13).

$A_{1,n+6},\ A_{n+6,n+6}$	$A_{2,n+6},\ A_{n+5,n+6}$	$A_{3,n+6}\ ,\ A_{n+4,n+6}$	$A_{k,n+6},\ 4\le k\le n+3$
$\dfrac{3}{8n}$	$-\dfrac{1}{2n}$	$\dfrac{1}{8n}$	$\dfrac{1}{n}$

$\tau_{1,n+6}$	$\tau_{2,n+6}$	$\tau_{3,n+6}$	$\tau_{k,n+6},\ 4\le k\le n+3$	$\tau_{n+4,n+6}$	$\tau_{n+5,n+6}$	$\tau_{n+6,n+6}$
$x_{0,n}$	$x_{1,6n}$	$x_{1,3n}$	$y_{k-3,n}$	$x_{3n-2,3n}$	$x_{6n-1,6n}$	$x_{n,n}$

$c_{3,\infty}(Q_{n+6})$	$c_{3,2}(Q_{n+6})$	$c_{3,1}(Q_{n+6})$
$\dfrac{1}{192\,n^3}\Big(1-\dfrac{4}{27\,n}\Big)$	$\dfrac{1}{12\sqrt{210}\,n^3}\Big(1+\dfrac{841}{1296\,n}\Big)^{1/2}$	$\dfrac{1}{72\sqrt{3}\,n^3}$

It is clear that quadrature formulae obtained in Sections 3.1 and 3.2 are of nearly the same quality as being asymptotically optimal in the Sobolev classes W_p^3, $1 < p \le \infty$. Nevertheless, it makes sense to compare their error constants in W_∞^3 and in W_2^3 under the assumption that they involve the *same number of nodes* n, $n \ge 7$. Interestingly, we have a clear winner in both W_∞^3 and W_2^3, namely, quadrature formula (3.12). The ranking of quadrature formulae (3.6), (3.8), (3.9), (3.10), (3.11), (3.12) and (3.13) according to the magnitude of their error constants $c_{3,\infty}(Q_n)$ and $c_{3,2}(Q_n)$ is given in Table 7 (the smaller error constant, the higher ranking).

Table 7. The ranking of quadrature formulae according to their error constants.

quadrature formula	(3.6)	(3.8)	(3.9)	(3.10)	(3.11)	(3.12)	(3.13)
position according to the size of $c_{3,\infty}(Q_n)$	2	3	6	4	5	1	7
position according to the size of $c_{3,2}(Q_n)$	6	2	4	7	3	1	5

The ranking is made assuming that n is big enough, e.g., $n \ge 59$. For small n, some small changes occur: in the ranking with respect to $c_{3,\infty}(Q_n)$, (3.10) overtakes (3.8) (if $n \le 58$) and even (3.6) (if $7 \le n \le 30$) whilst in the ranking with respect to $c_{3,2}(Q_n)$, (3.6) overtakes (3.13) if $7 \le n \le 9$.

4. ASYMPTOTICALLY OPTIMAL QUADRATURE FORMULAE IN W_1^4

In [2] the idea described in the beginning of the preceding section was exploited for the construction of asymptotically optimal quadrature formulae in the Sobolev classes W_∞^4 and W_2^4. To this, we add here two sequences of quadrature formulae, which are asymptotically optimal in the Sobolev class W_1^4.

The difference with the Sobolev classes W_p^3 is that, in the cases of W_p^4 there is a shift $d_{4,p}$ (depending on p) of the 1-periodic Bernoulli monospline $\widetilde{B}_4$ so that the shifted Bernoulli monospline has minimal L_q-deviation from zero ($1/p + 1/q = 1$), see (2.13). In particular,

$$d_{4,1} = \frac{1}{16}\, B_4(0)\,, \tag{4.1}$$

and

$$\inf_d \|B_4 - d\|_\infty = \|B_4 - 2^{-4}\, B_4(0)\|_\infty = \frac{1}{768}\,. \tag{4.2}$$

The Euler-MacLauren formulae (2.7) and (2.8) in the case $s = 4$ reduce to

$$\int_0^1 f(x)\,dx = Q^{Tr}_{n+1}[f] - \frac{1}{12\,n^2}\big[f'(1) - f'(0)\big] + \frac{1}{720\,n^4}\big[f'''(1) - f'''(0)\big] + \frac{1}{n^4}\int_0^1 \widetilde{B}_4(n\,x)\, f^{(4)}(x)\,dx\,,$$

$$\int_0^1 f(x)\,dx = Q^{Mi}_{n}[f] + \frac{1}{24\,n^2}\big[f'(1) - f'(0)\big] - \frac{7}{5760\,n^4}\big[f'''(1) - f'''(0)\big] + \frac{1}{n^4}\int_0^1 \widetilde{B}_4\big(n\,x - 1/2\big)\, f^{(4)}(x)\,dx\,,$$

and we rewrite these formulae in the form

$$\int_0^1 f(x)\,dx = Q^{Tr}_{n+1}[f] - \frac{1}{12\,n^2}\big[f'(1) - f'(0)\big] + \frac{1}{768\,n^4}\big[f'''(1) - f'''(0)\big] + \frac{1}{n^4}\int_0^1 \big[\widetilde{B}_4(n\,x) - 2^{-4}B_4(0)\big]\, f^{(4)}(x)\,dx\,, \tag{4.3}$$

$$\int_0^1 f(x)\,dx = Q^{Mi}_{n}[f] + \frac{1}{24\,n^2}\big[f'(1) - f'(0)\big] - \frac{1}{768\,n^4}\big[f'''(1) - f'''(0)\big] + \frac{1}{n^4}\int_0^1 \big[\widetilde{B}_4\big(n\,x - 1/2\big) - 2^{-4}B_4(0)\big]\, f^{(4)}(x)\,dx\,. \tag{4.4}$$

Definition 2. Given $0 \le t_1 < t_2 < t_3 < t_4 < 1$, we denote by $D_1(t_1, t_2, t_3)[f]$ and $D_3(t_1, t_2, t_3)[f]$ the interpolatory formulae for numerical differentiation with nodes $\{t_i\}_{i=1}^4$, which approximate $f'(0)$ and $f'''(0)$, respectively, i.e.

$$D_1[f] := D_1(t_1, t_2, t_3, t_4)[f] = \sum_{i=1}^{4} c_{i,1}\, f(t_i) \approx f'(0)\,,$$

$$D_3[f] := D_3(t_1, t_2, t_3, t_4)[f] = \sum_{i=1}^{4} c_{i,3}\, f(t_i) \approx f'''(0)\,.$$

We approximate derivatives $f'(0)$ and $f'''(0)$ appearing in (4.3)–(4.4) by $D_1[f]$ and $D_3[f]$, respectively. The derivatives $f'(1)$ and $f'''(1)$ are approximated by the formulae for numerical differentiation $\widetilde{D}_1[f]$ and $\widetilde{D}_3[f]$, respectively, which are obtained from $D_1[f]$ and $D_3[f]$ by a reflection, i.e.,

$$\widetilde{D}_1[f] = D_1[g], \quad \widetilde{D}_3[f] = D_3[g], \quad g(x) := -f(1-x)\,.$$

We observe that linear functionals $L_1[f] := f'(0) - D_1[f]$, $L_3[f] := f'''(0) - D_3[f]$, $\widetilde{L}_1[f] := f'(0) - \widetilde{D}_1[f]$ and $\widetilde{L}_3[f] := f'''(0) - \widetilde{D}_3[f]$ vanish on π_3, therefore, by Peano's theorem, for $f \in W_1^4$ they possess integral representations of the form

$$L[f] = \int_0^1 K_4(L;x) f^{(4)}(x)\,dx, \qquad \text{with} \;\; K_4(L;t) = L\big[(\cdot - t)_+^3/3!\big]\,.$$

Replacement of derivatives in (4.3) by the formulae for numerical differentiation yields a new quadrature formula Q,

$$\int_0^1 f(x)\,dx = Q[f] + \int_0^1 K_4(Q;x) f^{(4)}(x)\,dx\,,$$

where

$$\begin{aligned} Q[f] = Q_{n+1}^{Tr}[f] &+ \frac{1}{12\,n^2}\sum_{i=1}^{4} c_{i,1}\big[f(t_i) + f(1-t_i)\big] \\ &- \frac{1}{768\,n^4}\sum_{i=1}^{4} c_{i,3}\big[f(t_i) + f(1-t_i)\big]\,, \end{aligned} \tag{4.5}$$

and

$$\begin{aligned} K_4(Q;x) = \frac{1}{n^4}\big[\widetilde{B}_4(n\,x) - 2^{-4}B_4(0)\big] &+ \frac{1}{12\,n^2}\big[K_4(L_1;x) - K_4(\widetilde{L}_1;x)\big] \\ &- \frac{1}{768\,n^4}\big[K_4(L_3;x) - K_4(\widetilde{L}_3;x)\big]\,. \end{aligned} \tag{4.6}$$

Analogously, replacement of derivatives in (4.4) by the formulae for numerical differentiation yields a new quadrature formula Q,

$$\begin{aligned} Q[f] = Q_n^{Mi}[f] &- \frac{1}{24\,n^2}\sum_{i=1}^{4} c_{i,1}\big[f(t_i) + f(1-t_i)\big] \\ &+ \frac{1}{768\,n^4}\sum_{i=1}^{4} c_{i,3}\big[f(t_i) + f(1-t_i)\big]\,, \end{aligned} \tag{4.7}$$

and

$$\begin{aligned} K_4(Q;x) = \frac{1}{n^4}\big[\widetilde{B}_4(n\,x - 1/2) - 2^{-4}B_4(0)\big] &- \frac{1}{24\,n^2}\big[K_4(L_1;x) - K_4(\widetilde{L}_1;x)\big] \\ &+ \frac{1}{768\,n^4}\big[K_4(L_3;x) - K_4(\widetilde{L}_3;x)\big]\,. \end{aligned} \tag{4.8}$$

Here, as in the preceding section, it is assumed that $t_4 = O(n^{-1})$, and as a result, for $x \in [t_4, 1-t_4]$ the fourth Peano kernels of quadrature formulae (4.5) and (4.7) coincide with $n^{-4}\left[\widetilde{B}_4(n\,x) - 2^{-4}B_4(0)\right]$ and $n^{-4}\left[\widetilde{B}_4(n\,x-1/2) - 2^{-4}B_4(0)\right]$, respectively. Hence, for Q being either (4.5) or (4.7) we have

$$\|K_4(Q;\cdot)\|_{C[t_4,1-t_4]} = \frac{1}{n^4}\,\|B_4 - 2^{-4}B_4(0)\|_\infty = \frac{1}{768\,n^4}\,. \tag{4.9}$$

Both (4.5) and (4.7) are symmetric quadrature formulae with at most $n+9$ nodes. In view of (2.19), (4.9) and the obvious inequality

$$\mathcal{E}_n(W_1^4) \ge \mathcal{E}_n(\widetilde{W}_1^4) = \frac{1}{768\,n^4}\,,$$

a sufficient condition for either of (4.5) and (4.7) to generate a sequence of asymptotically optimal quadrature formulae in W_1^4 is

$$\|K_4(Q;\cdot)\|_{C[0,t_4]} \le \frac{1}{768\,n^4}\,. \tag{4.10}$$

Indeed, in such a case (4.10) and (4.9) imply

$$c_{4,1}(Q) = \|K_4(Q;\cdot)\|_{C[0,1]} = \frac{1}{768\,n^4}$$

and since Q has at most $n+9$ nodes, then for Q_n, the n-point quadrature formula of the same kind, with $n > 9$, we have

$$c_{4,1}(Q_n) \le \frac{1}{768\,(n-9)^4}\,.$$

Consequently,

$$1 \le \lim_{n\to\infty} \frac{c_{4,1}(Q_n)}{\mathcal{E}_n(W_1^4)} \le \lim_{n\to\infty} \frac{\frac{1}{768\,(n-9)^4}}{\mathcal{E}_n(\widetilde{W}_1^4)} = \lim_{n\to\infty} \frac{\frac{1}{768\,(n-9)^4}}{\frac{1}{768\,n^4}} = 1\,,$$

whence the asymptotical optimality holds.

4.1. ASYMPTOTICALLY OPTIMAL QUADRATURE FORMULAE BASED ON Q_{n+1}^{Tr}

We make use of the following formulae for numerical differentiation:

$$D_1(x_{0,n}, x_{1,3n}, x_{2,3n}, x_{1,n})[f] = \frac{n}{2}\big[-11f(x_{0,n}) + 18f(x_{1,3n}) - 9f(x_{2,3n}) + 2f(x_{1,n})\big]$$

$$D_3(x_{0,n}, x_{1,3n}, x_{2,3n}, x_{1,n})[f] = 27n^3\big[-f(x_{0,n}) + 3f(x_{1,3n}) - 3f(x_{2,3n}) + f(x_{1,n})\big].$$

The resulting quadrature formula (4.5) involves $n+5$ nodes,

$$Q_{n+5} = \sum_{k=1}^{n+5} A_{k,n+5}\, f(\tau_{k,n+5})\,. \tag{4.11}$$

Table 8. The weights and the nodes of quadrature formula (4.11).

$A_{1,n+5}, A_{n+5,n+5}$	$A_{2,n+5}, A_{n+4,n+5}$	$A_{3,n+5}, A_{n+3,n+5}$	$A_{4,n+5}, A_{n+2,n+5}$	$A_{k,n+5},\ 5 \le k \le n+1$
$\dfrac{59}{768\,n}$	$\dfrac{165}{256\,n}$	$-\dfrac{69}{256\,n}$	$\dfrac{805}{768\,n}$	$\dfrac{1}{n}$

$\tau_{1,n+5}$	$\tau_{2,n+5}$	$\tau_{3,n+5}$	$\tau_{k,n+5},\ 4 \le k \le n+2$	$\tau_{n+3,n+5}$	$\tau_{n+4,n+5}$	$\tau_{n+5,n+5}$
$x_{0,n}$	$x_{1,3n}$	$x_{2,3n}$	$x_{k-3,n}$	$x_{3n-2,3n}$	$x_{3n-1,3n}$	$x_{n,n}$

The weights and the nodes of Q_{n+5} are given in Table 8.

We shall show that the fourth Peano kernel of $Q = Q_{n+5}$ satisfies condition (4.10) with $[0, t_4] = [0, x_{1,n}]$. The latter Peano kernel is given by

$$K_4(Q_{n+5};x) = \frac{x^4}{24} - \frac{1}{6}\Big[\frac{59}{768n}\,x^3 + \frac{165}{256n}\Big(x - \frac{1}{3n}\Big)_+^3 - \frac{69}{256n}\Big(x - \frac{2}{3n}\Big)_+^3\Big],\ \ x \in [0, x_{1,n}].$$

We perform change of the variable $x = u/n$, with $u \in [0,1]$, to obtain

$$K_4(Q_{n+5};x) = \frac{1}{24\,n^4}\Big[u^4 - \frac{59}{192}\,u^3 - \frac{165}{64}\,(u-1/3)_+^3 + \frac{69}{64}\,(u-2/3)_+^3\Big] =: \frac{1}{24\,n^4}\,g(u).$$

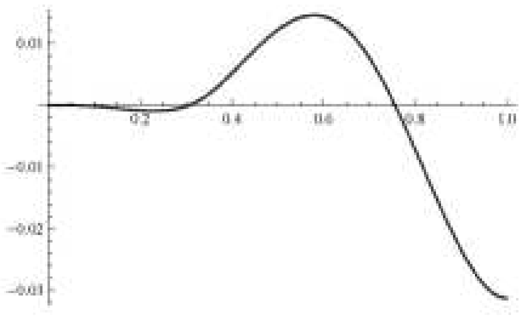

Figure. 3. The graph of $g(u)$, $u \in [0,1]$.

A straightforward analysis shows that g attains its uniform norm in $[0,1]$ at $u = 1$ (this is seen also from the graph of g, depicted on Figure 3). Hence,

$$\|K_4(Q_{n+5};\cdot)\|_{C[0,x_{1,n}]} = |K_4(Q_{n+5};x_{1,n})|\,.$$

Since

$$K_4(Q_{n+5};x) \equiv \frac{1}{n^4}\,\big[\widetilde{B}_4(n\,x) - 2^{-4}B_4(0)\big], \quad x \in [x_{1,n}, 1 - x_{1,n}]\,,$$

we have

$$\|K_4(Q_{n+5};\cdot)\|_{C[0,x_{1,n}]} = |K_4(Q_{n+5};x_{1,n})| = \frac{1}{n^4}\big|\widetilde{B}_4(n\,x_{1,n}) - 2^{-4}B_4(0)\big|$$
$$= \frac{1-2^{-4}}{n^4}\,\big|B_4(0)\big| = \frac{1}{768\,n^4}\,.$$

Thus, condition (4.10) is verified, and the asymptotical optimality in W_1^4 of the sequence of quadrature formulae $\{Q_{n+5}\}$ given by (4.11) is proved.

4.2. ASYMPTOTICALLY OPTIMAL QUADRATURE FORMULAE BASED ON Q_n^{Mi}

Here we apply formulae for numerical differentiation with nodes $x_{0,n}$, $y_{1,3n}$, $x_{1,3n}$ and $y_{1,n}$, namely

$$D_1(x_{0,n},y_{1,3n},x_{1,3n},1_{1,n})[f] = n\big[-11f(x_{0,n})+18f(y_{1,3n})-9f(x_{1,3n})+2f(y_{1,n})\big]$$
$$D_3(x_{0,n},y_{1,3n},x_{1,3n},y_{1,n})[f] = 216n^3\big[-f(x_{0,n})+3f(y_{1,3n})-3f(x_{1,3n})+f(y_{1,n})\big].$$

By (4.7) we obtain a quadrature formula with $n+6$ nodes,

$$Q_{n+6} = \sum_{k=1}^{n+6} A_{k,n+6}\,f(\tau_{k,n+6})\,. \tag{4.12}$$

The weights and the nodes of Q_{n+6} are given in Table 9.

Table 9. The weights and the nodes of quadrature formula (4.12).

$A_{1,n+6}, A_{n+6,n+6}$	$A_{2,n+6}, A_{n+5,n+6}$	$A_{3,n+6}, A_{n+4,n+5}$	$A_{4,n+6}, A_{n+3,n+6}$	$A_{k,n+6},\ 5\le k\le n+2$
$\dfrac{17}{96\,n}$	$\dfrac{3}{32\,n}$	$-\dfrac{15}{32\,n}$	$\dfrac{115}{96\,n}$	$\dfrac{1}{n}$

$\tau_{1,n+6}$	$\tau_{2,n+6}$	$\tau_{3,n+6}$	$\tau_{k,n+6},\ 4\le k\le n+3$	$\tau_{n+4,n+6}$	$\tau_{n+5,n+6}$	$\tau_{n+6,n+6}$
$x_{0,n}$	$y_{1,3n}$	$x_{1,3n}$	$y_{k-3,n}$	$x_{3n-1,3n}$	$y_{3n,3n}$	$x_{n,n}$

We proceed with showing that the sequence of quadrature formulae $\{Q_{n+6}\}_{n\in\mathbb{N}}$ defined in (4.12) is asymptotically optimal in W_1^4. To this end, we need to show that the fourth Peano kernel of $Q = Q_{n+6}$ satisfies condition (3.10), with $[0,t_4]$ replaced by $[0,y_{1,n}]$. We have

$$K_4(Q_{n+6};x) = \frac{x^4}{24} - \frac{1}{6}\Big[\frac{17}{96n}\,x^3 + \frac{3}{32n}\Big(x-\frac{1}{6n}\Big)_+^3 - \frac{15}{32n}\Big(x-\frac{1}{3n}\Big)_+^3\Big],\quad x\in[0,y_{1,n}],$$

or, after change of the variable, $x = u/n$ with $u\in[0,1/2]$,

$$K_4(Q_{n+6};x) = \frac{1}{24\,n^4}\Big[u^4 - \frac{17}{24}\,u^3 - \frac{3}{8}\,(u-1/6)_+^3 + \frac{15}{8}\,(u-1/3)_+^3\Big] =: \frac{1}{24\,n^4}\,h(u).$$

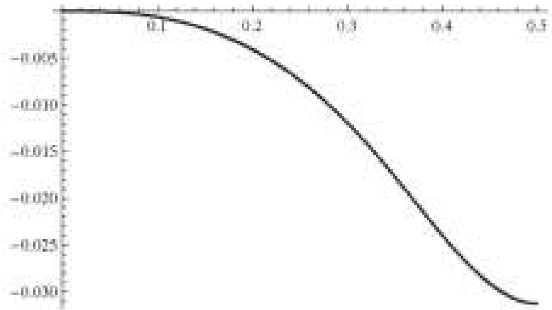

Figure. 4. The graph of $h(u)$, $u \in [0, 1/2]$.

By a straightforward analysis we see that h is monotone decreasing in the interval $[0, 1/2]$ (see Figure 4 with the graph of h), and therefore h attains its uniform norm in $[0, 1/2]$ at $u = 1/2$. Consequently,

$$\|K_4(Q_{n+6}; \cdot)\|_{C[0,y_{1,n}]} = |K_4(Q_{n+6}; y_{1,n})| .$$

Since

$$K_4(Q_{n+6}; x) \equiv \frac{1}{n^4} \left[\widetilde{B}_4(n\,x - 1/2) - 2^{-4} B_4(0)\right], \quad x \in [y_{1,n}, 1 - y_{1,n}] ,$$

we obtain

$$\begin{aligned}\|K_4(Q_{n+6}; \cdot)\|_{C[0,y_{1,n}]} &= |K_4(Q_{n+6}; y_{1,n})| = \frac{1}{n^4}\left|\widetilde{B}_4(n\,y_{1,n} - 1/2) - 2^{-4} B_4(0)\right| \\ &= \frac{1 - 2^{-4}}{n^4}\, |B_4(0)| = \frac{1}{768\, n^4} .\end{aligned}$$

The proof that $\{Q_{n+6}\}_{n\in\mathbb{N}}$ is a sequence of asymptotically optimal quadrature formulae in W_1^4 is accomplished.

As was seen, the fourth Peano kernels of (4.11) and (4.12) have the same L_∞-norm, namely, $\frac{1}{768\,n^4}$, however, quadrature formula (4.11) can be viewed as slightly better as it involves one node less than (4.12).

5. CONCLUSIONS

We have constructed certain sequences of quadrature formulae, which are asymptotically optimal in the Sobolev classes W_p^3, $1 \le p \le \infty$ and in W_1^4. Their weights and nodes are explicitly given, and their sharp error constants for $p = 1, 2$ and ∞ and are evaluated.

For the sake of simplicity, we have considered only symmetric quadrature formulae, however, sequences of non-symmetric asymptotically optimal quadrature formulae can be generated as well by making use of different formulae for numerical differentiation for approximation of the derivatives at the end points of integration interval.

The same approach can be applied for the construction of sequences of asymptotically optimal quadrature formulae in the Sobolev classes W_p^4, $r > 4$, though the calculation of their sharp error constants $c_{r,p}$, even for $p = 1, 2, \infty$, becomes rather elaborate.

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