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A numerical method for finite-part integrals

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Abstract

In the present paper we introduce and study an *extended product quadrature rule* to approximate Hadamard finite part integrals of the type

$$\mathbf{H}_p(fU,t) = \,=\!\!\!\!\!\!\int_0^{+\infty} \frac{f(x)}{(x-t)^{p+1}} U(x)dx, \quad t>0, \; p\in\mathbb{N}, \; U(x)=e^{-x}x^{\gamma}, \; \gamma\geq 0.$$

Hypersingular integrals arise in many contexts, such as singular and hypersingular boundary integral equations, which are tools for modeling many phenomena in different branches of the applied sciences. Here we derive an extended product rule and by a mixed combination with the *one weight product rule* introduced in [9], we propose a compound scheme of quadrature rules which allows a significant reduction in the number of evaluations of the density function f. Conditions assuring the stability and the convergence of the the mixed scheme in weighted uniform form are deduced. Some numerical experiments are also given, in order to highlight the efficiency of the mixed approach.

1 Introduction

This paper deals with the approximation of integral transforms of the type

$$\mathbf{H}_p(fU,t) = \,=\!\!\!\!\!\!\int_0^{+\infty} \frac{f(x)}{(x-t)^{p+1}} U(x)dx, \quad t>0, \; p\in\mathbb{N}, \; U(x)=e^{-x}x^{\gamma}, \; \gamma\geq 0, \tag{1}$$

where the integral on the right-hand side is defined as the finite part in the Hadamard sense. Integrals of this kind are also called "hypersingular integrals" and arise in many contexts, such as singular and hypersingular boundary integral equations, which are tools for modeling many phenomena in different branches of the applied sciences (see for instance [1], [14], [18], [27] and the references therein).

Here we propose an "extended product quadrature rule" obtained by replacing the function f by an extended Lagrange polynomial which interpolates f at two related sets of zeros of orthogonal polynomials. This rule, suitably combined with the one set product rule introduced in [9], allows to consider a compound scheme of quadrature formulae, organized so that a significant reduction in the number of samples of f is obtained. This mixed approach will find application in the construction of a fast numerical method for hypersingular integral equations, similar to that proposed in [23] for second kind Fredholm integral equations.

Then we determine conditions assuring the stability and the convergence of the the mixed scheme, in some weighted uniform spaces of functions. Despite the simplicity of the approach, the success of any product rule is based on the "exact" computation of the coefficients, topic that is not yet easy, since any kernel $k(x,t)$ appearing in the integral involves specific techniques. In the case of the *one weight product rule* (shortly OWPR) studied in [9] for the kernel $k(x,t)=(x-t)^{-p-1}$, the coefficients were constructed by means of the *modified moments* involving Laguerre polynomials, generated by some recurrence relations determined there. Unfortunately the same recurrence relations do not hold in the case of the extended rule coefficients, where some *generalized modified moments* appear, which involve the product of two Laguerre polynomials. Here we determine a recurrence relation for the generalized modified moments, whose construction starts from the ordinary modified moments.

Then we propose to employ the extended rule for composing a sequence of product rules organized in such a way that a significant reduction of samples of f is carried out. This saving is based on the representation of the extended Lagrange polynomial in terms of two ordinary Lagrange polynomials w.r.t. the weight w and the weight $\bar{w}$, separately (see (12)). As we will show, the mixed quadrature sequence allows to reduce of one third the number of samples of f.

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The plan of the paper is the following: next section contains some preliminary results and notations. In Section 3 we present a result of simultaneous approximation of a function f and its derivatives by means of a composite Lagrange polynomial sequence and results about the convergence are given in Sobolev-type weighted spaces of functions. In Section 4 we state the new product rule with some results about its stability, and an estimate of the error is obtained. Moreover, we will construct a mixed sequence of product rules which allows to approximate $\mathbf{H}_p(f)$ with a reduced number of evaluations of the density function f. In Section 5 we provide some details about the computation of the coefficients of the extended product rule and then we propose some numerical experiments, in order to show the efficiency of the mixed sequence of product rules also in comparison with the sequence of ordinary ones. Finally, in Section 6 the proofs of the main results are presented.

2 Definition and preliminary results

Throughout the paper the constant $\mathcal{C}$ will be used several times, having different meanings in different formulas. Moreover from now on we will write $\mathcal{C} \neq \mathcal{C}(a, b, \ldots)$ in order to say that $\mathcal{C}$ is a positive constant independent of the parameters $a, b, \ldots$, and $\mathcal{C} = \mathcal{C}(a, b, \ldots)$ to say that $\mathcal{C}$ depends on $a, b, \ldots$. Moreover, if $A, B \geq 0$ are quantities depending on some parameters, we will write $A \sim B$, if there exists a constant $0 < \mathcal{C} \neq (A, B)$ such that

$$\frac{B}{\mathcal{C}} \leq A \leq \mathcal{C}B.$$

Finally, $\mathbb{P}_m$ will denote the space of the algebraic polynomials of degree at most m.

2.1 Function spaces

With $U(x) = e^{-x}x^{\gamma},\ \gamma \geq 0$, we denote by C_U the following space of functions

$$C_U = \begin{cases} \left\{ f \in C^0((0,+\infty)) : \lim\limits_{\substack{x\to+\infty \\ x\to 0^+}} (fU)(x) = 0, \right\} & \text{if } \gamma > 0, \\ \left\{ f \in C^0([0,+\infty)) : \lim\limits_{x\to+\infty} (fU)(x) = 0, \right\} & \text{if } \gamma = 0, \end{cases}$$

equipped with the norm

$$\|f\|_{C_U} := \|fU\| = \sup_{x\geq 0} |(fU)(x)|_\infty .$$

In the case $\gamma = 0$, the space C_U consists of all continuous functions on $(0, +\infty)$.

For smoother functions, we introduce the Sobolev-type spaces of order $r \in \mathbb{N}$

$$W_r(U) = \left\{ f \in C_U \ :\ f^{(r-1)} \in AC((0,+\infty)) \text{ and } \|f^{(r)}\varphi^r U\| < +\infty \right\},$$

where $AC((0, +\infty))$ denotes the set of all functions which are absolutely continuous on every closed subset of $(0, +\infty)$ and $\varphi(x) = \sqrt{x}$. In what follows we will mean $W_0(U) = C_U$. We equip these spaces with the norm

$$\|f\|_{W_r(U)} := \|fU\| + \|f^{(r)}\varphi^r U\|.$$

Denoting by

$$E_m(f)_U = \inf_{P\in\mathbb{P}_m} \|(f - P)U\|_\infty,$$

the error of the best polynomial approximation of $f \in C_U$, we recall from [3] that for any $f \in W_r(U),\ r \geq 1$,

$$E_m(f)_U \leq \mathcal{C} \frac{\|f\|_{W_r(U)}}{(\sqrt{m})^r}, \quad 0 < \mathcal{C} \neq \mathcal{C}(m, f). \tag{2}$$

Analogously, by replacing the weight $U(x) = e^{-x}x^{\gamma},\ \gamma \geq 0$, with $u(x) = e^{-\frac{x}{2}}x^{\gamma},\ \gamma \geq 0$, the space C_u is defined. In the case the parameter γ is the same in u and U, we have $C_u \subset C_U$.

2.2 Orthogonal polynomials

Let $w(x) = e^{-x}x^{\alpha}$ be the Laguerre weight of parameter $\alpha > -1$ and let $\{p_m(w)\}_m$ be the corresponding sequence of orthonormal polynomials with positive leading coefficients

$$p_m(w, x) = c_m(w)x^m + \text{ terms of lower degree}, \quad c_m(w) > 0.$$

Denoting by $\{x_{m,k} =: x_k\}_{k=1}^m$ the zeros of $p_m(w)$ in increasing order, we have that

$$\frac{\mathcal{C}}{m} \leq x_1 < x_2 < \ldots x_m \leq 4m + 2\alpha + 2 - \mathcal{C}(4m)^{\frac{1}{3}}$$

and that

$$\Delta x_k := x_{k+1} - x_k \sim \sqrt{\frac{x_k}{4m - x_k}}, \quad k = 1, 2, \ldots, m-1.$$

From now on, for a fixed $0<\theta<1$, we will denote by $j=j(m)$ the index defined as

$$x_j = x_{j(m)} = \min\{x_k : x_k \geq \theta 4m, \quad k=1,2,..,m\}. \tag{3}$$

Moreover, related to the weight w, let us introduce the weight $\overline{w}(x)=xw(x)$. Denoting by $\{y_k\}_{k=1}^{m-1}$ the zeros of the corresponding $(m-1)$-th orthonormal polynomial $p_{m-1}(\overline{w})$, we recall that the zeros of $p_{m-1}(\overline{w})$ interlace those of $p_m(w)$ [19], i.e.,

$$x_k < y_k < x_{k+1}, \qquad k=1,2,\dots,m-1.$$

Thus the polynomial $Q_{2m-1} := p_m(w)p_{m-1}(\overline{w})$ has simple zeros and, setting

$$z_{2i-1} := x_i, i=1,2,\dots,m, \quad z_{2i} := y_i,\ i=1,2,\dots,m-1,$$

it follows that

$$\Delta z_k = z_{k+1} - z_k \sim \sqrt{\frac{z_{k+1}}{m}}, \quad k=1,2,\dots,2j,$$

with j defined as in (3), uniformly in $m\in\mathbb{N}$ [19].

3 Lagrange interpolation processes

Denote by $L_{m+1}(w,f)$ the *truncated Lagrange polynomial* [13], which interpolates a given function f at the zeros $\{x_k\}_{k=1}^m$ of $p_m(w,x)(4m-x)$, i. e. with j as defined in (3), let

$$L_{m+1}(w,f,x) = \sum_{k=1}^{j} \ell_{m,k}(w,x) f(x_k) \frac{4m-x}{4m-x_k}, \quad \ell_{m,k}(w,x) = \frac{p_m(w,x)}{p_m'(w,x_k)(x-x_k)}.$$

We recall that [13]

$$L_{m+1}(w,f) = f, \quad \forall f \in \mathcal{P}_m^*,$$

where

$$\mathcal{P}_m^* = \{q \in \mathbb{P}_m : q(4m) = 0 = q(x_i), \ \ i>j\} \subset \mathbb{P}_m.$$

About the simultaneous approximation of f in the weighted uniform norm, the following theorem was proven in [7].

Theorem 3.1. *Let $w(x)=x^\alpha e^{-x}$, $u(x)=e^{-\frac{x}{2}}x^\gamma, \gamma\geq 0$, and assume that*

$$\max\left(0, \frac{\alpha}{2}+\frac{1}{4}\right) \leq \gamma \leq \frac{\alpha}{2}+\frac{5}{4}. \tag{4}$$

If $f\in W_r(u)$, $r\geq 1$, then for $0\leq k\leq r-1$, it holds

$$\|(f-L_{m+1}(w,f))^{(k)}\varphi^k u\| \ \leq \ \mathcal{C}\frac{\log m}{(\sqrt{m})^{r-k}}\left\{\|f\|_{W_r(u)} + e^{-Am}\|fu\|\right\}, \quad 0<\mathcal{C}\neq\mathcal{C}(m,f). \tag{5}$$

In the case of the ordinary Lagrange polynomial interpolating f at the zeros of $p_m(w,x)(4m-x)$, the previous theorem was proved in [15].

Remark 1. By (5), under the assumptions (4), it follows for $f\in W_r(U)$, $r>1$,

$$\|L_{m+1}(w,f)\|_{W_{r-1}(u)} \leq \mathcal{C}\left(\|f\|_{W_r(u)} + \|f\|_{W_{r-1}(u)}\right). \tag{6}$$

Besides the one-weight Lagrange polynomial, consider the extended truncated Lagrange polynomial interpolating a function f at the zeros of $Q_{2m-1}(x)(4m-x)$ [19], i.e., with j defined as in (3),

$$L_{2m}(w,\overline{w},f,x) \quad = \quad \sum_{k=1}^{2j} \frac{Q_{2m-1}(x)(4m-x)}{(4m-z_k)Q_{2m-1}'(z_k)(x-z_k)} f(z_k) \in \mathbb{P}_{2m-1}. \tag{7}$$

Letting

$$\mathcal{P}_{2m-1}^* = \{q\in\mathbb{P}_{2m-1} : q(4m) = 0 = q(z_i), \ \ i>2j\} \subset \mathbb{P}_{2m-1}, \tag{8}$$

$L_{2m}(w,\bar{w})$ is a projector of C_U onto $\mathcal{P}_{2m-1}^*$. Moreover, setting

$$\widetilde{E}_{2m-1}(f)_U := \inf_{P\in\mathcal{P}_{2m-1}^*} \|(f-P)U\|,$$

the *quasi best approximation error* of f in C_U, it can be estimated by means of the best approximation error $E_M(f)_U$, where M is a proper fraction of $2m-1$, i.e. [16],

$$\widetilde{E}_{2m-1}(f)_U \leq \mathcal{C}\left\{E_M(f)_U + e^{-Am}\|fU\|\right\}, \quad \forall f\in C_U, \tag{9}$$

with $M=\left\lfloor (2m-1)\left(\frac{\theta}{1+\theta}\right)\right\rfloor$ and the constants $0<A\neq A(m,f)$, $0<\mathcal{C}\neq\mathcal{C}(m,f)$.

We recall here the following estimate of the error of best polynomial approximation $E_m(f)_U$, holding for any $f \in W_r(U)$ [3]

$$E_m(f)_U \leq \frac{\mathcal{C}}{(\sqrt{m})^r} E_{m-r}(f^{(r)})_{U\varphi^r}, \tag{10}$$

which gives

$$E_m(f)_U \leq \mathcal{C} \frac{\|f^{(r)}\varphi^r U\|}{(\sqrt{m})^r}, \tag{11}$$

where $\mathcal{C} \neq \mathcal{C}(m,f)$ in all estimates.

The polynomial $L_{2m}(w,\overline{w},f)$ can be represented in the following useful form

$$\begin{aligned} L_{2m}(w,\overline{w},f,x) &= p_{m-1}(\overline{w},x)L_{m+1}\left(w,\frac{f}{p_{m-1}(\overline{w})},x\right)+p_m(w,x)L_m\left(\overline{w},\frac{f}{p_m(w)},x\right) \\ &= p_{m-1}(\overline{w},x)(4m-x)\sum_{k=1}^{j}\ell_{m,k}(w,x)\frac{f(x_k)}{p_{m-1}(\overline{w},x_k)(4m-x_k)} \\ &+ p_m(w,x)(4m-x)\sum_{k=1}^{j}\ell_{m-1,k}(\overline{w},x)\frac{f(y_k)}{p_m(w,y_k)(4m-y_k)}, \\ \ell_{m,k}(w,x) &= \frac{p_m(w,x)}{p'_m(w,x_k)(x-x_k)}, \qquad \ell_{m-1,k}(\overline{w},x)=\frac{p_{m-1}(\overline{w},x)}{p'_{m-1}(\overline{w},y_k)(x-y_k)}, \end{aligned} \tag{12}$$

which will be employed in our successive results. Indeed, by this representation the samples of f involved in the extended polynomial are split into the sets $\{f(x_i)\}_{i=1}^{m}$ and $\{f(y_i)\}_{i=1}^{m-1}$. Thus, whenever the polynomial $L_{m+1}(w,f)$ (or $L_m(\overline{w},f)$) has been constructed, the computation of $L_{2m}(w,\overline{w},f)$ requires at most m new values of f (or $m+1$).

Next theorem is new and it deals with the simultaneous approximation of a function f by the extended Lagrange polynomial in (12)

Theorem 3.2. *Let $f \in W_r(U)$, with $r \in \mathbb{N}$ and let $0 \leq k \leq r-1$. If the parameters α,γ satisfy the assumption*

$$\alpha+1 \leq \gamma \leq \alpha+2,$$

then we have

$$\|(f-L_{2m}(w,\overline{w},f))^{(k)}\varphi^k U\| \leq \mathcal{C}\left(\log m \frac{\|f\|_{W_r(U)}}{(\sqrt{m})^{r-k}}+e^{-Am}\|fU\|\right), \tag{13}$$

where the constants $0<A \neq A(m,f)$, $0<\mathcal{C}\neq\mathcal{C}(m,f)$.

Remark 2. By (13) it follows for $f \in W_r(U)$, $r>1$

$$\|L_{2m}(w,\overline{w},f)\|_{W_{r-1}(U)} \leq \mathcal{C}\left(\|f\|_{W_r(U)}+\|f\|_{W_{r-1}(U)}\right). \tag{14}$$

Remark 3. For $k=0$, it was proved in [19].

Now we state a general result about the simultaneous approximation of functions by means of a suitable sequence of Lagrange interpolating polynomials, requiring a reduced number of samples of the function we want to approximate. Indeed, by the convergence results about the one-weight interpolation process and the extended one, we have two polynomial sequences $\{L_n(w,f)\}_{n\in\mathbb{N}}$ and $\{L_{2n}(w,\overline{w},f)\}_{n\in\mathbb{N}}$ that, under suitable common assumptions, uniformly converge to $f \in C_U$, with the same speed of convergence. Moreover, in view of (12), after having determined $L_{m+1}(w,f)$, the construction of $L_{2m}(w,\overline{w},f)$ requires only m evaluations of the function f, that can be of interest in approximation methods employing Lagrange polynomial sequences. Thus, for a fixed integer $m>1$, we consider the sequence $L_{m+1}(w,f), L_{2m}(w,\overline{w},f), L_{4m+1}(w,f), L_{8m}(w,\overline{w},f),\ldots$. Thus, for each integer $n \geq 0$, we define the following mixed polynomial sequence $\{\mathcal{L}_{2^n m}(f)\}_n$:

$$\mathcal{L}_{2^n m}(f,x)=\begin{cases} L_{2^n m+1}(w,f,x), & n=0,2,4,\ldots \\ L_{2^n m}(w,\overline{w},f,x), & n=1,3,5,\ldots \end{cases}. \tag{15}$$

About the convergence, we can claim the following

Theorem 3.3. *Under the assumption*

$$\alpha+1 \leq \gamma \leq \frac{\alpha}{2}+\frac{5}{4},$$

for any $f \in W_r(U), r \geq 1$ and $0 \leq k \leq r-1$ we have

$$\|[f-\mathcal{L}_{2^n m}(f)]^{(k)}\varphi^k U\|_\infty \leq \mathcal{C}\frac{\log 2^n m}{(\sqrt{2^n m})^{r-k}}\|f\|_{W_r(U)},$$

where $\mathcal{C} \neq \mathcal{C}(n,m,f)$.

Remark 4. We omit the proof of the previous theorem, since it can be easily deduced by combining the results of Theorems 3.1 and 3.2.

Remark 5. In some cases the sequence (15) can replace the usual sequence $\{L_{2^n+1}(w,f)\}_n$ commonly implemented in the approximation processes, with the considerable advantage of reducing of one third the global number of function evaluations. One application will be proposed in the next Section for the approximation of Hadamard integrals of the type (1). Similar mixed schemes have been employed in the construction of product rules for ordinary integrals in $(-1,1)$ [22] and in $(0,+\infty)$ [26]. We point out that similar constructions can also be implemented for the approximation of functions on the real line, since efficient extended Lagrange interpolating processes have been studied either in uniform norm and in mean weighted norm ([24], [25]).

4 Product integration rules for Hadamard integrals

In what follows we will consider hypersingular integrals defined as the finite part of divergent integrals, in the Hadamard sense. Many properties fulfilled by finite part integrals can be found in [17], [10], [18], [27] in the case of bounded intervals and in [7], [8], [6], [20] in the case of unbounded ones. Let us start by providing sufficient conditions on f to assure the existence of the integral (1). By [5, Th. 3.1], the following result immediately follows

Theorem 4.1. *Let $p \geq 1$, $\gamma \geq 0$. If $f \in W_{p+r}(U)$, $r \in \mathbb{N}, r \geq 1$ then for any $t > 0$*

$$t^p |\mathbf{H}_p(fU,t)| \leq \mathcal{C}\|f\|_{W_{p+r}(U)}, \qquad 0 < \mathcal{C} \neq \mathcal{C}(f,t).$$

Remark 6. The statement of the previous theorem is also valid under weaker assumptions on f, namely assuming f in weighted Zygmund-type spaces of functions.

About the approximation of integrals (1), we recall the following product rule, to whom we refer as the *one-weight product rule*:

$$\mathbf{H}_{p,m+1}(fU,t) = \sum_{k=1}^{j} f(x_k)\mathcal{C}_k(t), \quad \mathcal{C}_k(t) = \oint_0^{+\infty} \frac{4m-x}{4m-x_k}\frac{\ell_{m,k}(w,x)}{(x-t)^{p+1}}U(x)dx, \tag{16}$$

$$e_{p,m+1}(fU,t) = \mathbf{H}_p(fU,t) - \mathbf{H}_{p,m+1}(fU,t), \tag{17}$$

with j defined as in (3). The rule (16) is exact for the polynomials in $\mathcal{P}_m^*$, i.e.

$$e_{p,m+1}(fU,t) = 0, \quad \forall f \in \mathcal{P}_m^*.$$

Regarding the stability and the convergence of the rule (16) the following theorem can be deduced from [9, Th. 3.2]

Theorem 4.2. *For any $t > 0$, if $f \in W_{p+2}(U)$ and α, γ satisfy the assumption*

$$\max\left(0, \frac{\alpha}{2} + \frac{1}{4}\right) \leq \gamma \leq \frac{\alpha}{2} + \frac{5}{4}, \tag{18}$$

we have

$$t^p |\mathbf{H}_{p,m+1}(fU,t)| \leq \mathcal{C}\left(\|f\|_{W_{p+1}(U)} + \frac{\log m}{\sqrt{m}}\|f\|_{W_{p+2}(U)}\right) < \infty,$$

where $0 < \mathcal{C} \neq \mathcal{C}(m,f,t)$. Moreover, if $f \in W_{p+r}(U)$, $r \in \mathbb{N}, r \geq 2$, then we obtain

$$t^p |e_{p,m+1}(fU,t)| \leq \mathcal{C}\frac{\|f\|_{W_{p+r}(U)}}{(\sqrt{m})^{r-1}}\log m, \quad 0 < \mathcal{C} \neq \mathcal{C}(m,f,t). \tag{19}$$

One of the advanyages of this kind of approach is that no derivatives of the density function f are involved, unlike with other procedures require (see [11], [12] for bounded intervals and [4], [8] for unbounded ones.) The same good property is shared by the product integration rule we now propose, which is based on the extended Lagrange interpolating polynomial in (12). By approximating f in (1) by the Lagrange polynomial $L_{2m}(w,\bar{w},f)$, the following *extended product integration rule* can be deduced

$$\mathbf{H}_p(fU,t) = \mathcal{H}_{p,2m}(fU,t) + R_{p,2m}(fU,t), \quad \mathcal{H}_{p,2m}(fU,t) = \sum_{k=1}^{j}(f(x_k)\mathcal{A}_k(t) + f(y_k)\mathcal{B}_k(t)) \tag{20}$$

$$\mathcal{A}_k(t) = \frac{1}{p_{m-1}(\overline{w},x_k)(4m-x_k)}\oint_0^{+\infty} p_{m-1}(\overline{w},x)(4m-x)\frac{\ell_{m,k}(w,x)}{(x-t)^{p+1}}U(x)dx, \tag{21}$$

$$\mathcal{B}_k(t) = \frac{1}{p_m(w,y_k)(4m-y_k)}\oint_0^{+\infty} p_m(w,x)(4m-x)\frac{\ell_{m-1,k}(\overline{w},x)}{(x-t)^{p+1}}U(x)dx. \tag{22}$$

By definition of $L_{2m}(w,\bar{w},f)$, the rule is exact for any polynomial $P \in \mathcal{P}_{2m-1}^*$, $\mathcal{P}_{2m-1}^*$ being defined in (8). Moreover, performing its construction after that of the one- weight rule (16), only additional j function' evaluation are required. This allows to double the degree, by using only half new samples of f. About the stability and the convergence of the rule (20), we can claim the following

Theorem 4.3. *For any $t > 0$, if $f \in W_{p+2}(U)$, and α, γ satisfy*

$$\alpha + 1 \le \gamma \le \alpha + 2 \tag{23}$$

then

$$t^p |\mathcal{H}_{p,2m}(fU, t)| < \infty. \tag{24}$$

Moreover, assuming $f \in W_{p+r}(U)$, $r \in \mathbb{N}, r \ge 2$ one has

$$t^p |R_{p,2m}(fU, t)| \le \mathcal{C} \frac{\|f\|_{W_{p+r}(U)}}{(\sqrt{m})^{r-1}} \log m, \tag{25}$$

where $0 < \mathcal{C} \ne \mathcal{C}(m, f, t)$.

At first we observe that if the computation of $\mathcal{H}_{p,2m}(fU, t)$ follows that of $\mathbf{H}_{p,m+1}(fU, t)$, only j new function evaluations are needed, i.e. the degree of approximation is doubled by using the half number of required samples of f. Moreover, as we will show in the Section *Computational details* the coefficients of the product rules (16) and (20) are closely connected, since the latter can be obtained from the first.

By exploiting these properties, we now propose a mixed scheme of product rules, in order to obtain a significant saving in the approximation process of $\mathbf{H}_p(fU)$. Let $\{\mathcal{L}_{2^n m}(f)\}_n$ be the polynomial sequence defined in (15). By approximating the function f in $\mathbf{H}_p(fU)$ by the sequence $\{\mathcal{L}_{2^n m}(f)\}_n$, i.e.

$$\mathbf{H}_p(fU, t) = \,=\!\!\!\!\!\!\int_0^{+\infty} \frac{\mathcal{L}_{2^n m}(f, x)}{(x-t)^{p+1}} U(x)dx + R^{(p)}_{2^n m}(f, t) =: \mathcal{T}^{(p)}_{2^n m}(f, t) + R^{(p)}_{2^n m}(f, t), \tag{26}$$

define the sequence $\{\mathcal{T}^{(p)}_{2^n m}(f, t)\}_n$ as

$$\mathcal{T}^{(p)}_{2^n m}(f, t) = \begin{cases} \mathbf{H}_{p,2^n m+1}(fU, t), & n = 0, 2, 4, \dots \\ \\ \mathcal{H}_{p,2^n m}(fU, t), & n = 1, 3, 5, \dots \end{cases} \tag{27}$$

In the next theorem we state conditions assuring that the rule (26) is stable and that the sequence $\{\mathcal{T}^{(p)}_n(f, t)\}_n$ converges pointwise to $\mathbf{H}_p(fU, t)$.

Indeed, the following result about the stability and the convergence of the mixed sequence holds true

Theorem 4.4. *Under the assumptions $-1 < \alpha \le \frac{1}{2}$ and*

$$\alpha + 1 \le \gamma \le \frac{\alpha}{2} + \frac{5}{4}, \tag{28}$$

for any $f \in W_{p+2}(U)$ we get

$$t^p |\mathcal{T}^{(p)}_{2^n m}(fU, t)| < \infty. \tag{29}$$

Moreover, if $f \in W_{p+r}(U)$, $r \in \mathbb{N}, r \ge 2$, then

$$t^p |\mathbf{H}_p(fU, t) - \mathcal{T}^{(p)}_{2^n m}(fU, t)|| \le \mathcal{C} \frac{\|f\|_{W_{p+r}(U)}}{(\sqrt{2^n m})^{r-1}} \log(2^n m), \tag{30}$$

where $0 < \mathcal{C} \ne \mathcal{C}(f, t, n, m)$.

From the previous result we can conclude that when the assumptions of the Theorem 4.4 hold, the sequence $\{\mathcal{T}^{(p)}_{2^n m}(fU, t)\}_n$ can replace the commonly implemented sequence $\{\mathbf{H}_{p,2^n m+1}(fU, t)\}_n$, since they have the same rate of convergence. Moreover, a suitable algorithm for generating odd elements of the mixed sequence with the reuse of the samples employed in the even ones, allows to save one third w.r.t. the function evaluations necessary in computing corresponding elements of the sequence $\{\mathbf{H}_{p,2^n m+1}(fU, t)\}_n$.

5 Computational details and numerical tests

First we provide some details for computing the coefficients of the rules (16), (20). Indeed, as it is known, a large effort in the construction of product integration rules is due to the "exact" computation of the coefficients. Usually in the case of the one-weight product rule (16) the coefficients have been computed via modified moments. To be more precise, recalling the following expressions of the fundamental Lagrange polynomials

$$\ell_{m,k}(w, x) = \lambda_{m,k}(w) \sum_{i=0}^{m-1} p_i(w, x) p_i(w, x_k), \quad k = 1, 2, \dots, m, \tag{31}$$

the coefficients $\{\mathcal{C}_k(t)\}_{k=1}^{j}$ in (16) take the form

$$\mathcal{C}_k(t) = \frac{\lambda_{m,k}(w)}{(4m - x_k)} \sum_{i=0}^{m-1} p_i(w, x_k) \mathbf{H}_p((4m - \cdot) p_i(w) U, t),$$

where $\{\mathbf{H}_p((4m-\cdot)p_i(w)U,t)\}_{i=0}^{j}$ are the *Modified Moments* (MMs) w.r.t. the hypersingular kernel $k(x,t):=\frac{1}{(x-t)^{p+1}}$ and $\{\lambda_{m,k}(w)\}_{k=1}^{m}$ are the coefficients of the m−th Gauss-Laguerre rule. Since in [9] suitable recurrence relations for the modified moments were determined, we focus our attention on the computation of the coefficients in the rule (20), i.e. $\{\mathcal{A}_k,\mathcal{B}_k\}_{k=1}^{j}$.

In view of (31) and

$$\ell_{m-1,k}(\overline{w},x)=\lambda_{m-1,k}(\overline{w})\sum_{i=0}^{m-2}p_i(\overline{w},x)p_i(\overline{w},y_k),\quad k=1,2,\dots,m-1,$$

we have

$$\mathcal{A}_k(t) = \frac{\lambda_{m,k}(w)}{(4m-x_k)p_{m-1}(\overline{w},x_k)}\sum_{i=0}^{m-1}p_i(w,x_k)\mathbf{H}_p((4m-\cdot)p_i(w)p_{m-1}(\overline{w})U,t) \tag{32}$$

$$\mathcal{B}_k(t) = \frac{\lambda_{m-1,k}(\overline{w})}{(4m-y_k)p_m(w,y_k)}\sum_{i=0}^{m-2}p_i(\overline{w},y_k)\mathbf{H}_p((4m-\cdot)p_i(\overline{w})p_m(w)U,t). \tag{33}$$

Denoting by $M_{i,k}(t)$ the *Generalized Modified Moments* (GMMs) w.r.t. $k(x,t)$, i.e.

$$M_{i,k}(t)=\int_0^{+\infty}\frac{p_i(w,x)p_k(\overline{w},x)}{(x-t)^{p+1}}U(x)dx,\quad i=0,1,\dots,k=0,1,\dots$$

$(M_{i,k}(t)\neq M_{k,i}(t))$, the coefficients $\mathcal{A}_k,\mathcal{B}_k$ take the form

$$\mathcal{A}_k(t) = \frac{\lambda_{m,k}(w)}{(4m-x_k)p_{m-1}(\overline{w},x_k)}\sum_{i=0}^{m-1}p_i(w,x_k)\big((4m-b_{m-1}(\overline{w}))M_{i,m-1}(t)-a_m(\overline{w})M_{i,m}(t)-a_{m-1}(\overline{w})M_{i,m-2}(t)\big) \tag{34}$$

$$\mathcal{B}_k(t) = \frac{\lambda_{m-1,k}(\overline{w})}{(4m-y_k)p_m(w,y_k)}\sum_{i=0}^{m-2}p_i(\overline{w},y_k)\big((4m-b_m(w))M_{m,i}(t)-a_{m+1}(w)M_{m+1,i}(t)-a_m(w)M_{m-1,i}(t)\big), \tag{35}$$

where a_i, b_i are the coefficients of the *three term recurrence relation* for the orthonormal Laguerre polynomials

$$\begin{aligned} p_1(w,x)=0,\qquad & p_0(w,x)=\frac{1}{\sqrt{\Gamma(\alpha+1)}},\\ a_{i+1}(w)p_{i+1}(w,x) \;=\; & (x-b_i(w))p_i(w,x)-a_i(w)p_{i-1}(w,x)\\ a_i(w)=\sqrt{i(i+\alpha)},\qquad & b_i(w)=2i+\alpha+1. \end{aligned} \tag{36}$$

Assuming that the ordinary modified moments have been determined by the procedure described in [9], we show how to compute the GMMs starting from them. To be more precise denoting by $\{M_i(w)^{(p)}\}_{i=0}^{2m}$ the ordinary modified moments (MMs) w.r.t the kernel $k(x,t)$ and weights w, i.e.

$$M_i(w,t)^{(p)}=:M_i(w,t)=\int_0^{+\infty}\frac{p_i(w,x)}{(x-t)^{p+1}}U(x)dx,\quad i=0,1,\dots,$$

we give the algorithm for determining the GMMs.

Algorithm

Initialization: $\{M_{i,-1}(t)=0\}_{i=0}^{2m-1}$, $\{M_{i,0}(t)=p_0(\overline{w})M_i(w,t)\}_{i=0}^{2m-1}$;

for $0\le i\le 2m-1$, $0\le k\le 2m-1-i$

$$M_{i,k}(t)=\frac{1}{a_i(w)}\big(a_{k+1}(\overline{w})M_{i-1,k+1}(t)+a_{k-1}(\overline{w})M_{i-1,k-2}(t)+(b_k(\overline{w})-b_{i-1}(w))M_{i-1,k}(t)-a_{i-1}(w)M_{i-2,k}(t)\big).$$

Now we propose some numerical tests, to show the performance of the mixed sequence (27) w.r.t. the one-weight sequence (16). In each test we report the approximate values of the integral by means of the one-weight rule (**OWR**) and by the corresponding mixed sequence (**MixSeq**), for increasing values of n. Moreover, we specify the effective number # *f eval.* of function evaluations, corresponding to **OWR** and **MixSeq** in consequence of the truncation. We point out that all the computations have been performed in double-machine precision ($eps_D\approx 2.22044e-16$), except the routine for GMMs, performed in quadruple arithmetic precision in view of the mild instability of the algorithm.

Moreover, we will use the following definition of the truncation index (see [2, p. 781])

$$j=\min_{k=1,\dots,m}\left\{k\ :\ \lambda_{m,k}(w)<eps_D\right\}, \tag{37}$$

taking into account that $\lambda_{m,k}(w)\sim\Delta x_{m,k}w(x_k)$. The above definition is equivalent to (3) in the sense that there exists a $\theta\in(0,1)$ s.t. $x_{j-1}<4m\theta<x_j$, where j is defined in (37). To have an idea of the percentage of the knots involved in the truncation process, depending on the choice of θ, see [21].

Finally, we point out that the exponent α of the weight w will be selected according to

$$2\gamma - \frac{5}{2} \le \alpha \le \gamma - 1, \tag{38}$$

deduced by (28).

Example 1 Consider the integral

$$\mathbf{H}_0(fU,t) = \fint_0^{+\infty} \frac{\sinh(\frac{x}{8})|x-0.5|^{\frac{9}{2}}}{(x-t)} x^{\frac{3}{2}} e^{-x} dx,$$

where $\gamma = 1.5$, $p = 0$ and $f(x) = \sinh(\frac{x}{8})|x-0.5|^{\frac{9}{2}} \in W_4(U)$, then, according to (25), choosing $\alpha = 0.5$, the error behaves like $m^{-\frac{3}{2}}$. Thus, for $m = 1280$ we can expect 4 exact digits, even if the table shows much better numerical results. We observe, in addition, that the extended rule, besides the saving in the number of function computation, produces better results w. r.t the OPR.

Results		$t = 0.001$		
m	#	OWR	#	MixSeq.
33	32	$7.222685e+1$	32	$7.222685e+1$
64	47	$7.22268552e+1$	31	$7.2226855e+1$
129	67	$7.22268552e+1$	67	$7.22268552e+1$
256	95	$7.2226855260e+1$	63	$7.2226855260e+1$
513	134	$7.2226855260e+1$	134	$7.2226855260e+1$
1024	189	$7.2226855260e+1$	124	$7.22268552602e+1$

Results		$t = 1.5$		
m	#	OWR	#	MixSeq.
9	9	$9.49e+1$	9	$9.49e+1$
16	16	$9.49777e+1$	10	$9.497e+1$
33	32	$9.49777e+1$	32	$9.49777e+1$
64	47	$9.497777e+1$	31	$9.4977777e+1$
129	67	$9.4977777e+1$	67	$9.4977777e+1$
256	95	$9.49777778e+1$	66	$9.4977777813e+1$
513	134	$9.497777781e+1$	134	$9.497777781e+1$
1024	189	$9.497777781e+1$	126	$9.497777781811e+1$

Results		$t = 15$		
m	#	OWR	#	MixSeq.
9	9	$2.24e+3$	9	$2.24e+3$
16	16	$2.248551e+3$	10	$2.2485e+3$
33	32	$2.24855125e+3$	32	$2.24855125e+3$
64	47	$2.248551257e+3$	31	$2.2485512578e+3$
129	67	$2.2485512578e+3$	67	$2.2485512578e+3$
256	95	$2.2485512578e+3$	66	$2.2485512578e+3$
513	134	$2.248551257863e+3$	134	$2.248551257863e+3$
1024	189	$2.248551257863e+3$	124	$2.248551257863e+3$

Table 1: Example 1, for $t = 0.001, 1.5, 15$

Example 2

$$\mathbf{H}_1(fU,t) = \fint_0^{+\infty} \frac{\sin(x+5)}{(x-t)^2} \sqrt{x} e^{-x} dx,$$

where $\gamma = 0.5$, $p = 1$ and $f(x) = \sin(x+5)$. We have $f \in W_r(U), \forall r$, then, according to (25), choosing $\alpha = -0.5$, we expect a fast convergence, confirmed by the numerical results in Table 1.

Example 3

$$\mathbf{H}_2(fU,t) = \fint_0^{+\infty} \frac{x}{(5+x^2)(x-t)^3} x^{\frac{3}{2}} e^{-x} dx,$$

where $\gamma = 1.5$, $p = 2$ and $f(x) = \frac{x}{5+x^2}$. We have $f \in W_r(U), \forall r$, thus, according to (25), choosing $\alpha = 0.5$, a fast convergence is expected. However, the numerical results indicate a poor convergence order which may be explained by very large numbers of the seminorm $\|f^{(r)}\varphi^r U\|$.

Results		$t=0.5$		
m	#	OWR	#	MixSeq.
9	9	1.7	9	1.7
16	16	1.79	10	1.788473
33	25	1.78847	25	1.78847
64	35	1.7884716362	24	1.788471636285
129	50	1.7884716362853	50	1.7884716362853
256	68	1.7884716362853	48	1.7884716362853
Results		$t=5$		
m	#	OWR	#	MixSeq.
9	9	$6.e-2$	9	$6.e-2$
16	16	$6.e-2$	10	$6.976e-2$
33	25	$6.9766e-2$	25	$6.9766e-2$
64	35	$6.97661977219e-2$	24	$6.976619772188e-2$
129	50	$6.976619772188e-2$	50	$6.976619772188e-2$
256	68	$6.976619772188e-2$	48	$6.9766197721883e-2$
Results		$t=10$		
m	#	OWR	#	MixSeq.
9	9	$-1.1e-4$	9	$-1.1e-4$
16	16	$5.e-4$	10	$5.3e-4$
33	25	$5.352e-4$	25	$5.352e-4$
64	35	$5.3523475769e-4$	24	$5.35234757699e-4$
129	50	$5.352347576998e-4$	50	$5.352347576998e-4$
256	68	$5.352347576998e-4$	48	$5.352347576998e-4$

Table 2: Example 2, for $t=0.5,5,10$

Example 4

$$\mathbf{H}_0(fU,t) = \fint_0^{+\infty} \frac{e^{-\sqrt{x}}}{(x-t)} x^{\frac{3}{2}} e^{-x} dx,$$

where $\gamma=1.5$, $p=0$ and $f(x)=e^{-\sqrt{x}} \in W_4(U)$, then, according to (25), choosing $\alpha=0.5$, the error behaves like $m^{-\frac{3}{2}}$. Thus, for $m=1024$ we can have 4 exact digits but the numerical results displayed in Table 4 suggest that the accuracy can be higher.

Final remark As the Tables show, it seems that the extended product rule converges a little bit faster than the OWRA. As conjectured in [26] for the case of the ordinary product rule, the better performance of the extended rule depends on the greater number of quadrature nodes belonging to the truncated interval $(0,4m\theta)$.

6 The Proofs

Proof of Theorem 3.2. By arguments similar to those used in the proof of [7, Th.2.3] and taking into account the assumption on α,γ, we get

$$\|(f-L_{2m}(w,\overline{w},f))^{(k)}\varphi^k U\| \quad \le \mathcal{C}\left(m^{\frac{k}{2}}\log m E_M(f)_U + E_{2m-k}(f^{(k)})_{U\varphi^k} + e^{-Am}\|fU\|\right)$$

with $M=\left\lfloor (2m-1)\left(\frac{\theta}{1+\theta}\right)\right\rfloor$. Then, since by (10)

$$E_M(f)_U \le \mathcal{C}\frac{E_{M-k}(f^{(k)})_{U\varphi^k}}{(\sqrt{m})^k},$$

we have

$$\|(f-L_{2m}(w,\overline{w},f))^{(k)}\varphi^k U\| \quad \le \quad \mathcal{C}\left(\log m E_{M-k}(f^{(k)})_{U\varphi^k} + e^{-Am}\|fU\|\right),$$

and taking into account (11), under the assumption $f\in W_{r+1}(U)\equiv f^{(k)}\in W_{r+1-k}(U)$, the theorem is completely proven. □

Proof of Theorem 4.3. First we prove (24). By definition $\mathcal{H}_{p,2m}(fU,t)=\mathbf{H}_p(L_{2m}(w,\bar{w},f)U,t)$ and by using Theorem 4.1, it follows that

$$t^p|\mathcal{H}_{p,2m}(fU,t)| \le \mathcal{C}\|L_{2m}(w,\bar{w},f)\|_{W_{p+1}(U)}.$$

Then, taking into account the assumptions (23), by (14) we can conclude

$$t^p|\mathcal{H}_{p,2m}(fU,t)| \le \mathcal{C}\frac{\log m}{\sqrt{m}}\|f\|_{W_{p+2}(U)} + \|f\|_{W_{p+1}(U)} < \infty.$$

Results		$t = 0.001$		
m	#	OWR	#	MixSeq.
17	17	$3.e-1$	17	$3.e-1$
32	25	$3.2e-1$	24	$3.2e-1$
65	35	$3.236e-1$	35	$3.236e-1$
128	50	$3.2363613e-1$	48	$3.2363613e-1$
257	70	$3.236361328e-1$	70	$3.236361328e-1$
512	99	$3.236361328e-1$	97	$3.236361328e-1$
Results		$t = 1.5$		
m	#	OWR	#	MixSeq.
17	17	$3.9e-2$	17	$3.9e-2$
32	25	$3.94e-2$	24	$3.94e-2$
65	35	$3.949e-2$	35	$3.9491028e-2$
128	50	$3.9491028e-2$	48	$3.9491028e-2$
257	70	$3.949102877e-2$	70	$3.949102877e-2$
512	99	$3.94910287739e-2$	97	$3.94910287739e-2$
Results		$t = 15$		
m	#	OWR	#	MixSeq.
17	17	$-1.-4$	17	$-1.e-4$
32	25	$-1.8e-4$	24	$-1.8e-4$
65	35	$-1.7993e-4$	35	$-1.79935e-4$
128	50	$-1.7993501e-4$	48	$-1.799350113e-4$
257	70	$-1.79935011316e-4$	70	$-1.79935011316e-4$
512	99	$-1.79935011316e-4$	97	$-1.79935011316e-4$

Table 3: Example 3, for $t = 0.001, 1.5, 15$

To prove (25), by Theorem 4.1 again,

$$t^p |R_{p,2m}(fU,t)| = t^p \, |\mathbf{H}(f - L_{2m}(w,\bar{w},f)U,t)| \leq \mathcal{C} \|f - L_{2m}(w,\bar{w},f)\|_{W_{p+1}(U)}$$

and by (13), (25) follows. □

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Results		$t = 0.001$		
m	#	OWR	#	MixSeq.
9	5	$3.1e-1$	5	$3.1e-1$
16	10	$3.19e-1$	10	$3.19e+1$
33	16	$3.19e-1$	16	$3.19e-1$
65	24	$3.195e-1$	24	$3.195e-1$
129	34	$3.1954e-1$	34	$3.1954e-1$
256	48	$3.1954e-1$	48	$3.1954e-1$
513	68	$3.19544e-1$	68	$3.19544e-1$
1024	95	$3.19544e-1$	85	$3.19544e-1$

Results		$t = 1.5$		
m	#	OWR	#	MixSeq.
33	16	$-5.7e-2$	16	$-5.7e-2$
64	24	$-5.76e-2$	23	-5.766e-2
129	34	$-5.76e-2$	34	$-5.76e-2$
256	48	$-5.766e-2$	48	$-5.7666e-2$
513	68	$-5.7666e-2$	68	$-5.7666e-2$
1024	95	$-5.7666e-2$	95	$-5.76663e-2$

Results		$t = 15$		
m	#	OWR	#	MixSeq.
9	5	$-2.5e-2$	5	$-2.5e-2$
16	10	$-2.5e-2$	10	$-2.5e-2$
33	16	$-2.53e-2$	16	$-2.53e-2$
64	24	$-2.53e-2$	23	-2.53e-2
129	34	$-2.5309e-2$	34	$-2.5309e-2$
256	48	$-2.53091e-2$	48	$-2.53091e-2$
513	68	$-2.53091e-2$	68	$-2.53091e-2$
1024	95	$-2.53091e-2$	95	$-2.53091e-2$

Table 4: Example 4, for $t = 0.001, 1.5, 15$

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