Applied Numerical Mathematics 200 (2024) 309–317

Contents lists available at ScienceDirect

Applied Numerical Mathematics

journal homepage: www.elsevier.com/locate/apnum

Computing integrals with an exponential weight on the real axis in floating point arithmetic

Teresa Laudadio [a,*], Nicola Mastronardi [a,*], Donatella Occorsio [b,c]

[a] Istituto per le Applicazioni del Calcolo "M. Picone", Consiglio Nazionale delle Ricerche, Bari, Italy
[b] Department of Mathematics, Computer Science and Economics, University of Basilicata, Potenza, Italy
[c] Istituto per le Applicazioni del Calcolo "M. Picone", Consiglio Nazionale delle Ricerche, Napoli, Italy

ARTICLE INFO

Article history:
Received 12 December 2022
Received in revised form 28 May 2023
Accepted 30 May 2023
Available online 2 June 2023

Keywords:
Gaussian quadrature rules
Golub and Welsch algorithm
Singular Value Decomposition
Product integration rules

ABSTRACT

The aim of this work is to propose a fast and reliable algorithm for computing integrals of the type

$$\int_{-\infty}^{\infty} f(x)e^{-x^2-\frac{1}{x^2}}dx,$$

where $f(x)$ is a sufficiently smooth function, in floating point arithmetic. The algorithm is based on a product integration rule, whose rate of convergence depends only on the regularity of f, since the coefficients of the rule are "exactly" computed by means of suitable recurrence relations here derived. We prove stability and convergence in the space of locally continuous functions on $\mathbb{R}$ equipped with weighted uniform norm. By extensive numerical tests, the accuracy of the proposed product rule is compared with that of the Gauss–Hermite quadrature formula w.r.t. the function $f(x)e^{-\frac{1}{x^2}}$. The numerical results confirm the effectiveness of the method, supporting the proven theoretical estimates.

1. Introduction

The present paper deals with the computation of integrals

$$\int_{-\infty}^{\infty} f(x)\tilde{w}(x)dx, \tag{1}$$

where $\tilde{w}(x)=e^{-x^2-\frac{1}{x^2}}$ is a combination of the Pollaczek-type weight $e^{-\frac{1}{x^2}}$ and the Hermite weight e^{-x^2}, and f is a "smooth" function.

A straightforward approach to compute an approximation of (1) is to consider the Gauss quadrature rule (GQR) with weight function $w(x)=e^{-x^2}$ and integrand function $e^{-\frac{1}{x^2}}f(x)$. Unfortunately, the presence of the factor $e^{-\frac{1}{x^2}}$ as part of the

* Corresponding authors.
E-mail addresses: teresa.laudadio@cnr.it (T. Laudadio), nicola.mastronardi@cnr.it (N. Mastronardi), donatella.occorsio@unibas.it (D. Occorsio).

https://doi.org/10.1016/j.apnum.2023.05.025
0168-9274/

integrand function strongly reduces the convergence rate of GQR. On the other hand, the computation of integrals (1) is of interest in numerical methods for integral equations, which in turn are model for many applications arising in applied sciences. As an example, integral equations with the same weight function $\tilde{w}$, but extended to the positive real semiaxis, model some mathematical financial problems [7]. Approximation properties related to Pollaczek–Laguerre weights of the type $W(x) = x^\gamma e^{-x^\beta - \frac{1}{x^\alpha}}$ on the positive semiaxis, have been extensively studied in [11,12,15,16]. In particular in [5,6,11] the authors proposed a Gaussian quadrature rule for approximating integrals on the positive semiaxis with a Pollaczek–Laguerre weight and only with the use of the extended precision they were able to overcome the numerical instability in computing the corresponding zeros and weights [6, p. 230]. Such instability occurs only in computing the zeros and the coefficients of the Gaussian rule for a non standard weight, in applying the Chebyshev method of moments, and does not affect the stability of the Gaussian rule and the related methods considered there. Here, we deal with the Pollaczek–Hermite weight $\tilde{w}(x) = e^{-x^2 - \frac{1}{x^2}}$ proposing a fast and reliable algorithm for the efficient computation of integrals on $\mathbb{R}$ of type (1) without using extended precision. The product integration rule we propose is based on the approximation of f by means of a "truncated" Lagrange polynomial interpolating f, and hence on the exact computation of the rule coefficients, by means of suitable recurrence relations here derived. In view of the truncation, the rule requires a reduced number of function evaluations. Moreover, for functions f belonging to suitable spaces of locally continuous functions, endowed with weighted uniform norm, we prove the rule is stable and convergent. Since we will prove that the quadrature error has the same behavior of the best polynomial approximation of f, the more regular f is, the faster the convergence of the product rule is.

The paper is organized as follows. In Section 2 the main features of the Hermite polynomials are described. Section 3 is devoted to function spaces and to Lagrange interpolation processes associated to the considered product rule. In Section 4 the construction of the proposed product rule is described.

A number of numerical examples, confirming the stability properties of the proposed method, is provided in Section 5, followed by the proofs of the theorems stated in Section 6. The paper ends with the concluding remarks.

2. Computing the zeros of orthogonal polynomials

Let $\mathcal{H}_\ell(x) = k_\ell x^\ell + \sum_{j=0}^{\ell-1} c_j x^j$, $\ell = 0, 1, \ldots$, be the sequence of orthonormal Hermite polynomials with respect to the weight function $w(x) = e^{-x^2}$ in the interval $(-\infty, \infty)$, i.e.,

$$\int_{-\infty}^{\infty} \mathcal{H}_i(x)\mathcal{H}_j(x)w(x)dx = \delta_{ij}, \quad \text{with} \quad \delta_{ij} = \begin{cases} 1, & \text{if } i = j, \\ 0, & \text{if } i \neq j, \end{cases}$$

where $k_\ell, c_j \in \mathbb{R}$, $j = 0, 1, \ldots, \ell - 1$, and $k_\ell > 0$. Polynomials $\mathcal{H}_\ell(x)$ satisfy the following three–term recurrence relation [20]

$$\begin{cases} \mathcal{H}_{-1}(x) = 0, \\ \mathcal{H}_0(x) = k_0 = \sqrt[4]{\frac{1}{\pi}}, \\ \beta_{\ell+1}\mathcal{H}_{\ell+1}(x) = x\mathcal{H}_\ell(x) - \beta_\ell \mathcal{H}_{\ell-1}(x), \ \ \ell \geq 0, \end{cases} \tag{2}$$

where

$$\beta_0 = 0, \quad \beta_\ell = \frac{k_\ell}{k_{\ell-1}} = \sqrt{\frac{\ell}{2}}, \quad \ell = 1, 2, \ldots. \tag{3}$$

Using (2), we can write the n-step recurrence relation

$$J\mathbf{h}(x) = x\mathbf{h}(x) - \beta_n \mathcal{H}_n(x)\mathbf{e}_n,$$

where

$$J = \begin{bmatrix} 0 & \beta_1 & & & \\ \beta_1 & 0 & \beta_2 & & \\ & \beta_2 & \ddots & \ddots & \\ & & \ddots & 0 & \beta_{n-1} \\ & & & \beta_{n-1} & 0 \end{bmatrix}, \quad \mathbf{h}(x) = \begin{bmatrix} \mathcal{H}_0(x) \\ \mathcal{H}_1(x) \\ \vdots \\ \mathcal{H}_{n-2}(x) \\ \mathcal{H}_{n-1}(x) \end{bmatrix}. \tag{4}$$

The matrix J is called Jacobi matrix [2]. The following theorem was proved in [2, Th. 1.31].

Theorem 2.1. *Let $J = QXQ^T$ be the spectral decomposition of J, where $X \in \mathbb{R}^{n\times n}$ is a diagonal matrix and*

$$\boldsymbol{x} := \mathrm{diag}(X) = [x_1, \dots, x_n]^T, \quad x_1 < x_2 < \cdots < x_n,$$

and $Q \in \mathbb{R}^{n\times n}$ is an orthogonal matrix, i.e., $Q^TQ = I_n$. Then $\mathcal{H}_n(x_i) = 0,\ i = 1, \dots, n$, and $Q = VD$, with

$$V = [\mathbf{h}(x_1), \mathbf{h}(x_2), \dots, \mathbf{h}(x_n)], \quad D = \begin{bmatrix} \hat{w}_1 & & & \\ & \hat{w}_2 & & \\ & & \ddots & \\ & & & \hat{w}_n \end{bmatrix}, \tag{5}$$

and

$$\hat{w}_i = \frac{1}{\|\mathbf{h}(x_i)\|_2} = \frac{1}{\sqrt{\sum_{\ell=0}^{n-1} \mathcal{H}_\ell^2(x_i)}}.$$

The eigenvalues $x_i,\ i = 1, 2, \dots, n$, are the nodes of GQR and the corresponding weights w_i are defined as (see [20])

$$w_i := w_i(x_i) = \hat{w}_i^2 = \frac{1}{\sum_{\ell=0}^{n-1} \mathcal{H}_\ell^2(x_i)}, \qquad i = 1, \dots, n. \tag{6}$$

As shown in [21], the weights can be also obtained by the first row of Q as

$$w_i = \mu_0 q_{1,i}^2, \qquad i = 1, \dots, n, \tag{7}$$

where $\mu_0 = \int_{\mathbb{R}} e^{-x^2} dx$. The Golub and Welsch algorithm [3], relying on a modification of the QR–method [1], yields the nodes and the weights of GQR by computing only the eigenvalues of the Jacobi matrix and the first row of the associated eigenvector matrix.

A different way to compute the weights of GQR in a stable manner has been described in [8].

3. Function spaces and Lagrange interpolation processes

From now on, $\mathcal{C}$ will denote any positive constant having different meanings at different occurrences and the writing $\mathcal{C} \neq \mathcal{C}(a, b, ..)$ means that $\mathcal{C}$ does not depend on $a, b, \dots$

For a fixed $\delta \in \mathbb{R}^+$ let $w_\delta(x) = \sqrt{w(x)}(1 + |x|)^\delta$. Let us introduce the space C_{w_δ} defined as

$$C_{w_\delta} = \left\{ f \in C^0(\mathbb{R}) : \lim_{x\to\pm\infty} f(x) w_\delta(x) = 0 \right\},$$

equipped with the norm

$$\|f\|_{w_\delta} = \|f w_\delta\|_\infty = \sup_{x\in\mathbb{R}} |f(x) w_\delta(x)|.$$

Denoting by

$$E_n(f)_{w_\delta} := \inf_{P_n \in \mathbb{P}_n} \|(f - P_n) w_\delta\|_\infty, \tag{8}$$

the error of best polynomial approximation of $f \in C_{w_\delta}$, it can be proved that

$$\lim_{n\to\infty} E_n(f)_{w_\delta} = 0 \iff f \in C_{w_\delta},$$

[9] (see, e.g. [17, p. 275–276]). Note that functions in C_{w_δ} can grow exponentially as $|x| \to \infty$. For smoother functions, let us consider the following Sobolev subspaces of C_{w_δ}

$$W^r(w_\delta) = \left\{ f \in C_{w_\delta} :\ f^{(r-1)} \in AC(\mathbb{R}), \|f^{(r)} w_\delta\|_\infty < \infty \right\}, \quad r \in \mathbb{N},\ r \geq 1,$$

where $AC(\mathbb{R})$ denotes the set of all functions which are absolutely continuous on every closed subset of $\mathbb{R}$. Such spaces are equipped with the norm

$$\|f\|_{W^r(w_\delta)} = \|f w_\delta\|_\infty + \|f^{(r)} w_\delta\|_\infty.$$

For $f \in W^r(w_\delta)$, we recall that the following estimate holds [18,19,13]

$$E_n(f)_{w_\delta} \le \mathcal{C} \, \frac{\|f\|_{W^r(w_\delta)}}{(\sqrt{n})^r}, \quad \mathcal{C} \ne \mathcal{C}\,(n, f). \tag{9}$$

Let $\{x_k\}_{k=1}^n$ be the zeros of $\mathcal{H}_n$ and, for a fixed $0 < \theta < 1$, let $j = j(n)$ be the index of the zero of $\mathcal{H}_n$ such that

$$x_j = \min_{k=1,2,\dots,n} \{x_k : x_k > \theta\sqrt{2n}\}. \tag{10}$$

Moreover, let $\mathcal{P}_{n-1}$ the subspace of $\mathbb{P}_{n-1}$ defined as

$$\mathcal{P}_{n-1} := \{P \in \mathbb{P}_{n-1} : P(x_i) = 0, k > j, \text{ and } k < n+1-j\}.$$

Setting $\widetilde{P} \in \mathcal{P}_{n-1}$ the polynomial defined by

$$\|(f - \widetilde{P})w_\delta\|_\infty = \inf_{P \in \mathcal{P}_{n-1}} \|(f - P)w_\delta\|_\infty =: \widetilde{E}_{n-1}(f)_{w_\delta},$$

in [13, Lemma 3.1] (in a more general context) the following estimate was proved

$$\widetilde{E}_{n-1}(f)_{w_\delta} \le \mathcal{C}\left(E_N(f)_{w_\delta} + e^{-\mathcal{B}n}\|f w_\delta\|_\infty\right), \quad \mathcal{C} \ne \mathcal{C}\,(n, f), \tag{11}$$

with $N = \left\lfloor \left(\frac{\theta}{1+\theta}\right)^2 \frac{n}{2} \right\rfloor \sim n$, where $\lfloor \xi \rfloor$ denotes the largest integer not exceeding $\xi \in \mathbb{R}^+$, and $\mathcal{B} \in \mathbb{R}^+, \mathcal{B} \ne \mathcal{B}(n, f)$.

Let $L^1(\mathbb{R})$ be the space of all measurable functions f, equipped with the norm

$$\|f\|_{L^1(\mathbb{R})} = \int_{\mathbb{R}} |f(x)|\,dx,$$

and let $L^\infty(\mathbb{R}) =: C^0$.

3.1. *Truncated Lagrange interpolating polynomial*

For a given function f, with $j = j(n)$, defined in (10), the polynomial

$$\mathcal{L}_{n-1}(w, f, x) = \sum_{k=n-j+1}^{j} \ell_{n,k}(x) f(x_k), \quad \ell_{n,k}(x) = \frac{\mathcal{H}_n(x)}{\mathcal{H}_n'(x_k)(x - x_k)}, \tag{12}$$

is the *truncated Lagrange polynomial* interpolating f [13,14]. $\mathcal{L}_{n-1}(w, f) \in \mathcal{P}_{n-1}$, interpolates f at the zeros $\{x_k\}_{k=n+1-j}^{j} \in (-\theta\sqrt{2n}, \theta\sqrt{2n})$ and vanishes at $\{\{x_k\}_{\{k>j\}\cup\{k<n+1-j\}}\}$. Differently from the ordinary Lagrange polynomial interpolating f on all the zeros of $\mathcal{H}_n(x)$, $\mathcal{L}_{n-1}(w, f)$ is not a projector in $\mathbb{P}_{n-1}$, but it preserves polynomials belonging to the subspace $\mathcal{P}_{n-1}$, i.e., $\mathcal{L}_{n-1}(w, \mathcal{Q}) = \mathcal{Q}, \quad \mathcal{Q} \in \mathcal{P}_{n-1}$.

4. The Product rule

In this section we construct the product rule of interpolation type for computing an approximation of the integral (1). Hence, replacing f by $\mathcal{L}_{n-1}(w, f)$, we obtain the product rule

$$\begin{aligned} \int_{-\infty}^{\infty} \tilde{w}(x)\mathcal{L}_{n-1}(w, f, x)dx &= \sum_{k=n+1-j}^{j} C_k f(x_k) \\ &:= \sum_{k=n+1-j}^{j} f(x_k)\left[w_k \sum_{\ell=0}^{n-1} \mathcal{H}_\ell(x_k) \int_{-\infty}^{\infty} \tilde{w}(x)\mathcal{H}_\ell(x)dx\right] \\ &= \sum_{k=n+1-j}^{j} f(x_k) w_k \sum_{\ell=0}^{n-1} \mathcal{H}_\ell(x_k)\mathcal{M}_\ell, \end{aligned} \tag{13}$$

where, for $\ell = 0, 1, \dots$,

$$\mathcal{M}_\ell = \int_{-\infty}^{\infty} \mathcal{H}_\ell(x)\tilde{w}(x)dx, \tag{14}$$

are the so called *modified moments*.

4.1. Computing the Modified moments $\mathcal{M}_\ell$

In this subsection we construct the recurrence relations for computing the *modified moments* (14). Defining

$$\mathcal{N}_\ell := \int_{-\infty}^{\infty} \frac{\mathcal{H}_\ell(x)}{x^2}\tilde{w}(x)dx, \quad \ell = 0, 1, \dots,$$

the following lemma holds.

Lemma 4.1. *The sequences $\mathcal{M}_\ell$ and $\mathcal{N}_\ell$, $\ell = 0, 1, \dots$ satisfy the following recurrence relations*

$$\begin{cases} \mathcal{M}_0 = \frac{\sqrt[4]{\pi}}{e^2}, \\ \mathcal{M}_\ell = \frac{2-\ell}{\sqrt{\ell(\ell-1)}}\mathcal{M}_{\ell-2} + \frac{2}{\sqrt{\ell(\ell-1)}}\mathcal{N}_{\ell-2}, & \ell = 2, 4, 6, \dots, \\ \mathcal{M}_\ell = 0, & \ell = 1, 3, 5, \dots, \end{cases} \tag{15}$$

$$\begin{cases} \mathcal{N}_0 \quad = \frac{\sqrt[4]{\pi}}{e^2}, \\ \mathcal{N}_{\ell+2} = \frac{2}{\sqrt{(\ell+1)(\ell+2)}}\mathcal{M}_\ell - \left(\sqrt{\frac{\ell}{\ell+1}\frac{\ell}{\ell+2}} + \sqrt{\frac{\ell+1}{\ell+2}}\right)\mathcal{N}_\ell \\ \qquad -\sqrt{\frac{\ell-1}{\ell+1}\frac{\ell}{\ell+2}}\mathcal{N}_{\ell-2}, & \ell = 2, 4, 6, \dots, \\ \mathcal{N}_\ell \quad = 0, & \ell = 1, 3, 5, \dots. \end{cases} \tag{16}$$

4.2. Stability and error estimates

By means of the product rule (13), it is introduced the error

$$e_n(f) := \int_{\mathbb{R}} [f(x) - \mathcal{L}_{n-1}(w, f, x)]\tilde{w}(x)dx, \tag{17}$$

i.e.

$$\int_{\mathbb{R}} f(x)\tilde{w}(x)dx = \sum_{k=n+1-j}^{j} C_k f(x_k) + e_n(f), \tag{18}$$

being the rule exact for $P_{n+1} \in \mathcal{P}_{n+1}$.

Now we state the stability and the convergence of the formula in C_{w_δ}, providing error estimates in the spaces $W_r(w_\delta)$.

Theorem 4.2. *Under the assumption $\delta > \frac{1}{2}$, the rule (13) is stable in C_{w_δ}, i.e.,*

$$\sup_n \sum_{i=1}^{j} \frac{|C_i|}{w_\delta(x_i)} < \infty, \tag{19}$$

and

$$|e_n(f)| \le \mathcal{C}\left(E_N(f)_{w_\delta} + e^{-\mathcal{B}n}\|f w_\delta\|_\infty\right), \tag{20}$$

where $N = \left\lfloor \left(\frac{\theta}{1+\theta}\right)^2 n \right\rfloor \sim n$, and $0 < \mathcal{B} \neq \mathcal{B}(n, f)$, $\mathcal{C} \neq \mathcal{C}(n, f)$.

By combining (20) and (9), the following error estimate follows.

Corollary 4.3. *For any $f \in W^r(w_\delta)$, with $\delta > \frac{1}{2}$, the following error estimate holds*

$$|e_n(f)| \le \mathcal{C}\frac{\|f\|_{W^r(w_\delta)}}{(\sqrt{n})^r}, \quad \mathcal{C} \neq \mathcal{C}(n, f). \tag{21}$$

Table 1
Values of the approximations of the integral (22) obtained TPR and GQR, with $f(x) = \cos(x)$, and Mval $= 8.945397612471845 \times 10^{-2}$.

n	$2j-n$	TPR	$\lvert\frac{\text{TPR}-\text{Mval}}{\text{Mval}}\rvert$	GQR	$\lvert\frac{\text{GQR}-\text{Mval}}{\text{Mval}}\rvert$
8	8	$8.945098794037276 \times 10^{-2}$	3.34×10^{-5}	$6.949412400327926 \times 10^{-2}$	2.23×10^{-1}
16	16	$8.945397611011636 \times 10^{-2}$	1.63×10^{-10}	$9.723435717459904 \times 10^{-2}$	8.70×10^{-2}
32	32	$8.945397612471852 \times 10^{-2}$	6.21×10^{-16}	$8.918619331793731 \times 10^{-2}$	2.99×10^{-3}
64	48	$8.945397612471877 \times 10^{-2}$	3.41×10^{-15}	$8.936154227660445 \times 10^{-2}$	1.03×10^{-3}
128	68	$8.945397612471848 \times 10^{-2}$	1.55×10^{-16}	$8.945089722880344 \times 10^{-2}$	3.44×10^{-5}
256	90	$8.945397612471870 \times 10^{-2}$	2.64×10^{-15}	$8.945673065110885 \times 10^{-2}$	3.08×10^{-5}
512	124	$8.945397612471838 \times 10^{-2}$	9.31×10^{-16}	$8.945401734394182 \times 10^{-2}$	4.61×10^{-7}
1024	166	$8.945397612471874 \times 10^{-2}$	3.10×10^{-15}	$8.945397746086610 \times 10^{-2}$	1.49×10^{-8}
2048	242	$8.945397612471845 \times 10^{-2}$	0.00×10^{0}	$8.945397612351721 \times 10^{-2}$	1.34×10^{-11}
4096	404	$8.945397612471892 \times 10^{-2}$	6.05×10^{-15}	$8.945397612473283 \times 10^{-2}$	1.61×10^{-13}

Table 2
Values of the approximations of the integral (22) obtained applying TPR and GQR, with $f(x) = \arctan(\frac{1+x}{4})$, and Mval $= 5.427697244322335 \times 10^{-2}$.

n	$2j-n$	TPR	$\lvert\frac{\text{TPR}-\text{Mval}}{\text{Mval}}\rvert$	GQR	$\lvert\frac{\text{GQR}-\text{Mval}}{\text{Mval}}\rvert$
8	8	$5.427686729587454 \times 10^{-2}$	1.94×10^{-6}	$5.051927492275927 \times 10^{-2}$	6.92×10^{-2}
16	16	$5.427697240051552 \times 10^{-2}$	7.87×10^{-10}	$5.644085331675656 \times 10^{-2}$	3.99×10^{-2}
32	32	$5.427697244322757 \times 10^{-2}$	7.77×10^{-14}	$5.414250683007876 \times 10^{-2}$	2.48×10^{-3}
64	48	$5.427697244322347 \times 10^{-2}$	2.17×10^{-15}	$5.426208992962754 \times 10^{-2}$	2.74×10^{-4}
128	68	$5.427697244322358 \times 10^{-2}$	4.22×10^{-15}	$5.427544256103390 \times 10^{-2}$	2.82×10^{-5}
256	90	$5.427697244322337 \times 10^{-2}$	2.56×10^{-16}	$5.427767485244951 \times 10^{-2}$	1.29×10^{-5}
512	124	$5.427697244322327 \times 10^{-2}$	1.53×10^{-15}	$5.427698372784009 \times 10^{-2}$	2.08×10^{-7}
1024	166	$5.427697244322347 \times 10^{-2}$	2.17×10^{-15}	$5.427697278329974 \times 10^{-2}$	6.27×10^{-9}
2048	242	$5.427697244322321 \times 10^{-2}$	2.68×10^{-15}	$5.427697244286701 \times 10^{-2}$	6.57×10^{-12}
4096	407	$5.427697244322308 \times 10^{-2}$	4.99×10^{-15}	$5.427697244322690 \times 10^{-2}$	6.53×10^{-14}

5. Numerical Examples

In this section we state the numerical results obtained by approximating integrals

$$I(f) = \int_{-\infty}^{\infty} e^{-x^2 - \frac{1}{x^2}} f(x)dx, \tag{22}$$

for functions f belonging to different spaces of functions. We compare the results achieved by the proposed product rule (TPR) with those obtained by the truncated Gauss–Hermite quadrature rule (GQR) [10], considering e^{-x^2} as the Hermite weight and $g(x) = e^{-\frac{1}{x^2}} f(x)$ as function. In the tables n denotes the number of points involved in TPR and GQR, respectively.

For each test, the approximations of (22) obtained by the two methods, TPR and GQR, for $n = 2^i$, $i = 3, 4, \ldots, 12$, are computed in Matlab R2022a with machine precision $\epsilon \sim 2.22 \times 10^{-16}$ and compared with the value of the integral computed by the function NIntegrate of Mathematica, with a working precision of 500 digits (denoted by Mval), considered as the exact value of the integral. The computed approximations and the corresponding relative errors are reported in the associated tables.

It can be noticed that the ratio $(2j-n)/n$ becomes smaller and smaller as n increases. Therefore, the proposed truncated product rule has a computational cost much smaller than the non truncated one for large n.

Example 5.1. In this example, $f(x) = \cos(x)$ in (22) and Mval $= 8.945397612471845 \times 10^{-2}$. The results are displayed in Table 1. They show that the relative errors of TPR are close to the machine precision with $n \approx 32$, since $\cos(x)$ is a very regular function. About the slow convergence of GQR, we observe that, even though $g(x) := e^{-\frac{1}{x^2}} \cos(x) \in W_r(w_\delta)$ for any $r \geq 1$, the seminorms of g appearing in the error estimates becomes larger and larger as r increases, by slowing down the speed of convergence of GQR. For instance, $\|g\|_{W_r(w_\delta)} \sim 5 \times 10^3$ for $r = 5$, and $\|g\|_{W_r(w_\delta)} \sim 6 \times 10^{11}$ for $r = 10$.

Example 5.2. Here, $f(x) = \arctan\left(\frac{1+x}{4}\right)$ and Mval $= 5.427697244322335 \times 10^{-2}$. The results are displayed in Table 2. Similarly to Example 5.1, the relative errors of TPR are close to the machine precision with $n \approx 32$, being $\arctan\left(\frac{1+x}{4}\right)$ a regular function, while the convergence of GQR is almost linear since it is applied to $h(x) := e^{-\frac{1}{x^2}} \arctan\left(\frac{1+x}{4}\right) \in W_r(w_\delta)$ for any $r \geq 1$, and whose seminorms become larger and larger as r increases, strongly affecting the speed of convergence. For instance, $\|h\|_{W_r(w_\delta)} \sim 2 \times 10^{11}$, for $r = 10$.

Table 3
Values of the approximations of the integral (22) obtained applying TPR and GQR, with $f(x) = |\cos(x)|^{5/4}$, and Mval $=$ $9.105558869283804 \times 10^{-2}$.

n	$2j-n$	TPR	$\lvert\frac{\text{TPR}-\text{Mval}}{\text{Mval}}\rvert$	GQR	$\lvert\frac{\text{GQR}-\text{Mval}}{\text{Mval}}\rvert$
8	8	$9.485235885806660 \times 10^{-2}$	4.17×10^{-2}	$7.301487850488275 \times 10^{-2}$	1.98×10^{-1}
16	16	$9.074650084283779 \times 10^{-2}$	3.39×10^{-3}	$9.863496922603453 \times 10^{-2}$	8.32×10^{-2}
32	32	$9.182616784940598 \times 10^{-2}$	8.46×10^{-3}	$9.162629410875198 \times 10^{-2}$	6.27×10^{-3}
64	48	$9.079166478725698 \times 10^{-2}$	2.90×10^{-3}	$9.070205616732352 \times 10^{-2}$	3.88×10^{-3}
128	68	$9.121947847053928 \times 10^{-2}$	1.80×10^{-3}	$9.121708479806487 \times 10^{-2}$	1.77×10^{-3}
256	90	$9.104913976690782 \times 10^{-2}$	7.08×10^{-5}	$9.105186176595942 \times 10^{-2}$	4.09×10^{-5}
512	124	$9.109013869493021 \times 10^{-2}$	3.79×10^{-4}	$9.109017834749777 \times 10^{-2}$	3.80×10^{-4}
1024	166	$9.104375386675621 \times 10^{-2}$	1.30×10^{-4}	$9.104375504983463 \times 10^{-2}$	1.30×10^{-4}
2048	240	$9.106285825658801 \times 10^{-2}$	7.98×10^{-5}	$9.106285824155236 \times 10^{-2}$	7.98×10^{-5}
4096	404	$9.105641735268770 \times 10^{-2}$	9.10×10^{-6}	$9.105630563127487 \times 10^{-2}$	7.87×10^{-6}

Example 5.3. In this test $f(x) = |\cos(x)|^{5/4}$ and Mval $= 9.105558869283804 \times 10^{-02}$.

The results are displayed in Table 3. The function $|\cos(x)|^{5/4} \in W_1(w_\delta)$ and the speed of convergence of both the rules TPR and GQR is very slow.

6. Proofs

In this section, the proofs of Lemma 4.1 and Theorem 4.2 are outlined.

Proof of Lemma 4.1. Taking into account the three–term recurrence relation (2), we have

$$\beta_\ell \mathcal{M}_\ell = \int_{-\infty}^{\infty} x\mathcal{H}_{\ell-1}(x) e^{-x^2-\frac{1}{x^2}} dx - \beta_{\ell-1}\mathcal{M}_{\ell-2}, \quad \ell \geq 2. \tag{23}$$

Let us now compute the integral in (23). Since [20, p. 106],

$$e^{-x^2}\mathcal{H}_{\ell-1}(x) = -\frac{1}{\sqrt{2(\ell-1)}} \frac{d}{dx}\left(e^{-x^2}\mathcal{H}_{\ell-2}(x)\right), \tag{24}$$

integrating by parts (23) we obtain:

$$\begin{aligned}
\int_{-\infty}^{\infty} x\mathcal{H}_{\ell-1}(x)\tilde{w}(x)dx &= \frac{1}{\sqrt{2(\ell-1)}} \int_{-\infty}^{\infty} \mathcal{H}_{\ell-2}(x)\tilde{w}(x)dx \\
&\quad + \sqrt{\frac{2}{\ell-1}} \int_{-\infty}^{\infty} \frac{\mathcal{H}_{\ell-2}(x)}{x^2}\tilde{w}(x)dx \\
&= \frac{1}{\sqrt{2(\ell-1)}}\mathcal{M}_{\ell-2} + \sqrt{\frac{2}{\ell-1}}\mathcal{N}_{\ell-2}.
\end{aligned}$$

Therefore, the recurrence relation (15) for $\mathcal{M}_\ell$ holds, where the coefficients β_ℓ are given in (3).

To compute the sequence $\mathcal{N}_\ell$, $\ell = 0, 1, 2, \ldots$, we need the following lemma.

Lemma 6.1. *The sequence of even (odd) Hermite polynomials $\mathcal{H}_k(x)$, $k = 0, 2, 4, \ldots$ ($k = 1, 3, 5, \ldots$) satisfies the following three–recurrence relation*

$$\beta_{k+1}\beta_{k+2}\mathcal{H}_{k+2}(x) = \left(x^2 - (\beta_k^2 + \beta_{k+1}^2)\right)\mathcal{H}_k(x) - \beta_{k-1}\beta_k\mathcal{H}_{k-2}(x),$$

Proof. Let us consider (2) evaluated for $k = k+1$ and $k = k-1$, respectively,

$$\mathcal{H}_{k+1}(x) = \frac{\beta_{k+2}\mathcal{H}_{k+2}(x) + \beta_{k+1}\mathcal{H}_k(x)}{x} \tag{25}$$

and

$$\mathcal{H}_{k-1}(x) = \frac{\beta_k\mathcal{H}_k(x) + \beta_{k-1}\mathcal{H}_{k-2}(x)}{x}. \tag{26}$$

Replacing (25) and (26) into (2) for $\ell = k$, we then obtain:

$$\beta_{k+1}\frac{\beta_{k+2}\mathcal{H}_{k+2}(x)+\beta_{k+1}\mathcal{H}_k(x)}{x}+\beta_k\frac{\beta_k\mathcal{H}_k(x)+\beta_{k-1}\mathcal{H}_{k-2}(x)}{x}=x\mathcal{H}_k(x),$$

and thus

$$\beta_{k+1}\beta_{k+2}\mathcal{H}_{k+2}(x)=\left(x^2-(\beta_k^2+\beta_{k+1}^2)\right)\mathcal{H}_k(x)-\beta_{k-1}\beta_k\mathcal{H}_{k-2}(x), \tag{27}$$

i.e., we obtain a three–term recurrence relation for the odd and even polynomials extracted from the sequence $\mathcal{H}_\ell(x)$, $\ell = 0, 1, 2, \dots$. □

Therefore, the recurrence relation (16) is obtained dividing (27) by x^2 and considering the weighted integral, with weight $\tilde{w}$, on both sides.

The values of the modified moments $\mathcal{M}_0$ and $\mathcal{N}_0$ can be retrieved from [4, p. 337] and [4, p. 369], respectively.

Observe that $\mathcal{M}_\ell = 0$, ℓ even, since $\tilde{w}$ is an even function and $\mathcal{H}_\ell$ is an odd function for ℓ odd. □

Proof of Theorem 4.2. First of all we prove that for any $f \in C_{w_\delta}$,

$$\int_{\mathbb{R}} |\mathcal{L}_{n-1}(w,f,x)|\tilde{w}(x)dx \le \mathcal{C}\,\|fw_\delta\|_\infty, \quad \mathcal{C} \ne \mathcal{C}\,(n,f). \tag{28}$$

Since the factor $e^{-\frac{1}{x^2}} \in C^\infty(\mathbb{R})$ satisfies $0 \le e^{-\frac{1}{x^2}} < 1$, we have

$$\int_{\mathbb{R}} |\mathcal{L}_{n-1}(w,f,x)|e^{-x^2-\frac{1}{x^2}}dx \le \left(\int_{\mathbb{R}} w(x)dx\right)^{\frac12}\left(\int_{\mathbb{R}} (\mathcal{L}_{n-1}(w,f,x))^2w(x)dx\right)^{\frac12}.$$

By using the n-th Gauss-Hermite rule which is exact for the polynomial $(\mathcal{L}_{n-1}(w,f))^2 \in \mathbb{P}_{2n-2}$, we get

$$\left(\int_{\mathbb{R}} (\mathcal{L}_{n-1}(w,f,x))^2w(x)dx\right)^{\frac12} = \left(\sum_{k=1}^n w_k[f(x_k)]^2\right)^{\frac12} \times$$

$$\left(\sum_{k=1}^n \frac{w_k}{(1+|x_k|)^{2\delta}}[f(x_k)w_\delta(x_k)]^2\right)^{\frac12} \le \mathcal{C}\,\|fw_\delta\|_\infty \left(\sum_{k=1}^n \frac{w_k}{(1+|x_k|)^{2\delta}w(x_k)}\right)^{\frac12}$$

$$\le \mathcal{C}\,\|fw_\delta\|_\infty \left(\int_{\mathbb{R}} \frac{dx}{(1+|x|)^{2\delta}}\right)^{\frac12} \le \mathcal{C}\,\|fw_\delta\|_\infty,$$

taking into account the assumption $\delta > \frac12$.

We omit the proof of (19) since it can be easily deduced by standard arguments by (28). In order to prove (20), let $\widetilde{P} \in \mathcal{P}_{n-1}$, as defined in (11).

Then

$$\begin{aligned}|e_n(f)| &\le \int_{\mathbb{R}} \left|(f(x)-\widetilde{P}(x))\right|\tilde{w}(x)\,dx \\ &+ \int_{\mathbb{R}} \left|\mathcal{L}_{n+1}(w,f-\widetilde{P},x)\right|\tilde{w}(x)dx \\ &\le \|(f-\widetilde{P})w_\delta\|_\infty \int_{\mathbb{R}} \frac{w\rho(x)}{w_\delta(x)}dx + \mathcal{C}\,\|(f-\widetilde{P})w_\delta\|_\infty \\ &\le \mathcal{C}\,\tilde{E}_{n-1}(f)_{w_\delta}.\end{aligned}$$

The thesis follows by (11). □

7. Conclusions

The construction of a fast and reliable product rule for computing integrals involving functions of kind $e^{-x^2-\frac{1}{x^2}}f(x)$ on the whole real line in floating point arithmetic is considered.

It is shown that the convergence properties of the proposed method only rely on the regularity properties of $f(x)$ rather than those of $f(x)e^{-\frac{1}{x^2}}$.

The numerical experiments confirm the effectiveness of the proposed approach.

Declaration of competing interest

The authors declare that they have no conflict of interest.

Data availability

Data sharing not applicable to this article as no datasets were generated or analyzed during the current study.

Acknowledgements

This work was partially supported by Gruppo Nazionale Calcolo Scientifico (GNCS) of Istituto Nazionale di Alta Matematica (INdDAM). The authors thank the anonymous Referee for his/her comments and suggestions which helped to improve the paper. Third author is partially supported by INdAM GNCS project 2022 "Metodi e software per la modellistica integrale multivariata".

References

[1] H. Bowdler, R.S. Martin, C. Reinsch, J.H. Wilkinson, The QR and QL algorithms for symmetric matrices, Numer. Math. 11 (1968) 293–306.
[2] W. Gautschi, Orthogonal Polynomials: Computation and Approximation, Oxford University Press, Oxford, UK, 2004.
[3] G.H. Golub, J.H. Welsch, Calculation of Gauss quadrature rules, Math. Comput. 23 (106) (1969) 221–230.
[4] I.S. Gradshteyn, I.M. Ryzhik, Table of Integrals, Series, and Products, seventh edition, Academic Press, Boston, 2007.
[5] P. Junghanns, G. Mastroianni, I. Notarangelo, On Nyström and product integration methods for Fredholm integral equations, in: J. Dick, F.Y. Kuo, H. Woźniakowski (Eds.), Contemporary Computational Mathematics - a Celebration of the 80th Birthday of Ian Sloan, Springer International Publishing, 2018, pp. 645–673.
[6] P. Junghanns, G. Mastroianni, I. Notarangelo, Weighted Polynomial Approximation and Numerical Methods for Integral Equations, Pathways in Mathematics, Birkäuser–Springer, Cham, 2021.
[7] M. Kijima, Stochastic Processes with Applications to Finance, 2nd edn., Chapman & Hall/CRC Financial Mathematics Series, CRC Press, Boca Raton, 2013.
[8] T. Laudadio, N. Mastronardi, P. Van Dooren, Computing Gaussian quadrature rules with high relative accuracy, Numer. Algorithms 92 (2023) 767–793, https://doi.org/10.1007/s11075-022-01297-9.
[9] D.S. Lubinsky, Which weights on R admit Jackson theorems?, Isr. J. Math. 155 (2006) 253–280.
[10] G. Mastroianni, G.V. Milovanović, Interpolation Processes – Basic Theory and Applications, Springer Monographs in Mathematics, Springer, Berlin, Germany, 2008.
[11] G. Mastroianni, G.V. Milovanović, I. Notarangelo, Gaussian quadrature rules with an exponential weight on the real semiaxis, IMA J. Numer. Anal. 34 (2014) 1654–1685.
[12] G. Mastroianni, G.V. Milovanović, I. Notarangelo, A Nyström method for a class of Fredholm integral equations on the real semiaxis, Calcolo 54 (2017) 567–585.
[13] G. Mastroianni, I. Notarangelo, A Lagrange-type projector on the real line, Math. Comput. 79 (269) (2010) 327–352.
[14] G. Mastroianni, I. Notarangelo, Some Fourier-type operators for functions on unvounded interval, Acta Math. Hung. 127 (4) (2010) 347–375.
[15] G. Mastroianni, I. Notarangelo, Polynomial approximation with an exponential weight on the real semiaxis, Acta Math. Hung. 142 (1) (2014) 167–198.
[16] G. Mastroianni, I. Notarangelo, Lagrange interpolation at Pollaczek–Laguerre zeros on the real semiaxis, J. Approx. Theory 245 (1) (2019) 83–100.
[17] G. Mastroianni, M.G. Russo, Fourier sums in weighted spaces of functions. A survey, Jaen J. Approx. 1 (2) (2009) 257–291.
[18] G. Mastroianni, J. Szabados, Polynomial approximation on infinite intervals with weights having inner zeros, Acta Math. Hung. 96 (3) (2002) 221–258.
[19] G. Mastroianni, J. Szabados, Direct and converse polynomial approximation theorems on the real line with weights having zeros, in: Frontiers in Interpolation and Approximation, Dedicated to the Memory of A. Sharma, in: Pure Appl. Math. (Boca Raton), vol. 282, Chapman & Hall/CRC, Boca Raton FL, 2007, pp. 287–306.
[20] G. Szegö, Orthogonal Polynomials, 4th ed., American Mathematical Society, Providence, RI, 1975.
[21] H.S. Wilf, Mathematics for the Physical Sciences, Wiley, New York, 1962.