MATHEMATICAL MODELING AND COMPUTING, Vol. 9, No. 2, pp. 241–261 (2022)

High accurate method to calculate a singular integral related to Hankel transform

Assoudi R.[1,3], Bougtab S.[2], Allouche H.[2], Lamzoud K.[3], Feuillebois F.[4], Chaoui M.[3]

[1] *LGEMS Laboratory, National School of Applied Sciences, Ibn Zohr University, Agadir, Morocco*
[2] *Research Team MANTA, Department of Mathematics and Computer Sciences, Moulay Ismail University, Meknes, Morocco*
[3] *Department of Physics, Moulay Ismail University, Meknes, Morocco*
[4] *LIMSI–CNRS, Orsay, France*

(Received 17 September 2021; Accepted 7 February 2022)

In this paper we are interested in the approximation of the integral

$$I_0(f,\omega) = \int_0^{\infty} f(t)\, e^{-t}\, J_0(\omega t)\, dt$$

for fairly large ω values. This singular integral comes from the Hankel transformation of order 0, $f(x)$ is a function with which the integral is convergent.
For fairly large values of ω, the classical quadrature methods are not appropriate, on the other side, these methods are applicable for relatively small values of ω. Moreover, all quadrature methods are reduced to the evaluation of the function to be integrated into the nodes of the subdivision of the integration interval, hence the obligation to evaluate the exponential function and the Bessel function at rather large nodes of the interval $]0,+\infty[$.
The idea is to have the value of $I_0(f,\omega)$ with great precision for large ω without having to improve the numerical method of calculation of the integrals, just by studying the behavior of the function $I_0(f,\omega)$ and extrapolating it.
We will use two approaches to extrapolation of $I_0(f,\omega)$. The first one is the Padé approximant of $I_0(f,\omega)$ and the second one is the rational interpolation.

Keywords: *singular integral, Hankel transform, Gauss–Laguerre, extrapolation, Padé approximation, rational interpolation.*

2010 MSC: 42Axx, 42A10, 42A15, 65Dxx, 74Axx **DOI:** 10.23939/mmc2022.02.241

1. Introduction

Hankel transform, which appears when applying Fourier transform to problems with cylindrical symmetry, has various applications in Mathematical Physics. As an example, in Fluid Mechanics at low Reynolds number, it occurs when calculating the Green function of Stokes equations for the creeping flow near either a solid plane boundary [1] or a porous slab [2,3]. This Green function is then used for calculating Stokes flows either with the method of fundamental solution [4] or the boundary integral method [3,5]. In more recent work, we have studied the behaviour of a freely moving solid spherical particle in a shear flow near rough wall [6]. The roughness is periodic and of small amplitude compared with the sphere radius. The force and torque exerted on the particle are expanded for small roughness as:

$$\widetilde{\mathbf{F}} = \widetilde{\mathbf{F}}^{(0)} + \widetilde{\mathbf{F}}^{(1)}, \tag{1a}$$
$$\widetilde{\mathbf{C}} = \widetilde{\mathbf{C}}^{(0)} + \widetilde{\mathbf{C}}^{(1)}. \tag{1b}$$

This work is dedicated to the memory of our professor François Feuillebois.

The order (0) terms ($\widetilde{\mathbf{F}}^{(0)}, \widetilde{\mathbf{C}}^{(0)}$), representing the force and torque exerted on the spherical particle near smooth wall, were obtained from an analytical solution in bispherical coordinates [7]. The order (1) terms, showing the influence of roughness, were expressed as sums of integrals in the following form:

$$I_n(f,\omega) = \int_0^\infty f(x)\, e^{-x}\, J_n(\omega x)\, dx, \tag{2}$$

where J_n denotes the Bessel function of order n, $\omega = 2\pi/\widetilde{\mathrm{L}}$ is a positive constant in which $\widetilde{\mathrm{L}}$ is the roughness wavelength normalized by the sphere radius, and f is assumed to be bounded. For small $\omega \leqslant 2.5$, viz. large wavelength, the integral may be calculated numerically by Gauss–Laguerre method [8]. On the other hand, for fast oscillations when $\omega > 2.5$, this method does not provide satisfactory results. This may be observed with the simple example case of $f = 1$ and $n = 0$ in Figs. 1 and 2, where the exact result for the integral,

$$I_0^{\text{exact}}(1,\omega) = \frac{1}{\sqrt{1+\omega^2}}, \tag{3}$$

is compared with results of Gauss–Laguerre integration.

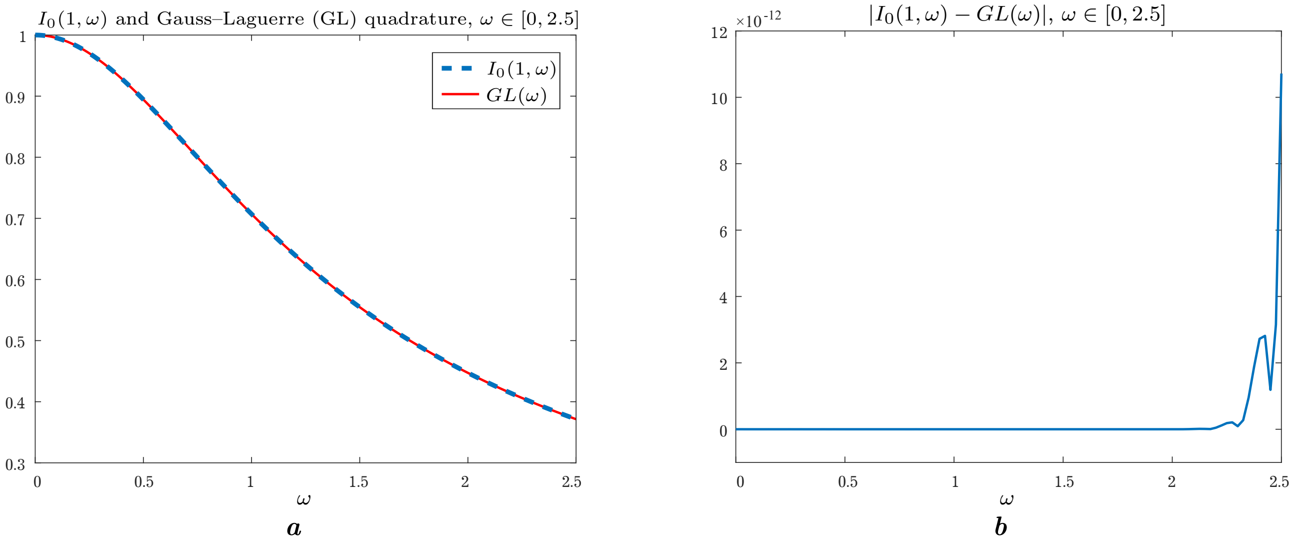


Fig. 1. (***a***) Overlapping of $I_0(1,\omega)$ and $GL(\omega)$: Gauss–Laguerre method's; (***b***) The error $|I_0(1,\omega) - GL(\omega)|$ for $\omega \in [0, 2.5]$.

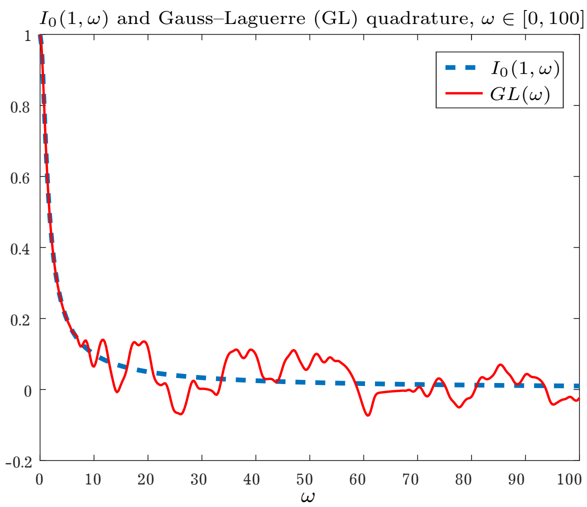


Fig. 2. $I_0(1,\omega)$ and $GL(\omega)$: Gauss–Laguerre method's over $[0, 100]$ with $f = 1$.

A method developed by [9] to treat such problems in the numerical calculation of the integrals $I_0(f,\omega)$ and $I_1(f,\omega)$ will be recalled in Section 2.1.

In this paper, we present two different extrapolation techniques to calculate numerically the integral $I_n(f,\omega)$. The first one, using Padé approximant, will be the subject of Section 3, and the second one, using rational interpolation, will be discussed in Section 4. Both approaches give results with a high accuracy and are simple to implement.

2. Preliminary

In this paragraph, we are going to describe what was done for the calculation of this integral and we will recall some of its properties to demonstrate some results that will be used.

2.1. Feuillebois approach

In [9], the Feuillebois approach concerns the computation of the integral involving the Bessel function of order 0, $I_0(f,\omega)$ and order 1, $I_1(f,\omega)$.

There is considered the integral form of Bessel function of order 0,

$$J_0(x) = \frac{1}{\pi}\int_{-1}^{1}\frac{1}{\sqrt{1-t^2}}\cos(xt)\,dt$$

that injected into the expression of $I_0(f,\omega)$

$$I_0(f,\omega) = \int_{-1}^{1}\frac{g_0(t)}{\sqrt{1-t^2}}\,dt, \tag{4}$$

$$g_0(t) = \frac{1}{\pi}\int_{0}^{\infty} f(x)\,e^{-x}\cos(x\omega t)\,dx.$$

Consider the following function

$$h_0(t) = \pi(1+\omega^2 t^2)\,g_0(t).$$

The integral $I_0(f,\omega)$ becomes

$$I_0(f,\omega) = \frac{1}{\pi}\int_{-1}^{1}(1-t^2)^{-1/2}h_0(t)\frac{dt}{1+\omega^2 t^2}.$$

By using asymptotic expansion, the integral $I_0(f,\omega)$ can be expressed in the following form:

$$I_0(f,\omega) = 2\left(\int_0^{\varepsilon} + \int_{\varepsilon}^{1}\right)$$

where ε is a number such that: $1 < \varepsilon^{-1} < |\omega|$.

So the decomposition of $I_0(f,\omega)$ as a sum of two integrals S_1 and S_2

$$I_0(f,\omega) = 2(S_1 + S_2)$$

with

$$S_1 = \int_0^{\frac{1}{\omega}\arctan(\omega\varepsilon)} f_1(y)\,dy \quad \text{and} \quad S_2 = \int_{\arcsin(\varepsilon)}^{\pi/2} f_2(\theta)\,d\theta,$$

f_1 and f_2 are regular functions

$$f_1(y) = \frac{1}{\pi}\left(1-\frac{\tan^2(\omega y)}{\omega^2}\right)^{-1/2} h_0\left(\frac{\tan(\omega y)}{\omega}\right) \quad \text{and} \quad f_2(\theta) = \frac{h_0(\sin(\theta))}{\pi(1+\omega^2\sin^2(\theta))}.$$

The standard Gauss–Legendre formulae can be used to calculate numerically the integrals S_1 and S_2.

Fig. 3 contains two superimposed curves $I_0(1,\omega)$ and that calculated by the Feuillebois method $I_{\text{Feu}}(\omega)$, over the interval $[5, 500]$ and the error curve.

The same approach is applied for the evaluation of $I_1(f,\omega)$, considering the integral form of Bessel function 1,

$$J_1(z) = \frac{z}{\pi}\int_{-1}^{1}(1-t^2)^{1/2}\cos(zt)\,dt.$$

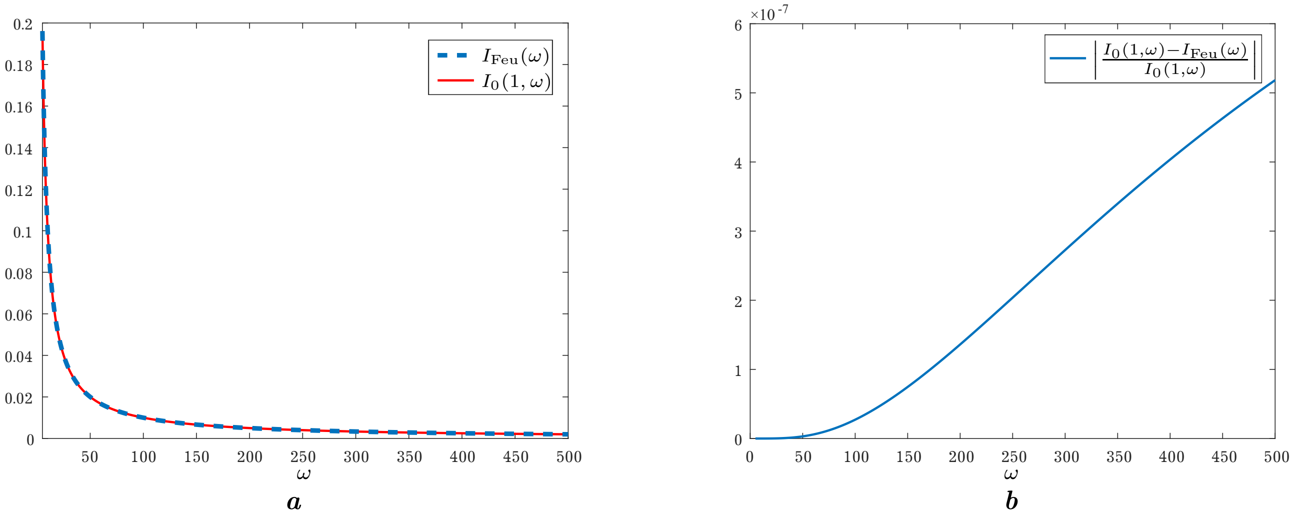


Fig. 3. (***a***) $I_0(1,\omega)$ and the Feuillebois method ($I_{\text{Feu}}(\omega)$) applicated to $f = 1$ over $[5, 500]$; (***b***) The normalized approximation error $\left|\frac{I_0(1,\omega)-I_{\text{Feu}}(\omega)}{I_0(1,\omega)}\right|$.

Then the expression for $I_1(f,\omega)$ is written:

$$I_1(f,\omega) = \int_{-1}^{1} (1-t^2)^{1/2} g_1(t)\, dt,$$

where

$$g_1(t) = \frac{\omega}{\pi} \int_0^\infty f(x)\, x\, e^{-x} \cos(\omega x t)\, dx.$$

Using derivative property for the Bessel functions $J_1(\omega x) = -\frac{1}{\omega}\frac{dJ_0(\omega x)}{dx}$, we obtain:

$$I_1(f,\omega) = -\frac{1}{\omega} I_0(f,\omega) + \frac{1}{\omega} I_0(f',\omega).$$

In the rest of this section, we will try to characterize $I_0(f,\omega)$ for the different classes of functions f with the aim to develop the methods of calculating $I_0(f,\omega)$.

2.2. Link with hypergeometric functions

The relation between Bessel functions and the hypergeometric functions is well known, particularly with the hypergeometric Gauss function

$${}_2F_1(a,b,c;x) = \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(c)_k} x^k,$$

where $(a)_k = a(a+1)\cdots(a+k-1)$, $(a)_0 = 1$.

For all $\alpha > 0$, let's look for the link between $I_0(x^\alpha,\omega) = \int_0^\infty x^\alpha e^{-x} J_0(\omega x)\, dx$ and the hypergeometric Gauss function.

We have

$$\forall x,\omega \in [0,+\infty[, \quad x^\alpha J_0(\omega x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(n!)^2} \left(\frac{\omega}{2}\right)^{2n} x^{2n+\alpha},$$

which gives

$$I_0(x^\alpha,\omega) = \int_0^\infty \sum_{n=0}^{\infty} e^{-x} \frac{(-1)^n}{(n!)^2} \left(\frac{\omega}{2}\right)^{2n} x^{2n+\alpha} dx.$$

We can interchange $\int$ and $\sum$ inside the convergence domain of a power series $|x| < R$ (it is uniformly convergent on $|x| < R$), and since the radius of convergence of the power series of the Bessel function is $R = +\infty$ then

$$I_0(x^\alpha, \omega) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(n!)^2} \left(\frac{\omega}{2}\right)^{2n} \int_0^\infty e^{-x} x^{2n+\alpha}\, dx$$
$$= \sum_{n=0}^{\infty} \frac{\Gamma(2n+\alpha+1)}{2^{2n}(n!)^2} \left(-\omega^2\right)^n$$

since the gamma function is $\Gamma(t) = \int_0^\infty x^{t-1} e^{-x}\, dx$.

Due to the property of Γ,

$$I_0(x^\alpha, \omega) = 2^\alpha \frac{\Gamma\left(\frac{\alpha}{2}+\frac{1}{2}\right)\Gamma\left(\frac{\alpha}{2}+1\right)}{\Gamma\left(\frac{1}{2}\right)}\, {}_2F_1\left(\frac{\alpha}{2}+\frac{1}{2}, \frac{\alpha}{2}+1, 1; -\omega^2\right).$$

Using this formula, the function $I_0(f, x)$ is defined, where $f(t) = t^k$ with the mathematical code that we used for the calculation of $I_0(t^3, x)$

```
In[1]:= g[k_] := 2^k (Gamma[k/2 + 1/2] * Gamma[k/2+1] / Gamma[1/2])

In[2]:= u[k_, x_ ] := g[k] * Hypergeometric2F1[k/2+1/2, k/2+1, 1, -x^2]

In[3]:= u[3, x ]

Out[3]= 3 (2 - 3 x^2) / (1 + x^2)^(7/2)
```

Theorem 1. *For all k in $\mathbb{N}$, the expression*

$$(1+\omega^2)^{k+1/2} I_0(t^k, \omega) = (1+\omega^2)^{k+1/2} \int_0^\infty t^k e^{-t} J_0(\omega t)\, dt$$

is a polynomial in $\mathbb{R}[\omega]$ of degree at most k.

Proof. By recurrence on k.

For $k = 0$ and $k = 1$

$$(1+\omega^2)^{1/2} \int_0^\infty e^{-t} J_0(\omega t)\, dt = 1 \quad \text{and} \quad (1+\omega^2)^{3/2} \int_0^\infty t\, e^{-t} J_0(\omega t)\, dt = 1.$$

The property is true for $k = 0$ and for $k = 1$.

Suppose the property is true to order $k-1$,

$$I_0(t^k, \omega) = \int_0^\infty x^k e^{-x} J_0(\omega x)\, dx$$
$$= \frac{1}{\omega^{k+1}} \int_0^\infty t^k e^{-t/\omega} J_0(t)\, dt$$
$$= -\frac{1}{\omega^{k+1}} \int_0^\infty t^{k-1} e^{-t/\omega} \left(J_0'(t) + t J_0''(t)\right) dt$$
$$= -\frac{1}{\omega^{k+1}} \left(\int_0^\infty t^{k-1} e^{-t/\omega} J_0'(t)\, dt + \int_0^\infty t^k e^{-t/\omega} J_0''(t)\, dt\right), \tag{5}$$

since $J_0(t)$ is a solution of the differential equation $ty''(t) + y'(t) + ty(t) = 0$. Now

$$\int_0^\infty t^k e^{-t/\omega} J_0''(t)\,dt = \left[t^k e^{-t/\omega} J_0'(t)\right]_0^\infty - k\int_0^\infty t^{k-1} e^{-t/\omega} J_0'(t)\,dt + \frac{1}{\omega}\int_0^\infty t^k e^{-t/\omega} J_0'(t)\,dt$$

$$\begin{aligned}\int_0^\infty t^k e^{-t/\omega} J_0'(t)\,dt &= \left[t^k e^{-t/\omega} J_0(t)\right]_0^\infty - k\int_0^\infty t^{k-1} e^{-t/\omega} J_0(t)\,dt + \frac{1}{\omega}\int_0^\infty t^k e^{-t/\omega} J_0(t)\,dt \\ &= -k\omega^k \int_0^\infty x^{k-1} e^{-x} J_0(\omega x)\,dx + \omega^k \int_0^\infty x^k e^{-x} J_0(\omega x)\,dx \\ &= \omega^k \left(-k\, I_0(t^{k-1},\omega) + I_0(t^k,\omega)\right),\end{aligned}$$

then

$$\begin{aligned}\int_0^\infty t^k e^{-t/\omega} J_0''(t)\,dt &= -k(\omega^{k-1}(-(k-1)I_0(t^{k-2},\omega) + I_0(t^{k-1},\omega)) + \frac{1}{\omega}\omega^k(-kI_0(t^{k-1},\omega) + I_0(t^k,\omega)) \\ &= \omega^{k-1}\left(k(k-1)I_0(t^{k-2},\omega) - 2kI_0(t^{k-1},\omega) + I_0(t^k,\omega)\right).\end{aligned}$$

Replacing in the expression (5), we will have

$$\begin{aligned}I_0(t^k,\omega) = \frac{-1}{\omega^{k+1}}\Big(&\omega^{k-1}(-(k-1)I_0(t^{k-2},\omega) + I_0(t^{k-1},\omega)) \\ &+ \omega^{k-1}\big(k(k-1)I_0(t^{k-2},\omega) - 2k\, I_0(t^{k-1},\omega) + I_0(t^k,\omega)\big)\Big).\end{aligned}$$

Finally,

$$I_0(t^k,\omega) = \frac{-1}{1+\omega^2}\left((k-1)^2 I_0(t^{k-2},\omega) + (1-2k)I_0(t^{k-1},\omega)\right)$$

and since $(1+\omega^2)^{k-2+1/2} I_0(t^{k-2},\omega)$ and $(1+\omega^2)^{k-1+1/2} I_0(t^{k-1},\omega)$ are polynomials of degree at most $k-2$ and $k-1$ respectively, $(1+\omega^2)^{k+1/2} I_0(t^k,\omega)$ is a polynomial of degree at most k. ■

Corollary 1. *If $f(x) = P(x)e^{-ax}$, where $P(x)$ is a polynomial of degree k and $a \in]-1,+\infty[$, then $\left(1+\frac{\omega^2}{1+a}\right)^{k+1/2} I_0(f,\omega)$ is a polynomial of degree at most k.*

Proof. Just make the variable change $u = (1+a)t$ in the integral $\int_0^\infty f(t)e^{-t}J_0(\omega t)\,dt$. ■

2.3. Case of the functions from $L^2(]0,+\infty[, e^{-x})$

Let $f(x)$ be a function of $L^2(]0,+\infty[, e^{-x})$, space L^2 of $]0,+\infty[$ attached to the weight function e^{-x} is Hilbert space where Hilbert basis is Laguerre polynomials sequence $(L_n)_{n\geqslant 0}$

$$f(x) = \sum_{n=0}^{\infty} c_n L_n(x).$$

A polynomial approximation of $f(x)$ is $P_N(x) = \sum_{n=0}^{N} c_n L_n(x)$ then an approximation of $I(f,\omega)$ is $I(P_N,\omega)$ that leads to the following convergence result

Theorem 2. *If $f(x)$ be a function of $L^2(]0,+\infty[, e^{-x})$ and $P_N(x)$ is the truncated Laguerre expansion to the order N of f then*

$$\lim_{N\to\infty} I_0(P_N,\omega) = I_0(f,\omega).$$

Proof.

$$I_0(f,\omega) - I_0(P_N,\omega) = \int_0^\infty (f-P_N)(x)\, e^{-x} J_0(\omega x)\,dx.$$

Where b_n is the coefficient of Laguerre polynomial expansion of the function $J_0(\omega x)$, one can deduce that

$$I_0(f,\omega) - I_0(P_N,\omega) = \langle f - P_N, J_0(\omega\bullet)\rangle_{e^{-x}} = \sum_{n=N}^{\infty} c_n b_n.$$

Schwartz inequality gives

$$|I_0(f,\omega) - I_0(P_N,\omega)| \leqslant \sum_{n=N+1}^{\infty} |c_n|^2 \sum_{n=N+1}^{\infty} |b_n|^2,$$

which tends to 0 as N tends to the infinity given that two series $\sum_n |c_n|^2$ and $\sum_n |b_n|^2$ are convergent.

According to Theorem 1, $(1+\omega^2)^{N+1/2} I_0(P_N,\omega)$ is a polynomial of degree at most N, consequently, it can be recovered exactly by a polynomial interpolation at $N+1$ points $\{w_k\colon k = 0,\dots,N\}$.

This result can be exploited as follows: for different values of N, the expression $(1+\omega^2)^{N+1/2} I_0(P_N,\omega)$ will be calculated by interpolating it in $N+1$ small values ω_k and Theorem 2 allows us to conclude that $I_0(f,\omega) \simeq I_0(P_N,\omega)$ for large N. ■

Theorem 3. *Let f be a function of $L^2([0,+\infty[, e^{-x})$, then*

$$\lim_{\omega\to+\infty} I_0(f,\omega) = 0.$$

Proof. The integral $I_0(f,\omega)$ is nothing else than the scalar product $\langle f, J_0(\omega\bullet)\rangle$ in Hilbert space $L^2([0,+\infty[, e^{-x})$, Schwartz inequality gives

$$|I_0(f,\omega)|^2 = \left|\int_0^\infty e^{-x} f(x) J_0(\omega x)\,dx\right|^2 \leqslant \int_0^\infty e^{-x} f^2(x)\,dx \int_0^\infty e^{-x} J_0^2(\omega x)\,dx.$$

Let (ω_n) be a sequence such that $\lim_{n\to+\infty} \omega_n = +\infty$, we put $f_n(x) = J_0^2(\omega_n x)$.

Then $\forall x \in [0,+\infty[$, $\lim_{\omega\to+\infty} J_0^2(\omega x) = 0 \Longrightarrow \lim_{n\to+\infty} f_n = 0$, furthermore $\forall x \in [0,+\infty[$, $0 \leqslant J_0^2(x) \leqslant 1 \Longrightarrow \forall n \in \mathbb{N}$ and $x \geqslant 0$, $0 \leqslant f_n \leqslant 1$ then according to the dominated convergence theorem

$$\lim_{n\to+\infty} \int_0^{+\infty} e^{-x} f_n(x)\,dx = \int_0^{+\infty} e^{-x} \lim_{n\to+\infty} f_n(x)\,dx = 0.$$ ■

3. Extrapolation by Padé approximation

It is well known that the rational approximation is a very powerful tool for the approximation of the functions reason it is used in the implementation of algorithms for calculating elementary functions [10].

We will extend the use of this approximation to the function $I_0(f,\omega)$ evaluation.

Padé approximation is a tool that is often used to construct extrapolation methods. This is what we shall use to extrapolate a sequence of approximants as introduced in Theorem 2 for the integral $I_0(f,\omega)$ to speed up convergence.

Moreover, Padé approximants tend to zero at infinity when the degree of the denominator is greater than the degree of the numerator. And according to Theorem 3, $I_0(f,\omega)$ tend to zeros when ω at infinity then we will have the function and its approximants with the same behavior at infinity. One more reason why we use these approximants to extrapolate $I_0(f,\omega)$.

3.1. Padé Approximation

We introduce Padé approximations as presented in [11].

Definition 1. *Let $f(z)$ be a formal power series*

$$f(z)=\sum_{i=0}^{\infty} c_i z^i.$$

Padé approximation problem of order (n,m) consists of determining two polynomials

$$p(z)=\sum_{i=0}^{n} a_i z^i \quad \deg(p)\leqslant n \quad \text{and} \quad q(z)=\sum_{i=0}^{m} b_i z^i \quad \deg(q)\leqslant m,$$

such that

$$f(z)-\frac{p(z)}{q(z)}=O\left(z^{n+m+1}\right).$$

The linearized problem

$$\left(\sum_{i=0}^{\infty} c_i z^i\right)\left(\sum_{i=0}^{m} b_i z^i\right)-\left(\sum_{i=0}^{n} a_i z^i\right)=O\left(z^{n+m+1}\right)$$

is equivalent to

$$\sum_{i=0}^{\infty}\left(\sum_{k=0}^{m} c_{i-k} b_k\right) z^i-\sum_{i=0}^{n} a_i z^i=O\left(z^{n+m+1}\right)$$

with the convention $c_i=0$ if $i<0$, we obtain:

$$\begin{pmatrix} c_0 & 0 & \cdots & 0 \\ c_1 & c_0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ c_n & c_{n-1} & \cdots & c_{n-m} \end{pmatrix}\begin{pmatrix} b_0 \\ b_1 \\ \vdots \\ b_m \end{pmatrix}=\begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{pmatrix} \tag{6}$$

and

$$\begin{pmatrix} c_{n+1} & c_n & \cdots & c_{n-m+1} \\ c_{n+2} & c_{n+1} & \cdots & c_{n-m+2} \\ \cdots & \cdots & \cdots & \cdots \\ c_{n+m} & c_{n+m-1} & \cdots & c_n \end{pmatrix}\begin{pmatrix} b_0 \\ b_1 \\ \vdots \\ b_m \end{pmatrix}=\begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{7}$$

The system (7) is solved by fixing arbitrarily b_0 to obtain the denominator coefficients that we inject into (6) to obtain the numerator coefficients.

The pair $(p(z),q(z))$ is the solution of the problem (n,m).

In its irreducible form the rational fraction $\frac{p}{q}(z)$ is called the order (n,m) Padé approximation of $f(z)$, denoted by $[n/m]_f$.

In his thesis (1892) H. Padé (1822–1901) arranged the approximants $[n/m]_f$ in the table, called Padé table.

$$\begin{array}{cccc} [0/0] & [0/1] & [0/2] & \cdots \\ [1/0] & [1/1] & [1/2] & \cdots \\ [2/0] & [2/1] & [2/2] & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{array}$$

Axiom 1. If the homogeneous system (7) is of maximal rank, the approximant $[n/m]_f$ is said to be normal and is written in the form:

$$[n/m]_f(z) = \frac{\begin{vmatrix} z^m S_{n-m} & z^{m-1}S_{n-m+1} & \cdots & S_n \\ c_{n-m+1} & c_{n-m+2} & \cdots & c_{n+1} \\ \cdots & \cdots & \cdots & \cdots \\ c_n & c_{n+1} & \cdots & c_{n+m} \end{vmatrix}}{\begin{vmatrix} 1 & 1 & \cdots & 1 \\ c_{n-m+1} & c_{n-m+2} & \cdots & c_{n+1} \\ \cdots & \cdots & \cdots & \cdots \\ c_n & c_{n+1} & \cdots & c_{n+m} \end{vmatrix}}$$

with

$$S_k(z) = \sum_{i=0}^{k} c_i z^i \quad \text{for} \quad k \geqslant 0 \quad \text{and} \quad S_k = 0 \quad \text{for} \quad k < 0.$$

There are several recursive algorithms that are inexpensive in number of arithmetic operations, that are easy to implement and calculate the elements of this table recursively.

3.2. Application to the evaluation of the function $I_0(f,\omega)$

The data that will be used to calculate the Padé approximants for ω large are the coefficients of the formal power series of $I_0(f,\omega)$ in a neighborhood of a certain relatively small ω_0,

$$I_0(f,\omega) = \sum_{n=0}^{\infty} c_n(\omega-\omega_0)^n. \tag{8}$$

We propose two different techniques for calculating the series coefficients.

3.2.1. By the power series of $J_0(x)$

Consider the expression (4) of $I_0(f,\omega)$.

The n-th derivative of $g_0(u)$ at u_0 is

$$\begin{aligned} g_0^{(n)}(u_0) &= \frac{1}{\pi}\int_0^{\infty} f(x)e^{-x}\left(\frac{\partial^n \cos(xt)}{\partial t^n}\right)_{t=u_0} dx \\ &= \frac{1}{\pi}\int_0^{\infty} x^n f(x)\, e^{-x}\cos^{(n)}(xu_0)\, dx \\ &= \frac{1}{\pi}\int_0^{\infty} x^n f(x)\, e^{-x}\cos\left(x\,u_0 + n\frac{\pi}{2}\right) dx \end{aligned}$$

which amounts to calculating the integrals

$$\int_0^{\infty} x^{2n} f(x)\, e^{-x}\cos(xu_0)dx \quad \text{and} \quad \int_0^{\infty} x^{2n+1} f(x)\, e^{-x}\sin(xu_0)dx$$

or

$$\int_0^{\infty} x^n f(x)\, e^{x(-1+iu_0)}dx$$

which gives the formal power series of $I_0(f,\omega)$ in a neighborhood of ω_0

$$\begin{aligned} I_0(f,\omega) &= \sum_{n\geqslant 0}\frac{1}{n!}\int_{-1}^{1}\left(\frac{\partial^n g_0(\omega t)}{\partial \omega^n}\right)_{\omega=\omega_0}\frac{dt}{\sqrt{1-t^2}}(\omega-\omega_0)^n \\ &= \sum_{n\geqslant 0}\frac{1}{n!}\int_{-1}^{1} g_0^{(n)}(\omega_0 t)\frac{t^n}{\sqrt{1-t^2}}dt(\omega-\omega_0)^n \\ &= \sum_{n\geqslant 0} c_n(\omega-\omega_0)^n, \end{aligned}$$

where

$$c_n = \frac{1}{n!}\int_{-1}^{1} \frac{t^n g_0^{(n)}(\omega_0 t)}{\sqrt{1-t^2}}dt.$$

Let $g_0^{(n)}(\omega_0 t) = \sum_{k\geqslant 0} \alpha_k T_k(t)$ be Chebyshev series of the function $t \mapsto g_0^{(n)}(\omega_0 t)$ then the coefficient c_n can be written as

$$c_n = \frac{\alpha_n \pi}{n!\,2^n}.$$

The calculation of c_n by Gauss–Chebyshev quadrature method and Gauss–Laguerre method consists of calculating the following quantities

$$\begin{aligned} c_n &\simeq \frac{1}{Nn!}\sum_{k=1}^{N} t_k^n \int_0^\infty x^n f(x)\, e^{-x} \cos\left(x\omega_0 t_k + n\frac{\pi}{2}\right) dx \\ &\simeq \frac{1}{Nn!}\sum_{k=1}^{N} t_k^n \sum_{l=1}^{M} w_l f(x_l) \cos\left(x_l\omega_0 t_k + n\frac{\pi}{2}\right), \end{aligned}$$

where $t_k = \cos\left(\frac{2k-1}{2N}\pi\right)$, w_l are the weights of Gauss–Laguerre quadrature method and x_l are the roots of $L_M^{(n)}(x)$ which is the generalized Laguerre polynomial of degree M. Since the numbers t_k^n are small and w_k are large, while the cosines are bounded by 1, the weights have moderate magnitude.

We have

$$w_l = \frac{\Gamma(M+n+1)x_l}{M![(M+1)L_{M+1}^{(n)}(x_l)]^2} = \frac{(M+n)!x_l}{M![(M+1)L_{M+1}^{(n)}(x_l)]^2} \quad \text{and} \quad \binom{M+n}{n} = \frac{(M+n)!}{M!n!},$$

which gives

$$c_n \simeq \binom{M+n}{n}\frac{1}{N(M+1)^2}\sum_{k=1}^{N}\sum_{l=1}^{M}\frac{t_k^n x_l}{L_{M+1}^{(n)}(x_l)^2} f(x_l)\cos\left(x_l\omega_0 t_k + n\frac{\pi}{2}\right).$$

3.2.2. By calculation of the successive derivatives of Bessel functions

Successive derivatives of Bessel functions can be computed recursively thanks to the recursion relation verified by Bessel functions derivatives, which are

$$\begin{aligned} J_0'(x) &= -J_1(x), \\ J_n'(x) &= \frac{1}{2}\left(J_{n-1} - J_{n+1}\right) \quad \text{for} \quad n = 1, 2, \ldots. \end{aligned}$$

Axiom 2. For all $n \in \mathbb{N}$, the derivative of order $2n$ and order $2n+1$ is given by

$$\begin{aligned} J_1^{(2n+1)} &= C_0^{(2n+1)} J_0 + C_1^{(2n+1)} J_2 + \cdots + C_k^{(2n+1)} J_{2k} + \cdots + C_{n+1}^{(2n+1)} J_{2n+2}, \quad n = 0, 1, \ldots; \\ J_1^{(2n)} &= C_0^{(2n)} J_1 + C_1^{(2n)} J_3 + \cdots + C_k^{(2n)} J_{2k+1} + \cdots + C_n^{(2n)} J_{2n+1}, \quad n = 1, 2, \ldots \end{aligned}$$

where the coefficients $C_k^{(n)}$ are calculated by $C_0^{(1)} = \frac{1}{2}$, $C_1^{(1)} = -\frac{1}{2}$ and

$$\begin{cases} C_0^{(2n)} = \frac{1}{2}C_1^{(2n-1)} - C_0^{(2n-1)}, \\ C_k^{(2n)} = \frac{1}{2}\left(C_{k+1}^{(2n-1)} - C_k^{(2n-1)}\right), \ k = 1, \ldots, n-1, \\ C_n^{(2n)} = -\frac{1}{2}C_n^{(2n-1)}, \end{cases} \qquad \begin{cases} C_0^{(2n+1)} = \frac{1}{2}C_0^{(2n)}, \\ C_k^{(2n+1)} = \frac{1}{2}\left(C_k^{(2n)} - C_{k-1}^{(2n)}\right), \ k = 1, \ldots, n, \\ C_{n+1}^{(2n+1)} = -\frac{1}{2}C_n^{(2n)}, \end{cases}$$

so can be arranged in the following recursive scheme:

$$\begin{array}{ccccccc} C_0^{(1)} & C_0^{(2)} & C_0^{(3)} & C_0^{(4)} & C_0^{(5)} & C_0^{(6)} & \cdots \\ C_1^{(1)} & C_1^{(2)} & C_1^{(3)} & C_1^{(4)} & C_1^{(5)} & C_1^{(6)} & \cdots \\ & & C_2^{(3)} & C_2^{(4)} & C_2^{(5)} & C_2^{(6)} & \cdots \\ & & & & C_3^{(5)} & C_3^{(6)} & \ddots \end{array}$$

Using MAPLE there are calculated the first coefficients $C_i^{(j)}$

$$\begin{array}{cccccccc}
\frac{1}{2} & \frac{-3}{4} & \frac{-3}{8} & \frac{5}{8} & \frac{5}{16} & -\frac{35}{64} & \cdots \\
 & & & & & & \cdots \\
\frac{-1}{2} & \frac{1}{4} & \frac{1}{2} & \frac{-5}{16} & \frac{-15}{32} & \frac{21}{64} & \cdots \\
 & & & & & & \cdots \\
 & & \frac{-1}{8} & \frac{1}{16} & \frac{3}{16} & \frac{-7}{64} & \cdots \\
 & & & & & & \cdots \\
 & & & & \frac{-1}{32} & \frac{1}{64} & \ddots
\end{array}$$

Axiom 3. Let ω be a positive real number, we put

$$I_{n,k} = \int_0^\infty x^k f(x)\, e^{-x} J_n(\omega x)\, dx$$

the n-th derivative of $I_0(f,\omega)$ is

$$\frac{d^{2n+1} I_0}{d\omega^{2n+1}}(f,\omega) = -C_0^{(2n)} I_{2n+1,1} - C_1^{(2n)} I_{2n+1,3} - \cdots - C_k^{(2n)} I_{2n+1,2k+1} - \cdots$$
$$- C_n^{(2n)} I_{2n+1,2n+1}; \quad n = 0, 1, \ldots,$$
$$\frac{d^{2n} I_0}{d\omega^{2n}}(f,\omega) = -C_0^{(2n-1)} I_{2n,0} - C_1^{(2n-1)} I_{2n,2} - \cdots - C_k^{(2n-1)} I_{2n,2k} - \cdots$$
$$- C_n^{(2n-1)} I_{2n,2n}; \quad n = 1, 2, \ldots.$$

Proof. Taking into consideration the conditions on f, we can do a derivation under the integral sign,

$$\frac{d^n I_0}{d\omega^n}(f,\omega) = -\int_0^\infty x^n f(x)\, e^{-x} J_1^{(n-1)}(\omega x)\, dx.$$

The approach consists of calculating Taylor series of $I_0(f,\omega)$ at the order $n+m$ for ω in neighborhood of ω_0 by approximating $I_{n,k}(\omega_0)$. This development will be used to calculate Padé approximation $[n/m]_I(\omega)$ as the estimate of $I_0(f,\omega)$,

$$I_0(f,\omega) = \sum_{k=0}^{n+m} \frac{1}{k!} \frac{d^k I_0}{d\omega^k}(f,\omega_0)(\omega-\omega_0)^k + o(\omega-\omega_0)^{n+m} = \sum_{k=0}^{n+m} c_k(\omega-\omega_0)^k + o(\omega-\omega_0)^{n+m}. \qquad \blacksquare$$

3.3. Numerical illustration

Example 1. Consider the case where $f = 1$, it is well known that the exact value of $I_0(1,\omega)$ is

$$I_0(1,\omega) = \int_0^\infty e^{-x} J_0(\omega x)\, dx = \frac{1}{\sqrt{1+\omega^2}}.$$

After calculation by Gauss–Laguerre quadrature method of the following integrals

$$\int_0^\infty x^k e^{-x} J_n(1.5x)\, dx, \quad k = 0, 1, \ldots, 16 \quad \text{et} \quad n = 0, 1, \ldots, 16,$$

we were able to obtain the Taylor series expansion of $I_0(1,\omega)$ in a neighborhood of $\omega_0 = 1.5$ up to order 16 as follows

$$\begin{aligned}
I_0(1,\omega) = {} & 5.54700196225229 \cdot 10^{-1} - 2.56015475180875 \cdot 10^{-1} X + 9.1902991090571 \cdot 10^{-2} X^2 \\
& - 1.8178613622311 \cdot 10^{-2} X^3 - 6.525656172111 \cdot 10^{-3} X^4 + 9.896050019246 \cdot 10^{-3} X^5 \\
& - 6.700335613180 \cdot 10^{-3} X^6 + 3.133197553474 \cdot 10^{-3} X^7 - 9.074844484962812 \cdot 10^{-4} X^8 \\
& - 6.580263217565992 \cdot 10^{-5} X^9 + 3.090072324144975 \cdot 10^{-4} X^{10} \\
& - 2.538657762042806 \cdot 10^{-4} X^{11} + 1.374176851918851 \cdot 10^{-4} X^{12} \\
& - 4.986447053828060 \cdot 10^{-5} X^{13} + 5.122662622074508 \cdot 10^{-6} X^{14}
\end{aligned}$$

$$+ 9.749061814785698 \cdot 10^{-6} X^{15} - 1.019560218693597 \cdot 10^{-5} X^{16} + O(X)^{17},$$

where $X = (\omega - 1.5)$, that will be used for calculating the following Padé approximation:

$$[7/9]_I(\omega) = \frac{\begin{array}{c} 0.554700196225229 + 1.7682291741338456X + 2.495106085209317X^2 \\ +2.013852912601038X^3 + 1.0020120103338053X^4 + 0.30690119261384924X^5 \\ +0.05352423164033492X^6 + 0.004097718669029887X^7 \end{array}}{\begin{array}{c} 1 + 3.649258938593925X + 6.016709346873545X^2 + 5.83562875765282X^3 \\ +3.6342763755021776X^4 + 1.486052551099337X^5 + 0.38923641509797025X^6 \\ +0.059670806993630324X^7 + 0.004097718992997817X^8 - 2.1686226449190713 \cdot 10^{-11} X^9 \end{array}}.$$

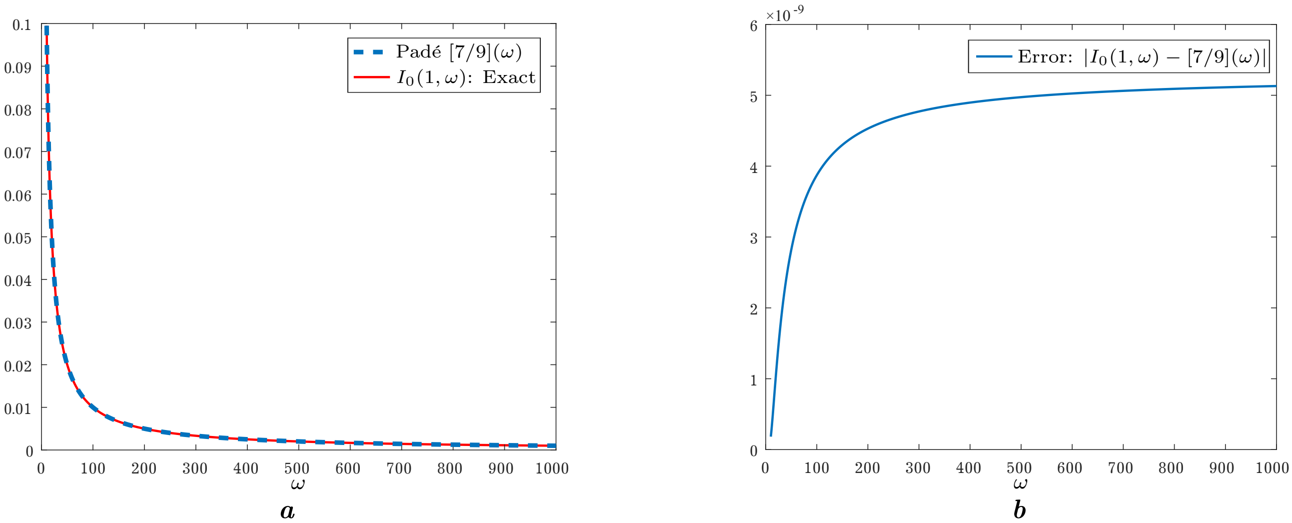


Fig. 4. (***a***) Overlapping of $I_0(1,\omega)$ and $[7/9](\omega)$; (***b***) The absolute Error: $|I_0(1,\omega) - [7/9](\omega)|$.

The figure 4 contains two superimposed curves, $I_0(1,\omega)$ and $[7/9]_I(\omega)$, on the interval $[10, 1000]$ and the error curve.

By calculating the integrals

$$\int_0^{\infty} x^k e^{-x} J_n(\omega_0 x)\, dx, \quad k = 0, 1, \ldots, 16 \quad \text{and} \quad n = 0, 1, \cdots, 16$$

with $\omega_0 = 1.5$, we are able to estimate the integrals $I_0(1,\omega)$ for all $\omega \in]1.5, 1000]$.

The Taylor series coefficients of $I_0(1,\omega)$ that we use are not accurate. They are the results of numerical calculation of integrals. In reality, instead of computing Padé approximants by $\sum_{k=0}^{n+m} c_k(\omega-\omega_0)^k$, they are calculated using $\sum_{k=0}^{n+m} \tilde{c}_k(\omega-\omega_0)^k$ where $c_i \simeq \tilde{c}_i$.

In [12, 13] the following Theorem 4, shows that the error order of the coefficients remains the same when we compare the calculated Padé approximants by the exact coefficients and those computed by the approximate coefficients.

Theorem 4. *If $c_i = \tilde{c}_i + O(h)$ then*

$$\left|[n/m]_{\tilde{I}}(\omega) - [n/m]_I(\omega)\right| = O(h),$$

where

$$\tilde{I}(\omega) = \sum_{k=0}^{n+m} \tilde{c}_k(\omega-\omega_0) + o(\omega-\omega_0)^{n+m}.$$

The accuracy of c_i by $\tilde{c}_i$ will not be lost with the use of Padé approximation. In other words, the difference between Padé approximants with the perturbed coefficients and those with the exact coefficients is of the same order as the difference between the perturbed and exact coefficients. Provided that Padé approximants can be calculated because the perturbation on the coefficients could cause the system (7) to have a bad conditioning which means a strong perturbation of the denominator, while it is still that the approximation $[n/m]_I$ is still good, see [12].

In the previous example, we could estimate up to $\omega = 1000$ using development near $\omega_0 = 100$. Can we go beyond $\omega > 1000$?

We know that Taylor series is a good approximation in a small neighborhood of ω_0 and Padé approximant has a larger convergence reason, but not enough large. There is a threshold where even this method fails due to rounding errors.

Given this remark, we can say that the utility and performance of this method lies in the fact that if numerical computation methods of integrals achieve their limit for a threshold ω_s. For $\omega > \omega_s$ the computation methods of the integrals are faulty then this method is an alternative to exceed this threshold.

Remark 1. We initially had to calculate the integral $I_0(f,\omega)$ which contains Bessel function $J_0(\omega t)$. For the calculation of derivative of $I_0(f,\omega)$, we need to calculate integrals $I_{n,k} = \int_0^\infty x^k e^{-x} J_k(\omega x)\,dx$ for $k = 1,\dots,n$ containing Bessel functions $J_k(\omega x)$. This gives the impression that we have complicated more the calculation instead of simplifying it. But the initial calculation $I(\omega)$ we want to perform is for ω rather large by the computation of integrals intervening in the derivatives of $I_0(f,\omega)$ are quite small ω.

3.4. Another approach

We know that Padé approximation reproduces the rational fractions set. In other words, if f is a rational fraction of degree m/n then for all $i > m$ and $j > n$, Padé approximants $[i/j]_f$ are identical to f.

Considering this remark and Theorem 1, it would be wise not to apply Padé approximation directly to $I_0(f,\omega)$ but to the function $\sqrt{1+\omega^2}I_0(f,\omega)$. Given that if f is a polynomial, $\sqrt{1+\omega^2}I_0(f,\omega)$ will be a rational fraction that Padé approximation will be able to finding and therefore the approximation of $I_0(f,\omega)$ by this approach will be exact on all the polynomials.

Let us return to the previous example, Taylor series expansion of $\sqrt{1+\omega^2}I_0(f,\omega)$ in the neighborhood of $\omega_0 = 1.5$ calculated by the product of Taylor series of $\sqrt{1+\omega^2}$ and that of $I_0(1,\omega)$ computed using the results of Proposition 3:

$$\begin{aligned}\sqrt{1+\omega^2}I_0(1,\omega) = {} & 0.9999999999999998 - 1.1102230246251565\cdot 10^{-16}X \\ & + 8.326672684688674\cdot 10^{-16}X^2 - 2.0122792321330962\cdot 10^{-16}X^3 \\ & + 6.730727086790012\cdot 10^{-16}X^4 + 3.157196726277789\cdot 10^{-16}X^5 \\ & - 7.042977312465837\cdot 10^{-16}X^6 + 2.3765711620882257\cdot 10^{-16}X^7 \\ & + 4.7271214720367993\cdot 10^{-17}X^8 - 1.1439688172437679\cdot 10^{-16}X^9 \\ & - 3.913969842672671\cdot 10^{-17}X^{10} - 1.303753112413819\cdot 10^{-16}X^{11} \\ & - 1.6149191359171589\cdot 10^{-16}X^{12} + 1.5806312422123048\cdot 10^{-16}X^{13} \\ & - 1.216305430939285\cdot 10^{-16}X^{14} - 1.3667046010537587\cdot 10^{-16}X^{15} \\ & - 2.1785687403380605\cdot 10^{-18}X^{16} + o(X)^{16}.\end{aligned}$$

Note that all the coefficients other than the constant coefficient are zero with an error of the 10^{-16} order so we have found the exact value of $I_0(1,\omega)$ with an error of the 10^{-16} order.

Remark 2. If the function $f(x)$ is written as $f(x) = g(x)\,e^{-ax}$ with $a > -1$ then instead of applying Padé approximation to $\sqrt{1+\omega^2}I_0(f,\omega)$, we can apply it to $\sqrt{1+(\alpha\omega)^2}I_0(f,\omega)$ where $\alpha = \frac{1}{1+a}$ and the approach will be exact on the spaces of the functions:

$$V_a = P(x)\,e^{-ax}, \quad a > -1,$$

where $P(x)$ is a polynomial.

In fact, according to Corollary 1 $\sqrt{1+(\alpha\omega)^2}I_0(Pe^{-ax},\omega)$, where P is a polynomial and $a > -1$ is a rational fraction that Padé approximation is able to find exactly.

4. Extrapolation by rational interpolation

Extrapolation by rational interpolation is another alternative that allows $I_0(f,\omega)$ to be approached for fairly wide ω knowing $I_0(f,\omega)$ for relatively small values of ω. Since by Theorem 3, $I_0(f,\omega)$ tends to zero at infinity, a polynomial approximation is not appropriate since all polynomials are unbounded at infinity. Approximation by a rational function of type (n,m) with $n<m$ will be much better since these functions will tend to zero at infinity.

Moreover considering Theorem 1, which shows that $\sqrt{1+\omega^2}I_k(f,\omega)$ is a rational fraction, then the use of rational fractions to extrapolate the value of $I_0(f,\omega)$ is justified.

The steps to follow are the next: we will calculate $I_0(f,\omega_i)$, for $i=0,\dots,N$ for relatively small values of ω_i using Gauss–Laguerre method or the method described in [9]. We can do this calculation with accurate precision. Then we will interpolate $\sqrt{1+\omega^2}I_0(f,\omega)$ by a rational fraction $r_{mn}(\omega)=\frac{p_{mn}(\omega)}{q_{mn}(\omega)}$ such that $r_{mn}(\omega_i)=\sqrt{1+\omega_i^2}I_0(f,\omega_i)$, $i=0,\dots,m+n$ where $m+n=N$,

$$I_0(f,\omega)\simeq\frac{1}{\sqrt{1+\omega^2}}r_{mn}(\omega),\quad \omega\gg\max_i\omega_i.$$

4.1. Rational interpolation

We present the rational interpolation as in [14].

Let $f(x)$ be a function known at abscissae $x_0\leqslant x_2\leqslant\dots\leqslant x_N$. We call rational fraction of order (m,n) denoted $r_{mn}(x)$ the rational fraction $r_{mn}(x)=\frac{p_{mn}(x)}{q_{mn}(x)}$ as degree of numerator is less than or equal to m and that of denominator is less than or equal to n such that $r_{mn}(x_i)=f(x_i)$, $i=0,\dots,m+n$ and $m+n\leqslant N$.

When the abscissae x_i are distinct two by two, the divided differences of $f(x)$ at the abscissae $x_0,\dots,x_n$ are defined by the following recurrence relation: $[x_i]f=f(x_i)$, for $i=0,\dots,N$ and

$$[x_i,\dots,x_{i+k}]f=\frac{[x_i,\dots,x_{i+k-1}]f-[x_{i+1},\dots,x_{i+k}]f}{x_i-x_{i+k}}$$

and if $x_{i-1}<x_i=x_{i+1}=\ldots=x_{i+k}<x_{i+k+1}$, les divided differences are defined by

$$[x_i,\dots,x_{i+l}]f=\frac{d^lf}{dx^l}(x_i),\quad l=1,\dots,k.$$

Let $B_i(x)$ be Newton basis polynomials: $B_0=1$ and $B_i(x)=B_{i-1}(x)(x-x_{i-1})$.

Let be $(m,n)\in\mathbb{N}^2$ such as $m+n\leqslant N$, the rational interpolation problem of order (m,n) amounts to looking for two polynomials $p_{m,n}(x)=\sum_{i=0}^m a_iB_i(x)$ and $q_{m,n}(x)=\sum_{i=0}^n b_iB_i(x)$ of respective degree m and n such that

$$(fq_{m,n}-p_{m,n})(x_i)=0,\quad i=0,\dots,m+n.$$

Condition that we can express it by

$$(fq_{m,n}-p_{m,n})(x)=B_{m+n+1}v(x),$$

where v is a function defined on an open set containing the x_i.

Which is expressed by

$$[x_0,\dots,x_i](fq_{m,n})=[x_0,\cdots,x_i]p_{n,m},\quad i=0,\dots,m, \tag{9}$$

$$[x_0,\dots,x_i](fq_{m,n})=0,\quad i=m+1,\dots,m+n. \tag{10}$$

Leibniz formula. Let $f(x)$ and $g(x)$ be two known functions at abscissa x_i for $i=0,\dots,N$, then the divided differences of the product $(fg)(x)$ are

$$[x_i,\dots,x_{i+k}](fg)=\sum_{l=0}^{k}[x_i,\dots,x_{i+l}]f[x_{i+l},\dots,x_{i+k}]g.$$

Let's put $c_{ij}=[x_i,\cdots,x_j]f$ for $i\leqslant j$ and agree to write $c_{ij}=0$ for $j<i$.

These notations and the Leibniz formula allow writing the expressions (9) and (10) in the form

$$\sum_{j=0}^{n}[x_0,\ldots,x_j]q_{m,n}[x_j,\ldots,x_i]f=\sum_{j=0}^{n}b_jc_{ji}=a_i,\quad i=0,\ldots,m \tag{11}$$

$$\sum_{j=0}^{n}[x_0,\ldots,x_j]q_{m,n}[x_j,\ldots,x_i]f=\sum_{j=0}^{n}b_jc_{ji}=0,\quad i=m+1,\ldots,m+n. \tag{12}$$

We solve the homogeneous linear system (13)

$$\begin{pmatrix} c_{0,m+1} & c_{1,m+1} & \cdots & c_{n,m+1}\\ c_{0,m+2} & c_{1,m+2} & \cdots & c_{n,m+2}\\ \cdots & \cdots & \cdots & \cdots\\ c_{0,m+n} & c_{1,m+n} & \cdots & c_{n,m+n} \end{pmatrix}\begin{pmatrix} b_0\\ b_1\\ \vdots\\ b_n\end{pmatrix}=\begin{pmatrix}0\\0\\ \vdots\\ 0\end{pmatrix} \tag{13}$$

and replace coefficients b_i by the solution of the previous system to evaluate the coefficients a_i

$$\begin{pmatrix} c_{0,1} & c_{1,1} & \cdots & c_{n,1}\\ c_{0,2} & c_{1,2} & \cdots & c_{n,2}\\ \cdots & \cdots & \cdots & \cdots\\ c_{0,m} & c_{1,m} & \cdots & c_{n,m} \end{pmatrix}\begin{pmatrix} b_0\\ b_1\\ \vdots\\ b_n\end{pmatrix}=\begin{pmatrix}a_0\\a_1\\ \vdots\\ a_m\end{pmatrix} \tag{14}$$

the pair $(p_{m,n},q_{m,n})$ is called solution of the problem (m,n).

In its irreducible form the rational fraction $r_{mn}=\frac{p_{m,n}}{q_{m,n}}$ is called Newton Padé approximation at points (x_i,y_i), $i=0,\ldots,n+m$.

4.2. Numerical Illustration

Example 2. Take the example where $f=x^3$, the exact value of $I_0(f,\omega)$ is:

$$I_0(f,\omega)=\int_0^{\infty}x^3e^{-x}J_0(\omega x)\,dx=\frac{6-9\omega^2}{(1+\omega^2)^{7/2}}.$$

We calculated the value of $\sqrt{1+\omega^2}I_0(f,\omega)$ at points $\omega_i=i\frac{20}{10}$; $i=0,\ldots,10$ with a precision of 10^{-16}.

The corresponding systems (13) and (14) are:

$$\left(\begin{matrix} -0.0113356182420733 & 0.002083029929847342 & -0.001235127117018606 & 0.001269709812597944\\ 0.0010397308318536 & -0.000216946556299759 & 0.000154616096071708 & -0.000204353143207220\\ -0.0000793441970716 & 0.000018191795767885 & -0.000014815492212148 & 0.000022922831963725\\ 5.1828452389633052\text{E-}6 & -1.2778399789307833 10\text{E-}6 & 1.1539293821411881 32\text{E-}6 & -1.9940546328015974 81\text{E-}6\\ -2.9588148539742620\text{E-}7 & 7.727005699093842339\text{E-}8 & -7.586131462729672394\text{E-}8 & 1.4244518711056514 60\text{E-}7\\ 1.4999246055318725\text{E-}8 & -4.103435708948302369\text{E-}9 & 4.320088831857492375\text{E-}9 & -8.659932798402398111\text{E-}9 \end{matrix}\right.$$

$$\left.\begin{matrix} -0.001376532756853854 & 0 & 0\\ 0.000361473620565857 & -0.000573258044485283 & 0\\ -0.000051534263449056 & 0.000132432449681166 & -0.000278963711860471\\ 5.197901894377090178\text{E-}6 & -0.000016881584153208 & 0.000057403186778018\\ -4.113303315730958593\text{E-}7 & 1.541632280394015873\text{E-}6 & -6.604035617248117009\text{E-}6\\ 2.697941646519983783\text{E-}8 & -1.115590375153198834\text{E-}7 & 5.499963913689502434\text{E-}7 \end{matrix}\right)\begin{pmatrix}b_0\\b_1\\b_2\\b_3\\b_4\\b_5\\b_6\end{pmatrix}=\begin{pmatrix}0\\0\\0\\0\\0\\0\end{pmatrix},$$

$$\left(\begin{matrix} 6 & 0 & 0 & 0\\ -2.7826163360674363 & -0.1835918579276362 & 0 & 0\\ 0.6427314807560272 & 0.0739680228482402 & -0.1921847382448180 & 0\\ -0.0986780211108042 & -0.0151219933160009 & 0.0067591636660140 & -0.004198110118182618 \end{matrix}\right.$$

$$\left.\begin{matrix} 0 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0 \end{matrix}\right)\begin{pmatrix}b_0\\b_1\\b_2\\b_3\\b_4\\b_5\\b_6\end{pmatrix}=\begin{pmatrix}a_0\\a_1\\a_2\\a_3\end{pmatrix}.$$

We solved the first system after fixing $b_0 = 1$, then we replaced the solution obtained in the second system. The rational interpolant $r_{3,6}(\omega)$ obtained is

$$r_{3,6}(\omega) = \frac{6 - 20.0000000000000007B_1(\omega) - 9.00000000000000057B_2(\omega) + 1.3\text{E-}17B_3(\omega)}{\begin{array}{c}1 + 93.780758353232065B_1(\omega) + 862.68602347203175B_2(\omega) + 1027.6543209876544B_3(\omega)\\ +323.98765432098767B_4(\omega) + 33.333333333333335B_5(\omega) + 1.0000000000000001B_6(\omega)\end{array}} = \frac{6 - 9\omega^2}{1 + 3\omega^2 + 3\omega^4 + \omega^6}.$$

By rational interpolation, we found again the exact value of $I_0(x^3, \omega)$.

Remark 3. Rational interpolation is able to reproduce the value of $I_0(f,\omega)$ when f is a polynomial function. It is obvious that the more the values of $I_0(f,\omega)$ at the interpolation points are computed with great precision, more $I_0(f,\omega)$ is found with great precision.

Example 3. In this example, we consider the function $f(x) = x^2\sin(x)$, we do not know the exact value of $I_0(f,\omega)$. The function to integrate $f(x)\,e^{-x}J_0(\omega x)$ presents oscillations and decreases rapidly towards 0 as can be seen in Fig. 5. It is about to integrate this kind of functions on $[0,+\infty[$ for the different values of ω.

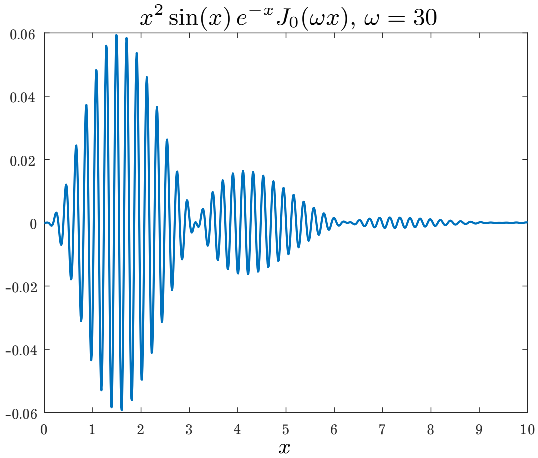


Fig. 5. The graph of function $x^2\sin(x)\,e^{-x}J_0(30x)$ over $[0,10]$.

For large ω, the oscillations of the function $f(x)\,e^{-x}J_0(\omega x)$ are very small, to see the effects of these oscillations on the value of the integral $I_0(f,\omega)$, we have to perform the calculation with high accuracy.

The stopping test will be taken on the relative error when the difference between two approximants is less than a fixed tolerance.

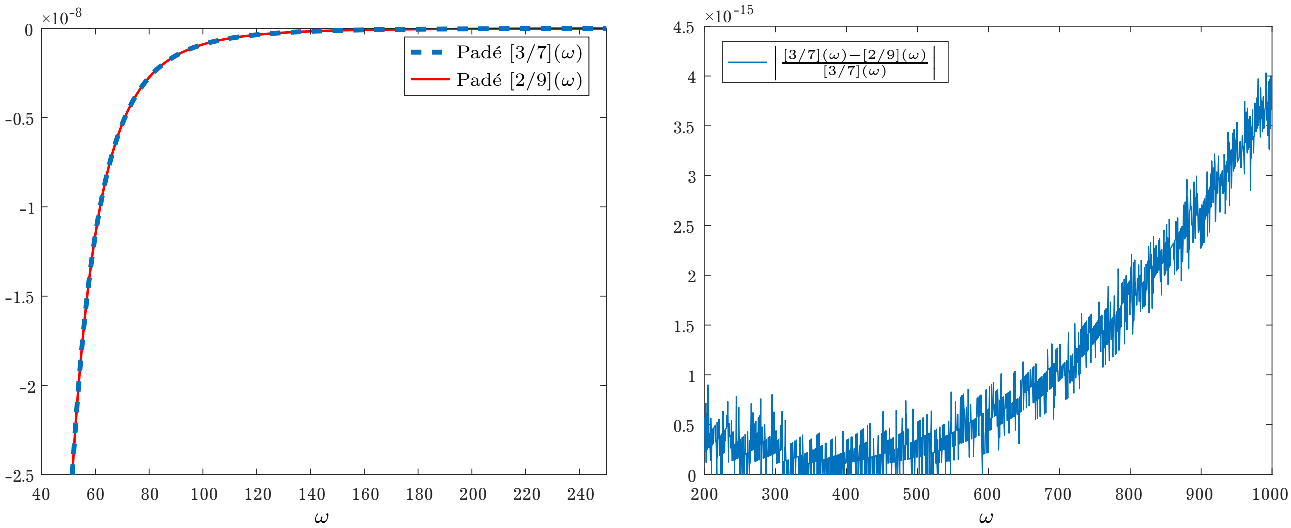
1. By Padé approximation:
   the power series expansion of $I_0(f,\omega)$ in the neighborhood of 100 calculated using the results of the Section 4 is:

$$\begin{aligned} S(\omega) = 10^{-10}\big(&-8.9999987750000952875 + 4.4999988975001238737\cdot10^{-1}X\\ &- 1.3499994487500867116\cdot10^{-2}X^2 + 3.1499979787504335581\cdot10^{-4}X^3\\ &- 6.2999939362517342322\cdot10^{-6}X^4 + 1.1339984234255896389\cdot10^{-7}X^5\\ &- 1.8899963213267689167\cdot10^{-9}X^6 + 2.9699921171298013451\cdot10^{-11}X^7\\ &- 4.4549842342620033619\cdot10^{-13}X^8 + 6.4349702202780078426\cdot10^{-15}X^9\\ &- 9.0089463965116172487\cdot10^{-17}X^{10} + 1.2284907412178836054\cdot10^{-18}X^{11}\\ &-1.6379845687007672081\cdot10^{-20}X^{12}\big), \end{aligned}$$

where $X = (\omega - 100)$,

$$[3/7]_I(\omega) = \frac{\begin{array}{c}10^{-10}(-8.9999987750000952875 - 1.9799983912574046926\cdot10^{-1}X\\ -1.0999976926096351538\cdot10^{-3}X^2 + 1.5877737314850609655\cdot10^{-21}X^3)\end{array}}{\begin{array}{c}1 + 7.1999979675080121990\cdot10^{-2}X + 2.2222209825687163937\cdot10^{-3}X^2\\ +3.8111079222604691833\cdot10^{-5}X^3 + 3.9222178029078275217\cdot10^{-7}X^4\\ +2.4222187510981534838\cdot10^{-9}X^5 + 8.3110965047839775848\cdot10^{-12}X^6\\ +1.2222196584551487595\cdot10^{-14}X^7\end{array}},$$

$$[2/9]_I(\omega) = \frac{\begin{array}{c}-8.9999987750000952875\cdot 10^{-10} - 1.9636342369141050301\cdot 10^{-11}X \\ -1.0799970405840839856\cdot 10^{-13}X^2\end{array}}{\begin{array}{c}1 + 0.071818155713184088 4X + 0.0022109074904918605X^2 \\ +0.000037818140548956 8X^3 + 3.8818124624979933921\cdot 10^{-7}X^4 \\ +2.3909046075457080652\cdot 10^{-9}X^5 + 8.1817993775939180636\cdot 10^{-12}X^6 \\ +1.1999967117600924513\cdot 10^{-14}X^7 + 4.3303161476595500476\cdot 10^{-32}X^8 \\ -1.4434428464760682279\cdot 10^{-34}X^9\end{array}}.$$



a ***b***

Fig. 6. (***a***) The Padé approximants $[3/7](\omega)$ and $[2/9](\omega)$ superposed; (***b***) The normalized relative error $\left|\frac{[3/7](\omega)-[2/9](\omega)}{[3/7](\omega)}\right|$.

Given that the normalized relative error $\left|\frac{[3/7](\omega)-[2/9](\omega)}{[3/7](\omega)}\right| < 4.5\cdot 10^{-15}$ as shown in the figure 6 is very small, we can decide that $I_0(f,\omega) \simeq [2/9]_I(\omega)$.

Table 1. Estimation of $I_0(f,300)$ and $I_0(f,500)$ by the sequence of Padé approximation $([1/n]_I)_n$.

n	$[1/n]_I(300)$	n	$[1/n]_I(500)$
1	$3.8571427321429632946\cdot 10^{-10}$	1	$4.8461537664202498399\cdot 10^{-10}$
2	$3.1034483195599147956\cdot 10^{-11}$	2	$2.7835052132265919293\cdot 10^{-11}$
3	$3.5724323120431271660\cdot 10^{-25}$	3	$1.9607843166329273292\cdot 10^{-12}$
4	$-3.4047919241226675 84\cdot 10^{-12}$	4	$-1.2463647693058681 99\cdot 10^{-13}$
5	$-3.7037036974799017 67\cdot 10^{-12}$	5	$-2.8799999993720941 99\cdot 10^{-13}$
6	$-3.7037036974800578 85\cdot 10^{-12}$	6	$-2.8799999993727966 99\cdot 10^{-13}$
7	$-3.7037036974800610 71\cdot 10^{-12}$	7	$-2.8799999993728134 25\cdot 10^{-13}$
8	$-3.7037036974800546 47\cdot 10^{-12}$	8	$-2.8799999993727455 74\cdot 10^{-13}$
9	$-3.7037036974800675 78\cdot 10^{-12}$	9	$-2.8799999993730200 97\cdot 10^{-13}$
10	$-3.7037036974800415 77\cdot 10^{-12}$	10	$-2.8799999993719115 53\cdot 10^{-13}$

2. By rational interpolation:
   The data to be interpolated are given by the table 2.
   The rational interpolants $r_{4,7}, r_{5,9}$ and $r_{7,13}$ are

$$r_{4,7}(\omega) = \frac{\begin{array}{c}-12801.1109960405344 + 6587.51374583276525\,\omega - 65.9492500687815791\,\omega^2 \\ -6.08022793792171594\cdot 10^{-13}\omega^3 + 7.78845289295888383\cdot 10^{-15}\omega^4\end{array}}{\begin{array}{c}-4.3838831790378849598\cdot 10^2 + 1.9395672958284531074\cdot 10^4\omega \\ -9.9640318148317067608\cdot 10^3\omega^2 + 99.773277506404582625\,\omega^3 \\ -5.7505458110699951969\cdot 10^{-4}\omega^4 + 1.4223456726257934167\cdot 10^3\omega^5 \\ -7.3194597180736612478\cdot 10^2\omega^6 + 7.3276944523222563912\,\omega^7\end{array}},$$

Table 2. The interpolation data $(\omega_i, I_0(f, \omega_i))$.

i	ω_i	$I_0(x^2\sin(x),\omega_i)$	i	ω_i	$I_0(x^2\sin(x),\omega_i)$
1	52	$-2.367145660847615621\cdot 10^{-8}$			
2	57	$-1.495779824667872412\cdot 10^{-8}$	19	142	$-1.558837242221159135\cdot 10^{-10}$
3	62	$-9.823893867087002936\cdot 10^{-9}$	20	147	$-1.311160396833317617\cdot 10^{-10}$
4	67	$-6.666044408976445536\cdot 10^{-9}$	21	152	$-1.109237539054592803\cdot 10^{-10}$
5	72	$-4.651358431400013164\cdot 10^{-9}$	22	157	$-9.435050687845589383\cdot 10^{-11}$
6	77	$-3.324977535413527886\cdot 10^{-9}$	23	162	$-8.066171064699103363\cdot 10^{-11}$
7	82	$-2.427577573770022920\cdot 10^{-9}$	24	167	$-6.928833831006382060\cdot 10^{-11}$
8	87	$-1.805702266491429080\cdot 10^{-9}$	25	172	$-5.978610604912353987\cdot 10^{-11}$
9	92	$-1.365536428080646926\cdot 10^{-9}$	26	177	$-5.180553602000757216\cdot 10^{-11}$
10	97	$-1.048054269066695896\cdot 10^{-9}$	27	182	$-4.506979307387018237\cdot 10^{-11}$
11	102	$-8.151576263444116048\cdot 10^{-10}$	28	187	$-3.935813145499952867\cdot 10^{-11}$
12	107	$-6.416874949034220817\cdot 10^{-10}$	29	192	$-3.449342834398048321\cdot 10^{-11}$
13	112	$-5.106841259720135773\cdot 10^{-10}$	30	197	$-3.033272129440746786\cdot 10^{-11}$
14	117	$-4.105000072854733818\cdot 10^{-10}$	31	202	$-2.675997224517686465\cdot 10^{-11}$
15	122	$-3.329993067538656782\cdot 10^{-10}$	32	207	$-2.368049514234511567\cdot 10^{-11}$
16	127	$-2.724105242070831996\cdot 10^{-10}$	33	212	$-2.101663597024152677\cdot 10^{-11}$
17	132	$-2.245809082831983374\cdot 10^{-10}$	34	217	$-1.870440241517230513\cdot 10^{-11}$
18	137	$-1.864831759229707714\cdot 10^{-10}$	35	222	$-1.669081850811516161\cdot 10^{-11}$

$$r_{5,9}(\omega) = \frac{\begin{array}{c} -36.922974666133073819\cdot 10^{7} + 36.719894684322817323\cdot 10^{6}\omega \\ -9.759225087778284241\,9\cdot 10^{5}\omega^2 + 9.918786190110692151\,9\cdot 10^{3}\omega^3 \\ -34.577455822338253003\,\omega^4 - 12.875242914303055989\cdot 10^{-15}\omega^5 \end{array}}{\begin{array}{c} -4.0771543453518027019\cdot 10^{5} + 5.5843500761934390426\cdot 10^{8}\omega \\ -5.5534349097166618986\cdot 10^{7}\omega^2 + 1.4759588732103918332\cdot 10^{6}\omega^3 \\ -1.5001046437997136563\cdot 10^{4}\omega^4 + 4.1025579704396603913\cdot 10^{7}\omega^5 \\ -4.0799882982931623064\cdot 10^{6}\omega^6 + 1.0843583430883748905\cdot 10^{5}\omega^7 \\ -1.1020873544574265673\,2\cdot 10^{3}\omega^8 + 3.8419395358168302805\,\omega^9 \end{array}},$$

$$r_{7,13}(\omega) = \frac{\begin{array}{c} -6.1780876874580232449\cdot 10^{10} + 7.5903175833249574003\cdot 10^{9}\omega \\ -3.2581668527941485652\cdot 10^{8}\omega^2 + 7.0134345325262674211\cdot 10^{6}\omega^3 \\ -8.5127909385503465429\cdot 10^{4}\omega^4 + 5.9473426837625185631\cdot 10^{2}\omega^5 \\ -2.2410525087374838636\,\omega^6 + 3.5399710224764226372\cdot 10^{-3}\omega^7 \end{array}}{\begin{array}{c} 6.0884090773555800580\cdot 10^{7} + 9.3440256675331218087\cdot 10^{10}\omega \\ -1.1479482111186115503\cdot 10^{10}\omega^2 + 4.9275637783993947706\cdot 10^{8}\omega^3 \\ -1.0606923261700306505\cdot 10^{7}\omega^4 + 6.8646706206197633344\cdot 10^{9}\omega^5 \\ -8.4336951984591605116\cdot 10^{8}\omega^6 + 3.6201857309466624452\cdot 10^{7}\omega^7 \\ -7.7927050896958013612\cdot 10^{5}\omega^8 + 9.4586565983986156465\cdot 10^{3}\omega^9 \\ -6.6081585375172516709\cdot 10^{1}\omega^{10} + 0.2490058343042467263\,\omega^{11} \\ -3.9333011360861424396\cdot 10^{-4}\omega^{12} + 8.5229359953197712895\cdot 10^{-20}\omega^{13} \end{array}}.$$

Fig. 8 shows that, the relative errors $\|r_{4,7} - r_{5,9}\| \leqslant 4.5\cdot 10^{-23}$ and $\|r_{5,9} - r_{7,13}\| \leqslant 1.4\cdot 10^{-26}$ decrease, also in Fig. 9 the normalized relative error $\left\|\frac{r_{4,7}-r_{5,9}}{r_{4,7}}\right\| \leqslant \cdot 10^{-11}$ and $\left\|\frac{r_{5,9}-r_{7,13}}{r_{5,9}}\right\| \leqslant \cdot 10^{-13}$ also decreases, we can take $r_{7,13}(\omega)$ as an approximation of $I_0(f,\omega)$ with an error of the order of 10^{-13} based on the normalized relative error that is significant.

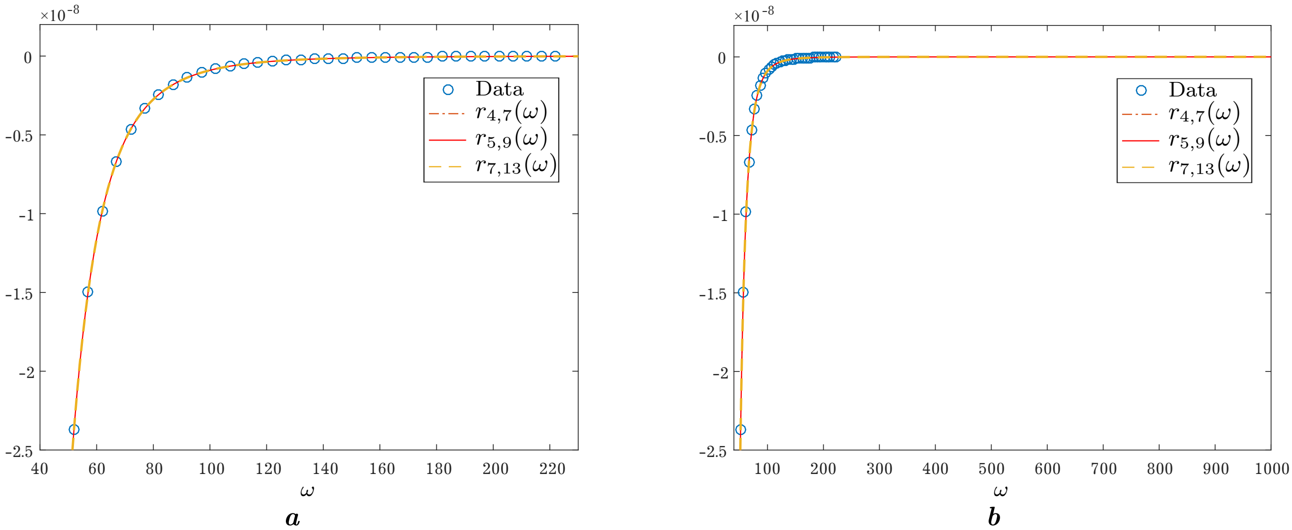


Fig. 7. Rational Interpolation $r_{4,7}(\omega)$, $r_{5,9}(\omega)$ and $r_{7,13}(\omega)$ on the data interval and outside data interval.

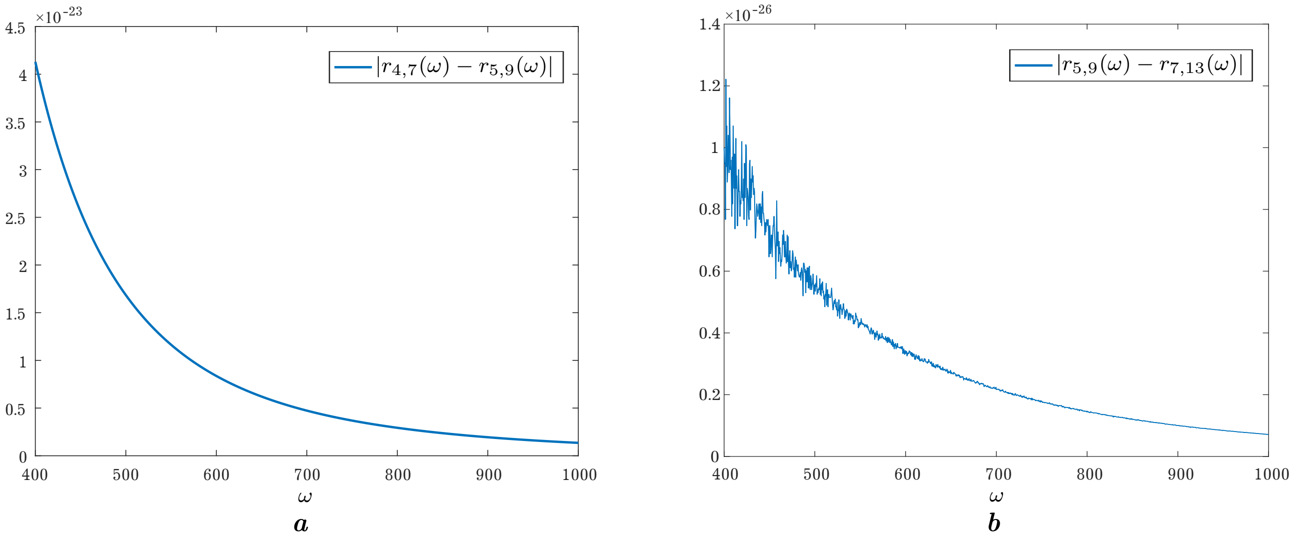


Fig. 8. Relative errors of rational interpolants: $|r_{4,7}(\omega) - r_{5,9}(\omega)|$ and $|r_{5,9}(\omega) - r_{7,13}(\omega)|$.

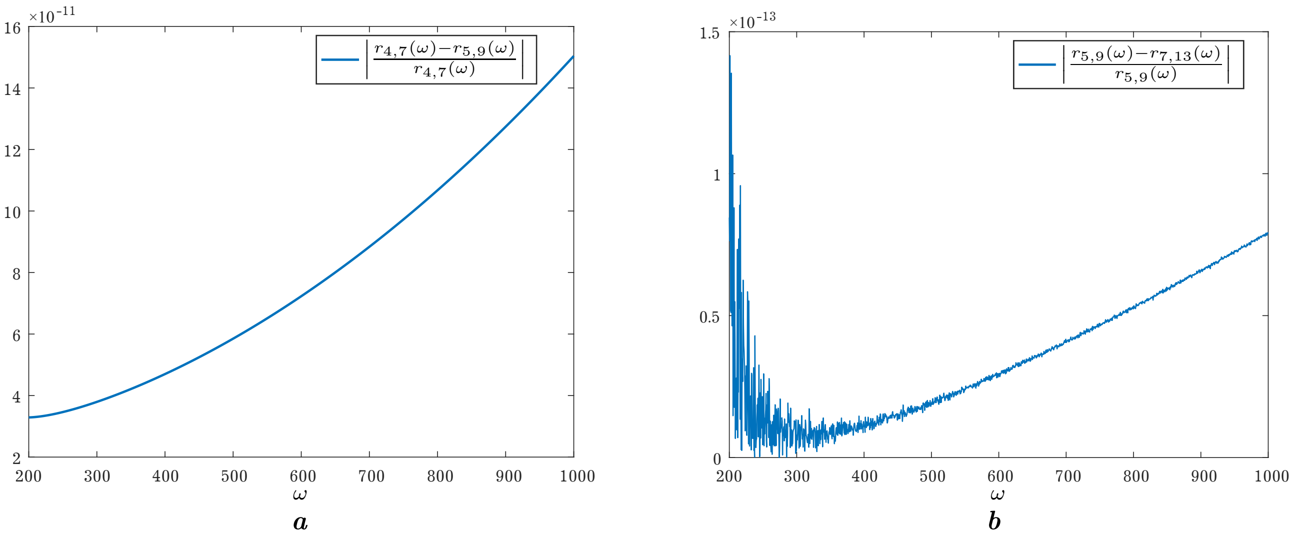


Fig. 9. Normalized relative errors of rational interpolants $\left|\frac{r_{4,7}(\omega)-r_{5,9}(\omega)}{r_{4,7}(\omega)}\right|$ and $\left|\frac{r_{5,9}(\omega)-r_{7,13}(\omega)}{r_{5,9}(\omega)}\right|$.

5. Conclusion

In the introduction, we explained the need to evaluate the integral

$$\int_0^\infty f(t)\, e^{-t} J_0(\omega t)\, dt$$

with fairly wide values of ω. This evaluation can not be done by classical quadrature methods even the most powerful among them, that of Gauss–Laguerre. We did not look for improving the existing quadrature methods but to exploit it to estimate the value of this integral considered as a function of the variable ω with a large values of ω. Thus, we have exploited the method developed by Feuillebois to evaluate this integral with relatively small values of ω that we used in Padé approximation or the rational interpolation. The use of this data effectively relies on a result that we have demonstrated in this paper. The extrapolation that we have proposed is an alternative to surpass the limits ω_0 of the other methods of computation of this integral for $\omega > \omega_0$.

[1] Blake J. R. A note on the image system for a Stokeslet in a no-slip boundary. Mathematical Proceedings of the Cambridge Philosophical Society. **70** (2), 303–310 (1971).

[2] Elasmi L., Feuillebois F. Green function for a Stokes flow near a porous slab. ZAMM – Journal of Applied Mathematics and Mechanics. **81** (11), 743–752 (2001).

[3] Khabthani S., Sellier A., Elasmi L., Feuillebois F. Motion of a solid particle in a shear flow along a porous slab. Journal of Fluid Mechanics. **713**, 271–306 (2012).

[4] Debbech A., Elasmi L., Feuillebois F. The method of fundamental solution for the creeping flow around a sphere close to a membrane. ZAMM – Journal of Applied Mathematics and Mechanics. **90** (12), 920–928 (2010).

[5] Elasmi L., Feuillebois F. Integral equation method for creeping flow around a solid body near a porous slab. The Quarterly Journal of Mechanics and Applied Mathematics. **56** (2), 163–185 (2003).

[6] Assoudi R., Chaoui M., Feuillebois F., Allouche H. Motion of a spherical particle along a rough wall in a shear flow. Zeitschrift für angewandte Mathematik und Physik. **69** (5), Article number: 112 (2018).

[7] Chaoui M., Feuillebois F. Creeping flow around a sphere in a shear flow close to a wall. The Quarterly Journal of Mechanics and Applied Mathematics. **56** (3), 381–410 (2003). Corrigendum: ibid. **65** (4), 581 (2012).

[8] Abramovitz M., Stegun I. A. Handbook of Mathematical Functions with Formulas Graphs and Mathematical Tables. A.M.S. (1964).

[9] Feuillebois F. Numerical calculation of singular integrals related to Hankel transform. Computers & Mathematics with Applications. **21** (2–3), 87–94 (1991).

[10] Muller J.-M. Elementary Functions Algorithms and Implementation. Birkhäuser Basel (2016).

[11] Baker G. A., Graves–Morris P. R. Padé approximants. Cambridge University Press (1996).

[12] Werner H., Wuytack L. On the continuity of the Padé operator. SIAM Journal on Numerical Analysis. **20** (6), 1273–1280 (1983).

[13] Allouche H., Tazdayte A. Numerical solution of singular boundary value problems with logarithmic singularities by Padé approximation and collocation methods. Journal of Computational and Applied Mathematics. **311**, 324–341 (2017).

[14] Claessens G. On the Newton–Padé approximation problem. Journal of Approximation Theory. **22** (2), 150–160 (1978).

Високоточний метод обчислення сингулярного інтеграла, пов'язаного з перетворенням Ганкеля

Ассуді Р.[1,3], Бугтаб С.[2], Алуш Х.[2], Ламзуд К.[3], Фейлбуа Ф.[4], Чауї М.[3]

[1] *Лабораторія LGEMS, Національна школа прикладних наук, Університет Ібн Зохра, Агадір, Марокко*
[2] *Наукова група MANTA, кафедра математики та комп'ютерних наук , Університет Мулая Ісмаїла, Мекнес, Марокко*
[3] *Кафедра фізики, Університет Мулая Ісмаїла, Мекнес, Марокко*
[4] *LIMSI–CNRS, Орсе, Франція*

У цій роботі нас цікавить апроксимація інтеграла

$$I_0(f,\omega) = \int_0^\infty f(t)\, e^{-t}\, J_0(\omega t)\, dt$$

для досить великих значень ω. Цей сингулярний інтеграл походить від перетворення Ганкеля порядку 0, $f(x)$ є функцією, з якою інтеграл є збіжним.
Для досить великих значень ω класичні квадратурні методи непридатні, а з іншого боку, ці методи застосовні для відносно малих значень ω. Більше того, усі квадратурні методи зводяться до оцінки функції, що інтегрується у вузлах розбиття інтервалу інтегрування, звідси випливає необхідність оцінювати експоненціальну функцію та функцію Бесселя у досить великих вузлах інтервалу $]0,+\infty[$.
Ідея полягає в тому, щоб мати значення $I_0(f,\omega)$ з великою точністю для великих ω без необхідності вдосконалювати чисельний метод обчислення інтегралів, просто вивчаючи поведінку функції $I_0(f,\omega)$ та екстраполюючи її.
Використовується два підходи до екстраполяції $I_0(f,\omega)$. Перший з них — це апроксимація Паде $I_0(f,\omega)$, а другий — раціональна інтерполяція.

Ключові слова: *сингулярний інтеграл, перетворення Ганкеля, Гаусс–Лагерра, екстраполяція, апроксимація Пад'е, раціональна інтерполяція.*