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An Accurate Numerical Method for the Computation of a class of Generalized Cosine Integrals

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Abstract. We develop an efficient and accurate method to compute the quadrature of an oscillatory integral arising in the discretization of the fractional Laplacian operator. The complete mathematical development is presented. The implementation, performed in modern C++, is provided as open-source software and proves to produce results with accuracy up to a few ulps.

Keywords. Generalized Cosine Integral, Numerical Quadratures, Asymptotic Approximations of Integrals, Double Exponential Quadrature, Numerical Methods in C++, Fractional Laplacian.

1 Introduction

This work aims to construct an accurate numerical method to compute the following oscillatory integrals $\boldsymbol{\mathcal{I}}_k(\alpha, h)$ depending on the parameters $\alpha, h \in \mathbb{R}$ and $k \in \mathbb{Z}$:

$$\boldsymbol{\mathcal{I}}_k(\alpha, h) = \frac{1}{\pi h^\alpha} \int_0^\pi \cos(k\theta)\, \theta^\alpha \,\mathrm{d}\theta = \frac{\mathrm{Ci}\,(\alpha+1, k\pi)}{\pi h^\alpha k^{\alpha+1}}\,, \quad \text{subject to } \alpha \in [0,2] \text{ and } h > 0\,. \tag{1}$$

The special function $\mathrm{Ci}\,(a, x)$ is the **Generalized Cosine Integral** [5, (8.21.7)], which has the representation

$$\mathrm{Ci}\,(a, x) = \int_0^x \cos(t)\, t^{a-1} \,\mathrm{d}t\,, \quad \text{for } a > 0\,. \tag{2}$$

(In what follows, we will write $\boldsymbol{\mathcal{I}}_k$ instead of $\boldsymbol{\mathcal{I}}_k(\alpha, h)$. Also, k will be considered belonging to the naturals $\mathbb{N} = \{0,\, 1,\, 2,\, \ldots\}$ since the integrals in equation (1) are invariant under change of sign in k.) Such integrals arise in spectral numerical methods to approximate the one-dimensional fractional Laplacian operator of band limited functions [7, p. 10]; this hypersingular operator being the focus of our current research. To be more precise to the reader, the power θ^α in equation (1) is the Fourier multiplier of the referred operator, $\mathcal{F}((-\nabla^2)^{\alpha/2} f)(\omega) = |\omega|^\alpha \widehat{f}(\omega)$, where $(-\nabla^2)^{\alpha/2}$ represents the fractional Laplacian.

For $k = 0$, the expression in equation (1) reduces to $\boldsymbol{\mathcal{I}}_0 = \pi^\alpha / \big(h^\alpha(\alpha+1)\big)$. In the general case, one can represent the integrals in terms of the generalized hypergeometric function ${}_1F_2$ as

$$\frac{h^\alpha(\alpha+1)\,\boldsymbol{\mathcal{I}}_k}{\pi^\alpha} = {}_1F_2\left(\frac{\alpha+1}{2}; \frac{1}{2}, \frac{3+\alpha}{2}; -\frac{k^2\pi^2}{4}\right), \tag{3}$$

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which is defined as a power series on k whose radius of convergence is infinite. However, power series are not suitable for calculating numerically the values of $\boldsymbol{\mathcal{I}}_k$ when k goes to infinity: as the argument $-k^2\pi^2/4$ decreases, the series of ${}_1F_2$ converges more slowly[5].

Remark 1.1. *Aside from the Generalized Cosine Integral in equation* (2)*, we also need to use the standard* **Sine and Cosine Integrals** $\mathrm{Si}\,(x)$ [2, (5.2.1)] *and* $\mathrm{Ci}\,(x)$ [2, (5.2.27)] *defined as*

$$\mathrm{Si}\,(x) = \int_0^x \frac{\sin(t)}{t}\,\mathrm{d}t \quad \textit{and} \quad \mathrm{Ci}\,(x) = -\int_x^\infty \frac{\cos(t)}{t}\,\mathrm{d}t\,, \tag{4}$$

and the relation (*which can be verified using the identities given in* [2, p. 231])

$$-k\int_0^\pi \sin(k\theta)\ln(\theta)\,\mathrm{d}\theta = \int_0^{k\pi} \frac{1-\cos(\theta)}{\theta}\,\mathrm{d}\theta = \gamma + \ln(k\pi) - \mathrm{Ci}\,(k\pi)\,, \quad \textit{for } k>0 \textit{ even}, \tag{5}$$

where γ *is the* **Euler-Mascheroni constant***.*

2 Asymptotic expressions for large k

To accurately compute the values of $\boldsymbol{\mathcal{I}}_k$ for large k, we start by looking for an asymptotic expression for it. We begin with the following lemma, which can be easily proved integrating by parts $\int_0^\pi \cos(k\theta)\,\theta^\alpha\,\mathrm{d}\theta = -\alpha k^{-1-\alpha}\int_0^{k\pi}\sin(\theta)\,\theta^{\alpha-1}\,\mathrm{d}\theta$:

Lemma 2.1. *Suppose* $\alpha > -1$ *and* $k > 0$*. Therefore,*

$$\mathrm{Ci}\,(\alpha+1, k\pi) = k^{\alpha+1}\int_0^\pi \cos(k\theta)\,\theta^\alpha\,\mathrm{d}\theta = -\alpha I_k(\alpha)\,, \tag{6}$$

where we define the function I_k *by*

$$I_k(\alpha) := \int_0^{k\pi} \sin(\theta)\,\theta^{\alpha-1}\,\mathrm{d}\theta\,, \quad \textit{for } \alpha > -1 \textit{ and } k \textit{ a positive integer}. \tag{7}$$

Remark 2.1. *We remark that the integral in equation* (7) *is well-defined despite the singularity near the origin because* $\left|\int_0^{k\pi}\sin(\theta)\,\theta^{\alpha-1}\,\mathrm{d}\theta\right| \le \left.\frac{\theta^{\alpha+1}}{\alpha+1}\right|_0^{k\pi} = \frac{(k\pi)^{\alpha+1}}{\alpha+1} < \infty$*, since* $|\sin(\theta)| \le \theta$ *for* $\theta \ge 0$*.*

It is worth:

Lemma 2.2. *Let* $\beta < 0$ *and define*

$$J_k(\beta) := (-1)^k (k\pi)^{-\beta}\int_0^\infty \sin(\theta)\,\theta^\beta\,\mathrm{d}\theta\,. \tag{8}$$

[5] In fact, the implementation available in the current release of **Boost Math Library** [8] for the hypergeometric function fails with the exception `"Cancellation is so severe that no bits in the result are correct..."` in calculating the value of ${}_1F_2$ in equation (3) for k large (depending on α) using double-precision arithmetic. To show this failure we present the example source code available at `https://github.com/gffrnl/generalized-cosine-integrals-kpi/blob/main/misc/boost_1F2_failure.cpp`. The details for compilation and usage are available in the source code. Unfortunately, the current release of Boost Math Library (1.84.0) does not furnish a specialized method to compute ${}_1F_2$, so we had to use the general purpose method to compute the generalized hypergeometric function ${}_pF_q$. We refer to `https://www.boost.org/doc/libs/1_84_0/libs/math/doc/html/math_toolkit/hypergeometric.html` for further details.

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(The convergence of this improper integral is guaranteed by the Dirichlet test, noting that the function θ^β is monotonically decreasing and converges to zero as $\theta \to \infty$, while $\left|\int_{k\pi}^{t} \sin(\theta)\, \mathrm{d}\theta\right| \leq 2$ for all $t \geq k\pi$.) Thus, J_k satisfies the recurrence relation

$$J_k(\beta) = 1 - \frac{\beta(\beta-1)}{(k\pi)^2}\, J_k(\beta-2)\,. \tag{9}$$

(The recurrence identity in equation (9) is obtained integrating by parts twice.)

Remark 2.2. *The recurrence relation (9) allows us to extend the definition of $J_k(\beta)$ to $\beta \geq 0$, even if the integral in equation (8) is not well-defined for $\beta > 0$. In addition to its computational practicality, this observation will be used to prove the following proposition.*

Proposition 2.1. *Suppose $\alpha \in (0, 2)$ and $k > 0$. Thus, we have*

$$I_k(\alpha) = \Gamma(\alpha)\, \sin\left(\frac{\pi\alpha}{2}\right) - (-1)^k (k\pi)^{\alpha-1} J_k(\alpha-1) \tag{10}$$

and, consequently,

$$\mathrm{Ci}\,(\alpha+1, k\pi) = -\alpha\, \Gamma(\alpha)\, \sin\left(\frac{\pi\alpha}{2}\right) + (-1)^k (k\pi)^{\alpha-1} \alpha\, J_k(\alpha-1)\,. \tag{11}$$

Proof. We first look the case $0 < \alpha < 1$, i.e., in which the following identity holds [4, (5.9.7)]:

$$\int_0^\infty \sin(y)\, \theta^{\alpha-1} \mathrm{d}y = \Gamma(\alpha)\, \sin\left(\frac{\pi\alpha}{2}\right), \quad \text{for } \alpha \in (0, 1)\,.$$

By the last identity, we are allowed to write $I_k(\alpha) = \Gamma(\alpha)\, \sin\left(\frac{\pi\alpha}{2}\right) - \int_{k\pi}^{\infty} \sin(\theta)\, \theta^{\alpha-1}\, \mathrm{d}\theta$ and, using the definition of J_k in Lemma 2.2, the equation (10) holds.

The case $\alpha \in (1, 2)$ is treated similarly. We apply integration by parts to the definition of $I_k(\alpha)$ to obtain

$$\begin{aligned} I_k(\alpha) &= (-1)^{k+1}(k\pi)^{\alpha-1} + (\alpha-1) \int_0^{k\pi} \cos(\theta)\, \theta^{\alpha-2}\, \mathrm{d}\theta \\ &= \Gamma(\alpha)\, \sin\left(\frac{\pi\alpha}{2}\right) + (-1)^{k+1}(k\pi)^{\alpha-1} - (\alpha-1) \int_{k\pi}^{\infty} \cos(\theta)\, \theta^{\alpha-2}\, \mathrm{d}\theta\,, \end{aligned} \tag{12}$$

where we used the fact that for $\alpha \in (1, 2)$ the following identity holds [4, (5.9.6)]:

$$\int_0^\infty \cos(\theta)\, \theta^{\alpha-2}\, \mathrm{d}\theta = \Gamma(\alpha-1) \cos(\pi(\alpha-1)/2) = \frac{\Gamma(\alpha)}{\alpha-1}\, \sin\left(\frac{\pi\alpha}{2}\right).$$

We can now use the recurrence relation given in equation (9) in the extended domain of definition for $\beta > 0$ (see Remark 2.2) to obtain

$$J_k(\alpha-1) = 1 - \frac{(\alpha-1)(\alpha-2)}{(k\pi)^2}\, J_k(\alpha-3)\,,$$

which can be used to write the integral involving the cosine function in equation (12) in terms of $J_k(\alpha-1)$ as

$$\begin{aligned} \int_{k\pi}^{\infty} \cos(\theta)\, \theta^{\alpha-2}\, \mathrm{d}\theta = -(\alpha-2) \int_{k\pi}^{\infty} \sin(\theta)\, \theta^{\alpha-3}\, \mathrm{d}\theta &= (-1)^{k+1}(\alpha-2)(k\pi)^{\alpha-3} J_k(\alpha-3) \\ &= \frac{(-1)^{k+1}(k\pi)^{\alpha-1}}{\alpha-1}\big[1 - J_k(\alpha-1)\big]\,. \end{aligned} \tag{13}$$

Finally, one proves the claim by substituting equation (13) in equation (12). □

Asymptotics of $J_k(\beta)$

The function $J_k(\beta)$ was defined in equation (8) for $\beta < 0$ and satisfies the recurrence relation given in equation (9), which allowed us to extend its domain of definition to $\beta \geq 0$. We now claim the following estimate for J_k:

Proposition 2.2. *If $k > 0$ and $\beta < 0$, then $|J_k(\beta)| \leq 2$.*

Proposition 2.2 implies the following asymptotic behavior for J_k, obtained by substituting (9) recursively:

$$J_k(\beta) = 1 - \frac{(\beta)_2}{(k\pi)^2} + \frac{(\beta)_4}{(k\pi)^4} - \cdots + (-1)^n \frac{(\beta)_{(2n)}}{(k\pi)^{2n}} + O\left(k^{-2n-2}\right), \quad k \to \infty . \tag{14}$$

The symbol $(a)_n$ in equation (14) denotes the **Pochhammer Symbol** for the descending factorial, defined as $(\beta)_n := \beta(\beta-1)\cdots(\beta-n+1)$.

Remark 2.3. *Note that the series in equation* (14) *converges in k for all fixed β and number of terms n. Nonetheless, the series is divergent in n for fixed β, as the terms in the numerators grow factorially.*

Proof of Proposition 2.2. We first note that

$$\begin{aligned}\int_{n\pi}^{(n+2)\pi} \sin(\theta)\,\theta^\beta \,\mathrm{d}\theta &= \int_0^\pi \left[(n\pi+\theta)^\beta - ((n+1)\pi+\theta)^\beta\right] \sin(n\pi+\theta)\,\mathrm{d}\theta \\ &= (-1)^n \int_0^\pi \left[(n\pi+\theta)^\beta - ((n+1)\pi+\theta)^\beta\right] \sin(\theta)\,\mathrm{d}\theta\,.\end{aligned}$$

Since $\beta < 0$, then $f(\theta) := (n\pi+\theta)^\beta - ((n+1)\pi+\theta)^\beta$ is a non-negative decreasing function in the interval $[0,\pi]$; therefore, using that $n \geq k > 0$, we have the following estimate:

$$\left|\int_{n\pi}^{(n+2)\pi} \sin(\theta)\,\theta^\beta \,\mathrm{d}\theta\right| \leq \int_0^\pi \left[(n\pi)^\beta - ((n+1)\pi)^\beta\right] \sin(\theta)\,\mathrm{d}\theta = 2\pi^\beta \left[(n)^\beta - (n+1)^\beta\right].$$

We now sum all periods to obtain an alternating series, which is bounded by its first term, and get the estimate

$$\left|\int_{k\pi}^{\infty} \sin(\theta)\,\theta^\beta \,\mathrm{d}\theta\right| \leq 2\pi^\beta \left[(k)^\beta - (k+1)^\beta + (k+2)^\beta - (k+3)^\beta + \cdots\right] \leq 2\pi^\beta k^\beta\,,$$

which proves the claim. □

When k is large enough, we can simply truncate the expansion in equation (14) when the term in the summation is smaller than the machine precision or than a given tolerance fixed beforehand. As the terms are alternating and decreasing, the truncation error is bounded by the first omitted term.

3 Numerical quadrature for small k

While the integrals $\boldsymbol{\mathcal{I}}_k$ for large k may be obtained by using the asymptotic expansion given in equation (14), those for which k is small must be calculated by other means, such as numerical quadrature. In order to create a standalone code, i.e., which does not require extended precision quadrature, we approximate the integrals involved by rational functions. When using the double-precision floating-point arithmetic (**IEEE Std 754-2008 "binary64"** [1]), all digits can be obtained solely by the asymptotic formula when $k > 10$.

The representation of $\boldsymbol{\mathcal{I}}_k(\alpha, h)$ in terms of the hypergeometric function in equation (3) motivated us to implement a function in the following form:

$$\int_0^\pi \cos(k\theta)\,\theta^\alpha\,\mathrm{d}\theta = \begin{cases} \pi^\alpha \alpha\, f_k(\alpha)\,, & \text{if } k \text{ is odd}\,, \\ \pi^\alpha \alpha(\alpha-1)\, f_k(\alpha)\,, & \text{if } k \text{ is even}\,. \end{cases} \tag{15}$$

where $f_k(\alpha)$ is a rational function on α. We remark that in equation (15) the zeros of the functions were factorized in the expression so we retain relative accuracy close to those points. We supplement this problem with the following condition:

$$f_k(0) = \lim_{\alpha\to 0} \frac{1}{\alpha} \int_0^\pi \cos(k\theta)\,\theta^\alpha\,\mathrm{d}\theta = \lim_{\alpha\to 0} \int_0^\pi \cos(k\theta) \left(\frac{\theta^\alpha - 1}{\alpha}\right) \mathrm{d}\theta = -\frac{\mathrm{Si}(k\pi)}{k}\,. \tag{16}$$

Moreover, when k is even, we impose:

$$\begin{aligned} f_k(1) &= \lim_{\alpha\to 1} \frac{1}{\alpha(\alpha-1)\pi} \int_0^\pi \cos(k\theta)\,\theta^\alpha\,\mathrm{d}\theta = \lim_{\alpha\to 1} \frac{1}{\alpha\pi} \int_0^\pi \cos(k\theta) \left(\frac{\theta^\alpha - 1}{\alpha - 1}\right) \mathrm{d}\theta \\ &= \frac{1}{\pi} \int_0^\pi \cos(k\theta)\,\theta \ln(\theta)\,\mathrm{d}\theta = -\frac{1}{k\pi} \int_0^\pi \sin(k\theta) \ln(\theta)\,\mathrm{d}\theta = \frac{\gamma + \ln(k\pi) - \mathrm{Ci}(k\pi)}{k^2\pi}\,. \end{aligned} \tag{17}$$

(The last identity holds by equation (5).) We refer the reader to equation (4) in Remark 1.1 for the definitions of $\mathrm{Si}(x)$ and $\mathrm{Ci}(x)$.

4 Software availability and implementation details

The software for the method was implemented in the **C++ programming language** in a single header file `gcikpi.hpp`[6], and we also provided a **Python interface**. All software is publicly available in a repository at `https://github.com/gffrnl/generalized-cosine-integrals-kpi`[7] licensed under **MIT License** to be permissive regarding code reuse and modification[8].

The quadrature for small k mentioned in Section 3 was performed using the **Double Exponential Method** (tanh-sinh) [3, 11] *in multiple-precision arithmetic*, and the coefficients of the rational functions were computed by the **Remez Algorithm** [10]. All numerical methods employed are available in the **Boost Libraries' Math Toolkit 4.1.1** [9]. After implementation in machine precision arithmetic, we systematically tested all the procedures by comparing them against high-precision quadratures, which demonstrated a relative error of approximately the machine epsilon on the whole range $\alpha \in [0, 2]$.

[6]Which stands for "`generalized-cosine-integrals-kpi`". We implemented the method as single C++ Callable Type `GzedCosineIntegralskPi` (up to this moment only in double-precision floating-point arithmetic) whose constructor `GzedCosineIntegralskPi(double alpha, double h)` takes only the parameters α and h. After the object's instantiation, the values of $\boldsymbol{\mathcal{I}}_k$ for each k can be obtained by the overloaded operator `()` with signature `double operator()(size_t k)`.

[7]See the `README.md` file in the repository for software requirements and the usage of the Python interface.

[8]The Python interface to the software easily allows the creation of **Jupyter® Notebooks** and, consequently, **Google Colaboratory™ (Colab) Notebooks**. Therefore, to show the usage of the software this way, we have also made Colab Notebooks publicly available at `https://drive.google.com/drive/folders/1jCwQQR_jWTeCUMxnlZLj4kNO4MoWjbLu?usp=sharing` (see, e.g., the file `test-suit-1.ipynb` for an example of how to clone the repository to a Notebook and use the Python interface).

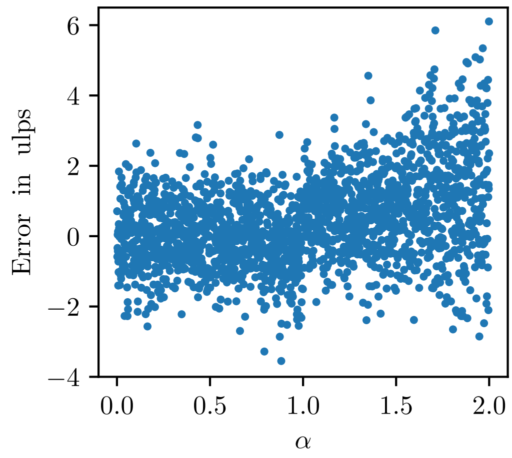

Figure 1: Error in ulps against α for $k = 100$. Source: The authors.

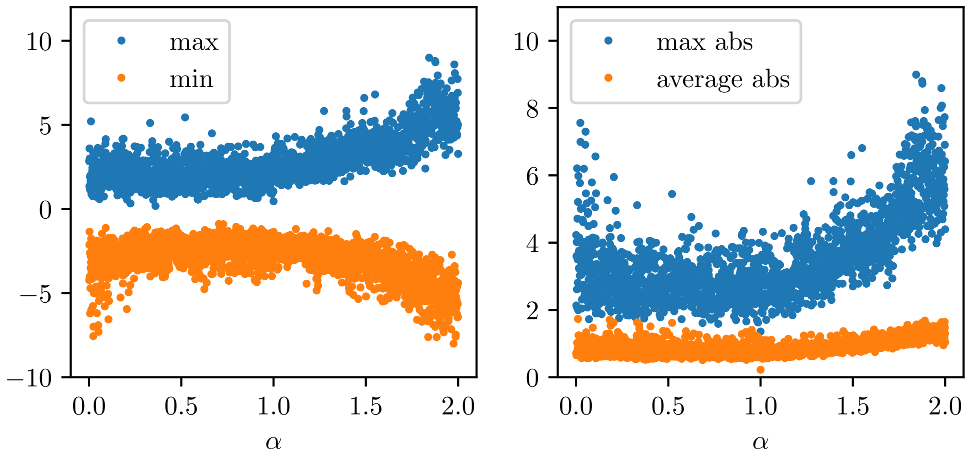

Figure 2: Error in ulps against α for $k = 1, \dots, 100$. Left: maximum and minimum errors. Right: maximum absolute and average absolute errors. Source: The authors.

5 Accuracy tests and final comments

To perform independent accuracy tests, we compared the values generated by our implementation with those obtained in **MapleSoft™ 15** software using multiple precision. The results are summarized in Figures 1 and 2, which present plots with the error in **ulps (units in the last place)** [6]. A testing unit is available along with the software in a Jupyter file, can be executed remotely from Google Colab, and reproduces the reported results.

Finally, we remark that the expression in equation (10) is ill-conditioned when k is even, especially when α is close to 1. To solve the problem, we rewrote the expression as

$$I_k(\alpha) = \big[\Gamma(\alpha) - 1\big]\sin\left(\frac{\pi\alpha}{2}\right) + \left[\sin\left(\frac{\pi\alpha}{2}\right) - 1\right] + \big[1 - (k\pi)^{\alpha-1}\big] + (k\pi)^{\alpha-1}\big[1 - J_k(\alpha - 1)\big], \quad (18)$$

since $J_k(\beta) - 1$ is obtained directly from the definition of $J_k(\beta)$. One may obtain the other terms from the following identities: $\Gamma(\alpha) - 1 = \texttt{expm1}(\texttt{lgamma}(\alpha))$, $\sin\left(\frac{1}{2}\pi\alpha\right) - 1 = -\dfrac{\cos^2\left(\frac{1}{2}\pi\alpha\right)}{1 + \sin\left(\frac{1}{2}\pi\alpha\right)}$ and $1 - (k\pi)^{\alpha-1} = -\,\texttt{expm1}\left((\alpha - 1)\ln(k\pi)\right)$ ($\texttt{expm1}(x)$ and $\texttt{lgamma}(x)$ stand for implementations of $\exp(x) - 1$ and $\ln(|\Gamma(x)|)$ in C-like programming languages, whose usage is more reliable and accurate than performing the naive compositions; for details, see `https://en.cppreference.com/w/cpp/numeric/math/expm1` and `https://en.cppreference.com/w/cpp/numeric/math/lgamma`).

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