The Hardy-Littlewood Function: An Exercise in Slowly Convergent Series

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Dedicated to Olav Njåstad on the occasion of his 70th birthday

Abstract

The function in question is $H(x) = \sum_{k=1}^{\infty} \sin(x/k)/k$. In deference to the general theme of this conference, a summation procedure is first described using orthogonal polynomials and polynomial/rational Gauss quadrature. Its effectiveness is limited to relatively small (positive) values of x. Direct summation with acceleration is shown to be more powerful for very large values of x. Such values are required to explore a (in the meantime disproved) conjecture of H. Alzer and C. Berg, according to which $H(x)$ is bounded from below by $-\pi/2$.

Key words:
Hardy-Littlewood function, slowly convergent series, summation by polynomial/rational Gauss quadrature, direct summation with acceleration

1 Introduction

Work on the complete monotonicity of certain functions involving the polygamma functions led H. Alzer et al. [2] to consider the function

$$H(x) = \sum_{k=1}^{\infty} \frac{1}{k} \sin \frac{x}{k} \tag{1}$$

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already studied by Hardy and Littlewood [7, §7] in connection with a summation procedure of Lambert. Hardy and Littlewood prove that the function is unbounded, there being infinitely many (though rare) positive values of x with $x \to \infty$ for which $H(x) > C(\log\log x)^{1/2}$. The complete monotonicity property alluded to above was shown by H. Alzer et al. [2] to be equivalent to the inequality $H(x) > -\pi/2$ for all $x > 0$. Although this inequality was eventually disproved by these authors, there may be some interest in studying the behavior of the function $H(x)$ numerically. Given the slow convergence of the series in (1), this is a challenging task in its own right.

We describe two procedures for computing $H(x)$. The first is one that has been used previously with some success (cf. [6, §4], and for further references [4, §3.2]) and employs Gaussian quadrature. In the present context, its effectiveness is somewhat limited, and does not allow us to go much beyond $x = 100$. We therefore develop another more direct method, which can deal with values of x that are considerably larger.

2 Summation by quadrature

Consider an infinite series

$$S = \sum_{k=1}^{\infty} a_k, \quad a_k = (\mathcal{L}f)(k), \tag{2}$$

whose general term is the Laplace transform

$$(\mathcal{L}f)(s) = \int_0^{\infty} \mathrm{e}^{-st} f(t)\mathrm{d}t$$

evaluated at $s = k$ of some known function f. Then we have

$$\begin{aligned} S &= \sum_{k=1}^{\infty} (\mathcal{L}f)(k) = \sum_{k=1}^{\infty} \int_0^{\infty} \mathrm{e}^{-kt} f(t)\mathrm{d}t = \int_0^{\infty} \sum_{k=1}^{\infty} \mathrm{e}^{-(k-1)t} \cdot \mathrm{e}^{-t} f(t)\mathrm{d}t \\ &= \int_0^{\infty} \frac{1}{1-\mathrm{e}^{-t}} \cdot \mathrm{e}^{-t} f(t)\mathrm{d}t, \end{aligned}$$

that is,

$$S = \int_0^{\infty} \frac{t}{1-\mathrm{e}^{-t}} \, \frac{f(t)}{t} \, \mathrm{e}^{-t}\mathrm{d}t. \tag{3}$$

In general, if $a_k \sim k^{-p}$ as $k \to \infty$, $p > 1$, then $f(t) \sim t^{p-1}$ as $t \to 0$.

To determine the function f in the case of the series (1) we note that [1, eqn 29.3.81]

$$\frac{1}{s}\,\mathrm{e}^{x/s} = (\mathcal{L}_{(t)} I_0(2\sqrt{xt}))(s),$$

where I_0 is the modified Bessel function of order zero. There follows, by Euler's formula,

$$\frac{1}{s}\,\sin(x/s) = \frac{1}{s}\,\frac{1}{2\mathrm{i}}\,(\mathrm{e}^{\mathrm{i}x/s} - \mathrm{e}^{-\mathrm{i}x/s}) = \frac{1}{2\mathrm{i}}\,\Big(\mathcal{L}_{(t)}[I_0(2\sqrt{\mathrm{i}xt}) - I_0(2\sqrt{-\mathrm{i}xt})](s)\Big)\,,$$

that is,

$$f(t) = f(t;x) = \frac{1}{2\mathrm{i}}\,[I_0(2\sqrt{\mathrm{i}xt}) - I_0(2\sqrt{-\mathrm{i}xt})]. \tag{4}$$

From the known power series expansion of I_0 one finds that

$$f(t;x) = \sum_{k=0}^{\infty}(-1)^k \frac{u^{2k+1}}{(2k+1)!^2}\,, \quad u = xt. \tag{5}$$

In particular, $\lim_{t\to 0} f(t;x)/t = x$. The series (5) is useful for computation as long as u is not too large, but is subject to severe cancellation errors otherwise. The number of decimal digits lost, owing to cancellation, is approximately 2, 6, 8, 17, and 25 for u respectively equal to 100, 500, 1,000, 5,000, and 10,000.

Alternatively, we may use the integral representation (cf. [1, eqn 9.6.16])

$$I_0(z) = \frac{1}{\pi}\int_0^{\pi} \mathrm{e}^{z\cos\theta}\mathrm{d}\theta,$$

and write (4) in the form

$$f(t;x) = \frac{1}{\pi}\int_0^{\pi} \mathrm{e}^{\sqrt{2u}\cos\theta}\sin(\sqrt{2u}\cos\theta)\mathrm{d}\theta, \quad u = xt. \tag{6}$$

Here, the integrand is a 2π-periodic even function of θ, so that integration, in effect, is over the full period. The fact that it is also an entire function makes the composite trapezoidal rule the method of choice for evaluating the integral. For the u-values considered above, there is practically no cancellation in calculating the trapezoidal sums, in stark contrast to the series in (5).

With regard to the integral in (3), Gauss quadrature relative to the Laguerre weight function e^{-t} on $[0,\infty)$ would seem to be an option. One can do better, however, by noting that the integrand has poles $\pm 2\nu \mathrm{i}\pi$, $\nu = 1, 2, 3, \ldots$. This suggests using Gauss-type formulae that are exact not only for polynomials, but also for rational functions having the same poles, or at least a few of those closest to the real axis. Such formulae have been developed in [3] and are implemented in [5]. Motivated by experience gained in [5], we choose, for $n = 5, 10, 15, \ldots$, an n-point quadrature rule that is exact for elementary rational functions corresponding to the first $m = 2\lfloor(n+1)/2\rfloor$ poles (taken in conjugate complex pairs) and for polynomials of degree $2n-1-m$. If $n_{\max}$ denotes the smallest n for which two consecutive quadratures agree within a tolerance of $\frac{1}{2}\,10^{-6}$, then, as a function of x, the value of $n_{\max}$ observed has the behavior shown in Table 1.

x	10	25	50	75	100
$n_{\max}$	20	35	55	75	95
d	1	4	10	15	20

Table 1. Number of Gauss points required in (3) for 6-digit accuracy, and severity of cancellation.

The table also shows the approximate number d of decimal digits lost, owing to cancellation errors in the quadrature sum for the integral in (3). (For $x = 100$, the error tolerance had to be lowered to $\frac{1}{2}\,10^{-3}$ to be able to achieve it.) All computations were done in quadruple precision. It is seen that values of x much beyond $x = 100$ are beginning to strain even quadruple-precision calculations. Results produced by these calculations in the range $0 \leq x \leq 100$ are shown in Fig. 1.

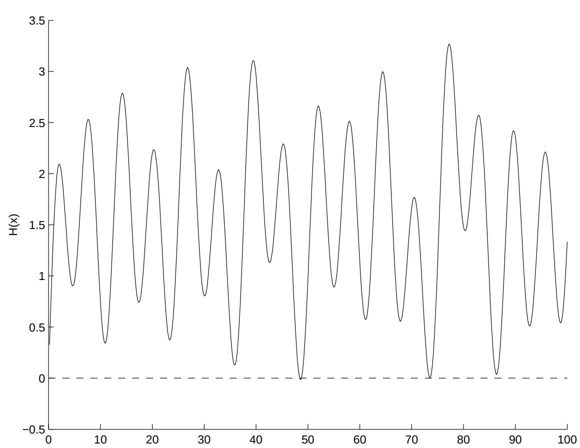

Fig. 1. The function $H(x)$ for $0 \leq x \leq 100$.

3 Direct summation

Summing the series in (1) directly, as is, would be too time-consuming if a reasonably high accuracy is desired. However, we may sum the first n terms directly, where $n \approx x$, and then observe that in the remaining terms $0 < x/k < 1$, so that a few terms in the Taylor expansion of $\sin(x/k)$ may be subtracted to speed up convergence and then added back for compensation. Thus, with $n = \lfloor x \rfloor$,

$$\begin{aligned} H(x) &= \sum_{k=1}^{n} \frac{1}{k} \sin\frac{x}{k} + \sum_{k=n+1}^{\infty} \frac{1}{k} \sin\frac{x}{k} \\ &= \sum_{k=1}^{n} \frac{1}{k} \sin\frac{x}{k} + \sum_{k=n+1}^{\infty} \frac{1}{k} \left(\sin\frac{x}{k} - \frac{x}{k} + \frac{1}{6}\left(\frac{x}{k}\right)^3 \right) \\ &\qquad + x\left(\frac{\pi^2}{6} - \sum_{k=1}^{n}\frac{1}{k^2}\right) - \frac{x^3}{6}\left(\frac{\pi^4}{90} - \sum_{k=1}^{n}\frac{1}{k^4}\right), \end{aligned} \tag{7}$$

where the well-known formulae $\zeta(2) = \pi^2/6$, $\zeta(4) = \pi^4/90$ for the zeta function $\zeta(s) = \sum_{k=1}^{\infty} k^{-s}$ have been used (cf. [1, eqs 23.2.24–25]). Since x will be very large, and $H(x)$ of the order of magnitude 1, the two remainder terms at the end of (7) must be calculated very accurately. As written, too much accuracy may be lost owing to cancellation. A better way to compute these terms is via the Euler-Maclaurin summation formula (cf. [1, eqn 3.6.28]). Thus,

$$\begin{aligned} &\frac{\pi^2}{6} - \sum_{k=1}^{n}\frac{1}{k^2} \\ &\quad \sim \frac{B_0}{n+1} - \frac{B_1}{(n+1)^2} + \frac{B_2}{(n+1)^3} + \frac{B_4}{(n+1)^5} + \cdots + \frac{B_{10}}{(n+1)^{11}}, \end{aligned} \tag{8}$$

and

$$\begin{aligned} \frac{\pi^4}{90} - \sum_{k=1}^{n}\frac{1}{k^4} \sim \frac{1}{3}\frac{B_0}{(n+1)^3} - \frac{B_1}{(n+1)^4} + \frac{2B_2}{(n+1)^5} + \frac{5B_4}{(n+1)^7} \\ + \frac{28}{3}\frac{B_6}{(n+1)^9} + \frac{3B_8}{(n+1)^{11}} + \frac{22B_{10}}{(n+1)^{13}}, \end{aligned} \tag{9}$$

where B_i are the Bernoulli numbers

$$B_0 = 1,\ B_1 = -\tfrac{1}{2},\ B_2 = \tfrac{1}{6},\ B_4 = -\tfrac{1}{30},\ B_6 = \tfrac{1}{42},\ B_8 = -\tfrac{1}{30},\ B_{10} = \tfrac{5}{66}\,.$$

The first seven terms in (8) and (9) will be ample to provide sufficient accuracy. Results thus produced are shown in Figs 2–3.

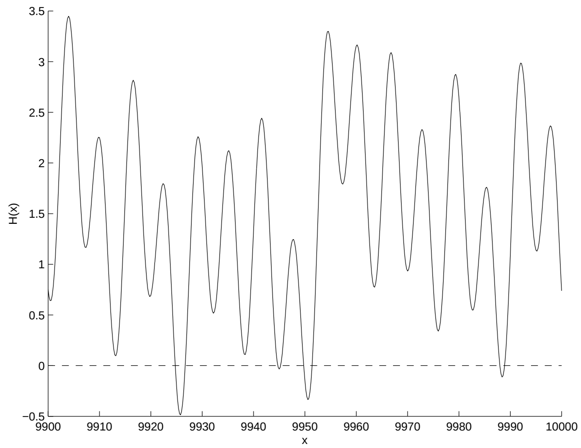

Fig. 2. The function $H(x)$ for $9,900 \le x \le 10,000$.

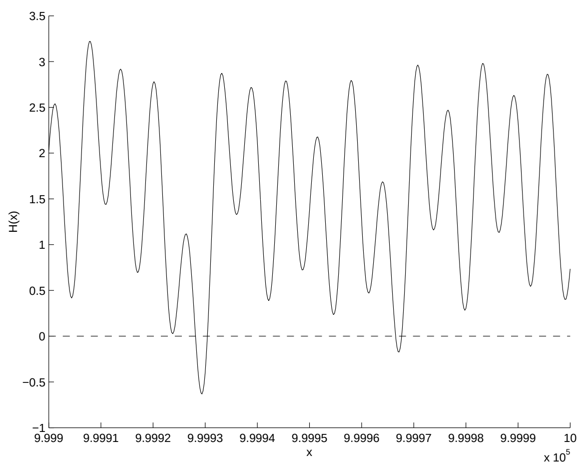

Fig. 3. The function $H(x)$ for $999,900 \le x \le 1,000,000$.

Evidently, neither the unboundedness of H from above nor the one from below can be as much as suggested by these calculations. To do so, in view of the $(\log \log x)^{1/2}$ behavior of $|H(x)|$, would require values of x so large as to not even be machine-representable, let alone be such that the summation procedure of this subsection would be feasible.

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