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# RIEMANN–SIEGEL SUMS VIA STATIONARY PHASE

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A new representation is obtained for the Riemann $\xi$ function, in the form of a series of integrals, multiplied by an exponential factor capturing the correct decay rate for large imaginary argument. Each term in this series then has a simple stationary-phase asymptote, the total agreeing with the Riemann–Siegel sum.

## INTRODUCTION

The fundamental series definition ([**1**, p. 807]) of the Riemann zeta function

$$\zeta(s) = \sum_{n=1}^{\infty} n^{-s} \tag{1}$$

converges only for $\sigma > 1$ where $s = \sigma + it$. Its analytic continuation to $\sigma < 1$ proceeds via a function proportional to $\zeta(s)$, for example,

$$\xi(s) = \pi^{-s/2}\,\Gamma\Big(\frac{s}{2}\Big)\zeta(s) \tag{2}$$

which satisfies

$$\xi(s) = \xi(1-s) \tag{3}$$

and is real on the critical line $\sigma = 1/2$. This function $\xi(s)$ was also defined by Riemann (see [**4**, p. 16 and Appendix]), except that he multiplied it by an extra factor $s(s-1)/2$ that we shall not need. Another similar function is the Hardy function ([**3**, equation (19)], [**4**, p. 119] and [**8**, p. 89])

$$Z(t) = \pi^{1/4-s/2}\Big[\Gamma\Big(\frac{s}{2}\Big)\Big]^{1/2}\Big[\Gamma\Big(\frac{1}{2}-\frac{s}{2}\Big)\Big]^{-1/2}\zeta(s) \tag{4}$$

$$= \pi^{1/4}\Big[\Gamma\Big(\frac{s}{2}\Big)\Gamma\Big(\frac{1}{2}-\frac{s}{2}\Big)\Big]^{-1/2}\xi(s) \tag{5}$$

where $s = 1/2 + it$.

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Many important studies on Riemann functions are for large argument $s$, specifically large imaginary part $t$, with real part $\sigma = 1/2$. In that case we can approximate the Gamma functions in (5) using Stirling's formula ([1, p. 257]) to give

$$\xi\Big(\frac{1}{2} + it\Big) = (2^{3/4}\pi^{1/4})\, t^{-1/4} e^{-\pi t/4}\, Z(t) \tag{6}$$

with error a factor $1 + O(t^{-1})$. In view of the fact that $Z(t)$ takes (more-or-less) order-one values for large $t$, this means that $\xi$ is asymptotically exponentially small for large $t$, and is then difficult to evaluate computationally with small relative error, for example, by direct numerical quadrature on formulae such as (8) below.

In fact, Riemann himself obtained a large-$t$ asymptote for $Z(t)$, in unpublished notes later discovered and published by Siegel (see [4, Chapter 7]). To leading order, with error of order $t^{-1/4}$, this asymptote is the finite sum

$$Z(t) = 2 \sum_{k=1}^{[\sqrt{t/(2\pi)}]} k^{-1/2} \cos\Big[t \log \frac{\sqrt{t/2\pi}}{k} - \frac{1}{2}t - \frac{\pi}{8}\Big] . \tag{7}$$

The Riemann–Siegel sum (7) plays a powerful role in modern analytical and computational studies ([3]) of Riemann functions. Especially when one or more correction terms for the $O(t^{-1/4})$ remainder are added, it enables accurate computation even for extremely large values of $t$. Most derivations of (7), including Riemann's original, are quite difficult, and the following almost elementary derivation might be found of interest.

## Fourier integral

For real $t$, the real-valued function $u(t) = \xi(1/2 + it)$ has the Fourier-cosine representation ([5, equation 2.5], [8, p. 36], and [4, p. 213])

$$u(t) = 4 \int_0^\infty \cos(tz)\, e^{z/2} \phi(e^{2z})\, dz \tag{8}$$

Here

$$\phi(\lambda) = \sum_{n=1}^{\infty} e^{-\pi n^2 \lambda} - \frac{1}{2}\lambda^{-1/2} \tag{9}$$

is related to an elliptic theta-function ([1, p. 576]), with the property

$$\phi(\lambda^{-1}) = \lambda^{1/2} \phi(\lambda) . \tag{10}$$

Note that $e^{z/2}\phi(e^{2z}) = e^{-z/2}\phi(e^{-2z})$, is an even function of $z$, so that we can also write

$$u(t) = 2 \int_{-\infty}^{\infty} e^{itz}\, e^{z/2} \phi(e^{2z})\, dz \tag{11}$$

## Shifted path and series representation

Since the integrand of (11) tends to zero in the complex $z = x + iy$ plane as $|x| \to \infty$ for $0 < y < \pi/4$, we can shift the path of integration, writing $z = i\pi/4 + X$, so

$$u(t) = 2e^{-\pi t/4} e^{i\pi/8} \int_{-\infty}^{\infty} e^{itX}\, e^{X/2} \phi(ie^{2X})\, dX \tag{12}$$

or, making use of symmetry,

$$u(t) = 4e^{-\pi t/4}\, \Re\, e^{i\pi/8} \int_{0}^{\infty} e^{itX}\, e^{X/2} \phi(ie^{2X})\, dX \tag{13}$$

Substituting the series (9) for $\phi$, we get

$$u(t) = e^{-\pi t/4} \sum_{k=0}^{\infty} v_k(t) \tag{14}$$

where

$$v_0(t) = -\frac{\cos \pi/8 + 2t \sin \pi/8}{1/4 + t^2} \tag{15}$$

and for $k = 1, 2, 3, \dots$

$$v_k(t) = 4 \int_0^{\infty} e^{X/2} \cos\Big(tX - \pi k^2 e^{2X} + \frac{\pi}{8}\Big)\, dX \tag{16}$$

with alternative forms

$$v_k(t) = 2 \int_1^{\infty} Y^{-3/4} \cos\Big(\frac{1}{2} t \log Y - \pi k^2 Y + \frac{\pi}{8}\Big)\, dY \tag{17}$$

$$= 8 \int_1^{\infty} \cos\Big(2t \log Z - \pi k^2 Z^4 + \frac{\pi}{8}\Big)\, dZ\,. \tag{18}$$

The series (14) subject to (15) and (16), which appears to be new, may be of interest in its own right. In particular, it has computational value at arbitrary (not necessarily large) $t$. Even for large $t$, numerical quadratures designed for rapidly oscillating integrands, mimicking stationary phase via an exponential fade factor decaying away from the point of stationary phase (for example, as in [**9**]), retain good accuracy, with the advantage of not needing correction terms. A somewhat similar approach was taken in [**2**], with a different series representation.

## Derivation of Riemann–Siegel sum

The Riemann–Siegel asymptote (7) for large $t$ now follows directly by Kelvin's method of stationary phase ([**7**, p. 163], and [**6**, p. 96]). Writing (16) in the form

$$v_k(t) = 4 \int_0^{\infty} e^{X/2} \cos \Psi(X)\, dX \tag{19}$$

where

$$\Psi(X) = tX - \pi k^2 e^{2X} + \frac{\pi}{8} \tag{20}$$

we have $\Psi'(X) = 0$ when $X = X_0 = \log\left[\sqrt{t/2\pi}/k\right]$. Then the integral in (19) is dominated by the neighbourhood of $X = X_0$, with the Taylor series

$$\begin{aligned}\Psi(X) &= \Psi(X_0) + \frac{1}{2}(X - X_0)^2\Psi''(X_0) + \cdots \\ &= \left[tX_0 - \frac{1}{2}t + \frac{\pi}{8}\right] - t(X - X_0)^2 + \cdots\end{aligned} \tag{21}$$

so

$$\begin{aligned}v_k(t) &= 4e^{X_0/2}\int_{-\infty}^{\infty}\cos\left(tX_0 - \frac{1}{2}t + \frac{\pi}{8} - t(X - X_0)^2\right)dX + \cdots \\ &= 2^{7/4}\pi^{1/4}t^{-1/4}k^{-1/2}\cos\left(tX_0 - \frac{1}{2}t - \frac{\pi}{8}\right) + \cdots\end{aligned} \tag{22}$$

Hence for large $t$ the series (14) is in agreement with the Riemann–Siegel sum (7), once (6) is used to relate $u(t) = \xi(1/2 + it)$ to $Z(t)$. Note that the infinite series (14) now truncates to a finite sum with $k < \sqrt{t/2\pi}$, because it is necessary that $X_0 > 0$ in order that the point of stationary phase lie within the range of the integral (19). Note also that $v_k = O(t^{-1/4})$ for $k = 1, 2, 3, \ldots$, so the term $v_0 = O(t^{-1})$ does not contribute, to leading order.

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