Fast Computation of the Riemann Zeta Function to Arbitrary Accuracy

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The Players

\[ s = \sigma + it \]

\[ \zeta(s) = \sum_{n=1}^{\infty} n^{-s}, \quad \sigma > 1 \]

\[ \chi(s) = \frac{\zeta(s)}{\zeta(1 - s)} \]

\[ = \pi^{s-1/2} \frac{\Gamma((1 - s)/2)}{\Gamma(s/2)} \]

Note \( \chi(s) \) has poles at \( s = 1, 3, \ldots 2n + 1, \ldots \)

\[ Z(t) = \frac{\zeta(1/2 + it)}{\sqrt{\chi(1/2 + it)}} \]

If \( t \in \mathbb{R} \) then \( |Z(t)| = |\zeta(1/2 + it)| \) and \( Z(t) \in \mathbb{R} \).
Motivation

The Lagarias-Odlyzko “analytic algorithm” for $\pi(x)$ [LO87, Gal99] requires many precise values of $\zeta(\sigma + it)$, with $\sigma$ fixed, $\sigma > 1$. E.g. to compute $\pi(10^{24})$ it would suffice to compute $\zeta(1.2 + ikh)$ to roughly 45 digit precision, with

$$h = 0.0075$$

$$0 \leq k \leq 1.6 \times 10^{15}$$

(i.e. $0 \leq t \leq 1.2 \times 10^{13}$)
Euler-Maclaurin Summation

\[ \zeta(s) = \sum_{n=1}^{N} n^{-s} + \frac{N^{1-s}}{s-1} \]
\[ + \sum_{m=1}^{M-1} \frac{B_m}{m} \binom{s+m-2}{m-1} N^{1-m-s} \]
\[ + O_M(s^M N^{1-M-s}) \]

Advantages

- Error analysis is straightforward [CO92].
- Allows arbitrary accuracy.
- \( O(t^{1+\epsilon} + d^{1+\epsilon}) \) operations to find \( d \) digits.

Disadvantages

- \( N \gtrsim t \).
- Needs Bernoulli numbers.
Riemann-Siegel Formula

\[ Z(t) = 2 \sum_{n=1}^{N} n^{-1/2-it} \sqrt[\chi(1/2 + it)]{ } + \sum_{m=0}^{M-1} \cdots + O(t^{-1/4-M/2}) \quad \text{as } t \to \infty, \]

where \( N = \lfloor \sqrt{t/(2\pi)} \rfloor \).

Advantages

- \( N \approx \sqrt{t/(2\pi)} \) for large \( t \).

Disadvantages

- Error analysis is difficult (currently only available for \( \sigma = 1/2 \)) [Gab79].
- Accuracy is limited.
Quadrature Near Saddle Point

Use numerical quadrature instead of the asymptotic expansion developed in the Riemann-Siegel formula:

Advantages

- $N \approx \sqrt{t/(2\pi)}$ for large $t$.
- Error analysis is straightforward.
- Allows arbitrary accuracy.

Disadvantages

- $O(t^{1/2+\epsilon} + d^{3/2+\epsilon})$ operations to find $d$ digits. [The Euler-Maclaurin formula wins when very high accuracy is needed.]
An Integral for $\zeta(s)$

Let

$$I_N(s) = \int_{N/N+1} \frac{\exp(i\pi z^2) z^{-s}}{e^{i\pi z} - e^{-i\pi z}} \, dz,$$

then

$$\zeta(s) = I_0(s) + \chi(s) \overline{I_0(1 - \bar{s})}.$$

We then use

$$I_0(s) = \sum_{n=1}^{N} n^{-s} + I_N(s)$$

and choose $N$ so the path is near the saddle point of $\exp(i\pi z^2) z^{-s}$ at $z = \sqrt{s/(2\pi i)}$. 
Location of saddle point(s)

\[ z = \sqrt{s/(2\pi i)} \]
\[
\log \left| \frac{\exp(i\pi z^2) \, z^{-s}}{e^{i\pi z} - e^{-i\pi z}} \right|
\]

\[s = 1.5 + 1000i, \ N = 12\]

\[0 \rightarrow 1 \text{ and } 12 \rightarrow 13\]
The Integrand

Absolute Value, Real and Imaginary Parts of

\[ f(s, z) = \frac{\exp(i\pi z^2) z^{-s}}{e^{i\pi z} - e^{-i\pi z}} \]

\[ z = x + i(x - 12.5) \]
Quadrature Analysis — a Tool

Let \( H(w) = \frac{1}{1 - e^{2i\pi w}}. \)

Note \( H(u - iv) = O(e^{-2\pi v}) \) as \( v \to \infty. \)
A Quadrature Formula

\[
\int_{C} f(z) \, dz = h \sum_{m \in \mathbb{Z}} f(z_0 + m \, h) \\
+ \int_{\mathcal{L}} f(z) H((z_0 - z)/h) \, dz \\
+ \int_{\mathcal{R}} f(z) H((z - z_0)/h) \, dz,
\]

Note that \( \int_{\mathcal{L}} = O_{\Delta}(e^{-2\pi \Delta/|h|}) \), similarly for \( \int_{\mathcal{R}} \).
“Left Error” for $I_0$ Integrand

$$h = 0.2(1 + i)$$

10 $\rightarrow$ 10.5, 12 $\rightarrow$ 12.5 and 12 $\rightarrow$ 13
5 Parameters for Quadrature

\[ N_{\mathcal{L}}, \ N, \ N_{\mathcal{R}}, \ W, \ \text{and} \ M, \ \text{where} \]
\[ 2W = \text{Width of sample interval, and with} \]
\[ M + 1 \ \text{sample points} \]
\[ z_0 = N + 1/2 - W(1 + i) \]
\[ h = 2W(1 + i)/M \]
Quadrature Formula for $I_0(s)$

\[
I_0(s) = \sum_{n=1}^{N} n^{-s} + h \sum_{m=0}^{M} f(s, z_0 + mh)
\]

\[
- \sum_{n=N_L}^{N} H\left(\frac{(N + 1/2 - n)}{h}\right) n^{-s}
\]

\[
+ \sum_{n=N+1}^{N_R} H\left(\frac{(n - N - 1/2)}{h}\right) n^{-s}
\]

\[
+ O(e^{-2\pi W^2 + \epsilon}) + O(e^{-\pi K M/W})
\]

where

\[
f(s, z) = \frac{\exp(i \pi z^2) z^{-s}}{e^{i\pi z} - e^{-i\pi z}}
\]

and

\[
K = \min\left(5/4 + N - N_L, 1/4 + N_R - N\right).
\]
Computing $\zeta(s)$ to 28 decimal places

\[
s = 1/2 + 10^5 i
\]
\[
N = 126
\]
\[
N_L = 121
\]
\[
N_R = 131
\]
\[
W = 2.5
\]
\[
M = 50
\]

Computation time using quadrature was 0.31 sec. in GP/PARI on a 300MHz Ultrasparc — vs 204 sec. (18 sec. after first computation) using PARI’s built-in routine based on Euler-Maclaurin summation.
Computing $\zeta(s)$ to 1000 decimal places

$$s = 1/2 + 10^5 i$$

$N = 126$

$N_L = 100$

$N_R = 152$

$W = 13$

$M = 1500$

Computation time using quadrature was 25 minutes in GP/PARI on 300MHz Ultrasparc.
Things to do

- Get explicit, tight, error bounds.
- Do a more careful complexity analysis.
- Generalize to other zeta functions and $L$-functions.
Literature

- For a good survey of methods for computing $\zeta(s)$, see the preprint [BBC].
- For a careful error analysis of the Euler-Maclaurin formula for $\zeta(s)$, see [CO92].
- For a careful error analysis of the Riemann-Siegel formula, when $\sigma = 1/2$, see [Gab79].
- Methods for efficient computation of $\zeta(\sigma + it)$ at many equally spaced values of $t$ are described in [OS88].
- For “smoothed” versions of the Riemann-Siegel formula, with better accuracy than the classical version, see [BK92].
- For further discussion of quadrature of saddle point integrals, see [Tem77].
References


