An Efficient Algorithm for the Riemann Zeta Function

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January 20, 1995

Abstract. A very simple class of algorithms for the computation of the Riemann-zeta function to arbitrary precision in arbitrary domains is proposed. These algorithms out perform the standard methods based on Euler-Maclaurin summation, are easier to implement and are easier to analyse.

Keywords: Riemann zeta function, computation, high-precision, algorithm
AMS (1991) subject classification: Primary 11Y16, Secondary 64D20, 11M99

*Research supported by NSERC

1 Introduction

We propose some very simple algorithms for the arbitrary precision calculation of the Riemann-zeta function which is the analytic continuation of

$$
\begin{aligned}
(1) \quad \zeta(s) : &= \sum_{n=1}^{\infty} \frac{1}{n^s} && \text{re(s)} > 1 \\
&= \frac{1}{(1-2^{1-s})} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^s} && \text{re(s)} > 0
\end{aligned}
$$

These algorithms do not compete with the Riemann-Siegel formula based algorithms for computations concerning zeros on the critical line (Im(s) = 1/2) where multiple low precision evaluations are required. (See [2,6].) They do however improve considerably on the standard algorithms for arbitrary precision computation of the zeta function in the major symbolic algebra packages (All of Maple, Mathematica and Pari use Euler-Maclaurin based algorithms [2,5,7]). They are easier to implement and far easier to analyse. Some additional comments on the computational aspects are offered at the end of this note.

2 Algorithms

We commence by presenting the algorithm in generic form and then offer two specializations.

Algorithm 1 *Let* $p_n(x) := \sum_{k=0}^{n} a_k x^k$ *be an arbitrary polynomial of degree* n *that does not vanish at -1. Let*

$$
(2) \qquad c_j := (-1)^j \left(\sum_{k=0}^{j} (-1)^k a_k - p_n(-1) \right)
$$

then

$$(3) \qquad \zeta(s) = \frac{-1}{(1-2^{1-s})p_n(-1)} \sum_{j=0}^{n-1} \frac{c_j}{(1+j)^s} \qquad + \qquad \xi_n(s)$$

where

$$(4) \qquad \xi_n(s) = \frac{1}{p_n(-1)(1-2^{1-s})} \frac{1}{\Gamma(s)} \int_0^1 \frac{p_n(x)|\log x|^{s-1}}{1+x} dx.$$

Here Γ *is the gamma function.*

Note that the c_j are (up to sign) just the coefficients of $\frac{p_n(x)-p_n(-1)}{1+x}$ which is a polynomial of degree $n-1$.

Proof of Algorithm l. We use the standard formulae.

$$(5) \quad \zeta(s) = \frac{1}{(1-2^{1-s})\Gamma(s)} \int_0^1 \frac{|\log x|^{s-1}}{1+x} dx \qquad \mathrm{re(s)} > 0$$

and

$$(6) \quad \frac{1}{(m+1)^s} = \frac{1}{\Gamma(s)} \int_0^1 x^m |\log x|^{s-1} dx \qquad re(s) > 0$$

See [1,7], though both follow easily from

$$(7) \quad \Gamma(s) = \int_0^\infty u^{s-1} e^{-u} du = \int_0^1 |\log x|^{s-1} dx \qquad re(s) > 0$$

which is just the definition of Γ and (1) .

We now write

$$\begin{aligned}
\xi_n(s) : \quad &= \frac{1}{p_n(-1)(1-2^{1-s})} \frac{1}{\Gamma(s)} \int_0^1 \frac{p_n(x)|\log x|^{s-1}}{1+x} dx \\
&= \frac{1}{p_n(-1)(1-2^{1-s})} \frac{1}{\Gamma(s)} \int_0^1 \frac{p_n(-1)|\log x|^{s-1}}{1+x} dx \\
&- \frac{1}{p_n(-1)(1-2^{1-s})} \frac{1}{\Gamma(s)} \int_0^1 \frac{p_n(-1)-p_n(x)}{1+x} |\log x 1^{s-1} dx
\end{aligned}$$

The first term above gives $\zeta(s)$ by (5) and the last term expands with (6) to give the series expansion in (3) $\square$

The trick now is to choose p_n so that the error in the integral for ξ_n divided by $p_n(-1)$ is as small as possible.

The Chebychev polynomial, shifted to $[0,1]$, and suitably normalized maximizes the value $p_n(-1)$ over all polynomials of comparable supremum norm on [0,1]. So the Chebychev polynomials are one obvious choice for p_n and give the next result.

Algorithm 2 *Let*

$$d_k := n \sum_{i=0}^{k} \frac{(n+i-1)!4^i}{(n-i)!(2i)!}$$

then

$$\zeta(s) = \frac{-1}{d_n(1-2^{1-s})} \sum_{k=0}^{n-1} \frac{(-1)^k(d_k - d_n)}{(k+1)^s} + \gamma_n(s)$$

where for $s = \sigma + it$ *with* $\sigma \geq \frac{1}{2}$

$$\begin{aligned} |\gamma_n(s)| &\leq \frac{2}{(3+\sqrt{8})^n} \frac{1}{|\Gamma(s)|} \frac{1}{|(1-2^{1-s})|} \\ &\leq \frac{3}{(3+\sqrt{8})^n} \frac{(1+2|t|)e^{\frac{|t|\pi}{2}}}{|(1-2^{1-s})|} \end{aligned}$$

Proof. The formula we need for the nth Chebychev polynomial on $[0,1]$ is

$$T_n(x) = (-1)^n n \sum_{k=0}^{n} (-1)^k \frac{(n+k-1)!}{(n-k)!(2k)!} 4^k x^k$$

from which the expression for d_k is deduced. To estimate the error we observe that, by Algorithm 1,

$$
\begin{aligned}
|\gamma_n(s)| &= \left|\frac{1}{d_n(1-2^{1-s})}\frac{1}{\Gamma(s)}\int_0^1 \frac{T_n(x)|\log x|^{s-1}}{1+x}dx\right| \\
&\le \frac{2}{(3+\sqrt{8})^n}\frac{1}{|(1-2^{1-s})\Gamma(s)|}\int_0^1 \frac{|\log x|^{s-1}}{1+x}dx
\end{aligned}
$$

since on $[0,1], |T_n(x)|$ is bounded by 1 and $|T_n(-1)| \ge \frac{1}{2}(3+\sqrt{8})^n$. We now compute that

$$
\int_0^1 \frac{|\log x|^{\frac{1}{2}}}{1+x}dx \le .68
$$

to deduce that

$$
|\gamma_n(s)| \le \frac{1.36}{(3+\sqrt{8})^n}\frac{1}{|(1-2^{1-s})\Gamma(s)|}.
$$

Now for $s = \sigma + it$ with $\sigma \ge \frac{1}{2}$

$$
|\frac{\Gamma(\sigma)}{\Gamma(\sigma+it)}|^2 = \prod_{n=0}^{\infty}(1+\frac{t^2}{(\sigma+n)^2}).
$$

So

$$
\begin{aligned}
\frac{1}{|\Gamma(s)|} &= \frac{\left(\prod_{n=0}^{\infty}(1+\frac{t^2}{(\sigma+n)^2})\right)^{\frac{1}{2}}}{|(\Gamma(\sigma)|} \\
&\le \frac{\left(\prod_{n=0}^{\infty}(1+\frac{t^2}{(\frac{1}{2}+n)^2})\right)^{\frac{1}{2}}}{|\Gamma(\sigma)|} \\
&\le \frac{(\frac{1+4t^2}{|t|\pi})^{\frac{1}{2}}\,(\sinh(\mathrm{t}\pi))^{\frac{1}{2}}}{|\Gamma(\sigma)|}.
\end{aligned}
$$

Since $|\Gamma(\sigma)|^{-1} \le 1.5$ on $[\frac{1}{2},\infty)$ we are done. $\square$

Since $(3+\sqrt{8}) = 5.828\ldots$ and this is the driving term in the estimate, we see that we require roughly (1.3)n terms for n digit accuracy, provided we are close to the real axis.

An even simpler algorithm, though not quite as fast, can be based on taking $p_n(x) := x^n(1-x)^n$.

Algorithm 3 *Let*

$$e_j = (-1)^j [\sum_{k=0}^{j-n} \frac{n!}{k!(n-k)!} - 2^n]$$

(where the empty sum is zero). Then

$$\zeta(s) = \frac{-1}{2^n(1-2^{1-s})} \sum_{j=0}^{2n-1} \frac{e_j}{(j+1)^s} + \gamma_n(s)$$

where for $s = \sigma + it$ *with* $\sigma > 0$

$$|\gamma_n(s)| \leq \frac{1}{8^n} \frac{(1+|\frac{t}{\sigma}|)e^{\frac{|t|\pi}{2}}}{|1-2^{1-s}|}.$$

If $-(n-1) \leq \sigma < 0$ *then*

$$|\gamma_n(s)| \leq \frac{1}{8^n|1-2^{1-s}|} \frac{4^{|\sigma|}}{|\Gamma(s)|}$$

(Note that the $\gamma_n(s) = 0$ for $s = -1, -2, \ldots, -n+1$.)

The details of this are very similar to those of Algorithm 2 on using $p_n(x) := x^n(1-x)^n$ and we omit them. The fact that convergence persists into the part of the half plane $\{re(s) < 0\}$ is a consequence of the fact that

$$\int_0^1 \frac{x^n(1-x)^n}{1+x} |\log x|^{s-1}\, dx$$

converges provided re(s) > −n. Thus Algorithm 3 gives another proof of the analytic continuation of the $\zeta(s)(1-s)$. (Note that $|e_j/2^n| = 1$ for $j = 0, \ldots, n$ and $|e_j/2^n| \leq 1$ for all j.)

Because $1/\Gamma(s) = 0$ for s a negative integer we have that $\gamma_n(s) = 0$ for $s = -1, -2, \ldots, -n+1$. However since

$$\zeta(-2n+1) = -\frac{\beta_{2n}}{2n}$$

the sum in Algorithm 2 computes Bernoulli numbers, for $s = -1, \ldots, -n+1$, exactly.

For modest precision (100 digits or less) Algorithm 3 above compares with Maple's inbuilt algorithm. It is marginally but not hugely faster. However, we were computing $\zeta(5)$ at lest ten times faster at 1000 digits precision. None of Maple, Mathematica nor Pari would compute 20,000 digits of $\zeta(5)$ on our SGI R4000 Challenges. Indeed none of them would compute 5,000 digits in a day. By comparison Algorithm 3, implemented in Maple, computed 20,000 digits in under two CPU hours. Algorithm 2 is faster again.

In order to make comparisons some care has to be taken. For an Euler-Maclaurin based computation, Bernoulli numbers have to be computed. If they are then stored a second evaluation will be much faster than an initial evaluation. Part of what makes Euler-Maclaurin unattractive for very large precision computations is that it is storage intensive and computationally expensive to compute the Bernoulli numbers, at least by usual methods. Roughly speaking, order of n Bernoulli numbers are required for n-digit precision and this requires in excess of order of n^2 storage.

The Binomial-like coefficients of Algorithms 2 and 3 are much easier to compute and if done sequentially require only one additional binomial coefficient per term which computes by a single multiplication and division.

3 Optimality

Algorithms 2 and 3 are nearly optimal in the following sense. There is no sequence of n-term exponential polynomials that can converge to $\zeta(s)$ on an interval $[a, b], a > 1$ very much faster than those of the algorithms. Precisely we have.

Theorem 1 *Let $1 < \alpha < \beta$ and let n be fixed. Then*

$$||\zeta(s)-\sum_{k=1}^{n}\frac{a_k}{b_k^s}||_{[\alpha,\infty)}\geq\frac{1}{\left(2^{\alpha}(3+\sqrt{8})^2\right)^n}$$

and

$$||\zeta(s)-\sum_{k=1}^{n}\frac{a_k}{b_k^s}||_{[\alpha,\beta)}\geq(D(\alpha,\beta))^n$$

for any real (a_k) *and* (b_k)*. Here* $D(\alpha,\beta)$ *is a positive constant that depends only on* α *and* β *and* $||.||_{[\alpha,\beta]}$ *denotes the supremum norm on* $[\alpha,\beta]$*.*

Proof. The proof follows the method of [4]. Under the change of variables $s\to-\log(x)/\log(2)$ for some real (c_k), (d_k) and (e_k)

$$||\zeta(s)-\sum_{k=1}^{n}\frac{a_k}{b_k^s}||_{[\alpha,\beta]}$$

$$=||\sum_{k=1}^{\infty}x^{log(k)/log(2)}-\sum_{k=1}^{n}a_kx^{c_k}||_{[2^{-\beta},2^{-\alpha}]}$$

$$\geq||\sum_{k=0}^{n}x^k-\sum_{k=1}^{n}d_kx^{e_k}||_{[2^{-\beta},2^{-\alpha}]}$$

where the last inequality follows by the comparison theorem (Corollary 2 of [4]). Now Theorem 8 of [4] gives the explicit estimate

$$||\sum_{k=0}^{n}x^k-\sum_{k=1}^{n}d_kx^{e_k}||_{[2^{-(\beta-\alpha)},1]}\geq\frac{1}{\left(C+\sqrt{C^2-1}\right)^{2n}}$$

where $C:=(3+2^{-(\beta-\alpha)})/(1-2^{-(\beta-\alpha)})$ and the result follows with the aid of Corollary 2 of [4] again. □

Another way in which Algorithms 2 and 3 are (somewhat) near optimal is the following. At even integers the algorithms generate rational approximations that satisfy, for each positive integer N,

$$||\zeta(2N) - \frac{p_n}{q_n}|| < \frac{1}{q_n^{\epsilon}}$$

for infinitely many integers $(p_n), (q_n)$ and some positive $\epsilon := \epsilon(N)$. But results of Mahler show that no such inequalities exist with arbitarily large ϵ and it is expected that in fact ϵ can be no greater than two. (See Chapter 11 of [3].)

References

[1] M. Abromowitz and I. Stegun, *Handbook of Mathematical Functions*, Dover, N.Y. 1972.

[2] M.V. Berry and J.P. Keating, *A new asymptotic representation for $\zeta(\frac{1}{2}+it)$ and quantum spectral determinants*. Proc. R. Soc. Lond. A, **437**(1992), 151-173.

[3] J. Borwein and P. Borwein, *Pi and the AGM*, Wiley N.Y. 1987.

[4] P. Borwein, *Uniform approximation by polynomials with variable exponents*, Canadian J. Math. **35**(1983), 547-557.

[5] H. Cohen and M. Olivier, *Calcul des valeurs de la function zêta de Riemann en multiprécision*, C.R. Acad. Sci. Paris, Série 1, **314** (1992), 427-430.

[6] A. Odlyzko and A. Schönhage, *Fast algorithms for multiple evaluations of the Riemann zeta-function*, Trans. A.M.S. **309** (1988), 797-809.

[7] E.C. Titchmarsh, *The Theory of the Riemann Zeta-function*, Second ed. Oxford Scientific. Publication, 1986.

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