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An Efficient Algorithm for the Riemann Zeta Function

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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 compete with the standard methods based on Euler-Maclaurin summation, are easier to implement and are easier to analyze.

1. Introduction

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

$$(1.1)\qquad \zeta(s) := \sum_{n=1}^{\infty} \frac{1}{n^s} \qquad \text{re(s)} > 1$$
$$= \frac{1}{(1-2^{1-s})} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^s} \qquad \text{re(s)} > 0$$

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 can however improve 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.

2. Algorithms

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

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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

$$c_j := (-1)^j \left(\sum_{k=0}^{j} (-1)^k a_k - p_n(-1) \right) \tag{2.1}$$

then

$$\zeta(s) = \frac{-1}{(1-2^{1-s})p_n(-1)} \sum_{j=0}^{n-1} \frac{c_j}{(1+j)^s} \quad + \quad \xi_n(s) \tag{2.2}$$

where

$$\xi_n(s) = \frac{1}{p_n(-1)(1-2^{1-s})} \frac{1}{\Gamma(s)} \int_0^1 \frac{p_n(x)|\log x|^{s-1}}{1+x} dx. \tag{2.3}$$

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. We use the standard formulae.

$$\zeta(s) = \frac{1}{(1-2^{1-s})\Gamma(s)} \int_0^1 \frac{|\log x|^{s-1}}{1+x} dx \qquad \text{re(s)} > 0 \tag{2.4}$$

and

$$\frac{1}{(m+1)^s} = \frac{1}{\Gamma(s)} \int_0^1 x^m |\log x|^{s-1} dx \qquad re(s) > 0 \tag{2.5}$$

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

$$\Gamma(s) = \int_0^\infty u^{s-1} e^{-u} du = \int_0^1 |\log x|^{s-1} dx \qquad re(s) > 0 \tag{2.6}$$

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

We now write

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

The first term above gives $\zeta(s)$ by (2.4) and the last term expands with (2.5) to give the series expansion in (2.2). □

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,

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

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

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

to deduce that

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

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

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

So

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

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

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 $\zeta(s)(1-s)$. (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 $s = -1, -2, \dots, -n+1$. However since

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

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

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 3.1. *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)

$$\begin{aligned} &||\zeta(s) - \sum_{k=1}^{n} \frac{a_k}{b_k^s}||_{[\alpha,\beta]} \\ &= ||\sum_{k=1}^{\infty} x^{log(k)/log(2)} - \sum_{k=1}^{n} a_k x^{c_k}||_{[2^{-\beta},2^{-\alpha}]} \\ &\geq ||\sum_{k=0}^{n} x^k - \sum_{k=1}^{n} d_k x^{e_k}||_{[2^{-\beta},2^{-\alpha}]} \end{aligned}$$

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

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

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 arbitrarily large ϵ and it is expected that in fact ϵ can be no greater than two. (See Chapter 11 of [3].)

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