EFFICIENT ALGORITHMS FOR THE ZETA FUNCTION

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Abstract.

A very simple class of algorithms for the computation of the Riemann-zeta function

$$\zeta(s) := \sum_{n=1}^{\infty} \frac{1}{n^s}$$

to arbitrary precision in arbitrary domains is proposed.

These algorithms far out perform the standard methods based on Euler-Maclaurin summation.

They do not compete with the Riemann-Siegel formula based algorithms for computations concerning zeros on the critical line ($\mathrm{Im}(s) = 1/2$) where multiple low precision evaluations are required.

They are easier to implement and are far easier to analyse.

Algorithm 1. Let $p_n(x) := \sum_{k=0}^{n} a_k x^k$ be any polynomial of degree n not zero at -1. Let

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

then

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

where

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

Here Γ is the gamma function.

Proof. We use the standard formulae.

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

and

$$\frac{1}{(m+1)^s} = \frac{1}{\Gamma(s)} \int_0^1 x^m |\log x|^{s-1} dx$$

Now

$$\xi_n(s)$$

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

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

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

The first term above gives $\zeta(s)$ and the last term expands to give the series expansion in the algorithm □

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 maximize 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.

Another obvious choice is $p_n(x) := x^n(1-x)^n$.

Both have interesting features.

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 $\sigma \geq \frac{1}{2}$

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

$$\leq \frac{3}{(3+\sqrt{8})^n} \frac{(1+2|t|)e^{\frac{|t|\pi}{2}}}{|(1-2^{1-s})|}$$

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 by Algorithm 1

$$|\gamma_n(s)| = \left| \frac{1}{d_n(1-2^{1-s})} \frac{1}{\Gamma(s)} \int_0^1 \frac{T_n(x)|\log x|^{s-1}}{1+x} dx \right|$$

$$\leq \frac{2}{(3+\sqrt{8})^n} \frac{1}{|(1-2^{1-s})\Gamma(s)|} \int_0^1 \frac{|\log x|^{s-1}}{1+x} dx.$$

Now use

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

and

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

$\square$

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

The fact that convergence persists into the part of the half plane $\{re(s) < 0\}$ is a consequence of the fact that

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

converges provided $\mathrm{Re}(s) > -n$.

Thus Algorithm 3 gives another proof of the analytic continuation of the $\zeta(s)(1-s)$.

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 3 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. However, we were computing $\zeta(5)$ at lest ten times faster at 1000 digits precision.

Neither Maple nor Mathematica would compute 5,000 digits of $\zeta(5)$ on SGI R4000 Challenges.

By comparison Algorithm 3, implemented in Maple, computed 20,000 digits in under two CPU hours.

For Euler-Maclaurin Bernoulli numbers have to be computed. If they are then stored a second evaluation will be much faster. Euler-Maclaurin is unattractive for very large precision computations. It is storage intensive to compute Bernoulli numbers. (Pari crashes with a 40 mb stack on 5000 digits.)

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

Optimality

Algorithms 2 and 3 are nearly optimal in the following sense. There is no sequence of n-term exponential polynomials that essentially better.

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. Under the change of variables $s \to -\log(x)/\log(2)$ for some real (c_k), (d_k) and (e_k)

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

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

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

where the last inequality follows by a comparison theorem. Now we have 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 $C := (3 + 2^{-(\beta-\alpha)})/(1 - 2^{-(\beta-\alpha)})$ $\square$