EXTENDED COMPUTATION OF THE RIEMANN ZETA-FUNCTION

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In 1955 a programme of study of the first 10000 zeros of the Riemann Zeta-function

$$\zeta(s) = \sum_{n=1}^{\infty} n^{-s} \quad (s = \sigma + it)$$

was completed. Use was made of the high-speed digital computer SWAC and a report of this programme has appeared recently [**1**]. More recently still, the programme has been extended to the first 25000 zeros. All these zeros have $\sigma = \frac{1}{2}$. The purpose of this paper is to summarize the methods needed for this (and possibly future) work from the high-speed computer point of view.

The bulk of the programme, representing only a few hours of machine time, was based on the Riemann-Siegel asymptotic formula as developed by Titchmarsh with numerical bounds for the error. In the great majority of cases this formula was sufficiently accurate to demonstrate by means of sign changes the existence of roots in certain intervals of the line $\sigma = \frac{1}{2}$. In a few cases, however, more accuracy was needed to decide whether a sign change actually occurs. The exceptional cases do not decrease in frequency in spite of the fact that the asymptotic formula improves as $t \to \infty$. In fact the behaviour of $\zeta(s)$ becomes more irregular as t increases. Future investigations of the function will, no doubt, be directed towards isolated intervals on the critical line in which $\zeta(s)$ may be expected to behave capriciously. At such places an especially accurate determination of the values of $\zeta(s)$ is required. A further asymptotic development of the function suitable for considerable accuracy and applicable at great distances up the critical line is thus needed. Four terms in the asymptotic expansion are given below. [See equation (10).]

Another possibility is the use of the Euler-Maclaurin formula as actually used by Hutchinson [**2**]:

$$\zeta(s) = \sum_{\nu=1}^{n-1} \nu^{-s} + \tfrac{1}{2} n^{-s} + (s-1)^{-1} n^{1-s} + \sum_{\mu=1}^{k} T_\mu(s) + R(k, n, s), \tag{1}$$

where
$$(2\mu)!\ T_\mu(s) = B_{2\mu} n^{1-s-2\mu} \prod_{j=0}^{2\mu-2} (s+j)$$

and
$$|R(k, n, s)| < |T_{k+1}(s)|\,|s+2k+1|/|\sigma+2k+1|.$$

The substitution $s = \frac{1}{2} + it$ into (1) gives the following formulas for the

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real and imaginary parts of $\zeta(\frac{1}{2}+it)$:

$$\begin{aligned}\mathrm{Re}\Big(\zeta(\tfrac{1}{2}+it)\Big) = 1+\sum_{\nu=2}^{n-1} \nu^{-1/2}\cos(t\log\nu)+\tfrac{1}{2}n^{-1/2}\cos(t\log n)\\ -n^{1/2}(t^2+\tfrac{1}{4})^{-1}\{t\sin(t\log n)+\tfrac{1}{2}\cos(t\log n)\}\\ +\sum_{\mu=1}^{k}\mathrm{Re}(T_\mu)+\mathrm{Re}\Big(R(k,n,s)\Big),\end{aligned}$$

$$\begin{aligned}\mathrm{Im}\Big(\zeta(\tfrac{1}{2}+it)\Big) = -\sum_{\nu=2}^{n-1} \nu^{-1/2}\sin(t\log\nu)-\tfrac{1}{2}n^{-1/2}\sin(t\log n)\\ -n^{1/2}(t^2+\tfrac{1}{4})^{-1}\{t\cos(t\log n)-\tfrac{1}{2}\sin(t\log n)\}\\ +\sum_{\mu=1}^{k}\mathrm{Im}(T_\mu)+\mathrm{Im}\Big(R(k,n,s)\Big).\end{aligned}$$

The terms $\mathrm{Re}(T_\mu)$ and $\mathrm{Im}(T_\mu)$ can be computed recursively by the formulae

$$\left.\begin{aligned} n^2 b_\mu \mathrm{Re}(T_{\mu+1}) &= (t^2-4\mu^2+\tfrac{1}{4})\,\mathrm{Re}(T_\mu)+4\mu t\,\mathrm{Im}(T_\mu),\\ n^2 b_\mu \mathrm{Im}(T_{\mu+1}) &= (t^2-4\mu^2+\tfrac{1}{4})\,\mathrm{Im}(T_\mu)-4\mu t\,\mathrm{Re}(T_\mu),\end{aligned}\right\} \tag{2}$$

where the numbers b_μ are given by

$$\left.\begin{aligned} b_1 = 60,\quad b_2 = 42,\quad b_3 = 40,\quad b_4 = 39{\cdot}5,\\ b_\mu = (2\mu+1)(2\mu+2)\,B_{2\mu}/B_{2\mu+2} \to 4\pi^2 = 39{\cdot}4784176\ldots\end{aligned}\right\} \tag{3}$$

as $\mu\to\infty$. The initial conditions for (2) are

$$12\,\mathrm{Re}(T_1) = n^{-3/2}\{t\sin(t\log n)+\tfrac{1}{2}\cos(t\log n)\},$$

$$12\,\mathrm{Im}(T_1) = n^{-3/2}\{t\cos(t\log n)-\tfrac{1}{2}\sin(t\log n)\}.$$

A dozen of the b's may be stored in the computer. The appropriate choice of n and k for a given t is a problem in "machine economics". The programmer will find that n must be of the order of magnitude of t. In fact (2) and (3) show that n should exceed $t/2\pi = \tau$.

A few thousand terms of the series

$$\Sigma\,\nu^{-1/2}\cos(t\log\nu),\quad \Sigma\,\nu^{-1/2}\sin(t\log\nu) \tag{4}$$

take a minute or so. Hence this method should be used only when it is necessary to obtain high accuracy. However, the logarithms involved must then be computed with care since information is lost in taking the fractional parts of $\tau\log\nu$ to form $\cos(t\log\nu)$ and $\sin(t\log\nu)$. There is a good case for using double precision for $\log\nu$. A number of nearby values of t should be used to determine the noise level of the round-off error in the series (4). For checking purposes it is worth-while to compute both the real and imaginary parts of $\zeta(\frac{1}{2}+it)$ since they must satisfy the extra condition

$$-\mathrm{Im}\Big(\zeta(\tfrac{1}{2}+it)\Big)\Big/\mathrm{Re}\Big(\zeta(\tfrac{1}{2}+it)\Big) = \tan\vartheta,$$

where

$$\vartheta = \mathrm{Im}\left(\log\Gamma(\tfrac{1}{4}+\tfrac{1}{2}it)\right) - \tfrac{1}{2}t\log\pi$$

$$\sim \tfrac{1}{2}t\log(t/2\pi) - \tfrac{1}{2}t - \pi/8 + (48t)^{-1} + 7(5760t^3)^{-1} + \dots. \qquad (5)$$

In spite of such controls on the calculations the use of (1) for $t > 100000$ is rather questionable because of the large number of terms required.

The more elaborate Riemann-Siegel formula based on the so-called approximate functional equation, requires only $m = [t^{1/2}]$ cosine terms of the type

$$\nu^{-1/2}\cos(t\log\nu - \vartheta),$$

where ϑ is given in (5). In fact we approximate the real-valued function

$$f(\tau) = e^{i\vartheta}\,\zeta(\tfrac{1}{2}+2\pi i\tau)$$

by the sum

$$f_1(\tau) = 2\sum_{\nu^2\leqslant\tau}\nu^{-1/2}\cos 2\pi\{\tau\log\nu - \gamma\},$$

where by (5)

$$\gamma = \vartheta/(2\pi) = \tfrac{1}{2}\tau(\log\tau - 1) - \tfrac{1}{16} + \frac{1}{192\pi^2\tau} + \frac{7}{92160\pi^4\tau^3} + O(\tau^{-5}).$$

If we define $R(\tau)$ by

$$f(\tau) = f_1(\tau) + (-1)^{m-1}\tau^{-1/4}R(\tau), \qquad (6)$$

then $R(\tau)$ has an asymptotic expansion in powers of $\tau^{-1/2}$; the first four terms are given in what follows.

Following Titchmarsh we define the functions $a_r(t)$ by the generating function

$$\sum_{r=0}^{\infty} a_r(t)\,z^r = \exp\{(it-\tfrac{1}{2})\log(1+zt^{-1/2}) - izt^{1/2} + \tfrac{1}{2}z^2 i\}$$

so that, if we write x for $t^{-1/2}$,

$$\begin{aligned}
a_0(t) &= 1, & a_5(t) &= 9ix^3/20 + O(x^5),\\
a_1(t) &= -\tfrac{1}{2}x, & a_6(t) &= -x^2/18 + O(x^4),\\
a_2(t) &= 3x^2/8, & a_7(t) &= x^3/9 + O(x^5),\\
a_3(t) &= ix/3 - 5x^3/16, & a_8(t) &= O(x^4),\\
a_4(t) &= -5ix^2/12 + O(x^4), & a_9(t) &= -ix^3/162 + O(x^5).
\end{aligned}$$

In general

$$(r+1)\,a_{r+1}(t) = x\left(ia_{r-2}(t) - (r+\tfrac{1}{2})\,a_r(t)\right)$$

and $$a_r(t) = O(x^4) \quad (r > 9).$$

Next let $$\theta = 2(\tau^{1/2} - m)$$

be twice the fractional part of the square root of τ and write

$$\psi(z) = (\sec \pi z) \cos \pi(\tfrac{1}{8} + z - \tfrac{1}{2}z^2). \tag{7}$$

Taking derivatives we write

$$Q_k(z) = (2/\pi)^{k/2} \psi^{(k)}(z),$$

and define

$$S_N(t) = \sum_{\mu=0}^{N-1} \mu!\,(2i)^{-\mu} a_\mu(t) \sum_{\nu=0}^{\infty} i^\nu [\nu!(\mu-2\nu)!]^{-1} Q_{\mu-2\nu}(\theta). \tag{9}$$

If in Titchmarsh's Theorem 4.16 we multiply throughout by $e^{i\vartheta}$ and expand the result in descending powers of t we find for $R(\tau)$ in (6) the expression

$$R(\tau) = \{S_N(t) + O(t^{-N/6})\} \exp\Big((48it)^{-1} + O(t^{-3})\Big).$$

Setting $N = 12$ and substituting from (9) and the list of a's we obtain

$$R(\tau) = Q_0 - xQ_3/24 + \frac{x^2}{16}\Big[Q_2 + \frac{Q_6}{72}\Big] - \frac{x^3}{16}\Big[Q_1 + \frac{Q_5}{15} + \frac{Q_9}{5184}\Big] + O(x^4),$$

where the arguments of the Q's are all equal to θ, or in other words from (8)

$$R(\tau) = \psi(\theta) - \frac{\tau^{-1/2}}{12\pi^2}\psi^{(3)}(\theta) + \frac{\tau^{-1}}{16\pi^2}\Big[\psi^{(2)}(\theta) + \frac{1}{18\pi^2}\psi^{(6)}(\theta)\Big]$$
$$- \frac{\tau^{-3/2}}{32\pi^2}\Big[\psi'(\theta) + \frac{4}{15\pi^2}\psi^{(5)}(\theta) + \frac{1}{324\pi^4}\psi^{(9)}(\theta)\Big] + O(\tau^{-2}). \tag{10}$$

This gives us, *via* (6), four terms in the asymptotic development of $f(\tau)$ with an error of order $t^{-9/4}$.

However, the function $\psi(z)$ when expressed by its definition (7) becomes indeterminate at $z = \frac{1}{2}$ and its derivatives are even more unstable there. The higher derivatives become extremely complicated combinations of trigonometric functions so that (10) is practically useless as it stands. On the other hand ψ is an entire function, symmetric about $z = 1$, so that we may introduce the even function

$$\phi(z) = \psi(1+z) = \sec \pi z \cos \pi\{(4z^2+3)/8\}$$

and expand $\phi(z)$ in powers of z^2, evaluating ϕ and its derivatives for use in (10) at the point θ_1 where

$$-1 < \theta_1 = 1 - \theta \leqslant 1.$$

Carrying out this expansion with double precision so as to avoid destructive cancellation we obtain after substituting into (10)

$$R(\tau) = \phi(\theta_1) + \tau^{-1/2}\phi_1(\theta_1) + \tau^{-1}\phi_2(\theta_1) + \tau^{-3/2}\phi_3(\theta_1) + O(\tau^{-2}),$$

where the power series coefficients of ϕ, ϕ_1, ϕ_2, and ϕ_3 are given in the accompanying table.

ϕ	ϕ_1	ϕ_2	ϕ_3
$\cdot 3826834324$	$+\cdot 02682510\, z$	$+\cdot 00518854$	$+\cdot 001340\, z$
$+\cdot 4372404681\, z^{2}$	$-\cdot 01378477\, z^{3}$	$+\cdot 00030947\, z^{2}$	$-\cdot 003744\, z^{3}$
$+\cdot 1323765754\, z^{4}$	$-\cdot 03849125\, z^{5}$	$-\cdot 01133594\, z^{4}$	$+\cdot 001330\, z^{5}$
$-\cdot 0136050260\, z^{6}$	$-\cdot 00987107\, z^{7}$	$+\cdot 00223305\, z^{6}$	$+\cdot 002265\, z^{7}$
$-\cdot 0135676220\, z^{8}$	$+\cdot 00331076\, z^{9}$	$+\cdot 00519664\, z^{8}$	$-\cdot 000955\, z^{9}$
$-\cdot 0016237253\, z^{10}$	$+\cdot 00146478\, z^{11}$	$+\cdot 00034399\, z^{10}$	$-\cdot 000600\, z^{11}$
$+\cdot 0002970535\, z^{12}$	$+\cdot 00001321\, z^{13}$	$-\cdot 00059106\, z^{12}$	$+\cdot 000101\, z^{13}$
$+\cdot 0000794330\, z^{14}$	$-\cdot 00005923\, z^{15}$	$-\cdot 00010230\, z^{14}$	$+\cdot 000069\, z^{15}$
$+\cdot 0000004645\, z^{16}$	$-\cdot 00000598\, z^{17}$	$+\cdot 00002089\, z^{16}$	$-\cdot 000001\, z^{17}$
$-\cdot 0000014327\, z^{18}$	$+\cdot 00000096\, z^{19}$	$+\cdot 00000593\, z^{18}$	
$-\cdot 0000001035\, z^{20}$	$+\cdot 00000018\, z^{21}$	$-\cdot 00000017\, z^{20}$	
$+\cdot 0000000124\, z^{22}$			
$+\cdot 0000000018\, z^{24}$			

It is not necessary to store all these coefficients in the high-speed memory of the machine. The first two functions will in general suffice for all but the most delicate situations since

$$\cdot 00116 < \phi_2(\theta_1) < \cdot 00519.$$

Beyond the 25000-th zero, where $\tau > 3492\cdot 43956$, the contribution of the term $\pm\phi_2\tau^{-5/4}$ to the value of $f(\tau)$ does not exceed $1\cdot 933 \,.\, 10^{-7}$ in absolute value. As a numerical example we may consider the calculation of $\zeta(s)$ at the value $s = \frac{1}{2} + 17143\cdot 803905i$, where $\tau = 2728\cdot 5211352546932$ and where $f(\tau)$ has the least maximum for all $\tau < 3492$. Here

$$\tau^{1/2} = 52\cdot 2352480156,$$

so $\theta_1 = \cdot 5295039688$. The principal term $f_1(\tau)$ and the first four terms of the remainder are

$$\begin{array}{r} \cdot 073478610 \\ -\cdot 071297360 \\ -\cdot 000027686 \\ -\cdot 000000227 \\ +\cdot 000000001 \\ \hline f(\tau) = +\cdot 002153336 \end{array}$$

In the neighbourhood of this low maximum the two roots of $\zeta(s)$ are closer together than any other pair among the first 25000 roots. They are

$$\tfrac{1}{2}+17143{\cdot}7319i, \quad \tfrac{1}{2}+17143{\cdot}7673i,$$

which differ by only ·0354i. The previous record was held by the roots numbered 6707 and 6708, which are

$$\tfrac{1}{2}+7005{\cdot}0629i, \quad \tfrac{1}{2}+7005.1006i,$$

differing by ·0377i.

In our previous report we gave an account of the failures of what is called Gram's Law among the first 10000 zeros. In anticipation of an increase in the number of failures of Gram's Law among the next 15000 roots, the SWAC was instructed to examine and merely count minor failures and to report in detail on the major failures only, these latter being then examined in greater detail in a subsequent run. The SWAC's census of failures is given below.

In explanation of these results, we define the n-th Gram interval I_n as comprising those values of τ for which

$$\tau_n \leqslant \tau \leqslant \tau_{n+1},$$

where τ_n is the real positive root τ of

$$\tau \log \tau - \tau = n + \tfrac{1}{8}.$$

The length of I_n is nearly $1/\log \tau_n$. Gram's Law states, in effect, that the n-th root of $\zeta(\tfrac{1}{2}+2\pi i\tau) = 0$ lies in I_n. Of the 800 or more failures among the first 10000 Gram intervals a great majority were minor ones; that is, ones in which the missing root lies inside the extended interval

$$\tau_{n-\frac{1}{4}} \leqslant \tau \leqslant \tau_{n+\frac{5}{4}}.$$

Minor failures are of two types depending on whether the missing root lies outside to the left of I_n or to the right. We have then three kinds of failures of Gram's Law

Type A: left minor failure,

Type B: right minor failure,

Type C: major failure.

In studying the 15000 roots beyond the first 10000 the SWAC was instructed to report out after every 500 roots the numbers of failures of Types A, B and C among these roots. For convenience of presentation we consider 15 sets, S_1, S_2, …, S_{15} of 1000 roots each, beginning, as the SWAC did, with root number 9892 (in order to overlap the previous run).

We denote by A_k, B_k, C_k the numbers of failures of Types A, B and C among the roots of S_k. The results obtained are then as follows:

k	A_k	B_k	C_k	$A_k+B_k+C_k$
1	48	51	6	105
2	45	42	9	96
3	47	42	9	98
4	38	53	13	104
5	42	43	11	96
6	44	40	13	97
7	44	53	13	110
8	40	40	7	87
9	49	54	14	117
10	49	44	12	105
11	45	37	16	98
12	45	44	14	103
13	43	50	9	102
14	51	49	13	113
15	44	48	9	101
Averages	45	46	11	102

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