POWER SERIES EXPANSIONS
OF RIEMANN'S ξ FUNCTION

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ABSTRACT. We show how high-precision values of the coefficients of power series expansions of functions related to Riemann's ζ function may be calculated. We also show how the Stieltjes constants can be evaluated using this scheme and how the Riemann hypothesis can be expressed in terms of the behavior of two of the sequences of coefficients. High-precision values for the coefficients of these power series are found using *Mathematica* ™ .

1. INTRODUCTION

The functional equation for the ζ function is normally expressed [3, p. 16] as

$$(1) \qquad \xi(s) = \xi(1 - s),$$

where

$$(2) \qquad \xi(s) = \frac{s}{2}(s - 1)\pi^{-s/2}\Gamma\left(\frac{s}{2}\right)\zeta(s).$$

It is this function ξ and related functions which we will examine via power series expansions.

Riemann showed [5] that

$$(3) \qquad 2\xi(s) = 1 + \int_1^\infty \left(\sum_{n=1}^\infty e^{-n^2\pi t}\right)\frac{s(s-1)}{t}(t^{(1-s)/2} + t^{s/2})\,dt$$

and suggested that ξ can be expanded as a power series in $(s - 1/2)^2$ "which converges very rapidly." We will instead look at the power series expansion about the point $s = 1$.

In addition to $\xi(s)$ we also look at the expansions of $\xi'(s)/\xi(s)$, $\xi'(1/s)/\xi(1/s)$, and $\log\xi(1/s)$. Note that the zeros of ξ, i.e., the nontrivial zeros of ζ, are singularities of the functions $\log\xi(s)$ and $\xi'(s)/\xi(s)$ and that the mapping $s \mapsto 1/s$ maps the critical line to the circle of radius 1 centered at $s = 1$. Thus, the Riemann hypothesis can be expressed in terms of the growth of the coefficients of the power series expansion of $\xi'(1/s)/\xi(1/s)$ or of

$\log \xi(1/s)$: the Riemann hypothesis is equivalent to the radius of convergence being 1.

2. Power series expansion of $\xi(s)$ about $s = 1$

To find the power series coefficients of $\xi(s)$, we examine the derivatives of $\xi(s)$ at $s = 1$. In particular, if we let

$$(4) \qquad 2\xi(s) = \sum_{j=0}^{\infty} \alpha_j (s-1)^j,$$

then by induction on (3), we get

$$(5) \qquad \alpha_0 = 1 \quad \text{and} \quad \alpha_j = \beta_{j-2} + \beta_{j-1} \quad \text{for } j \geq 1,$$

where

$$(6) \qquad \beta_{-1} = 0, \qquad \beta_0 = 1 + \frac{\gamma}{2} - \log(2\sqrt{\pi}),$$

and

$$(7) \qquad \beta_j = \frac{1}{j!} \int_1^{\infty} \left(\sum_{n=1}^{\infty} e^{-n^2 \pi t} \right) \frac{(\log \sqrt{t})^j}{t} (\sqrt{t} + (-1)^j) \, dt \quad \text{for } j \geq 1.$$

3. Power series expansion of $\xi'(s)/\xi(s)$

We also wish to get the values of σ_{k+1}, where

$$(8) \qquad \frac{\xi'(s)}{\xi(s)} = \sum_{k=0}^{\infty} \sigma_{k+1} (1-s)^k.$$

(The reason for the factor of $(-1)^k$ and the subscript of $k+1$ will become apparent below.) To find the values of σ_{k+1}, we can multiply the power series expansion of $2\xi'(s)$ by that of $1/(2\xi(s))$. We note that the power series expansion of $1/(2\xi(s))$ is given by

$$(9) \qquad 1/(2\xi(s)) = \sum_{n=0}^{\infty} a_n (s-1)^n,$$

where

$$(10) \qquad a_0 = 1 \quad \text{and} \quad a_n = -\sum_{j=1}^{n} \alpha_j a_{n-j},$$

as can be seen by examining the product of the expansions of $2\xi(s)$ and $1/(2\xi(s))$.

For small values of k this method of computing the coefficients σ_{k+1} works well. However, the cost of computing each coefficient increases linearly with the index. Because, as we shall see below, there is another method whose cost per term does not increase at all, we only use this method for small k. There is also an issue of numerical ill-conditioning in the calculation of the σ_{k+1} from the β_j. However, this ill-conditioning is not nearly so bad as that of Lehmer's method, which loses nearly 0.85 digits per coefficient [4, equation (12)].

We use a different approach for large k. From the well-known product over all nontrivial zeros of the ζ function [3, p. 20],

$$(11) \qquad \xi(s) = \frac{1}{2} \prod_\rho \left(1 - \frac{s}{\rho} \right),$$

we get

$$(12) \qquad \log \xi(s) = -\log 2 + \sum_\rho \log \left(\frac{\rho - 1}{\rho} \right) + \sum_\rho \log \left(1 - \frac{s - 1}{\rho - 1} \right)$$

$$(13) \qquad = -\log 2 + \sum_\rho \log \left(1 - \frac{1}{\rho} \right) - \sum_{k=1}^\infty \frac{1}{k} \left(\sum_\rho \left(\frac{s - 1}{\rho - 1} \right)^k \right).$$

Note that at $s = 1$ we get the identity $\sum_\rho \log(1 - 1/\rho) = 0$ since $\xi(1) = 1/2$.
   Differentiating (13), we get

$$(14) \qquad \frac{\xi'(s)}{\xi(s)} = \sum_{k=1}^\infty \left[\sum_\rho \frac{1}{(1 - \rho)^k} \right] (1 - s)^{k-1},$$

and we see that

$$(15) \qquad \sigma_k = \sum_\rho \frac{1}{(1 - \rho)^k} = \sum_\rho \frac{1}{\rho^k}.$$

Note that the functional equation for ξ applied to (13) at $s = 1$ yields

$$(16) \qquad \sum_{k=1}^\infty \frac{1}{k} \sigma_k = 0,$$

and applied to (14) at $s = 1$ yields

$$(17) \qquad \sigma_1 = -\sum_{k=1}^\infty \sigma_k.$$

In general, the functional equation applied to the jth derivative of (14) yields

$$(18) \qquad \sigma_{j+1} = (-1)^{j+1} \sum_{k=1}^\infty \binom{k - 1}{j} \sigma_k.$$

We can use these identities as consistency checks on the values of σ_k.
   For k large, the sum of the $-k$ powers of the nontrivial zeros of the zeta function is rapidly convergent. For k small we must get the values of σ_k from the values of α_j.

4. Power Series Expansions of Related Functions

To get the power series expansions for

$$(19) \qquad \frac{\xi'(1/s)}{\xi(1/s)} = \sum_{k=0}^\infty \tau_k (1 - s)^k$$

and

$$(20) \qquad \log(2\xi(1/s)) = \sum_{k=0}^\infty \lambda_k (1 - s)^k,$$

we need the following: if

$$(21) \qquad f(z) = \sum_{n=0}^{\infty} a_n (z-1)^n,$$

then

$$(22) \qquad f\left(\frac{1}{z}\right) = a_0 + \sum_{m=1}^{\infty} \left[\sum_{n=1}^{m} \binom{m-1}{n-1} a_n \right] (1-z)^m,$$

which can be seen from the fact that

$$(23) \qquad \left(\frac{1}{z} - 1\right)^n = \frac{(1-z)^n}{[1-(1-z)]^n} = (1-z)^n \left[\sum_{k=0}^{\infty} (1-z)^k \right]^n$$

and collecting like powers of $(1-z)$. Using this, we get the following expressions for the coefficients:

$$(24) \qquad \tau_0 = \sigma_1,$$

$$(25) \qquad \tau_k = \sum_{j=1}^{k} \binom{k-1}{j-1} (-1)^j \sigma_{j+1} \quad \text{for } k \geq 1,$$

$$(26) \qquad \lambda_0 = 0,$$

$$(27) \qquad \lambda_k = \sum_{j=1}^{k} \frac{(-1)^{j-1}}{j} \binom{k-1}{j-1} \sigma_j \quad \text{for } k \geq 1.$$

As with σ_k, further identities can be derived, which can be used for checking consistency. In particular, substituting (18) into the expressions for τ_k and λ_k, we get

$$(28) \qquad \tau_k = -\sum_{j=2}^{\infty} \binom{j+k-2}{k} \sigma_j,$$

$$(29) \qquad \lambda_k = \frac{-1}{k} \sum_{j=1}^{\infty} \binom{j+k-1}{k-1} \sigma_j.$$

5. Further observations

From (28) we see that

$$(30) \qquad \tau_{m-1} = -\sum_{j=m}^{\infty} \binom{j-1}{m-1} \sigma_{j-m+2}$$

$$(31) \qquad = -\sum_{\rho} \left[\sum_{j=m}^{\infty} \binom{j-1}{m-1} \rho^{-j} \right] \rho^{m-2}$$

$$(32) \qquad = -\sum_{\rho} (\rho-1)^{-m} \rho^{m-2}$$

$$(33) \qquad = -\sum_{\rho} \left(\frac{\rho}{\rho-1}\right)^m \rho^{-2}.$$

Likewise, from (29), λ_k can be expressed in terms of a sum over ρ, namely

$$(34) \qquad \lambda_m = \frac{1}{m} \sum_\rho \left[1 - \left(\frac{\rho}{\rho - 1} \right)^m \right].$$

In fact, τ_m is just the second central difference of $m\lambda_m$:

$$(35) \qquad \tau_m = (m+1)\lambda_{m+1} - 2m\lambda_m + (m-1)\lambda_{m-1}.$$

From (33) it is clear that the Riemann hypothesis implies that the values of $|\tau_k|$ are bounded by

$$(36) \qquad \sum_\rho |\rho|^{-2} = 0.04619141793224206762862\ldots.$$
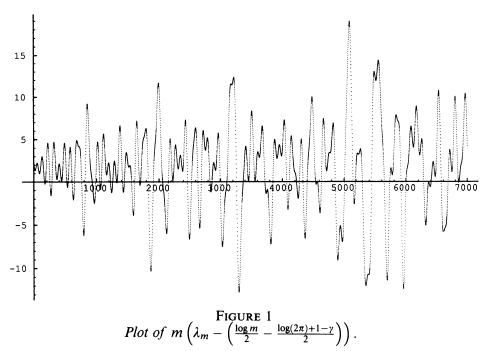
Conversely, if the $|\tau_k|$ are bounded, then by (19) the Riemann hypothesis must be true. It is also clear that the failure of the Riemann hypothesis (if such is the case) would be rather difficult to observe in the growth of the numerical values of the coefficients τ_k, since k would have to be *extremely* large before a (large) ρ which is off the critical line would yield $|\rho/(\rho - 1)|^k$ large.

Likewise, from (34) it is clear that the Riemann hypothesis implies that $\lambda_m > 0$ for all positive m. In fact, if we assume the Riemann hypothesis, and further that the zeros are very evenly distributed, we can show that

$$(37) \qquad \lambda_m \approx \frac{\log m}{2} - \frac{\log(2\pi) + 1 - \gamma}{2}.$$

This comes from the fact [3, p. 132] that the number of zeros ρ in the critical strip with $0 < \operatorname{Im} \rho < T$ is

$$(38) \qquad N(T) \sim \frac{T}{2\pi} \log \frac{T}{2\pi} - \frac{T}{2\pi}$$

FIGURE 1

Plot of $m\left(\lambda_m - \left(\frac{\log m}{2} - \frac{\log(2\pi) + 1 - \gamma}{2} \right) \right).$

and (34). Note that this asymptotic conjecture is much stronger than the Riemann hypothesis. Even the coefficient of the log m (not to mention the constant term) could be altered by a slight preference of the zeros to cluster at, or avoid, the points $1/2 + 2i \tan((2k+1)\pi/(2m))$. This approximation to λ_m agrees rather well with the observed behavior of these numbers (cf. Figure 1).

6. STIELTJES CONSTANTS

The Stieltjes constants are the numbers γ_n in the Laurent expansion

$$(39) \qquad \zeta(s) = \frac{1}{s-1} + \sum_{n=0}^{\infty} (-1)^n \frac{\gamma_n}{n!} (s-1)^n.$$

In this section we show how the coefficients σ_j can be used efficiently to evaluate the Stieltjes constants.

Taking the logarithm of both sides of (2), we see that

$$(40) \qquad \log(s-1)\zeta(s) = \log 2\xi(s) + \frac{1}{2}\log \pi - \frac{1-s}{2}\log \pi - \log\left[s\Gamma\left(\frac{s}{2}\right)\right].$$

Employing equation 6.1.33 (p. 256) of [1] with $1 + z = s/2$, we find that

$$(41) \qquad \begin{aligned} \log\left[s\Gamma\left(\frac{s}{2}\right)\right] &= \left(\log 2 + \frac{\gamma-1}{2}\right) + \frac{\gamma-1}{2}(1-s) \\ &\quad + \sum_{n=2}^{\infty} \frac{\zeta(n)-1}{n2^n}[1 + (1-s)]^n. \end{aligned}$$

Substituting this into (40), we get that

$$(42) \qquad \begin{aligned} \log(s-1)\zeta(s) &= \log 2\xi(s) + \left[\frac{1}{2}\log \pi - \log 2 + \frac{1-\gamma}{2} - \sum_{n=2}^{\infty} \frac{\zeta(n)-1}{n2^n}\right] \\ &\quad - \left[\frac{1}{2}\log \pi + \frac{\gamma-1}{2} + \sum_{n=2}^{\infty} \frac{\zeta(n)-1}{2^n}\right](1-s) \\ &\quad - \sum_{j=2}^{\infty} \frac{1}{j}\left[\sum_{n=j}^{\infty} \binom{n-1}{j-1} \sum_{k=2}^{\infty} \frac{1}{(2k)^n}\right](1-s)^j. \end{aligned}$$

Now we know that

$$\log(s-1)\zeta(s) = \gamma(s-1) + \cdots$$

and that

$$\log 2\xi(s) = -\sum_{j=1}^{\infty} \frac{1}{j}\sigma_j(1-s)^j.$$

Hence, to get the coefficients of the constant and linear terms to be correct, we must have that

$$(43) \qquad \sum_{n=2}^{\infty} \frac{\zeta(n)-1}{n2^n} = \frac{1-\gamma}{2} + \log\frac{\sqrt{\pi}}{2}$$

and

$$(44) \qquad \sum_{n=2}^{\infty} \frac{\zeta(n)-1}{2^n} = \log 2 - \frac{1}{2}.$$

Furthermore, since for large x

$$(45) \qquad \sum_{n=j}^{\infty} \binom{n-1}{j-1} x^{-n} = (x-1)^{-j},$$

we get that (42) simplifies to

$$(46) \qquad \log(s-1)\zeta(s) = \gamma(s-1) - \sum_{j=2}^{\infty} \frac{1}{j}\left[\sigma_j + \sum_{k=2}^{\infty}(2k-1)^{-j}\right](1-s)^j.$$

By taking the exponential of this series we get that $\gamma_0 = \gamma$ and

$$(47) \qquad \begin{aligned} \frac{\gamma_k}{k!} = \frac{1}{k+1}\Bigg(& \sigma_{k+1} + \frac{\zeta(k+1,3/2)}{2^{k+1}} - \gamma\frac{\gamma_{k-1}}{(k-1)!} \\ & - \sum_{j=1}^{k-1}\frac{\gamma_{j-1}}{(j-1)!}\left[\sigma_{k+1-j} + \frac{\zeta(k+1-j,3/2)}{2^{k+1-j}}\right]\Bigg). \end{aligned}$$

It should be noted that we could also map s to $1/s$ in (46) and get the series expansion of $\log(1/s - 1)\zeta(1/s)$ about $s = 1$. If we do this, we find that the behavior of these coefficients is very similar to the behavior of the λ_m. In particular, we empirically find that these coefficients are approximated by $\lambda_m - (0.75 - 0.134/m)/m$. Since the evaluation of these coefficients is much more ill-conditioned than that of the λ_m, and the results are so similar, we do not pursue this further.

We note here that the values we found for the Stieltjes constants are not consistent with those presented in Table 2 of [2]. In particular, the number of correct digits presented there decreases linearly from about ten for γ_{36} to about three for γ_{50}. The value for γ_{55} is correct to ten digits, however. (It is clear that the error is not in our values, since we can use (39) to evaluate $\zeta(30)$ with an absolute error of less than 10^{-26} while the term involving γ_{50} has magnitude greater than 10^{10}.)

7. PRACTICAL CONSIDERATIONS

The computations associated with this paper were performed over a period of several months using *Mathematica*™ on a Sun SPARC-station 1. (A few of the results are presented in the appendix. More complete results are available by e-mail from the author.) With careful coding these computations can probably be extended by at least an order of magnitude, more on a more powerful computer. Here we discuss some of the practical considerations in such computations.

A major difficulty is the evaluation of β_j using (7). In fact there are two things that can be done here to make the computation efficient. First the theta function $\sum_{n=1}^{\infty} e^{-n^2\pi t}$ can be evaluated for any t with a single evaluation of the exponential function and relatively few multiplications. The sum converges rapidly and we include only the significant initial terms. The terms c_n in the sum are evaluated as follows:

    1. Let $c_1 = e^{-\pi t}$, $a = c_1^2$, and $b_1 = ac_1$.
    2. Let $c_{n+1} = c_n b_n$ and $b_{n+1} = b_n a$.

This algorithm is based on the fact that the differences of successive square integers are the successive odd integers.

The other thing that can be done to make (7) efficient is to use a double-exponential quadrature routine. In particular, by reparametrizing the integral with $t = 1 + e^\tau$ and using the trapezoid rule with sufficiently small stepsize (i.e., progressively halving the stepsize until the estimated error is sufficiently small), the error converges to 0 faster than any power of the stepsize. Since we have (17) and (18), we can check for consistency in the values of σ_k and do not need to go to great lengths to estimate the error incurred in the quadrature routine.

Another point to be aware of is that, as mentioned in §3, only the first several hundred values of σ_k can be efficiently calculated by dividing the series expansion of $\zeta'(s)$ by the series expansion of $\zeta(s)$; for larger values of k, σ_k is best evaluated by directly summing inverse powers of the zeros of the ζ function.

Finally, for very extensive calculations, λ_k calculated using (27) suffers from ill-conditioning. Since λ_k can also be calculated using (34), we can combine these two formulae and express λ_k using (34), where only the first several hundred zeros are included, and (27), where the first several hundred zeros are *not* included in the σ_j. In particular,

$$(48) \qquad m\lambda_m = \sum_{i=1}^{N}\left[1 - \left(\frac{\rho_i}{\rho_i - 1}\right)^m\right] - \sum_{j=1}^{m}(-1)^j\binom{m}{j}\sigma_{j,N},$$

where

$$\sigma_{j,N} = \sigma_j - \sum_{i=1}^{N}\rho_i^{-j} = \sum_{i=N+1}^{\infty}\rho_i^{-j}.$$

This splitting was not used in the calculations presented in the appendix.

APPENDIX

k	α_k	
0	+1.000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000	(0)
1	+2.30957089661210338143102479064952916219321271520507595253920722129713564767245799708O	(-2)
2	+2.3343864534226183134882356885810481045268880440781352993486966445261162746796961339 46	(-2)
3	+4.97938499229486723511717743894883531533405119031116449729736222496716951590001579428	(-4)
4	+2.5318173031652700505612108411637347812162476124680516932004525099666232551497055973 7	(-4)
5	+5.050254792219174169585235225013184802155949855115946521610652948278792216309485432300	(-6)
6	+1.720987041861535577780154973904094132086757701702736404927326535419947612327570256219	(-6)
7	+3.2378414616810769603480659196734062089420122269004286279830767694635723758098590749485	(-8)
8	+8.315968250027721630708768786514767520775647323890266412483461676055203222011449340850	(-9)
9	+1.4852419214918940045225838489643707531590973645045046236458745172051470454227592811777777	(-10)
10	+3.0655602327633313510279499968476071335101043951727736679477527584247165585867914345 23	(-11)
20	+1.2134779622875435113559662535132616827196429736894369228229583513642325232287489188071	(-24)
50	+1.0704290691548383133857306575485850593602625031782153709141131169592725884659059315 5	(-71)
100	+1.2408628236250662089303729152648266523679878218011497183515101627403718622727312716 96	(-161)
150	+9.3041337135495779411068526784254542152542124147332195033491904715398670891206461849O	(-260)

k	λ_k	
0	−6.9314718055994530941723212145817656807550013436025525412066000949333936219696947156059	(-1)
1	+2.3095708966121033814310247906495291621932127152050750952539207221297135647672457997080	(-2)
2	+4.6172867614023335192864243096033943387066108314123254699816298966992694601558057705AG	(-2)
3	+6.9212973518108267930497348872601068994212026393200243617482708163383628392849455363 37	(-2)
4	+9.2197619873060409647627872409439018065541673490213201205779714212736563306644475C5730	(-2)
5	+1.1510854289223549048622128109857276671349132303595990790584951638719090042767247281564	(-1)
6	+1.37927668713729882904167137003416663561389660786544834323414299364966399173221286G017	(-1)
7	+1.6063715965299421294040287257385366292282442046162616303548680222624890164945086103 57	(-1)
8	+1.8321945964338257908193931774721859846998098273431805825307322192294743785654454743098	(-1)
9	+2.0565733867091704617028938742134330474123655341004356019608497727988730141462823206002	(-1)
10	+2.2793393631931577436930340573684453380748385942738127649614843069730829981011373724070	(-1)
20	+4.3846384360466075647997306767236011141956127351909716142162815565338406971636804217GC	(-1)
50	+8.7062192976748038597903939969723137228880910048998112057837447733612870824896593S24 30	(-1)
100	+1.1860377537679132992736469839793792693298702359322787634218936590623426250365758172 37	(0)
200	+1.5332788242567238320636127578534097200400424785844995385899349906090065948305997665939	(0)
500	+1.983800185984489894093667592662983365128441521939691632641423273119401230747101292110	(0)
1000	+2.3260531616864664574065046940832238158044982041692942226890632508476422953640417G3830	(0)
2000	+2.675879760190751756905349140785670258231690602747867042182960870731022804306868201118	(0)
4000	+3.0176169058992665676759081907061326908349640730306161346167017387441342216815616873 22	(0)

k	σ_k	
1	+2.3095708961210338143102479064952916219321271520507595253920722129713564767245799708	(-2)
2	-4.6154317295804602757107990379077303530267962324144990348848453508042676249660955470	(-2)
3	-1.1115823145210592276266823891457847396418924898651877027345267289121300062624022668	(-4)
4	+7.3627221261689518326771307030600151131283159627410029044634235763037817581718916822	(-5)
5	+7.1509335576260773580109391313245132240664933152756876892430773499738867953433453798	(-7)
6	-2.8143641693876626160671564047612376758597264230790495720326720006075168134498338302	(-7)
7	-4.5741911497047721111626925898888290675003535399088094208405330642824417045059579692	(-9)
8	+1.2688681100507607190125475731981339303292111145778642933676333984922328502032097983	(-9)
9	+2.8274371550558870893343968780614040360549272896412393916344242726721990405274763716	(-11)
10	-5.9977148471518745948920262897913945377265261620475444135700980718512411277037635141	(-12)
20	+1.4823993296629079281479369921172610527471499707044927574926928515355605179386555369	(-23)
50	+1.1616791579794980951159713056759983513336040727451525659854941509929317023859530785	(-58)
100	-1.6235337791320460137199270264220270565006396396878996768158905294998178171908173392	(-115)
200	+1.0897295987775098651196942181107217046672649587050437821739970196065104721692114782	(-230)
400	-7.7519974395984675115926991862936751337244546944474772622803612990099633364630822424	(-463)

k	Stieltjes constants γ_k	
0	+5.7721566490153286060651209008240243104215933593992359880576723488486772677664670936	(-1)
1	-7.2815845483676724860586375874901319137736338334337952599006559741401433571511484878	(-2)
2	-9.6903631928723184845303860352125293590658061013407498807013654518507538228041417198	(-3)
3	+2.0538344203033458661600465427533842857158044454106182454814833691383449211297005357	(-3)
4	+2.3253700654673000574681701775260680009044694137848509907580409071246841005315521900302	(-3)
5	+7.9332381730106270175333487744444483073153940458488707573425626982314821180171520237	(-4)
6	-2.3876934543019960987242184190800427778371515635807863147642530739106755999296387143	(-4)
7	-5.2728956705775104607409750547885828199625347296989533101340422688568273246514118214	(-4)
8	-3.5212335380303950960205216500120874172918053379235035665733150736506065301060	(-4)
9	-3.4394774418088048177914623798227390620789538594441629759291904843150103344615283709	(-5)
10	+2.0533281490906479468372228923706530295985377416676430384020871435300902407106017519	(-4)
20	+4.6634356151159494900594824433550525113143473926588997670726628098544582130032900701	(-4)
50	+1.2682360265132271659672525364865755553848357594489017019809569934697325440412714190	(2)
100	-4.2534015711708026962311443851972783582470289310534734689716243198563624487106798672	(17)
150	+8.0288537315068429932566464259898920148424673878973112390001195006142409263025740	(35)

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