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AN EFFECTIVE ASYMPTOTIC FORMULA FOR THE STIELTJES CONSTANTS

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ABSTRACT. The Stieltjes constants γ_k appear in the coefficients in the regular part of the Laurent expansion of the Riemann zeta function $\zeta(s)$ about its only pole at $s = 1$. We present an asymptotic expression for γ_k for $k \gg 1$. This form encapsulates both the leading rate of growth and the oscillations with k. Furthermore, our result is effective for computation, consistently in close agreement (for both magnitude and sign) for even moderate values of k. Comparison to some earlier work is made.

1. INTRODUCTION AND MAIN RESULT

The Riemann zeta function has but one simple pole, at $s = 1$ in the complex plane [13, 15]. In the Laurent series about that point,

$$\zeta(s) = \frac{1}{s-1} + \sum_{k=0}^{\infty} \frac{(-1)^k \gamma_k}{k!}(s-1)^k, \tag{1.1}$$

γ_k are called the Stieltjes constants [2, 3, 5, 7, 8, 12, 14, 16], where $\gamma_0 = \gamma$, the Euler constant. These constants have many uses in analytic number theory and elsewhere. Among other applications, estimates for γ_n may be used to determine a zero-free region of the zeta function near the real axis in the critical strip $0 < \mathrm{Re}\ s < 1$.

In this paper, we are interested in the leading asymptotic form of these constants for $k \gg 1$. Throughout we write $f(n) \sim g(n)$ when the limit relation $\lim_{n\to\infty} \frac{f(n)}{g(n)} = 1$ holds. We have

Theorem 1. *Let $v = v(n)$ be the unique solution of the equation*

$$2\pi \exp[v \tan v] = n\frac{\cos v}{v}, \tag{1.2}$$

in the interval $(0, \pi/2)$, with $v \to \pi/2$ as $n \to \infty$. Let $u = v\tan v$ with $u(n) \sim \log n$ as $n \to \infty$. Then we have for $n \gg 1$,

$$\gamma_n \sim \frac{B}{\sqrt{n}} e^{nA} \cos(an + b), \tag{1.3}$$

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where

$$A = \frac{1}{2}\log(u^2+v^2) - \frac{u}{u^2+v^2},$$
$$B = \frac{2\sqrt{2\pi}\sqrt{u^2+v^2}}{[(u+1)^2+v^2]^{1/4}},$$
$$a = \tan^{-1}\left(\frac{v}{u}\right) + \frac{v}{u^2+v^2},$$

and

$$b = \tan^{-1}\left(\frac{v}{u}\right) - \frac{1}{2}\tan^{-1}\left(\frac{v}{u+1}\right).$$

Formula (1.3) holds as long as we stay bounded away from zeros of the cosine factor. We note that, in view of (1.2), the functions A, B, a, b depend weakly on n as $\log n$ and $\log\log n$. To leading order, $A \sim \log\log n$ and $B \sim \frac{\pi}{2}(\log n)^{-1}$.

The result (1.3) has many advantages. It captures both the basic growth rate $\exp(n\log\log n)$ and the oscillations $\cos[n(\pi/2)/\log n]$. It therefore has implications for the sign changes observed in γ_n with increasing n. Furthermore, (1.3) is found to be numerically accurate for even modest values of n. After the proof of Theorem 1 in the next section, we describe numerical results in Section 3. There, we also compare and contrast our result with earlier work of Matsuoka [9, 10]. Although Matsuoka has given an asymptotic series to high order, it does not appear to be effective for computation. This is because the fractional part of the argument of the cosine factor modulo 2π in his result is not sufficiently controlled.

It has been known for some time that the Stieltjes constants of both even and odd indices are both positive and negative infinitely often [2, 12, 10]. This is one corollary of Theorem 1.

Recent analytic results for the Stieltjes constants may be found in [3] and [4]. The latter includes an addition formula for the constants together with series representations. Many open questions concerning the Stieltjes constants remain, including characterizing their arithmetic properties.

Proof of Theorem 1. We begin with the integral representation ([17], pp. 153-154; [6], pp. 5) for $n \geq 1$,

$$\gamma_n = \int_1^\infty P_1(x)\frac{\log^{n-1} x}{x^2}(n-\log x)dx. \tag{2.1}$$

Here, $P_1(x) = B_1(x-[x]) = x-[x]-1/2$ is the first periodized Bernoulli polynomial, and it has the standard Fourier series [1, p. 805],

$$P_1(x) = -\sum_{j=1}^\infty \frac{\sin(2\pi jx)}{\pi j}. \tag{2.2}$$

With the change of variable $t = \log x$, from (2.1) and (2.2) we then have

$$\begin{aligned}\gamma_n &= -\sum_{L=1}^\infty \int_0^\infty \frac{\sin(2L\pi e^t)}{\pi L} t^{n-1}e^{-t}(n-t)dt \\ &= -\mathrm{Im}\left\{\sum_{L=1}^\infty \frac{1}{L\pi}\int_0^\infty \exp[i2L\pi e^t + n\log t]e^{-t}\left(\frac{n}{t}-1\right)dt\right\}. \qquad (2.3)\end{aligned}$$

We apply the saddle point method, and find that the $L = 1$ term in (2.3) dominates the others. With the function $h(t) \equiv i2L\pi e^t + n \log t$, the saddle points occur for $h'(t) = 0$. Therefore, they satisfy

$$te^t = \frac{ni}{2L\pi}, \tag{2.4}$$

and are asymptotically given by $t \sim \log n - \log\log n + \alpha + \beta$. For integers M, we have $\alpha = \left(2M + \frac{1}{2}\right)\pi i - \log(2L\pi)$ and $\beta = \log\log n/\log n - \alpha/\log n = o(1)$. This gives

$$\begin{aligned} t_M = \log n - \log\log n - \log(2L\pi) + \left(2M + \frac{1}{2}\right)\pi i \\ + \frac{\log\log n}{\log n}[1 + o(1)],\ M = 0, \pm 1, \pm 2, \ldots. \end{aligned} \tag{2.5}$$

We find that $|e^{h(t_M)}|$ as a function of M is maximized at $M = 0$, and as a function of L, at $L = 1$.

More precisely, we have the estimate

$$\begin{aligned} \log|e^{h(t_M)}| &= \mathrm{Re}[h(t_M)] \\ = n\log\log n &- \frac{n}{\log n}[\log\log n + 1 + \log(2L\pi)] - \frac{1}{2}\frac{n}{\log^2 n}\left(2M + \frac{1}{2}\right)^2 \pi^2 \\ &+ \frac{1}{2}\frac{n}{\log^2 n}[\log\log n + \log(2L\pi)]^2 + O_R\left(\frac{n}{\log^3 n}\right), \end{aligned} \tag{2.6}$$

where the O_R "rough" error term may omit some factors of $\log\log n$. From the second term in the right-hand side of (2.6) we see that the terms in (2.3) with $L \geq 2$ are roughly exponentially smaller than the first term. In terms of M, (2.6) is largest at $M = 0$, but we can also easily show that the original contour ($t \in [0, \infty)$) can be deformed to a steepest descent contour that passes only through the saddle t_0. In Figure 1 we plot the curves $\mathrm{Re}[h'(t)] = 0$ and $\mathrm{Im}[h'(t)] = 0$ in the (x, y) plane, with $L = 1$ and $t = x + iy$. The intersection points of these curves are the saddle points, and the figure captures 3 saddles in the range $y = \mathrm{Im}(t) \in [-2\pi, 3\pi]$ (here we used $n = 1,000$). The steepest descent (SD) curve through the saddle $t_0 = u + iv$ is given by $\mathrm{Im}[h(t)] = \mathrm{Im}[h(t_0)]$ so that

$$n\tan^{-1}\left(\frac{y}{x}\right) + 2\pi e^x \cos y = \frac{nv}{u^2 + v^2} + n\tan^{-1}\left(\frac{v}{u}\right). \tag{2.7}$$

The right side of (2.7), for $n \to \infty$, is approximately $n\pi/(2\log n)$ so that the SD contour starts at the origin roughly at the slope $y/x = \pi/(2\log n)$, traverses the saddle in a nearly horizontal direction (since $h''(t_0)$ is to leading order real and negative) and winds up at $t = \infty + i\pi/2$. In Figure 2 we sketch the SD contour when $n = 1,000$, along with the steepest ascent (SA) contour that is also a branch of (2.7), and which orthogonally intersects the SD contour at the saddle t_0 (here $t_0 \approx 3.706 + 1.246i$).

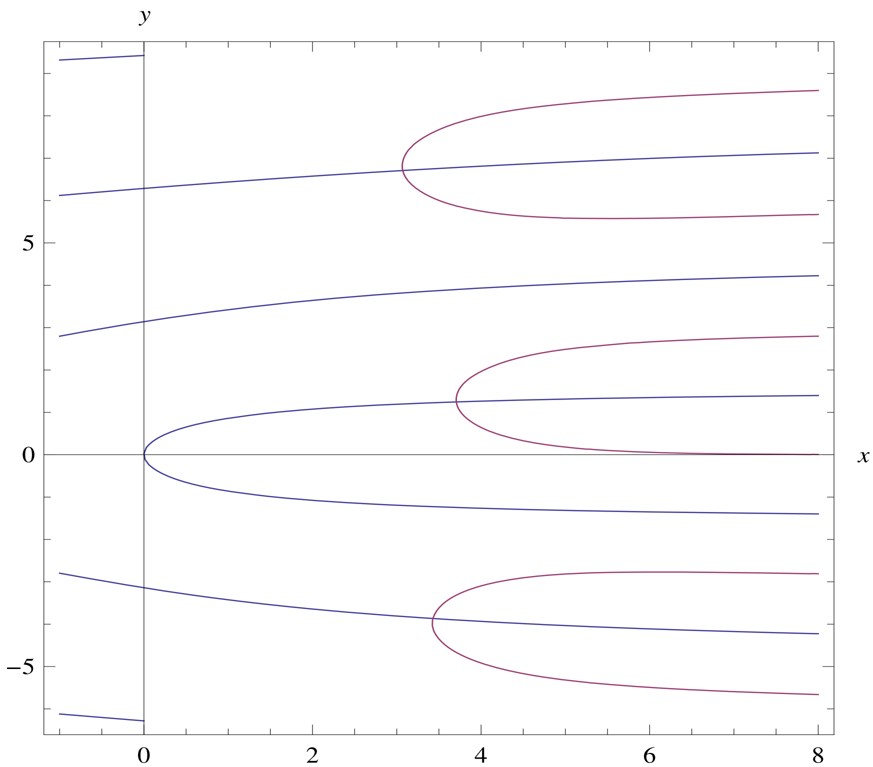

FIGURE 1. The real and imaginary parts of the saddle point equation $h'(t) = 0$ are plotted in the (x, y) plane, with $L = 1$ and $t = x + iy$. Three saddle points are present in the range $y = \text{Im}(t) \in [-2\pi, 3\pi]$. Here, $n = 1,000$ in (2.4).

We have $h''(t) = 2L\pi i e^t - n/t^2$, so that $h''(t_0) = -n/t_0 - n/t_0^2$. We therefore have

$$\int_0^\infty e^{h(t)} \left(\frac{n}{t} - 1\right) e^{-t} dt \sim \left(\frac{n}{t_0} - 1\right) \frac{\sqrt{2\pi}}{\sqrt{\frac{n}{t_0} + \frac{n}{t_0^2}}} e^{h(t_0)} e^{-t_0}$$

$$\sim n\sqrt{\frac{2\pi}{n}} \frac{e^{-t_0}}{\sqrt{t_0 + 1}} e^{h(t_0)}. \tag{2.8}$$

Then we have

$$e^{h(t_0)} = \exp\left[n\left(\log t_0 - \frac{1}{t_0}\right)\right] = e^{n[A(n)+ia(n)]}, \tag{2.9}$$

where $A(n) = \text{Re}[\log t_0 - 1/t_0]$ and $a(n) = \text{Im}[\log t_0 - 1/t_0]$. From (2.3), (2.8), and (2.9) we then have

$$\gamma_n \sim -\sqrt{\frac{2n}{\pi}} e^{nA(n)} \text{Im}\left[\frac{e^{-t_0}}{\sqrt{t_0 + 1}} e^{ina(n)}\right]. \tag{2.10}$$

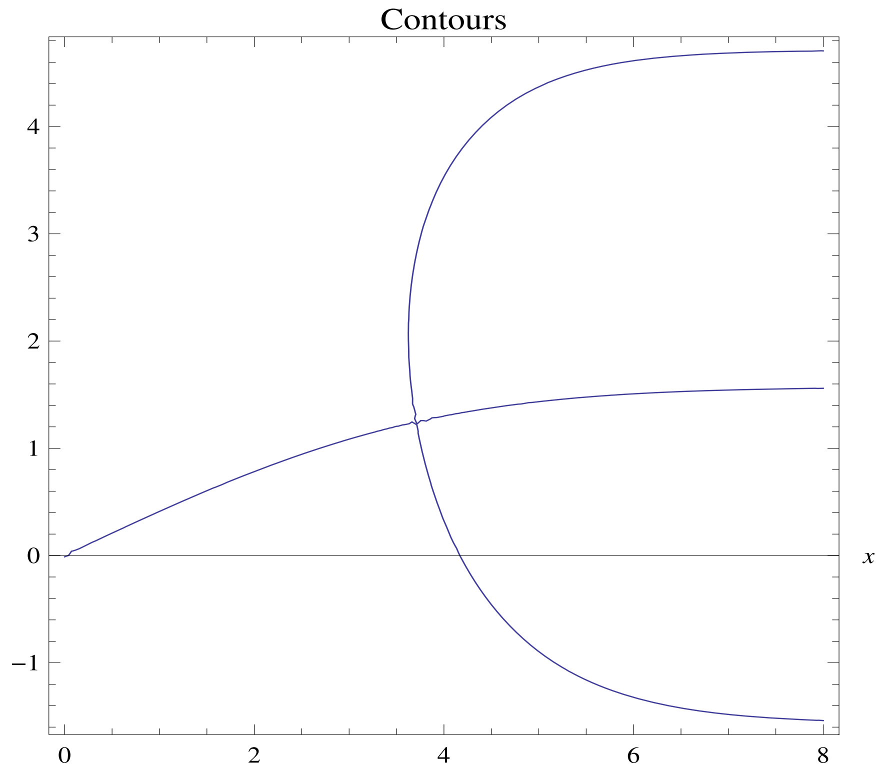

FIGURE 2. The steepest descent and ascent contours intersecting at the saddle point t_0 are shown. Here, $n = 1,000$.

Finally, putting $t_0 = u + iv$ in the relation (2.4) at $L = 1$ gives the pair of equations

$$2\pi e^u \cos v = \frac{nv}{u^2 + v^2}, \tag{2.11a}$$

$$u \cos v = v \sin v. \tag{2.11b}$$

Since u can be eliminated through the relation $2\pi e^u = n(\cos v)/v$, the single equation (1.2) for v follows. □

Remarks. The representation (2.1) may be readily verified by substitution in the defining relation (1.1). Then we obtain

$$\zeta(s) = \frac{1}{s-1} + \frac{1}{2} - s\int_1^\infty x^{-(s+1)} P_1(x)dx, \tag{2.12}$$

and this is equivalent to [15, p. 14].

As a byproduct of the proof of Theorem 1, we have the $n \to \infty$ forms (cf. (2.5)) $u \sim \log n - \log\log n - \log(2\pi)$ and $v \sim (\pi/2)(1 - 1/\log n)$.

The above calculations also show that to refine Theorem 1, the terms in (2.3) with $L \geq 2$ will play no role, and the full asymptotic series will come from refining the Taylor expansion of $h(t)$, as well as the "slowly varying" factors $e^{-t}(n/t - 1)$, about $t = t_0$. Computing the first correction term would refine (1.3) by changing the amplitude factor $B/\sqrt{n}$ to $(B + C/n)/\sqrt{n}$ and the argument of the cosine to $an+b+c/n$, where c and C would again depend only weakly on n. Such corrections should be numerically significant if $an + b$ is close to a zero of the cosine, which occurs, for example, when $n = 137$.

From Theorem 1, the leading order frequency of γ_n is given by $\tan^{-1}\left(\frac{\pi}{2}\frac{1}{\log n}\right)$. In turn, this implies that the scale for sign changes is $2\log n$. Then subsequences γ_{n+j} with $j < 2\log n$ with the same sign will appear infinitely often. Similarly, subsequences γ_{kn+j} with $0 \le j < k$ will change sign infinitely often, and for $j < 2\log n$ can have the same sign.

2. Numerical results and comparisons

The formula (1.3) was implemented in Mathematica and the ratio of γ_n to this asymptotic expression was examined for n from 2 to 35,000. In only one instance, at $n = 137$, was a difference in sign found to occur. In this case, the cosine factor is small, approximately 0.000169881. For larger values of n, typically (1.3) gives γ_n to approximately 1%.

The short table below displays known values of γ_n together with values obtained from (1.3). The level of agreement for such small values of n is remarkable. Later in the table we observe the start of the exponential growth.

n	γ_n	γ_n from (1.3)
3	0.00205383	0.00190188
4	0.00232537	0.00231644
5	0.000793324	0.000812965
6	-0.000238769	-0.000242081
7	-0.00052729	-0.000541476
8	-0.000352123	-0.00036176
9	-0.0000343948	-0.0000350704
10	0.000205333	0.000210539
15	-0.000283469	-0.000288108
20	0.000466344	0.000471981
25	-0.00107459	-0.00108588
30	0.00355773	0.00359535
35	-0.020373	-0.0205982
40	0.248722	0.251108
45	-5.07234	-5.10969
50	126.824	127.549

Matsuoka [9, 10] determined an asymptotic series for γ_k and developed interesting consequences from it. From $\gamma_n = \frac{n!}{2\pi i}\int_C z^{-n-1}\zeta(1-z)dz$, with C a contour encircling 0, he wrote and decomposed another contour integral expression. He then applied the saddle point method to the main term. However, his result presents some difficulties.

At the leading order, we have ([10, p. 281]; [11])

$$\gamma_n = \sqrt{\frac{2n}{\pi}}\frac{e^{G(n)}}{\log n!}\left[\cos F(n) + O\left(\frac{\log\log n}{\log n}\right)\right], \tag{3.1}$$

where

$$F(n) = -\frac{\pi}{2}\frac{n}{\log n} + O\left(\frac{n \log\log n}{\log^2 n}\right). \tag{3.2}$$

Perhaps surprisingly, we have as $n \to \infty$ [10, p. 286],

$$G(n) = -n\log n + n\log\log n + n + o(n). \tag{3.3}$$

Then for sufficiently large n, the factor e^G in (3.1) is a decreasing rather than an increasing exponential.

We have implemented (3.1) in Mathematica as well as the subsidiary quantities $a_0 = a_0(n)$, $b_0 = b_0(n)$, $F(n)$, and $G(n)$. Here $x = a_0$ and $y = b_0$ are the solutions of the pair of equations

$$-(n+1)\frac{y}{x^2+y^2} + \frac{\pi}{2} - \text{Im}\ \psi(x+iy) = 0, \tag{3.4a}$$

$$-(n+1)\frac{x}{x^2+y^2} - \log 2\pi - \text{Re}\ \psi(x+iy) = 0, \tag{3.4b}$$

where $x > y > 0$ and $\psi = \Gamma'/\Gamma$ is the digamma function. We have numerically observed the expected behaviour of all quantities. As it stands, (3.1) is problematic in that both e^G does not grow with n and the $\cos F(n)$ factor is too imprecise.

On the other hand, Matsuoka also showed that for $n \geq 10$ [10, Theorem 6]

$$|\gamma_n| < 0.0001 e^{n \log\log n}. \tag{3.5}$$

Our Theorem 1 is consistent with this result.

We may also compare the magnitudes $|\gamma_n|$ with the upper bound found by Zhang and Williams [17],

$$|\gamma_n| \leq \frac{[3+(-1)^n](2n)!}{n^{n+1}(2\pi)^n} \sim [3+(-1)^n]\frac{\sqrt{\pi n}\,2^n n^{n-1}}{e^{2n}\pi^n}. \tag{3.6}$$

Owing to the factor $n^n = \exp(n\log n) \gg \exp(n\log\log n)$, the right side of this inequality gives a considerable overestimation. This is not surprising, as the upper bound originates without taking into account cancellation due to an oscillating integrand. We also note that if $|\gamma_n|$ had roughly n^n growth, with some geometric factors as in (3.6), then the series in (1.1) would have a finite radius of convergence, contradicting the fact that $\zeta(s) - 1/(s-1)$ is an entire function.

3. Summary

We have given an asymptotic expression for the Stieltjes constants γ_n that is complementary to earlier work by Matsuoka [9, 10]. Our result is very suitable for computation, and indeed it provides useful results for even moderate values of n.

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