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Relations and positivity results for the derivatives of the Riemann ξ function

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Abstract

We present and evaluate the integer-order derivatives of the Riemann xi function. These derivatives contain logarithmic integrals of powers multiplying a specific Jacobi theta function and as such can be alternatively viewed as certain Mellin transforms at integer argument. We describe how the derivatives at $s=0$, $s=\frac{1}{2}$, and $s=1$ can be evaluated exactly. We further show, based upon a novel representation, that the even order derivatives at $s=\frac{1}{2}$ are all positive, as are all derivatives at $s=1$. An expression is presented for the derivatives on the critical line, which may be useful in studying the zeros of the function $\Xi(t)=\xi(\frac{1}{2}+it)$.

Keywords: Theta function; Functional equation; Riemann zeta function; Riemann xi function; Derivatives; Li criterion

Knowing about the signs of derivatives of a function can be very useful information in localizing its zeros [9]. It is in this spirit that the present investigation considers the derivatives of the Riemann ξ function [3,6,8–11]. In particular, the properties of the function $\Xi(t)=\xi(\frac{1}{2}+it)$ of a complex variable t further motivate such a study. The function ξ is determined from the Riemann zeta function ζ by way of the relation $\xi(s)=(s/2)(s-1)\pi^{-s/2}\Gamma(s/2)\zeta(s)$, where Γ is the Gamma function. The function $\Xi(t)$ is known to be an even entire function of first-order taking real values for real values of t.

In this paper, we mainly present and evaluate a relation for successive integer-order derivatives of the xi function. These derivatives contain logarithmic integrals of powers multiplying a specific theta function and as such can be alternatively viewed as certain Mellin transforms at integer argument. Various forms of these integrals can be used to demonstrate positivity at specific points. Indeed, we are able to show that all derivatives of the xi function are nonnegative for $s\geqslant\frac{1}{2}$. We then describe the structure of certain integrals arising from individual terms of the theta function.

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Various Jacobi theta functions are useful in the theory of the Riemann Zeta function [3,6,8,10,11]. In particular, the functional equations of these infinite series can be used in deriving the fundamental functional equation of the zeta function. Sometimes the relation between a theta function and its first derivative at unit argument has been used in writing the functional equation [3,10]. In fact, there is an infinite set of such identities at unit argument, which has been presented explicitly [2].

If we first write the theta series [3,10,11]

$$\omega(x)=\sum_{n=1}^{\infty}\mathrm{e}^{-\pi n^2 x},\quad \mathrm{Re}\ x>0, \tag{1}$$

the corresponding functional equation is $2\sqrt{x}\omega(x)+\sqrt{x}=2\omega(1/x)+1$, $x>0$. Of special importance here, an analytic continuation of the Riemann zeta function ζ to the whole complex plane is given by [3, p. 16; 10]

$$\pi^{-s/2}\Gamma(s/2)\zeta(s)=\int_1^{\infty}\omega(x)[x^{s/2}+x^{(1-s)/2}]\,\frac{\mathrm{d}x}{x}-\frac{1}{s(1-s)}. \tag{2}$$

In turn, this implies that we have the integral representation

$$\xi(s)=\frac{1}{2}+\frac{s}{2}(s-1)\int_1^{\infty}(x^{s/2-1}+x^{-s/2-1/2})\omega(x)\,\mathrm{d}x. \tag{3}$$

We demonstrate that the general jth derivative of the xi function is given by

$$\begin{aligned}\xi^{(j)}(s)=&\frac{j(j-1)}{2^{j-1}}\int_1^{\infty}\omega(x)(x^{s/2-1}\mp x^{-s/2-1/2})\ln^{j-2}x\,\mathrm{d}x\\&+\frac{j}{2^{j-1}}\left(s-\frac{1}{2}\right)\int_1^{\infty}\omega(x)(x^{s/2-1}\pm x^{-s/2-1/2})\ln^{j-1}x\,\mathrm{d}x\\&+\frac{s(s-1)}{2^{j+1}}\int_1^{\infty}\omega(x)(x^{s/2-1}\mp x^{-s/2-1/2})\ln^{j}x\,\mathrm{d}x,\end{aligned} \tag{4}$$

where the top sign holds for the odd order derivatives and the bottom sign for the even order ones. By successive differentiation of Eq. (3) with respect to s, we find that a suitable form is given by

$$\begin{aligned}\xi^{(j)}(s)=&a_j\int_1^{\infty}\omega(x)(x^{s/2-1}\mp x^{-s/2-1/2})\ln^{j-2}x\,\mathrm{d}x\\&+b_j\left(s-\frac{1}{2}\right)\int_1^{\infty}\omega(x)(x^{s/2-1}\pm x^{-s/2-1/2})\ln^{j-1}x\,\mathrm{d}x\\&+\frac{s(s-1)}{2^{j+1}}\int_1^{\infty}\omega(x)(x^{s/2-1}\mp x^{-s/2-1/2})\ln^{j}x\,\mathrm{d}x,\end{aligned} \tag{5}$$

where the coefficients satisfy the recursion relations

$$a_{j+1}=a_j/2+b_j,\quad b_{j+1}=b_j/2+2^{-j}, \tag{6}$$

and $b_1 = 1$ and $a_1 = 0$. The solution of Eq. (6), $a_j = j(j-1)2^{-j+1}$ and $b_j = j2^{-j+1}$, furnishes the result (4). By using integration by parts twice, we may instead write

$$\xi^{(j)}(s) = \frac{1}{2^{j-1}} \int_1^\infty [x^{3/2}\omega'(x)]'(x^{s/2-1/2} \mp x^{-s/2}) \ln^j x \, \mathrm{d}x. \tag{7}$$

This relation is very useful in deriving positivity results for the derivatives, as seen in the following.

The xi function satisfies the functional equation $\xi(s) = \xi(1-s)$. Therefore, we have that $\xi^{(j)}(0) = \mp\xi^{(j)}(1)$, where the top sign holds for odd order derivatives and the bottom sign for even order ones. The general expressions (4) and (7) give the explicit value of the derivative at the origin:

$$\xi^{(j)}(0) = \frac{j(j-1)}{2^{j-1}} \int_1^\infty \omega(x)(x^{-1} \mp x^{-1/2}) \ln^{j-2} x \, \mathrm{d}x - \frac{j}{2^j} \int_1^\infty \omega(x)(x^{-1} \pm x^{-1/2}) \ln^{j-1} x \, \mathrm{d}x. \tag{8}$$

Approximate numerical values for the first few derivatives at $s = 0$ are: $\xi'(0) \simeq -0.011547854$, $\xi''(0) \simeq 0.0233438645$, and $\xi'''(0) \simeq -0.0014939515$. One way to obtain such numerical values is to use high precision values of the zeta function and its derivatives. In turn, this means having high precision values of the Stieltjes constants γ_k given in Eq. (15) below.

In addition, the result of Eq. (7) immediately shows that all derivatives of ξ at $s = 1$ are positive. We have

$$\xi^{(j)}(1) = \frac{1}{2^{j-1}} \int_1^\infty [x^{3/2}\omega'(x)]'(1 \mp x^{-1/2}) \ln^j x \, \mathrm{d}x. \tag{9}$$

The function

$$[x^{3/2}\omega'(x)]' = \pi x^{1/2} \sum_{n=1}^\infty \left(\pi x n^2 - \frac{3}{2}\right) n^2 \mathrm{e}^{-\pi n^2 x} \tag{10}$$

is strictly positive for $x \geqslant 1$; in fact, every term on the right-hand side of Eq. (10) is strictly positive. Since the factor $1 \mp x^{-1/2}$ is nonnegative for $x \geqslant 1$, it follows that all the values $\xi^{(j)}(1)$ are positive. In turn, all odd order derivatives at $s = 0$ are negative, and all even order derivatives at $s = 0$ are positive. Similar reasoning readily shows that all derivatives of the xi function are nonnegative when $s \geqslant \frac{1}{2}$.

In particular, the quantities of Eqs. (8) and (9) enter the Li equivalence for the Riemann hypothesis [1]. If the sequence $\{\lambda_n\}_{n=1}^\infty$ is defined by

$$\lambda_n = \frac{1}{(n-1)!} \frac{\mathrm{d}^n}{\mathrm{d}s^n} [s^{n-1} \ln \xi(s)]_{s=1}, \tag{11}$$

then Li's criterion for the Riemann hypothesis to hold is that all $\{\lambda_n\}_{n=1}^\infty$ are non-negative [9]. We note that Li's convention for the xi function has a factor of two difference: $\xi_{Li}(s) = 2\xi(s)$, although this is immaterial in logarithmic derivatives such as λ_j. We also have

$$\lambda_n = \frac{(-1)^n}{(n-1)!} \frac{\mathrm{d}^n}{\mathrm{d}s^n} [(1-s)^{n-1} \ln \xi(s)]_{s=0}, \tag{12}$$

and $\xi(0) = -\zeta(0) = \frac{1}{2}$. (Hence $\xi_{Li}(0) = 1$.) The approximate numerical values for the first few λ_j's are: $\lambda_1 \simeq 0.0230957$, $\lambda_2 \simeq 0.0923457$, and $\lambda_3 \simeq 0.207639$. Further numerical values are given at the end of the Appendix. In fact, we have $\lambda_1 = -B$, where $B \equiv \ln 2 + (\frac{1}{2})\ln\pi - 1 - \gamma/2 \simeq -0.0230957$, and $\gamma \simeq 0.5772156649$ is the Euler constant. This follows from the logarithmic derivative [6]

$$\frac{\xi'(s)}{\xi(s)} = B + \sum_\rho \left(\frac{1}{s-\rho} + \frac{1}{\rho}\right), \tag{13}$$

where ρ runs over all the nontrivial zeros of the zeta function. Thus $\xi'(s)/\xi(s) = \sum_\rho (s-\rho)^{-1}$, which is consistent with $\xi_{Li}(s) = \Pi_\rho(1 - s/\rho)$. In general, the λ_j's are connected to sums over the nontrivial zeros of $\zeta(s)$ by way of [9]

$$\lambda_n = \sum_\rho \left[1 - \left(1 - \frac{1}{\rho}\right)^n\right]. \tag{14}$$

By using the Laurent expansion of the zeta function about $s = 1$,

$$\zeta(s) = \frac{1}{s-1} + \sum_{n=0}^{\infty} \frac{(-1)^n}{n!}\gamma_n (s-1)^n, \tag{15}$$

where the γ_k are the Stieltjes constants [5,6], it is possible to write a closed form for the λ_j's. The Stieltjes constants can be evaluated from the expression

$$\gamma_k = \lim_{N\to\infty}\left(\sum_{m=1}^{N}\frac{1}{m}\ln^k m - \frac{\ln^{k+1} N}{k+1}\right), \tag{16}$$

and several other forms have been given [5]. For instance, we have

$$\lambda_2 = 1 + \gamma - \gamma^2 + \pi^2/8 - 2\ln 2 - \ln\pi - 2\gamma_1, \tag{17}$$

and

$$\lambda_3 = \tfrac{1}{2}\left[2 + \tfrac{3}{4}\pi^2 - 6\ln 2 - 3\ln\pi - 12\gamma_1 + \gamma[3 + 2(\gamma - 3)\gamma + 6\gamma_1] + 3\gamma_2 - \tfrac{7}{4}\zeta(3)\right]. \tag{18}$$

It is not difficult to determine that λ_j contains the term $-(-1)^j[j/(j-1)!]\gamma_{j-1}$. The successive λ_j's can be related in several different ways, including simply

$$\lambda_{n+1} = \lambda_n + \frac{1}{n!}\left[\frac{\mathrm{d}^n}{\mathrm{d}s^n} s^n \frac{\xi'(s)}{\xi(s)}\right]_{s=1}. \tag{19}$$

Alternatively, in the particular case of λ_2, one can write $\lambda_2 = 2\lambda_1 - \lambda_1^2 + \lim_{s\to 1} s\xi''(s)/\xi(s)$. Such exact values and partial recursion relations indicate some possibility for direct verification and not of the Li criterion. Moreover, in the Appendix we give an alternative finite sum representation of the λ_j constants.

Additionally, we may evaluate the derivatives of the xi function at $s = \frac{1}{2}$, where the odd order derivatives vanish. Using the bottom sign in Eq. (4), we have

$$\xi^{(j)}\left(\frac{1}{2}\right) = \frac{4j(j-1)}{2^j}\int_1^\infty \omega(x)x^{-3/4}\ln^{j-2} x\,\mathrm{d}x - \frac{1}{2^{j+2}}\int_1^\infty \omega(x)x^{-3/4}\ln^j x\,\mathrm{d}x, \quad j \text{ even}. \tag{20}$$

Approximate numerical values for the first few even order derivatives at $s=\frac{1}{2}$ are: $\xi''(\frac{1}{2}) \simeq 0.0229719443$, $\xi^{(4)}(\frac{1}{2}) \simeq 0.0029628484$, and $\xi^{(6)}(\frac{1}{2}) \simeq 0.0005992959$. Below, we indicate how these derivatives may be evaluated exactly as an infinite series. Again, the result of Eq. (7),

$$\xi^{(j)}\left(\frac{1}{2}\right) = \frac{1}{2^{j-2}} \int_1^\infty [x^{3/2}\omega'(x)]' x^{-1/4} \ln^j x \, \mathrm{d}x, \tag{21}$$

immediately shows that all even order derivatives at $s=\frac{1}{2}$ are positive.

As far as values on the critical line, we have for $s=\frac{1}{2}+it$ and t real,

$$\begin{aligned} \xi^{(j)}\left(\frac{1}{2}+it\right) &= \frac{4j(j-1)}{2^j} \int_1^\infty x^{-3/4} \begin{bmatrix} i\sin\left(\frac{t}{2}\ln x\right) \\ \cos\left(\frac{t}{2}\ln x\right) \end{bmatrix} \ln^{j-2} x\omega(x)\, \mathrm{d}x \\ &\quad +4\frac{j}{2^j} it \int_1^\infty x^{-3/4} \begin{bmatrix} \cos\left(\frac{t}{2}\ln x\right) \\ i\sin\left(\frac{t}{2}\ln x\right) \end{bmatrix} \ln^{j-1} x\omega(x)\, \mathrm{d}x \\ &\quad -\frac{(t^2+1/4)}{2^j} \int_1^\infty x^{-3/4} \begin{bmatrix} i\sin\left(\frac{t}{2}\ln x\right) \\ \cos\left(\frac{t}{2}\ln x\right) \end{bmatrix} \ln^{j} x\omega(x)\, \mathrm{d}x, \end{aligned} \tag{22}$$

where the top line of the integrands holds for odd order derivatives and the bottom line for even order derivatives. The reduction of this equation to Eq. (20) for $t=0$ and j even is obvious. Alternatively, by way of Eq. (7) we obtain

$$\xi^{(j)}\left(\frac{1}{2}+it\right) = \frac{1}{2^{j-1}} \int_1^\infty [x^{3/2}\omega'(x)]' x^{-1/4} \begin{bmatrix} i\sin\left(\frac{t}{2}\ln x\right) \\ \cos\left(\frac{t}{2}\ln x\right) \end{bmatrix} \ln^j x \, \mathrm{d}x. \tag{23}$$

This equation can be used to write a Fourier transform representation of the xi function derivatives on the critical line, with the substitution $x \to \exp(2u)$:

$$\xi^{(j)}\left(\frac{1}{2}+it\right) = \int_0^\infty \Phi_j(u) \begin{bmatrix} i\sin(ut) \\ \cos(ut) \end{bmatrix} \mathrm{d}u, \tag{24}$$

where we put

$$\Phi_j(u) = 8\pi \sum_{n=1}^\infty \left(\pi n^2 \mathrm{e}^{2u} - \frac{3}{2}\right) n^2 \mathrm{e}^{-\pi n^2 \mathrm{e}^{2u}} \mathrm{e}^{5u/2} u^j. \tag{25}$$

Before showing how to evaluate the individual terms of Eq. (4), we remark on some other aspects of Eqs. (4) and (7). By either using the former equation, or by operating directly on Eq. (2), the results here for the xi function can be carried over to the zeta function. This means that derivatives of the xi function can be related to those of the zeta function, with the appearance of terms with $\ln \pi$ and the polygamma function.

The two terms on the right side of Eq. (4) may be thought of as certain Mellin transforms evaluated at integer argument. This interpretation can be realized by putting $x=\ln u$ in the transform

$F(s)=\int_0^\infty x^{s-1} f(x)\,dx$, giving $F(s)=\int_1^\infty \ln^{s-1} u f[x(u)](du/u)$. The choice of $f(x)=\exp(x/4)\omega(\exp x)$ can then be used.

When the theta series is inserted into Eq. (4) or special cases such as Eq. (8) or (20), we have terms of the form $\int_1^\infty x^a \ln^m x e^{-\pi n^2 x}\,dx$. Such integrals can be evaluated for a given integer m by using the incomplete Gamma function $\Gamma(x,y)$ [4]:

$$\int_1^\infty x^{v-1} e^{-\mu x} \ln^m x\,dx = \frac{\partial^m}{\partial v^m}[\mu^{-v}\Gamma(\mu,v)], \quad \operatorname{Re}\mu > 0,\ \operatorname{Re} v > 0. \tag{26}$$

The incomplete Gamma function [1,4] is given for $\operatorname{Re} x > 0$ by

$$\Gamma(\alpha,x) = \int_1^\infty e^{-t} t^{\alpha-1}\,dt = \frac{2x^\alpha e^{-x}}{\Gamma(1-\alpha)} \int_0^\infty \frac{t^{1-2\alpha} e^{-t^2}}{t^2+x}\,dt, \tag{27}$$

where the latter form holds for $\operatorname{Re}\alpha < 1$. As an illustration, we have from Eqs. (20) and (27) that

$$\xi''\left(\frac{1}{2}\right) = \sum_{n=1}^\infty (\pi n^2)^{-1/4} \left\{ \left[2 - \frac{1}{16}\ln^2(\pi n^2)\right] \Gamma\left(\frac{1}{4}, \pi n^2\right) \right.$$
$$\left. -\frac{1}{16}\left[\frac{\partial^2}{\partial\alpha^2}\Gamma(\alpha,\pi n^2)\bigg|_{\alpha=1/4} - 2\ln(\pi n^2)\frac{\partial}{\partial\alpha}\Gamma(\alpha,\pi n^2)\big|_{\alpha=1/4}\right]\right\}. \tag{28}$$

Another way to evaluate integrals of the form of Eq. (26) is to start with the relation

$$\Gamma(\alpha,x) = \Gamma(\alpha) - \frac{x^\alpha}{\alpha}\,{}_1F_1(\alpha;\alpha+1;-x), \quad -\alpha \notin N, \tag{29}$$

which connects the incomplete Gamma function to the confluent hypergeometric function ${}_1F_1$ [1,4]. From the derivative of the ratio of Pochhammer symbols

$$\frac{d}{d\alpha}\frac{(\alpha)_k}{(\alpha+1)_k} = \frac{1}{\alpha}\frac{(\alpha)_k}{(\alpha+1)_k}\left[1 - \frac{(\alpha)_k}{(\alpha+1)_k}\right], \tag{30}$$

it is not difficult to show that

$$\frac{d}{d\alpha}\,{}_1F_1(\alpha;\alpha+1;-x) = \frac{1}{\alpha}[{}_1F_1(\alpha;\alpha+1;-x) - {}_2F_2(\alpha,\alpha;\alpha+1,\alpha+1;-x)], \tag{31}$$

where ${}_pF_q$ is the generalized hypergeometric function [1,4]. It follows from Eqs. (29) and (31) that

$$\frac{d}{d\alpha}\Gamma(\alpha,x) = \Gamma(\alpha)\psi(\alpha) + \frac{x^\alpha}{\alpha^2}[-\alpha\ln x\,{}_1F_1(\alpha;\alpha+1;-x) + {}_2F_2(\alpha,\alpha;\alpha+1,\alpha+1;-x)], \tag{32}$$

where $\psi = \Gamma'/\Gamma$ is the digamma function [4]. Then, from $\int_1^\infty x^a e^{-\pi n^2 x}\,dx = (n^2\pi)^{-1-a}\Gamma(1+a,n^2\pi)$ and Eq. (32) it follows that

$$\int_1^\infty x^a \ln x e^{-\pi n^2 x}\,dx = (n^2\pi)^{-1-a}\Gamma(1+a)[\psi(a+1) - \ln(n^2\pi)]$$
$$+\frac{1}{(a+1)^2}\,{}_2F_2(a+1,a+1;a+2,a+2;-n^2\pi). \tag{33}$$

A generalization of Eq. (31) is

$$\frac{d}{d\alpha}\,{}_mF_m(\alpha,\ldots,\alpha;\alpha+1,\ldots,\alpha+1;-x) = \frac{m}{\alpha}[{}_mF_m(\alpha,\ldots,\alpha;\alpha+1,\ldots,\alpha+1;-x)$$
$$-{}_{m+1}F_{m+1}(\alpha,\ldots,\alpha;\alpha+1,\ldots,\alpha+1;-x)]. \tag{34}$$

Then we may determine, for example, that

$$\int_1^\infty x^a \ln^2 x e^{-\pi n^2 x}\,dx = (n^2\pi)^{-1-a}\Gamma(1+a)$$
$$\times[-2\ln(n^2\pi)\psi(a+1)+\ln^2(n^2\pi)+\psi^2(a+1)+\psi'(a+1)]$$
$$-\frac{2}{(a+1)^3}\,{}_3F_3(a+1,a+1,a+1;a+2,a+2,a+2;-n^2\pi). \tag{35}$$

One sees that in general the evaluation of $\int_1^\infty x^a \ln^j x e^{-\pi n^2 x}\,dx$ contains ${}_{j+1}F_{j+1}(a+1,\ldots,a+1;a+2,\ldots,a+2;-n^2\pi)$. In applying equations such as (33) and (35) to Eqs. (8) and (20), one puts $a=-1$ and $a=-\frac{1}{2}$ for the former equation and $a=-\frac{3}{4}$ for the latter equation.

In conclusion, we have presented various explicit formulas for the integer order derivatives of the Riemann xi function. Representation (7) is particularly illuminating, as it directly shows that the derivatives are positive for $s \geqslant \frac{1}{2}$. In regard to the (positive) derivatives at $s=1$, we have related these to the specific logarithmic derivatives of ξ occurring in the Li criterion [9] for the Riemann hypothesis to hold. In turn, the sequence in Eq. (11) can be written exactly either with the Stieltjes constants γ_k, many of whose properties have been studied [5], or with the η_j constants (as given in the Appendix).

We have also illustrated how the derivatives of the xi function can be written as Fourier transforms. This provides another approach for investigating the signs of the derivatives in a given region.

With the use of special functions, we have shown how the xi function derivatives can be written as infinite series. These series arise as a result of summing over logarithmic integrals, with exponential factors due to individual terms in the Jacobi theta function ω. These, and the other analytic results presented, may provide a basis for further computational and theoretic investigation of the xi function. Indeed, we have obtained further analytic results which will be presented separately.

Appendix. Alternative representation of Li's λ_j's

Here we derive an alternative formula for the particular sequence of logarithmic derivatives of the Riemann xi function given in Eq. (11). We demonstrate the following representation,

$$\lambda_n = -\sum_{m=1}^{n}\binom{n}{m}\eta_{m-1} + \sum_{m=2}^{n}(-1)^m\binom{n}{m}(1-2^{-m})\zeta(m) + 1 - \frac{n}{2}(\gamma+\ln\pi+2\ln 2), \tag{A.1}$$

where the constants η_j can be written as

$$\eta_k = \frac{(-1)^k}{k!}\lim_{N\to\infty}\left(\sum_{m=1}^{N}\frac{1}{m}\Lambda(m)\ln^k m - \frac{\ln^{k+1}N}{k+1}\right), \tag{A.2}$$

and Λ is the von Mangoldt function [3,6,7[1],8,10,11]. From the expansion around $s=1$ of the logarithmic derivative of the zeta function,

$$\frac{\zeta'(s)}{\zeta(s)} = -\frac{1}{(s-1)} - \sum_{p=0}^{\infty} \eta_p (s-1)^p, \tag{A.3}$$

we have

$$\ln \zeta(s) = -\ln(s-1) - \sum_{p=1}^{\infty} \frac{\eta_{p-1}}{p} (s-1)^p, \tag{A.4}$$

giving

$$\ln \xi(s) = -\ln 2 + \ln s - \frac{s}{2} \ln \pi + \ln \Gamma\left(\frac{s}{2}\right) - \sum_{p=1}^{\infty} \frac{\eta_{p-1}}{p} (s-1)^p. \tag{A.5}$$

The radius of convergence of the expansion (A.3) is 3, as the first singularity encountered is the trivial zero of $\zeta(s)$ at $s=-2$. We then evaluate

$$\frac{\mathrm{d}^n}{\mathrm{d}s^n} [s^{n-1} \ln \xi(s)]_{s=1} = (n-1)! \sum_{j=0}^{n-1} \binom{n}{j} \frac{1}{(n-j-1)!} \left[\frac{\mathrm{d}^{n-j}}{\mathrm{d}s^{n-j}} \ln \xi(s) \right]_{s=1}, \tag{A.6}$$

using in particular the special values $\psi(\frac{1}{2}) = -\gamma - 2\ln 2$ and $\psi^{(n)}(\frac{1}{2}) = (-1)^{n+1} n! (2^{n+1}-1)\zeta(n+1)$ for $n \geqslant 1$, where $\psi = \Gamma'/\Gamma$ is the digamma function and $\psi^{(j)}$ is the polygamma function. Finally, the sum in Eq. (A.6) over j can be converted to a sum over $m = n-j$ and the simple result $-\sum_{m=1}^{n} (-1)^m \binom{n}{m} = 1$ used, yielding Eq. (A.1). According to the properties of the von Mangoldt function, Eq. (1) may give an alternative number theoretic interpretation of Li's constants [9].

The Laurent expansion of ζ'/ζ with the form of the constants η_j in Eq. (A.2) can be developed by applying Theorem 1 of Ref. [7]. In this case, the counting function $A(x) = -\sum_{n \leqslant x} \Lambda(n) = -\psi(x)$, where ψ is the Chebyshev function, and the error term is given by $u(x) = x - \psi(x)$.

One way to generate numerical values for the λ_j's is to develop a recursion relation between the Stieltjes constants of Eq. (15) and the constants η_k and then to evaluate Eq. (A.1). We have $\eta_0 = -\gamma_0 = -\gamma$ and

$$\eta_n = -(-1)^n \left[\frac{(n+1)}{n!} \gamma_n + \sum_{k=0}^{n-1} \frac{(-1)^{k-1}}{(n-k-1)!} \eta_k \gamma_{n-k-1} \right]. \tag{A.7}$$

This equation is equivalent to the statement $[\zeta'(s)/\zeta(s)]\zeta(s) = \zeta'(s)$. As an example, we present the following in Table 1.

[1] In Eq. (1.7), $(\log x)^x$ should be replaced with $(\log x)^k$ and on p. 25 "comparing with (1.15)" should be replaced with "comparing with (1.5)".

Table 1

k	λ_k	η_k
0		-0.577216
1	0.0230957	0.187546
2	0.0923457	-0.0516886
3	0.207639	0.0147517
4	0.368793	-0.00452448
5	0.575543	0.0014468
6	0.827566	-0.000471544
7	1.12446	0.00015518
8	1.46576	-0.0000513452
9	1.85092	0.0000170414
10	2.27934	-5.66605×10^{-6}
11	2.75036	1.88585×10^{-6}
12	3.26326	-6.28055×10^{-7}
13	3.81724	2.09241×10^{-7}
14	4.41148	-6.97247×10^{-8}
15	5.04508	2.32372×10^{-8}
16	5.71711	-7.74484×10^{-9}
17	6.42658	2.58144×10^{-9}
18	7.17248	-8.60444×10^{-10}
19	7.95374	2.86808×10^{-10}
20	8.76928	-9.56012×10^{-11}
21	9.61796	3.18668×10^{-11}
22	10.4986	-1.06222×10^{-11}
23	11.4101	3.54072×10^{-12}
24	12.3513	-1.18024×10^{-12}
25	13.3210	3.93412×10^{-13}

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