A sharpening of Li’s criterion for the Riemann Hypothesis

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Abstract

Exact and asymptotic formulae are displayed for the coefficients $\lambda_n$ used in Li’s criterion for the Riemann Hypothesis. In particular, we argue that if (and only if) the Hypothesis is true, $\lambda_n \sim n(A \log n + B)$ for $n \to \infty$ (with explicit $A > 0$ and $B$). The approach also holds for more general zeta or $L$-functions.

Alternative expressions are presented for the coefficients $\lambda_n$ introduced by Li [7, 11] to recast the Riemann Hypothesis as $\lambda_n > 0$ ($\forall n$): a first representation [6] as a finite oscillatory sum, then a closely related integral representation [7], upon which the saddle-point method finally yields definite $n \to +\infty$ asymptotic estimates in one of two sharply distinct forms, [9] or [10], depending on the falsity or truth of the Riemann Hypothesis. (Only the main ideas are indicated here.)
1 Background.

The coefficients \( \lambda_n \) are defined as \( \lambda_n = \sum_\rho [1 - (1 - 1/\rho)^n] \), or equivalently via the generating function

\[
\frac{d}{dz} \log \Xi \left( \frac{1}{1 - z} \right) \equiv \sum_{n=1}^{\infty} \lambda_n z^{n-1}, \quad (\Xi(s) = s(s-1)\Gamma(s/2)\pi^{-s/2}\zeta(s)).
\] (1)

The Riemann zeros are listed in pairs, as

\[ \{\rho = \frac{1}{2} \pm i\tau_k\}_{k=1,2,...}; \quad \{\Re \tau_k\} \text{ positive and non-decreasing}; \] (2)

sums and products over zeros are performed with \( \rho \) and \( 1 - \rho \) paired together, as usual; we parametrize each such pair by the single number \( x_k = \rho(1 - \rho) = \frac{1}{4} + \tau_k^2 \). A “secondary” zeta function is

\[ Z(\sigma) = \sum_{k=1}^{\infty} x_k^{-\sigma}, \quad \Re \sigma > \frac{1}{2}. \] (3)

It extends to a meromorphic function in \( \mathbb{C} \), and all its poles lie at the negative half-integers except \( \sigma = +\frac{1}{2} [6] \), which has the polar part \([9]\]

\[ Z(\frac{1}{2} + \varepsilon) = R_{-2} \varepsilon^{-2} + R_{-1} \varepsilon^{-1} + O(1)_{\varepsilon \to 0}, \quad R_{-2} = \frac{1}{8\pi}, \quad R_{-1} = -\frac{\log 2\pi}{4\pi}. \] (4)

2 Exact forms.

To reexpress the \( \lambda_n \), we use a symmetrical Hadamard product form of \( \Xi(s) \) [4, Sec.1.10][9], namely \( \Xi(s) = \prod_{k=1}^{\infty} [1 - s(1 - s)/x_k] \), instead of the standard form [2, chap. 12]. Hence,

\[ \Xi \left( \frac{1}{1 - z} \right) = \prod_{k=1}^{\infty} \left[ 1 + \frac{z}{(1 - z)^2 x_k} \right], \quad \log \Xi \left( \frac{1}{1 - z} \right) = -\sum_{j=1}^{\infty} \frac{(-1)^j}{j} \left[ \frac{z}{(1 - z)^2} \right]^j Z(j); \] (5)

then, expanding \( (1 - z)^{-2j} \) by the generalized binomial formula, reordering in powers of \( z \) and identifying the output with (1), we get as first result

\[ \lambda_n = -n \sum_{j=1}^{n} \frac{(-1)^j}{j} \binom{n + j - 1}{2j - 1} Z(j). \] (6)

Remark: other such linear relations already exist, involving the cumulants of the Stieltjes constants [11] and/or the sums \( Z_j = \sum_\rho \rho^{-j} \) instead of \( Z(j) \); see [11, Sec.3.3] and references therein. An advantage of \([3]\) is that the lesser known factors \( Z(j) \) are positive, and smooth (they sample the holomorphic function \( Z(\sigma) \)). Still, this evaluation of \( \lambda_n \) involves cancellations that increase with \( n \).

An integral representation equivalent to (6) simply by residue calculus, but much more manageable, is

\[ \lambda_n = \frac{(-1)^n n i}{\pi} \int_C I(\sigma) \, d\sigma, \quad I(\sigma) = \frac{\Gamma(\sigma + n)\Gamma(\sigma - n)}{\Gamma(2\sigma + 1)} Z(\sigma), \] (7)

where \( C \) is a positive contour encircling (only) the subset of poles \( \sigma = +1, \cdots, +n \) of the integrand \( I(\sigma) \).
3  Asymptotic forms.

The integral formula readily suggests an asymptotic \((n \to \infty)\) evaluation by the classic saddle-point method \([5] \text{ Sec.2.5}\). First, the contour \(C\) is deformed in the direction of decreasing \(|I(\sigma)|\) until it crosses the nearest saddle-points of \(|I(\sigma)|\). Among these saddle-points, the one(s) where \(|I(\sigma)|\) is the largest give the dominant large-\(n\) contributions to the integral, through local formulae at each such saddle-point (the integrand itself may be asymptotically approximated as well: e.g., by a Stirling formula for \(\Gamma(z)\)).

We caution that our subsequent assertions, involving an integrand which cannot be described in fully closed form, partly retain an experimental character and would warrant further confirmation.

In the present problem and for large \(n\), the landscape of the function \(|I(\sigma)|\) near the contour \(C\) is dominantly controlled by the \(\Gamma\)-ratio: the resulting deformation is a dilation of \(C\) away from the segment \([1,n]\), then the nearest saddle-points can be of two types here (once \(n\) is large enough).

1) For \(\sigma\) on the segment \((\frac{1}{2}, 1)\), \(|I(\sigma)| \sim \pi [\sin \pi \sigma \Gamma(2\sigma + 1)]^{-1} n^{2\sigma-1} Z(\sigma)\) always has one real minimum \(\sigma_c(n)\) (tending to \(\frac{1}{2}\) as \(n \to \infty\); other real saddle-points lie below \(\sigma = \frac{1}{2}\), and are subdominant).

2) There may exist complex saddle-points \(\sigma_c(n)\), with imaginary parts proportional to \(n\); we may focus just on the upper half-plane, as the lower half-plane gives complex-conjugate ("c.c." ) contributions. Wherever \(Z(\sigma)\) is dominated by the term \(x_k^{-\sigma}\) from one Riemann zero \(x_k\) (naively, \(x_1\)), the saddle-point equation (in the Stirling approximation for the \(\Gamma\)-ratio) is \(0 = \frac{d}{d\sigma} \log |I(\sigma)| \sim \log(\sigma^2 - n^2) - 2 \log 2\sigma - \log x_k\), yielding the formal saddle-point location

\[
\sigma_c(n) = n i / 2\tau_k. \tag{8}
\]

Here, any zero \(x_k\) on the critical axis (\(\tau_k\) real) yields a purely imaginary \(\sigma_c(n)\), not eligible: it lies outside the domain of convergence of \([3]\), and its contribution would be subdominant in any case. The discussion then fundamentally splits depending on the presence or absence of zeros off the critical axis.

[RH false] If the zero \(x_k\) lies off the critical axis (and selecting \(\arg \tau_k > 0\)), the associated complex saddle-point \(\sigma_c(n)\) is relevant: it lies inside the domain of convergence \(\{|\Re \sigma| > \frac{1}{2}\}\) as soon as \(n |\Im 1/\tau_k| > 1\), and it will exponentially dominate the real saddle-point (as seen later): by the standard calculation, its asymptotic contribution to \(\lambda_n\) is \((|\tau_k + i/2|/|\tau_k - i/2|)^n\), which grows exponentially in modulus and fluctuates in phase. This result can also be rigorously confirmed directly from \([1]\): by a conformal mapping argument \([1]\), the function \(\frac{d}{dz} \log \Xi(z)\) has precisely the points \(z_k = (\tau_k - i/2)(\tau_k + i/2)^{-1}\) and \(z_{-k} = \bar{z}_k\) as simple poles of residue 1 in the unit disk; by a general Darboux theorem \([3]\) chap. VII \(\S 2\), this implies the asymptotic form \(\sum_k (z_{\pm k})^{-n}\) for the Taylor coefficients \(\lambda_n\) of that function, i.e.,

\[
\lambda_n \sim \sum_{\{\arg \tau_k > 0\}} \left( \frac{\tau_k + i/2}{\tau_k - i/2} \right)^n \quad [\text{c.c.}] \quad (\text{mod } o(e^{cn}) \forall c > 0), \quad n \to \infty. \tag{RH false}
\]
(An infinite set of these zeros poses no extra problem: their contributions form an asymptotic sequence.)

On the other hand, the Darboux approach does not resolve the case [RH true], in which the poles $z_{\pm k}$ all lie at the same (unit) distance, and cluster at $z = 1$!

[RH true] By contrast, the saddle-point analysis of (7) still appears to work. Now all the $\tau_k$ are real, $Z(\sigma) = O(Z(\text{Re } \sigma)) \text{ Im } \sigma^{-3/2}$ in $\{\text{Re } \sigma > \frac{1}{2}\}$, and the contour $C$ can be freely moved towards the boundary of the half-plane without crossing any of the $\sigma_c(n)$ (all purely imaginary). Hence the only dominant saddle-point in this case is $\sigma_c(n) \in (\frac{1}{2}, 1)$; it is shaped by the double pole of $Z(\sigma)$ at $\frac{1}{2}$ (itself generated by the totality of Riemann zeros), in the form $\sigma_c(n) \sim \frac{1}{2} + \frac{1}{\log n}$. One may then proceed as usual in the quadratic approximation of $\log I(\sigma)$ around $\sigma_c(n)$, but this is not so fit for a confluent case ($\sigma = \frac{1}{2}$ is a singular point). Here, it is at once simpler and more accurate to keep on deforming a portion of the contour $C$ nearest to $\sigma = \frac{1}{2}$ until it fully encircles this pole (now clockwise), and to note that the resulting additions to the integral are asymptotically negligible. Hence for [RH true], the result is

$$\lambda_n \sim (-1)^n 2n \text{ Res}_{\sigma=1/2} \left[ \frac{\Gamma(\sigma + n)\Gamma(\sigma - n)}{\Gamma(2\sigma + 1)} Z(\sigma) \right] \sim 2\pi n \left[ 2R_{-2} \log n - 2R_{-2}(1 - \gamma) + R_{-1} \right];$$

(\gamma = \text{Euler’s constant}); specifically for the Riemann zeros, using the explicit values (4),

$$\lambda_n \sim \frac{1}{2} n (\log n - \log 2\pi - 1 + \gamma), \quad n \to \infty. \quad \text{[RH true]} \quad (11)$$

The form (10) covers more general situations: the zeros of, e.g., Dedekind zeta functions and some Dirichlet $L$-functions (11), in their [RH true] case ($R_{-2}$ is always positive, in agreement with Li’s criterion).

We see a good agreement of (11) with numerical data (8) for $n < 3300$ — still a bit short to give full confidence in (11), however. (This agreement is even improved in the mean if we include the contribution like (10) but from the next pole,

$$\delta\lambda_n = (-1)^n 2n \text{ Res}_{\sigma=0} \left[ \frac{\Gamma(\sigma + n)\Gamma(\sigma - n)}{\Gamma(2\sigma + 1)} Z(\sigma) \right] = 2Z(0) = + \frac{7}{4},$$

although this term should not be asymptotically meaningful — larger oscillatory terms are also present.)

Finally, the result becomes even simpler for some pure linear combinations of the Stieltjes cumulants. The latter may be defined in degree $n$ as

$$g_n^c = (-1)^{n-1} \frac{d^n}{ds^n} \left[ \log(s \zeta(1 + s)) \right]_{s=0} = - \lim_{M \to +\infty} \left\{ \sum_{m=1}^{M} \frac{\Lambda(m)(\log m)^{n-1}}{m} - \frac{(\log M)^n}{n} \right\} \quad (13)$$

(cf. formula (4.1) in (11): this relates to the Euler factorization of $\zeta(s)$ over the primes). Our $g_n^c$ corresponds to $(-1)^n(n - 1)! \eta_{n-1}$ in (11): e.g., $g_1^c = \gamma = -\eta_0$. Theorem 2 in (11) evaluates the differences $(\lambda_n - S_n)$ where $S_n = -\sum_{j=1}^{n} \left( \frac{n}{j} \right) \eta_{j-1} = \sum_{j=1}^{n} \frac{(-1)^{j-1}}{j(j-1)!} \left( \frac{n}{j} \right) g_j^c$. As a consequence for $n \to \infty$, (11) implies

$$S_n = o(n); \quad \text{[RH true]} \quad (14)$$
whereas in the opposite case, we expect $S_n \sim \lambda_n$ as in [9]: it will oscillate between exponentially large values, negative and positive, but appreciable in absolute size only beyond $n \approx \min_{\{\arg \tau_k > 0\}} \{[\text{Im } 1/\tau_k]^{-1}\}$.

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