An Explicit Quintic Obstruction for the Riemann Theta Kernel

An Independent Rational Reconstruction

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Luminary Oddities

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Abstract

We give a complete rational reconstruction of an explicit obstruction to positive definiteness for a fixed-center product of the Riemann theta density. At $s_0 = \frac{1}{4}\log(13/(4\pi))$, the signed derivative functional evaluated on the square of $P(X) = X^5 - 264X^3 + 10952X$ lies in the exact rational interval

$$[-1412370791.837791749,\ -1412370791.837791748].$$

The proof constructs derivatives by formal power series, retains twelve theta summands, bounds the entire remaining series, and encloses exponentials by range-reduced alternating series. A printed table of rational moment intervals proves the negative contraction. The odd derivative Hankel block is indefinite, and the six-point translation Gram has a negative direction at every sufficiently small positive spacing.

Keywords. Riemann theta density; positive definite functions; Hankel matrices; rational interval arithmetic.

We use the Riemann theta density in the normalization of Rodgers and Tao [1]. The object studied here is the normalized product at one fixed real center. The reconstruction below specifies the finite arithmetic that certifies the obstruction and includes the complete infinite-series remainder.

1 The kernel and the obstruction

Define the Riemann theta density by

$$\Phi(s) = \sum_{n=1}^{\infty} (2\pi^2 n^4 e^{9s} - 3\pi n^2 e^{5s}) e^{-\pi n^2 e^{4s}}, \qquad s \in \mathbb{R}. \tag{1}$$

This series and each of its derivatives converge uniformly on compact real intervals. Indeed, on any such interval, the absolute value of a fixed derivative of a summand is bounded by a polynomial in n times e^{-cn^2}, for some $c > 0$.

For completeness, let

$$\vartheta(y) = \sum_{n\in\mathbb{Z}} e^{-\pi n^2 y}, \qquad F(s) = e^s \vartheta(e^{4s}).$$

The identity $\vartheta(y) = y^{-1/2}\vartheta(1/y)$ implies $F(s) = F(-s)$, and direct differentiation gives

$$\Phi(s) = \frac{F''(s) - F(s)}{16}.$$

Thus the complete density is even. No individual summand in (1) is required to be even.

At any center s for which $\Phi(s) \neq 0$, set

$$p_s(t) = \frac{\Phi(s + t/2)\Phi(s - t/2)}{\Phi(s)^2}. \tag{2}$$

This is a smooth, even function of t, with $p_s(0) = 1$. For $0 \leq j \leq 5$, put

$$m_{2j}(s) = (-1)^j p_s^{(2j)}(0),$$

and set $m_{2j+1}(s) = 0$ for $0 \leq j \leq 4$. These values define a real linear functional $\mathcal{L}_s$ on real polynomials of degree at most ten by $\mathcal{L}_s(X^k) = m_k(s)$. This definition makes no assumption that $\mathcal{L}_s$ is represented by a positive measure.

Theorem 1. *Let*

$$x_0 = \frac{13}{4}, \qquad s_0 = \frac{1}{4}\log\frac{13}{4\pi}, \qquad P(X) = X^5 - 264X^3 + 10952X.$$

Then $s_0 > 0$, $\Phi(s_0) > 0$, and

$$-1412370791.837791749 \;\leq\; \mathcal{L}_{s_0}(P^2) \;\leq\; -1412370791.837791748. \tag{3}$$

Every finite decimal in this statement denotes its exact rational value. The moment block on $\{X, X^3, X^5\}$ and the full moment matrix on $\{1, X, \ldots, X^5\}$ are indefinite. Moreover, for every sufficiently small $h > 0$, the matrix

$$\left(p_{s_0}((j-k)h)\right)_{j,k=0}^{5}$$

has a negative direction. In particular, p_{s_0} is not positive definite.

The following sections prove the theorem.

2 Derivatives from a formal power series

The positivity of the selected center can be established without a numerical value of π. Integrating

$$\frac{1}{1+u^2} = \sum_{j=0}^{10}(-1)^j u^{2j} - \frac{u^{22}}{1+u^2}, \qquad 0 \leq u \leq 1,$$

gives

$$\pi < 4\sum_{j=0}^{10}\frac{(-1)^j}{2j+1} = \frac{47028692}{14549535} < \frac{13}{4}.$$

Thus $s_0 > 0$. At this center, each summand of (1) has the strictly positive factor $2n^2x_0 - 3$, so $\Phi(s_0) > 0$.

To construct the required derivatives, introduce an indeterminate z and expand formally in u:

$$(2ze^{4u} - 3)\exp\!\big(5u - z(e^{4u} - 1)\big) = \sum_{k=0}^{\infty}\frac{Q_k(z)}{k!}u^k. \tag{4}$$

The coefficients through $k = 10$ can be constructed by a finite recurrence in the polynomial ring $\mathbb{Q}[z]$. Define

$$A_1(z) = 5 - 4z, \qquad A_r(z) = -\frac{4^r}{r!}z \quad (r \geq 2), \qquad E_0(z) = 1,$$

and, for $1 \le k \le 10$, set

$$E_k(z) = \frac{1}{k} \sum_{r=1}^{k} r A_r(z) E_{k-r}(z). \tag{5}$$

Also set

$$C_0(z) = 2z - 3, \qquad C_r(z) = \frac{2\,4^r}{r!} z \quad (r \ge 1),$$

and define

$$Q_k(z) = k! \sum_{r=0}^{k} C_r(z) E_{k-r}(z), \qquad 0 \le k \le 10. \tag{6}$$

Indeed, differentiating the formal exponential of $\sum_{r\ge1} A_r(z)u^r$ gives (5), while multiplication by $\sum_{r\ge0} C_r(z)u^r$ gives (6). Equivalently, these polynomials satisfy

$$Q_0(z) = 2z - 3, \qquad Q_{k+1}(z) = (5 - 4z)Q_k(z) + 4zQ_k'(z). \tag{7}$$

Consequently Q_k has integer coefficients and degree $k + 1$.

Write $x = \pi e^{4s}$. A summand of (1) is $\pi n^2 e^{5s}(2n^2x - 3)e^{-n^2x}$. Applying (4) to its value at $s + u$, and differentiating the normally convergent series, yields

$$\Phi^{(k)}(s) = \pi e^{5s-x} B_k(x), \qquad B_k(x) = \sum_{n=1}^{\infty} n^2 Q_k(n^2x) e^{-(n^2-1)x}. \tag{8}$$

In particular, with $B_k = B_k(x_0)$ and $v_k = B_k/B_0$,

$$m_{2j}(s_0) = \frac{(-1)^j}{2^{2j}} \sum_{r=0}^{2j} (-1)^r \binom{2j}{r} v_r v_{2j-r}, \qquad 1 \le j \le 5, \tag{9}$$

and $m_0(s_0) = 1$. The factors 2^{-2j} and $(-1)^r$ in (9) come from differentiating the two shifted arguments in (2).

3 A complete tail bound

For the rest of the proof write $x = x_0 = 13/4$, and write $Q_k(z) = \sum_{j=0}^{k+1} q_{k,j} z^j$. Retain twelve terms:

$$U_k = \sum_{n=1}^{12} n^2 Q_k(n^2x) e^{-(n^2-1)x}. \tag{10}$$

For $n \ge 13$ and $0 \le j \le 11$, the successive ratio of the positive monomial majorants is

$$\frac{(n+1)^{2j+2} e^{-((n+1)^2-1)x}}{n^{2j+2} e^{-(n^2-1)x}} = \left(1 + \frac{1}{n}\right)^{2j+2} e^{-(2n+1)x} \le \rho,$$

where

$$\rho = \left(\frac{14}{13}\right)^{24} e^{-27x} < 1. \tag{11}$$

The last inequality follows, for example, from the exact integer comparison $14^{24} < 9\,13^{24}$ and $9 < 1 + 27x < e^{27x}$. Thus the complete omitted theta tail satisfies

$$|B_k - U_k| \le T_k, \qquad T_k = \frac{e^{-168x}}{1 - \rho} \sum_{j=0}^{k+1} |q_{k,j}| x^j 13^{2j+2}. \tag{12}$$

This follows by applying one geometric majorant to each absolute monomial contribution and then summing. No sign assumption is made about any omitted summand.

4 Rational enclosure algorithm

The following finite arithmetic specifies enclosures for all quantities in (8)–(12). For an interval with rational endpoints, define the outward rounding operation

$$\mathcal{R}([a,b]) = \left[\frac{\lfloor 10^{100}a\rfloor}{10^{100}}, \frac{\lceil 10^{100}b\rceil}{10^{100}}\right]. \tag{13}$$

All polynomial operations in (5) and (6) are exact rational operations. For interval operations, a rational constant is enclosed by $\mathcal{R}([a,a])$; addition uses the sums of corresponding endpoints, subtraction reverses the endpoints of the subtracted interval, and multiplication takes the minimum and maximum of the four endpoint products. A reciprocal of $[a,b]$ is $[1/b, 1/a]$, and is used only when $0 \notin [a,b]$. Apply $\mathcal{R}$ after every interval operation.

To enclose exponentials, define

$$S_N(u) = \sum_{r=0}^{N} \frac{(-u)^r}{r!}.$$

For $0 \le u < 1$, the alternating-series estimate gives

$$0 < S_{119}(u) \le e^{-u} \le S_{120}(u). \tag{14}$$

For each required rational $t \in [0, 1024)$, start with

$$J_0(t) = \mathcal{R}([S_{119}(t/1024), S_{120}(t/1024)]),$$

and perform ten interval squarings,

$$J_{r+1}(t) = \mathcal{R}(J_r(t)J_r(t)), \qquad 0 \le r \le 9.$$

Write $\mathcal{E}(t) = J_{10}(t)$. It follows from (14) that $e^{-t} \in \mathcal{E}(t)$. The required arguments are $(n^2-1)x$ for $1 \le n \le 12$, $168x = 546$, and $27x = 351/4$. All lie in $[0, 1024)$.

For $0 \le k \le 10$, evaluate (10) by replacing each exponential by $\mathcal{E}((n^2-1)x)$, giving an interval $\widehat{U}_k$. Evaluate the right-hand side of (12) with e^{-168x} replaced by $\mathcal{E}(168x)$ and ρ replaced by $(14/13)^{24}\mathcal{E}(27x)$, giving an interval $\widehat{T}_k$. Its denominator has a strictly positive lower endpoint. Enclose B_k by

$$\widehat{B}_k = \widehat{U}_k + [-\sup \widehat{T}_k, \sup \widehat{T}_k]. \tag{15}$$

The lower endpoint of $\widehat{B}_0$ is strictly positive. Hence the interval quotients $\widehat{B}_k/\widehat{B}_0$ and the interval evaluation of (9) are defined. Set the zeroth moment to $[1,1]$ exactly.

Every step uses finite integer or rational arithmetic. In particular, the exponential sums have 120 or 121 rational terms, the polynomial recurrences stop at index ten, and the explicit theta sums have twelve terms. Applying these operations and then rounding the final moment intervals outward to 21 decimal places gives the following table. Its decimal endpoints are exact rationals.

Moment	Lower endpoint ℓ_{2j}	Upper endpoint u_{2j}
m_0	1.000000000000000000000	1.000000000000000000000
m_2	37.494948632526286288836	37.494948632526286288837
m_4	3932.027580671382208032879	3932.027580671382208032880
m_6	627047.936215875601827601711	627047.936215875601827601712
m_8	122418538.750248794464511260609	122418538.750248794464511260610
m_{10}	24027209085.312836732144002587110	24027209085.312836732144002587111

5 Contraction and finite translation Grams

The exact square of the declared polynomial is

$$P(X)^2 = X^{10} - 528X^8 + 91600X^6 - 5782656X^4 + 119946304X^2. \tag{16}$$

The sign-aware contraction of the printed moment intervals has lower endpoint

$$L = \ell_{10} - 528u_8 + 91600\ell_6 - 5782656u_4 + 119946304\ell_2$$

and upper endpoint

$$U = u_{10} - 528\ell_8 + 91600u_6 - 5782656\ell_4 + 119946304u_2.$$

Exact rational arithmetic gives

$$L = \frac{-14123707918377917480924533545 06}{10^{21}} = -1412370791.837791748092453354506,$$
$$U = \frac{-14123707918377917480923275334 17}{10^{21}} = -1412370791.837791748092327533417.$$

Consequently

$$-1412370791.837791749 \le L \le \mathcal{L}_{s_0}(P^2) \le U \le -1412370791.837791748 < 0,$$

which proves (3). Thus the printed 21-place moment intervals suffice for the stated nine-place witness enclosure.

Let

$$H_{\mathrm{odd}} = (m_{a+b}(s_0))_{a,b\in\{1,3,5\}}, \qquad H_5 = (m_{a+b}(s_0))_{a,b=0}^{5}.$$

For $c_{\mathrm{odd}} = (10952, -264, 1)^\top$, $c_{\mathrm{odd}}^\top H_{\mathrm{odd}} c_{\mathrm{odd}} = \mathcal{L}_{s_0}(P^2) < 0$. The first coordinate direction is positive because $m_2(s_0) > 0$. Hence H_{odd} is indefinite, and so is H_5, which contains it as a principal block.

To pass from derivatives to finite translation Grams, abbreviate $p = p_{s_0}$ and define, for $h > 0$,

$$G_h = (p((j-k)h))_{j,k=0}^{5}, \qquad (F_h)_{a,r} = \begin{cases} h^{-a}(-1)^{a-r}\binom{a}{r}, & 0 \le r \le a, \\ 0, & r > a. \end{cases}$$

These forward differences give the entrywise limit

$$F_h G_h F_h^\top \longrightarrow K = \left((-1)^b p^{(a+b)}(0)\right)_{a,b=0}^{5}, \qquad h \longrightarrow 0^+. \tag{17}$$

Only derivatives through order ten are required for this limit. With $D = \mathrm{diag}(1, i, i^2, \dots, i^5)$,

$$(D^* K D)_{a,b} = (-i)^{a+b} p^{(a+b)}(0) = m_{a+b}(s_0).$$

Here odd derivatives vanish, and for $a + b = 2j$ the coefficient is $(-i)^{2j} = (-1)^j$. Thus $D^* K D = H_5$.

Set $c = (0, 10952, 0, -264, 0, 1)^\top$. By (17),

$$c^* D^* F_h G_h F_h^\top D c \longrightarrow c^\top H_5 c = \mathcal{L}_{s_0}(P^2) < 0.$$

The left-hand side is therefore negative for every sufficiently small $h > 0$. It is the quadratic value of G_h on the vector $F_h^\top D c$, so each such six-node Gram has a negative direction. This contradicts the defining Gram condition for a positive definite function and completes the proof.

Remark. The conclusion concerns the specified fixed-center product.

Reproducibility

The supplementary file `verify_reconstruction.py` implements the formal polynomial construction, complete tail estimate, exponential enclosures, and outward rational arithmetic stated above using only the Python standard library. Its exact output is retained in `certificate.json`; `moment_table.json` records the printed table and its sign-aware contraction. The verifier reconstructs the intervals from the formulas rather than assuming the certificate values. A checksum manifest identifies the distributed files.

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References

[1] B. Rodgers and T. Tao, *The de Bruijn–Newman constant is non-negative*, Forum of Mathematics, Pi **8** (2020), e6. doi:10.1017/fmp.2020.6.