

An Explicit Quintic Obstruction for the Riemann Theta Kernel

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Abstract. We exhibit an explicit polynomial square on which the signed derivative functional of a fixed-center Riemann theta product is negative. At the center $s_0 = \frac{1}{4}\log(13/(4\pi))$, the polynomial $P(X) = X^5 - 264X^3 + 10952X$ satisfies $\mathcal{L}_{s_0}(P^2) \leq -1\,351\,625\,671$. The certificate uses rational interval arithmetic for derivatives through order ten and an explicit bound on the complete infinite theta tail. It follows that the normalized product at this center is not positive definite and that its odd derivative Hankel block is indefinite.

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

1. Introduction

We use the classical Riemann theta density in the normalization of Rodgers and Tao [1]. Theta correlation kernels and their positive-definiteness properties are studied, for example, by Csordas [2]. For a fixed real center s , the object considered here is the normalized product $\Phi(s + t/2)\Phi(s - t/2)/\Phi(s)^2$.

The possibility of a failure of positivity is consistent with Hudson's classification of nonnegative pure-state Wigner functions [3]. An informal numerical report also observed negative Fourier values for individual theta-product slices [4, Section 6]. We give a rigorous certificate at an exact center, with an integer polynomial of degree five. The argument retains the full theta series and uses no spectral optimization to justify the chosen polynomial.

2. Definitions and main result

Let Φ be the smooth even Riemann theta density, given by the normally convergent series

$$\Phi(s) = \sum_{n=1}^{\infty} (2\pi^2 n^4 e^{9s} - 3\pi n^2 e^{5s}) e^{-\pi n^2 e^{4s}}. \quad (1)$$

Its evenness follows from the Jacobi theta transformation. For $s \geq 0$, every summand is positive, and hence $\Phi(s) > 0$. Define

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

The function p_s is smooth and even, and $p_s(0) = 1$. On real polynomials of degree at most ten, define the real linear functional $\mathcal{L}_s$ by

$$\mathcal{L}_s(X^{2j}) = (-1)^j p_s^{(2j)}(0), \quad 0 \leq j \leq 5, \quad (3)$$

$$\mathcal{L}_s(X^{2j+1}) = 0, \quad 0 \leq j \leq 4. \quad (4)$$

These are signed derivative moments; the definition does not assume a positive representing measure. The letter X denotes the polynomial variable, whereas χ below denotes a theta-series parameter.

Theorem 1.

Set

$$\chi_0 = \frac{13}{4}, \quad s_0 = \frac{1}{4} \log \frac{13}{4\pi}, \quad P(X) = X^5 - 264X^3 + 10952X. \quad (5)$$

Then $s_0 > 0$ and

$$\mathcal{L}_{s_0}(P^2) \leq -1\,351\,625\,671 < -10^9. \quad (6)$$

The derivative Hankel block on $\{X, X^3, X^5\}$ is indefinite. The full derivative Hankel matrix on $\{1, X, \dots, X^5\}$ is also indefinite, and p_{s_0} is not positive definite.

3. Derivative and tail enclosures

First, the selected center is positive. The finite geometric identity on $0 \leq u \leq 1$ gives

$$\frac{1}{1+u^2} = \sum_{j=0}^{10} (-1)^j u^{2j} - \frac{u^{22}}{1+u^2}. \quad (7)$$

After integration, the last term is strictly negative. Therefore

$$\pi < 4 \sum_{j=0}^{10} \frac{(-1)^j}{2j+1} = \frac{47\,028\,692}{14\,549\,535} < \frac{13}{4}. \quad (8)$$

This proves $s_0 > 0$. At s_0 , the factor $2n^2\chi_0 - 3$ is positive for every $n \geq 1$, so $\Phi(s_0) > 0$. On a compact neighborhood of s_0 , each fixed derivative of a theta summand is bounded by a polynomial in n times e^{-cn^2} for some $c > 0$. The bound is summable and justifies differentiation term by term through order ten.

Write $\chi = \pi e^{4s}$. Define integer polynomials by

$$Q_0(z) = 2z - 3, \quad Q_{k+1}(z) = (5 - 4z)Q_k(z) + 4zQ'_k(z). \quad (9)$$

Differentiating the entire summand, including its exponential factors, gives

$$\Phi^{(k)}(s) = \pi e^{5s - \chi} B_k(\chi), \quad (10)$$

$$B_k(\chi) = \sum_{n=1}^{\infty} n^2 Q_k(n^2 \chi) e^{-(n^2 - 1)\chi}. \quad (11)$$

The common positive factor is canceled only after the derivative has been formed. In the remainder of the proof, B_k denotes $B_k(\chi_0)$. For $0 \leq k \leq 10$, write

$$Q_k(z) = \sum_{j=0}^{k+1} q_{k,j} z^j. \quad (12)$$

Retain the first three theta terms:

$$A_k = Q_k(\chi_0) + 4Q_k(4\chi_0)e^{-3\chi_0} + 9Q_k(9\chi_0)e^{-8\chi_0}. \quad (13)$$

For a monomial of degree j , the ratio of successive absolute terms with $n \geq 4$ is bounded by

$$\frac{(n+1)^{2j+2}e^{-(n+1)^2-1)x_0}}{n^{2j+2}e^{-(n^2-1)x_0}} \leq (5/4)^{2j+2}e^{-9x_0}. \quad (14)$$

Here $2j+2 \leq 24$. All the ratios are strictly below one: $(5/4)^{24} < 256 < 1 + 9x_0 + (9x_0)^2/2 < e^{9x_0}$. Summing the resulting geometric majorants proves

$$|B_k - A_k| \leq T_k, \quad (15)$$

$$T_k = \sum_{j=0}^{k+1} \frac{|q_{k,j}|x_0^j 4^{2j+2} e^{-15x_0}}{1 - (5/4)^{2j+2} e^{-9x_0}}. \quad (16)$$

Thus every term with $n \geq 4$ is included. No sign is assigned to the omitted summands; their complete contribution is enclosed symmetrically.

4. Exact rational certificate

The primitive exponential enclosures use

$$S_{120}(t) = \sum_{j=0}^{120} \frac{t^j}{j!}, \quad R_{120}(t) = \frac{t^{121}}{121!} \frac{1}{1 - t/122}. \quad (17)$$

For $0 \leq t < 122$, the first omitted term and the bound on subsequent term ratios imply

$$S_{120}(t) \leq e^t \leq S_{120}(t) + R_{120}(t), \quad (18)$$

$$\frac{1}{S_{120}(t) + R_{120}(t)} \leq e^{-t} \leq \frac{1}{S_{120}(t)}. \quad (19)$$

The only arguments needed are $3x_0 = 39/4$, $8x_0 = 26$, $15x_0 = 195/4$, and $9x_0 = 117/4$. They are rational and all lie below 122.

All finite operations use inclusive rational interval arithmetic. With $G = 2^{192}$, an interval $[a, b]$ is enlarged after each operation to

$$\left[\frac{\lfloor Ga \rfloor}{G}, \frac{\lfloor Gb \rfloor}{G} \right]. \quad (20)$$

Addition adds corresponding endpoints. Multiplication takes the minimum and maximum of the four endpoint products. A reciprocal is taken only after the interval is proved to exclude zero. These rules enclose the exact expression at every step, including all divisions in the tail bound and the normalization.

The main certificate generates $Q_0, \dots, Q_{10}$ by the equivalent closed formula

$$Q_k(z) = \sum_{r=0}^k \binom{k}{r} 5^{k-r} 4^r \sum_{j=0}^r S(r, j) (-1)^j z^j (2z - 3 - 2j), \quad (21)$$

where $S(r, j)$ are Stirling numbers of the second kind. This identity follows by expanding $(5 + 4z d/dz)^k [(2z - 3)e^{-z}]$ and then multiplying by e^z . A second certificate instead generates the polynomials by the recurrence above and compares their coefficients with the closed expression.

Put $v_k = B_k/B_0$. Leibniz differentiation of the two shifted factors gives the exact signed moments

$$m_{2j} := \mathcal{L}_{s_0}(X^{2j}) = \frac{(-1)^j}{2^{2j}} \sum_{r=0}^{2j} (-1)^r \binom{2j}{r} v_r v_{2j-r}. \quad (22)$$

Set $m_0 = 1$ exactly. Applying the stated exponential, tail, and interval rules yields the enclosures in Table 1. The integer endpoints are outward enlargements of the complete rational moment intervals. The full endpoint ledger is supplied as `certificate_192bit.json`; a separate 160-bit calculation is supplied as `certificate_160bit.json`. The two standalone verifiers constitute the finite arithmetic part of the proof and require only the Python standard library.

Moment	Lower endpoint	Upper endpoint
m_0	1	1
m_2	37	38
m_4	3 932	3 933
m_6	627 047	627 048
m_8	122 418 538	122 418 539
m_{10}	24 027 208 770	24 027 209 433

Table 1. Integer enclosures for the signed derivative moments at the exact center s_0 .

5. Proof of Theorem 1

The exact square of the declared polynomial is

$$P(X)^2 = X^{10} - 528X^8 + 91600X^6 - 5\,782\,656X^4 + 119\,946\,304X^2. \quad (23)$$

For a positive coefficient, use the upper moment endpoint in Table 1; for a negative coefficient, use the lower endpoint. Linearity then gives

$$\mathcal{L}_{s_0}(P^2) \leq 24\,027\,209\,433 - 528(122\,418\,538) + 91\,600(627\,048) \quad (24)$$

$$- 5\,782\,656(3\,932) + 119\,946\,304(38) \quad (25)$$

$$= -1\,351\,625\,671 < -10^9. \quad (26)$$

Let H_{odd} denote the moment block on the three odd monomials, and let $c = (10952, -264, 1)^T$. Then $c^T H_{\text{odd}} c = \mathcal{L}_{s_0}(P^2) < 0$. On the other hand, the first coordinate direction has value $m_2 \geq 37 > 0$. Consequently H_{odd} is indefinite. The full matrix H_5 , with odd moments equal to zero, contains this block and is indefinite as well.

$$H_{\text{odd}} = (m_{a+b})_{a,b \in \{1,3,5\}}, \quad H_5 = (m_{a+b})_{a,b=0}^5. \quad (27)$$

To obtain the positive-definiteness conclusion, suppose that every finite translation Gram of p_{s_0} were positive semidefinite. Replace differentiation on each variable of the smooth kernel $p_{s_0}(u - v)$ by forward differences on the nodes $0, h, \dots, 5h$. Congruence preserves positive semidefiniteness. As $h \rightarrow 0$, the resulting matrices converge entrywise to the derivative Gram

$$\left((-1)^b p_{s_0}^{(a+b)}(0)\right)_{a,b=0}^5. \quad (28)$$

A diagonal unitary change of phases, with diagonal entries i^a , converts this matrix to H_5 : its (a, b) entry becomes $(-i)^{a+b} p_{s_0}^{(a+b)}(0) = m_{a+b}$. The limit would therefore make H_5 positive semidefinite, contrary to the negative direction above. Thus p_{s_0} is not positive definite. This completes the proof.

Remark. The confluence argument also shows that the six-node Gram on $0, h, \dots, 5h$ has a negative direction for all sufficiently small positive h . No numerical spacing is needed for Theorem 1. The result concerns this fixed-center product; it does not determine positive definiteness of kernels obtained by averaging over the center.

6. Supplementary material

The supplementary archive contains `verify_quintic_192bit.py` and `verify_quintic_160bit.py`, their retained exact rational certificates, and `integer_moment_bounds.json`. Both scripts reconstruct the full-tail enclosures, the signed moments, and the polynomial-square contraction. The first uses the closed Stirling formula; the second uses the polynomial recurrence and a separate implementation of the interval arithmetic. The scripts use integer and rational arithmetic throughout. A README provides reproduction commands, and SHA-256 manifests identify the distributed files.

Disclosure of AI assistance

Generative AI tools, including OpenAI's Codex, assisted with mathematical exploration and review, preparation of verification code, literature searches, and manuscript drafting and formatting. The author takes responsibility for the manuscript and supplementary materials, including all mathematical claims, computations, and references.

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