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Metric discrepancy results for geometric progressions with large ratios

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Abstract For geometric progressions with common ratios greater than 4, the speed of convergence to the uniform distribution is determined for almost all initial values.

Keywords Discrepancy · Lacunary sequence · Law of the iterated logarithm

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1 Introduction

A sequence $\{x_k\}$ of real numbers is said to be uniformly distributed mod 1 if

$$\frac{1}{N}{}^{\#}\{k \le N \mid \langle x_k \rangle \in [a, b)\} \to b - a, \quad (N \to \infty),$$

for all $0 \le a < b < 1$, where $\langle x \rangle$ denotes the fractional part $x - [x]$ of a real number x. Since the convergence is uniform in a and b, the following discrepancy is used to measure its speed.

Dedicated to Professor Norio Kôno on his 77th birthday.

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$$D_N\{x_k\} = \sup_{0\le a<b<1} \left| \frac{1}{N} {}^{\#}\{k \le N \mid \langle x_k \rangle \in [a,b)\} - (b-a) \right|.$$

For an arithmetic progression $\{n_k\}$, the order of convergence of $D_N\{n_k x\}$ was studied by Khintchin [9] and Kesten [8]. For uniformly distributed i.i.d. $\{U_k\}$, Chung-Smirnov theorem asserts the law of the iterated logarithm

$$\overline{\lim_{N\to\infty}} \frac{N D_N\{U_k\}}{\sqrt{2N \log\log N}} = \frac{1}{2}, \quad \text{a.s.}$$

By various studies on lacunary series, it is known that a sequence $\{n_k x\}$ behaves like uniformly distributed i.i.d. when $\{n_k\}$ diverges rapidly. Actually Philipp [10] followed Takahashi's method [11] and proved the result below by assuming the Hadamard gap condition $n_{k+1}/n_k \ge q > 1$.

$$\frac{1}{4\sqrt{2}} \le \overline{\lim_{N\to\infty}} \frac{N D_N\{n_k x\}}{\sqrt{2N \log\log N}} \le \frac{1}{\sqrt{2}} \left(166 + \frac{664}{q^{1/2}-1}\right), \quad \text{a.e.}$$

Dhompongsa [3] proved that the limsup equals to $\frac{1}{2}$ when $\{n_k\}$ satisfies very strong gap condition $\lim_{k\to\infty}(\log(n_{k+1}/n_k))/\log\log k = \infty$. Beside of these results, any concrete value of limsup for exponentially growing sequence was not determined before the recent results below on divergent geometric progressions $\{\theta^k x\}$.

Theorem 1 [4–7] *For any $\theta \notin [-1,1]$, there exists a constant $\Sigma_\theta \ge 1/2$ such that*

$$\overline{\lim_{N\to\infty}} \frac{N D_N\{\theta^k x\}}{\sqrt{2N \log\log N}} = \Sigma_\theta, \quad \text{a.e.}$$

If $\theta^j \notin \mathbf{Q}$ for any $j \in \mathbf{N}$, then $\Sigma_\theta = \frac{1}{2}$, and otherwise $\Sigma_\theta > \frac{1}{2}$. When θ satisfies $\theta^j \in \mathbf{Q}$ for some $j \in \mathbf{N}$, we take p, q, and r as below.

$$\theta^r = p/q \quad \text{where} \quad r = \min\{j \in \mathbf{N} \mid \theta^j \in \mathbf{Q}\}, \quad p \in \mathbf{Z}, \quad q \in \mathbf{N}, \quad \gcd(p,q) = 1. \tag{1}$$

If p and q are odd, then

$$\Sigma_\theta = \frac{1}{2}\sqrt{\frac{|p|q+1}{|p|q-1}}.$$

If $q = 1$, then

$$\Sigma_\theta = \frac{1}{2}\sqrt{\frac{|p|+1}{|p|-1}}, \quad \frac{1}{2}\sqrt{\frac{(|p|+1)|p|(|p|-2)}{(|p|-1)^3}}, \quad \frac{1}{9}\sqrt{42}, \quad \text{or} \quad \frac{1}{49}\sqrt{910},$$

according as p is odd, $|p| \ge 4$ is even, $p = 2$, or $p = -2$. If $p = \pm 5$ and $q = 2$, then

$$\Sigma_\theta = \frac{1}{9}\sqrt{22}.$$

For related works, see [1,2]. In this paper, we prove the next result and determine Σ_θ when θ is large.

Theorem 2 *Suppose that θ satisfies (1). If p is odd, q is even and $|p/q| \geq 9/4$, or if p is even, q is odd and $|p/q| \geq 4$, then*

$$\Sigma_\theta = \left(\frac{(|p|q)^I + 1}{(|p|q)^I - 1} v\left(\frac{|p| - q - 1}{2(|p| - q)}\right) + \frac{2(|p|q)^I}{(|p|q)^I - 1} \sum_{m=1}^{I-1} \frac{1}{(|p|q)^m} v\left(q^m \frac{|p| - q - 1}{2(|p| - q)}\right)\right)^{1/2}, \tag{2}$$

where $v(x) = \langle x\rangle(1 - \langle x\rangle)$ and $I = \min\{n \in \mathbf{N} \mid q^n = \pm 1 \mod |p| - q\}$.

By (2), we can calculate the concrete values of Σ_θ in the following way.

$$\Sigma_{\pm 7/2} = \frac{1}{5}\sqrt{\frac{1294}{195}}, \quad \Sigma_{\pm 9/2} = \frac{2}{49}\sqrt{\frac{18561}{119}},$$
$$\Sigma_{\pm 14/3} = \frac{1}{11}\sqrt{\frac{4096559910}{130691231}}, \quad \Sigma_{\pm 9/4} = \frac{1}{5}\sqrt{\frac{222}{35}}, \ldots$$

When $q = 1$ and $|p| \geq 4$ is even, we have $I = 1$, and (2) gives the values stated in Theorem 1. It also gives the value $\Sigma_{\pm 5/2}$ in Theorem 1.

We here emphasize that the values of Σ_θ are determined for large θ, say, that satisfying $|\theta| \geq 4$. On the other hand, we can find some smaller p/q for which (2) fails to hold. $\theta = \pm 2$ is one such example.

Before closing this section, we note that the conditions $|p/q| \geq 9/4$ and $|p/q| \geq 4$ are superfluous, and much weaker conditions are sufficient. Set

$$\begin{aligned}
A_1(p, q) &:= 2p^3 - (4q + 2)p^2 - (q^2 - 2q)p + 3q^2,\\
A_2(p, q) &:= (8q^2 - 6)p^3 + (-16q^3 + 4q + 24)p^2 + (-q^4 + 10q^2 - 24q - 24)p + q^3,\\
A_3(p, q) &:= p^3 - (4q + 1)p^2 + 2pq + 2q^2\\
A_4(p, q) &:= (6q^2 - 4)p^6 + (-4q^3 + 8q^2 + 2q + 16)p^5 + (-25q^4 - 24q - 16)p^4\\
&\quad + (12q^5 - 24q^4 + 25q^3 + 8q^2 - 2q)p^3 + (-4q^6 + 16q^5 - 12q^4 + 32q^3 - 8q^2)p^2\\
&\quad + (4q^5 - 32q^4 - 10q^3)p - 4q^4.
\end{aligned}$$

When p is odd and q is even, if the conditions $A_1(|p|, q) > 0$, $A_2(|p|, q) > 0$, and

$$|p/q| \geq 2, \tag{3}$$

are satisfied, then we have (2). The condition $|p/q| > 9/4$ implies these conditions. Although $A_1(9, 4) < 0$ and $A_2(9, 4) > 0$, we can still prove (2) for $p/q = \pm 9/4$.

We here note that $|p/q| \geq (2+\sqrt{6})/2 + 1/q$ also implies $A_1(|p|, q) > 0$ and $A_2(|p|, q) > 0$.

When p is odd and q is even, if (3), $A_3(|p|, q) > 0$ and $A_4(|p|, q) > 0$ are satisfied, then (2) holds. The condition $|p/q| \geq 4$ implies these conditions.

2 Preliminary

We prepare some results. Proofs can be found in [4,6,7]. For $a, b, a', b' \in [0, 1)$, put

$$V(a, a') = a \wedge a' - aa', \quad \widetilde{V}(a, b, a', b') = V(a, a') + V(b, b') - V(a, b') - V(b, a')$$

and

$$\sigma^2_{p/q}(a, b) = \widetilde{V}(a, b, a, b) + 2\sum_{k=1}^{\infty} \frac{1}{(pq)^k} \widetilde{V}(\langle p^k a\rangle, \langle p^k b\rangle, \langle q^k a\rangle, \langle q^k b\rangle). \tag{4}$$

Here we list general properties that we use.

$$\widetilde{V}(a, b, a', b') = \widetilde{V}(a', b', a, b) = -\widetilde{V}(b, a, a', b') = -\widetilde{V}(a, b, b', a'), \tag{5}$$

$$0 \leq \widetilde{V}(0, b, 0, b') = V(b, b') \leq V(b, b) \leq 1/4, \tag{6}$$

$$\widetilde{V}(a, b, a, b) = |b-a| - |b-a|^2 = v(b-a) = v(a-b), \tag{7}$$

$$\sigma^2_{p/q}(0, a) = V(a, a) + 2\sum_{k=1}^{\infty} \frac{1}{(pq)^k} V(\langle p^k a\rangle, \langle q^k a\rangle). \tag{8}$$

When θ satisfies (1), Σ_θ does not depend on r and is given by

$$\Sigma_\theta = \Sigma_{p/q} = \sup_{0\leq a' < a \leq 1} \sigma_{p/q}(a', a), \quad \text{and}$$
$$\Sigma_\theta = \Sigma_{p/q} = \sup_{0\leq a \leq 1/2} \sigma_{p/q}(0, a) \quad \text{if} \quad p > 0. \tag{9}$$

Put $b_i := \frac{i}{p-q}$, $c_1 := \frac{q-2}{2q}$, $c_2 := \frac{p-3}{2p}$, $c_3 := \frac{p-1}{2p}$, $c_4 := b_{(p-q-1)/2} = \frac{(p-q-1)/2}{p-q}$, $c_5 := \frac{q-1}{2q}$, $c_6 := \frac{p-2}{2p}$, and $c_7 := b_{(p-q-3)/2} = \frac{(p-q-3)/2}{p-q}$. When p and q are positive and satisfying $p/q \geq 2$, one can verify $c_1 < c_2 < c_4 < c_3$ and $c_5 \leq c_6 \leq c_4$. By $p = q \mod p-q$, we have

$$\langle p^k b_i\rangle = \langle q^k b_i\rangle \quad \text{and} \quad V\left(\langle p^k b_i\rangle, \langle q^k b_i\rangle\right) = v(p^k b_i) = v(q^k b_i). \tag{10}$$

Thanks to $v(-x) = v(x)$, we have $v(q^{m+nI} c_4) = v(\pm q^m c_4) = v(q^m c_4)$. Hence $\sigma_{p/q}(0, c_4)$ equals to the left hand side of (2).

In the next two sections, we prove $\Sigma_{p/q} = \sigma_{p/q}(0, c_4)$ in the case p is positive and p/q is large. By assuming this, we here prove $\Sigma_{-p/q} = \Sigma_{p/q}$. In [6] we proved

$\Sigma_{-p/q} \le \Sigma_{p/q}$. If we find $0 \le \widehat{b} < \widetilde{b} \le 1$ with $\sigma_{-p/q}(\widehat{b}, \widetilde{b}) = \sigma_{p/q}(0, c_4) = \Sigma_{p/q}$, we have the equality.

We put $\widehat{b} = (1-c_4)p/(p+q)$ and $\widetilde{b} = \widehat{b} + c_4$. It holds that $\langle(-p)^n\widehat{b}\rangle = \langle q^n\widehat{b}\rangle$ and $\langle(-p)^n\widetilde{b}\rangle = \langle q^n\widetilde{b}\rangle$ if n is even, and that $\langle(-p)^n\widehat{b}\rangle = \langle q^n\widetilde{b}\rangle$ and $\langle(-p)^n\widetilde{b}\rangle = \langle q^n\widehat{b}\rangle$ if n is odd. Actually, we have $(p+q)\widehat{b} = p - pc_4 = -pc_4 = -qc_4$ mod 1, which implies $-p\widehat{b} = q\widetilde{b}$, $-p\widetilde{b} = q\widehat{b}$ mod 1, and $(-p)^2\widehat{b} = -pq\widetilde{b} = q^2\widehat{b}$ mod 1, and so on. By noting (5), (7), and $\langle\langle q^n\widetilde{b}\rangle - \langle q^n\widehat{b}\rangle\rangle = \langle q^n c_4\rangle$, we have

$$\widetilde{V}(\langle(-p)^n\widehat{b}\rangle, \langle(-p)^n\widetilde{b}\rangle, \langle q^n\widehat{b}\rangle, \langle q^n\widetilde{b}\rangle) = -\widetilde{V}(\langle q^n\widetilde{b}\rangle, \langle q^n\widehat{b}\rangle, \langle q^n\widehat{b}\rangle, \langle q^n\widetilde{b}\rangle)$$
$$= -v(q^n c_4)$$

for odd n, and

$$\widetilde{V}(\langle(-p)^n\widehat{b}\rangle, \langle(-p)^n\widetilde{b}\rangle, \langle q^n\widehat{b}\rangle, \langle q^n\widetilde{b}\rangle) = v(q^n c_4)$$

for even n, to have $\sigma_{-p/q}(\widehat{b}, \widetilde{b}) = \sigma_{p/q}(0, c_4)$.

We prepare some inequalities to prove $\Sigma_{p/q} = \sigma_{p/q}(0, c_4)$. We denote $\sigma_{p/q}(0, a)$ simply by $\sigma(a)$.

Put

$$X_N(a) := V(a, a) + 2\sum_{n=1}^{N} \frac{1}{(pq)^n} V\left(\langle p^n a\rangle, \langle q^n a\rangle\right), \quad Y_N(a) := 2\sum_{n=N+1}^{\infty} \frac{v(q^n a)}{(pq)^n},$$
$$T_N := 2\sum_{n=N+1}^{\infty} \frac{1}{4(pq)^n},$$

$S_t(a) := 2v(t^2 a)/(pq)^2$, and $Z(a) := V(a, a) + 2v(qa)/pq$. Thanks to (6) and (10), we have

$$V\left(\langle p^k a\rangle, \langle q^k a\rangle\right) \le v(q^k a), \quad V\left(\langle p^k a\rangle, \langle q^k a\rangle\right) \le v(p^k a),$$
$$V\left(\langle p^k a\rangle, \langle q^k a\rangle\right) \le 1/4,$$

and

$$\sigma^2(a) \le W_j(a) \quad (1 \le j \le 6), \quad \text{and} \quad W_1(b_i) = W_2(b_i) = \sigma^2(b_i) \quad (0 \le i \le p-q), \tag{11}$$

where

$$W_1 := X_1 + Y_1, \qquad W_2 := X_2 + Y_2, \qquad W_3 := X_1 + T_1,$$
$$W_4 := Z + S_q + T_2, \qquad W_5 := Z + S_p + T_2, \qquad W_6 := Z + T_1.$$

By $\gcd(q, p-q) = 1$, $\langle p^k c_4\rangle = \langle q^k c_4\rangle \in \{b_1, \ldots, b_{p-q-1}\}$ and $v(b_i) \ge v(b_1)$, we have

$$\sigma^2(c_4) \geq Z(c_4) + 2\sum_{n=2}^{\infty} \frac{1}{(pq)^n} v(b_1) =: U.$$

Note that the evaluation of U strongly depends on the parity of p, since $\langle qc_4 \rangle = qc_4 - (q-2)/2$ or $\langle qc_4 \rangle = qc_4 - (q-1)/2$ according as q is even or odd.

We denote the derivative $\frac{d}{da} f$ of f by Df, the right derivative by $D^+ f$, and the left derivative by $D^- f$.

3 Odd *p* and even *q*

Assume that q is even, and that p is odd and positive. We divide $[0, 1/2)$ into subintervals $[0, c_1)$, $[c_1, c_2)$, $[c_2, c_3)$, and $[c_3, 1/2)$, and prove $\sigma^2(a) \leq \sigma^2(c_4)$ on each.

3.1 $[c_2, c_3)$ part

We assume (3), $A_1(p, q) > 0$, and $a \in [c_2, c_3)$. We have $\langle pa \rangle = pa - (p-3)/2$ and $\langle qa \rangle = qa - (q-2)/2$. Since $\langle pa \rangle < \langle qa \rangle$ holds on $[c_2, c_4)$, and $\langle pa \rangle \geq \langle qa \rangle$ on $[c_4, c_3)$, we can evaluate X_1 as

$$X_1(a) = \begin{cases} -3a^2 + (3 - 3/p)a + 3/2p - 1/2 & a \in [c_2, c_4], \\ -3a^2 + (3 - 2/q - 1/p)a - 1/pq + 1/q + 1/2p - 1/2 & a \in [c_4, c_3), \end{cases}$$

and verify that $DX_1(a)$ decreases on $[c_2, c_3)$. We also have $|Dv(q^n a)| \leq q^n$ a.e. a, and therefore $|DY_1| \leq 2/p(p-1)$ a.e. By combining these, we have

$$\begin{aligned} DW_1(a) &> D^- X_1(c_4) - 2/p(p-1) \\ &= (3pq - 2p - q)/p(p-1)(p-2) > 0 \quad \text{a.e. on} \quad (c_2, c_4], \end{aligned}$$

and

$$\begin{aligned} DW_1(a) &< D^+ X_1(c_4) + 2/p(p-1) \\ &= -A_1(p, q)/p(p-1)(p-2) < 0 \quad \text{a.e. on} \quad [c_4, c_3). \end{aligned}$$

Hence $\sigma^2(a) \leq W_1(a) \leq W_1(c_4) = \sigma^2(c_4)$ for $a \in [c_2, c_3)$. Here we note that functions appearing here are bounded and absolutely continuous, and the exceptional set of null measure for $DW_1(a) > 0$ or $DW_1(a) < 0$ does not harm the argument to show that c_4 is the maximal point.

Here we prove $A_1(p, q) > 0$ by assuming $p/q > 9/4$. Since $2p^2 - (4q+2)p + (q^2 - 2q)$ is increasing in $p \geq (9/4)q$, $A_1(p, q)$ also. Because of $A_1((9/4)q, q) = 3q^2(3q - 28)/32 > 0$ if $q \geq 10$, we see that $A_1(p, q) > 0$ if $q \geq 10$ and $p/q > 9/4$. Thanks to $A_1(5, 2) > 0$, $A_1(11, 4) > 0$, $A_1(17, 6) > 0$ and $A_1(19, 8) > 0$, we see that $A_1(p, q) > 0$ if $p/q > 9/4$.

We prove the case $p/q = 9/4$. Due to the above proof, we see that $\sigma^2(a) \leq \sigma^2(c_4)$ for $a \in [c_2, c_4]$. Since we have $T_1 = \frac{1}{2520}$ and X_1 is decreasing in $a \geq c_4$, we have

$\sigma^2(a) \le W_3(a) \le X_1(\frac{34}{81}) + \frac{1}{2520} < \frac{222}{875} = \sigma^2(c_4)$ on $[\frac{34}{81}, c_3)$. On $[c_4, \frac{33}{81})$, we have $\langle 16a\rangle \le \langle 81a\rangle$ and see DX_2 is decreasing and $|DY_2(a)| \le \frac{1}{324}$. Hence we have $DW_2(a) \le DX_2(c_4) + \frac{1}{324} < 0$ and $\sigma^2(c_4) = W_2(c_4) \ge W_2(a) \ge \sigma^2(a)$ on $[c_4, \frac{33}{81})$. Note that $Y_2 \le \frac{1}{90{,}720}$. On $[\frac{33}{81}, \frac{27}{65})$, by $\langle 16a\rangle \ge \langle 81a\rangle$ we see that X_2 equals to a quadratic function having axis at $\frac{881}{2160}$. Hence $\sigma^2(a) \le X_2(\frac{881}{2160}) + \frac{1}{90{,}720} < \sigma^2(c_4)$. On $[\frac{27}{65}, \frac{34}{81})$, by $\langle 16a\rangle < \langle 81a\rangle$, X_2 is decreasing. Hence $\sigma^2(a) \le X_2(\frac{27}{65}) + \frac{1}{90{,}720} < \sigma^2(c_4)$ for $a \in [\frac{27}{65}, \frac{34}{81})$.

3.2 $[c_3, 1/2)$ part

Let $a \in [c_3, 1/2)$. We have $\langle pa\rangle = pa - (p-1)/2$ and $\langle qa\rangle = qa - (q-2)/2$. We see $\langle qa\rangle - \langle pa\rangle = -(p-q)a + (p-q+1)/2 > 1/2$. Since $W_3(a)$ maximizes at $a_1 := (3p-1)/6p$, we have $W_3(a) \le W_3(a_1)$. By

$$U - W_3(a_1) = A_2(p,q)/(12p^2q(p-q)^2(pq-1)) > 0,$$

we have $\sigma^2(a) < U$ for $a \in [c_3, 1/2)$.

We derive $A_2(p,q) > 0$ from $p/q \ge 9/4$. Put $\widehat{A}_2(p,q) = (8q^2-6)p^2 + (-16q^3 + 4q)p - q^4$. We see

$$A_2(p,q) = p\widehat{A}_2(p,q) + (24p^2 - 24qp - 24p) + (10q^2p + q^3) > \widehat{A}_2(p,q).$$

We see $\widehat{A}_2(p,q)$ is increasing in p if $p \ge 2q$. By $\widehat{A}_2((9/4)q,q) = q^2(28q^2 - 171)/8 > 0$ $(q \ge 4)$, and by $\widehat{A}_2(5,2) > 0$, the proof is over.

3.3 $[0, c_1)$ part

We consider on $[0, c_1)$. We assume $q \ge 4$, since $c_1 = 0$ otherwise. Since $V(a,a)$ increases on $[0, c_1)$ and $W_4(a) - V(a,a)$ has period $1/q$, the first equality of

$$\sup_{a\in[0,c_1)} W_4(a) = \sup_{a\in[c_1-1/q,c_1)} W_4(a) = \sup_{a\in[c_1-1/q^2,c_1)} W_4(a) = W_4(c_1) < U \qquad (12)$$

holds. On $[c_1 - 1/q, c_1)$, we have $\langle qa\rangle = qa - (q-4)/2$, and we see Z equals to a quadratic function having axis at $a_2 := (2q+p-6)/(4q+2p)$. By $a_2 - c_1 = (p-q)/q(2q+p) > 0$, we see that it is increasing on $[c_1 - 1/q, c_1)$. Since $S_q(a)$ has period $1/q^2$, we verified the second equality of (12). On $[c_1 - 1/q^2, c_1)$, we have $\langle q^2 a\rangle = q^2a - q(q-2)/2 + 1$. We see that $W_4(a)$ equals to a quadratic function with axis $a_3 := (2q^2 + (2p-4)q + p^2 - 6p - 2)/(4q^2 + 4pq + 2p^2)$. By

$$a_3 - c_1 = (p^2 - pq - q)/(4q^2 + 4pq + 2p^2) > p(p-2q)/(2q^2 + 2pq + 1p^2) \ge 0,$$

we have the third equality. The rest is proved by

$$\begin{aligned}&4p^2q^2(p-q)^2(pq-1)(U-W_4(c_1))\\&\quad=4qp^5+(-8q^2-4)p^4+(7q^3+8q)p^3+(-6q^4-7q^2+8q-2)p^2\\&\qquad+(6q^3-8q^2-4q)p-2q^2,\end{aligned}$$

by noting

$$\begin{aligned}4qp^5-(8q^2+4)p^4+2p^3q^3&\geq 4qp^5-9q^2p^4+2p^3q^3\\&=p^3q^3(4p/q-1)(p/q-2)\geq 0,\\5q^3p^3-6q^4p^2\geq 0,\quad 8qp^3&-7q^2p^2>0,\quad (8q-2)p^2>0,\\(5q^3-8q^2-4q)p>0,&\quad q^3p-2q^2>0.\end{aligned}$$

3.4 $[c_1, c_2)$ part

Considering on $[c_1, c_2)$, we have $\langle qa\rangle = qa-(q-2)/2$. Since Z equals to a quadratic function with axis $a_4 := (2q+p-2)/(4q+2p)$, and since $a_4-c_2 = (6q+p)/2p(2q+p) > 0$, it is increasing on $[c_1, c_2)$.

First, we consider the case when $2q \leq p \leq \frac{3}{2}q^2+q$ holds. Since S_p has period $1/p^2$, and since

$$c_2-1/p^2-c_1=(2p+q)(p-2q)/2p^2q\geq 0,$$

we have the first equality of

$$\sup_{a\in[c_1,c_2)} W_5(a)=\sup_{a\in[c_2-1/p^2,c_2)} W_5(a)\leq W_5(a_5)<U. \tag{13}$$

On $[c_2-1/p^2, c_2)$, we have $\langle p^2a\rangle = p^2a-p(p-3)/2+1$, and we see that $W_5(a)$ equals to a quadratic function with axis $a_5 := (2q^3+(p-2)q^2+2p^3-6p^2-2p)/(4q^3+2pq^2+4p^3)$, hence we have the third inequality. We have the rest by

$$\begin{aligned}&4p^2q(p-q)^2(pq-1)(2q^3+pq^2+2p^3)(U-W_5(a_5))\\&\quad=-4p^6+(36q^3+4q^2+8q+16)p^5+(-79q^4+16q^3-40q^2\\&\qquad-20q-16)p^4+(44q^5-44q^4+79q^3-8q^2-2q)p^3+(-16q^6+24q^5\\&\qquad-44q^4+52q^3-8q^2)p^2+(16q^5-40q^4-10q^3)p-4q^4>0.\end{aligned}$$

Actually, when $q\geq 4$, we see

$$\begin{aligned}&-4p^6+(36q^3+4q^2+8q+16)p^5-79q^4p^4+16q^5p^3\\&\quad\geq(36q^3-2q^2)p^5-79q^4p^4+16q^5p^3\\&\quad\geq\frac{71}{2}q^3p^5-79q^4p^4+16q^5p^3\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{2}\left(\frac{p}{q}-2\right)\left(71\frac{p}{q}-16\right) \geq 0, \\
&(16q^3-40q^2-20q-16)p^4 \geq (16-10-5/4-1/4)q^3p^4 > 0, \\
&(12q^5-44q^4)p^3 \geq (12-11)q^5p^3 > 0, \quad 16q^5p^3-16q^6p^2 > 0, \\
&(24q^5+52q^3-8q^2)p^2 > 0, \\
&(79q^3-8q^2-2q)p^3-44q^4p^2 \geq (79-2-1/8)q^3p^3-44q^4p^2 > 0, \\
&(16q^5-40q^4-10q^3)p-4q^4 \geq (16-10-5/8)q^5p-4q^4 > 0.
\end{aligned}
$$

When $q = 2$, and $p = 5$ or 7, one can verify the above inequality.

Next, we consider the case $p > \frac{3}{2}q^2 + q$. We have already seen that Z and W_6 are increasing on $[c_1, c_2)$. Note that $p/q > \frac{3}{2}q + 1 \geq 4$ and $(c_2 - 1/p) - c_1 = (p/q - 5/2)/p > 0$. We can verify

$$
\begin{aligned}
&(U - W_6(c_2-1/p))(4p^3q(p-q)^2(pq-1)) \\
&\quad = (8q^2-2)p^4 + (34q^3-4q+8)p^3 + (-95q^4-36q^2-8q-8)p^2 \\
&\qquad + (50q^5+95q^3)p - 50q^4 > 0
\end{aligned}
$$

by $8p^3 - (8q+8)p^2 \geq 8p^3 - 12qp^2 > 0$ and

$$
\begin{aligned}
&(8q^2-2)p^4 + (34q^3-4q)p^3 + (-95q^4-36q^2)p^2 + 50q^4p \\
&\quad > \frac{15}{2}q^2p^4 + 33q^3p^3 - 104q^4p^2 + 50q^5p = q^5p\left(\frac{15}{2}\left(\frac{p}{q}\right)^3 + 33\left(\frac{p}{q}\right)^2\right. \\
&\quad \left. -104\left(\frac{p}{q}\right) + 50\right) =: q^5p \cdot g\left(\frac{p}{q}\right) > 0
\end{aligned}
$$

since $g'(t) > 0$ for $t \geq 2$ and $g(2) > 0$. Hence we see

$$
\sigma^2(a) \leq W_6(a) \leq W_6(c_2 - 1/p) \leq U \quad (a \in [c_1, c_2 - 1/p]).
$$

We consider on $[c_2 - 1/p, c_2)$. We have $\langle pa \rangle = pa - (p-5)/2$, $\langle qa \rangle = qa - (q-2)/2$, and can see that $\langle pa \rangle < \langle qa \rangle$ on $[c_2 - 1/p, c_7)$ and $\langle pa \rangle \geq \langle qa \rangle$ on $[c_7, c_2)$. By recalling the bound $|DY_1| \leq 2/p(p-1)$, we can verify that DX_1 is decreasing on $[c_2 - 1/p, c_2)$,

$$
\begin{aligned}
DW_1(a) &\geq D^- X_1(c_7) - 2/p(p-1) \\
&= (4p^2 + (5q-6)p - 3q)/p(p-q)(p-1) > 0,
\end{aligned}
$$

on $[c_2 - 1/p, c_7)$, and

$$
\begin{aligned}
DW_1 \leq D^+ X_1(c_7) + 2/p(p-1) = (&-2p^3 + (8q+2)p^2 \\
&+ (3q^2-6q)p - 5q^2)/p(p-q)(p-1) < 0
\end{aligned}
$$

on $[c_7, c_2)$. Actually, the first inequality is clear and the second is proved by

$$\begin{aligned}-2p^3 + (8q+2)p^2 + 3q^2 p &\le -2p^3 + 9qp^2 + 3q^2 p\\ &= pq^2\left(-2\left(\frac{p}{q}\right)^2 + 9\left(\frac{p}{q}\right) + 3\right) < 0\end{aligned}$$

by $\frac{p}{q} \ge 7$ if $q \ge 4$. In case $q = 2$, we have

$$-2p^3 + (8q+2)p^2 + (3q^2 - 6q)p - 5q^2 = -2(p+1)(p^2 - 10p + 10) < 0$$

for $p \ge 9$. Hence we see the second inequality of

$$\sigma^2(a) \le W_1(a) \le W_1(c_7) = \sigma^2(c_7) \le W_4(c_7) < \widetilde{U} < \sigma^2(c_4) \quad (a \in [c_2 - 1/p, c_2)).$$

Put $\widetilde{U} := Z(c_4) + S_q(c_4) < \sigma^2(c_4)$. Because of $0 < q^2/2(p-q) < 3q^2/2(p-q) < 1$,

$$\begin{aligned}q^2 c_4 &= (q^2/2 - 1) + (1 - q^2/2(p-q)), \quad \text{and}\\ q^2 c_7 &= (q^2/2 - 1) + (1 - 3q^2/2(p-q)),\end{aligned}$$

we see $\langle q^2 c_4\rangle = 1 - q^2/2(p-q)$ and $\langle q^2 c_7\rangle = 1 - 3q^2/2(p-q)$. Hence we can calculate $S_q(c_4)$ and $S_q(c_7)$, and can verify the rest by

$$\begin{aligned}&(\widetilde{U} - W_4(c_7))(2p^2q^2(p-q)^2(pq-1))\\ &\quad= (12q^4 - 4q^3 - 1)p^2 + (8q^5 + 4q^4 - 12q^3 + 4q^2 + 2q)p - 8q^4 - 4q^3 - q^2\\ &\quad\ge 9q^4p^2 + 7q^5p - 11q^4 > 0.\end{aligned}$$

4 Even *p* and odd *q*

Assume that q is odd and p is even and positive. We may assume $q \ge 3$.

4.1 $[c_6, 1/2)$ part

We consider on $[c_6, 1/2)$. We have $\langle pa\rangle = pa - (p-2)/2$, and by $c_5 \le c_6$, $\langle qa\rangle = qa - (q-1)/2$. Since $\langle pa\rangle < \langle qa\rangle$ holds on $[c_6, c_4)$, and $\langle pa\rangle \ge \langle qa\rangle$ on $[c_4, 1/2)$, we see that DX_1 is decreasing on $[c_6, 1/2)$. Recalling $|DY_1(a)| \le 2/p(p-1)$, we have

$$DW_1(a) \ge D^- X_1(c_4) - 2/p(p-1) = (2q^2 - 2q + p^2 - p)/(p-1)q(p-q) > 0$$

on $[c_6, c_4)$, and

$$DW_1(a) \le D^+ X_1(c_4) + 2/p(p-1) = -A_3(p,q)/(p-1)pq(p-q) < 0$$

on $[c_4, 1/2)$. Hence $W_1(a) \le W_1(c_4) = \sigma^2(c_4)$ for $a \in [c_6, 1/2)$.

We derive $A_3(p,q) > 0$ from $p/q \geq 4$. Because of $p \geq 4q$ and p and q are relatively prime, we see $p > 4q$ or $p \geq 4q+2$. Hence we have $A_3(p,q) = p^2(p - 4q - 1) + 2pq + 2q^2 > 0$.

4.2 $[0, c_5)$ part

We consider on $[0, c_5)$. The condition (3) implies $p \geq 2q+2$. Since $V(a,a)$ is increasing on $[0, c_5)$ and $W_4(a) - V(a,a)$ has period $1/q$, we have the first equality of

$$\sup_{a\in[0,c_5)} W_4(a) = \sup_{a\in[c_5-1/q,c_5)} W_4(a) = \sup_{a\in[c_5-1/q^2,c_5)} W_4(a) = W_4(c_5) < U. \tag{14}$$

On $[c_5 - 1/q, c_5)$, we have $\langle qa\rangle = qa - (q-3)/2$ and we see that Z equals to a quadratic function having axis at $a_6 := (p+2q-4)/(2p+4q)$. Because of

$$a_6 - c_5 = (p-2q)/(2q(2q+p)) > 0,$$

it is increasing on $[c_5 - 1/q, c_5)$. Since S_q has period $1/q^2$, we have the second equality of (14). On $[c_5 - 1/q^2, c_5)$, we have $\langle q^2 a\rangle = q^2 a - q(q-1)/2 + 1$ and we see that $W_4(a)$ equals to a quadratic function having axis at $a_7 := (2q^2 + (2p-2)q + p^2 - 4p - 2)/(4q^2 + 4pq + 2p^2)$. Because of

$$a_7 - c_5 = ((p+1)(p-2q-1)+1)/(2q(2q^2+2pq+p^2)) > 0,$$

$W_4(a)$ is increasing on $[c_5 - 1/q^2, c_5)$ and the third equality of (14) is proved. The rest is by

$$\begin{aligned}&(U - W_4(c_5))(4p^2q^2(p-q)^2(pq-1))\\&\quad = p(p-2q)\,(p(pq-1)(p+2q)+4q+2) + 4(q-2)p^2 + 2(2p^2-q^2) > 0.\end{aligned}$$

4.3 $[c_5, c_6)$ part

On $[c_5, c_6)$, we have $\langle qa\rangle = qa - (q-1)/2$ and we see that Z equals to a quadratic function having axis at $1/2$. Hence it is increasing on $[c_5, c_6)$. Since S_p has period $1/p^2$, we have the first equality of

$$\sup_{a\in[c_5,c_6)} W_5(a) = \sup_{a\in[(c_6-1/p^2)\vee c_5,c_6)} W_5(a) \leq W_5(a_8) < U. \tag{15}$$

On $[(c_6 - 1/p^2) \vee c_5, c_6)$, by $\langle p^2 a\rangle = p^2 a - p(p-2)/2 + 1$ we see that $W_5(a)$ is a quadratic function having axis at $a_8 := (2q^3 + pq^2 + 2p^3 - 4p^2 - 2p)/(4q^3 + 2pq^3 + 4p^3)$. Hence we have the middle of (15). Rest is by

$$U - W_5(a_8) = A_4(p,q)/4p^2q(q-p)^2(pq-1)(2q^3+pq^2+2p^3) > 0.$$

Finally, we prove $A_4(p,q) > 0$ by assuming

$$\frac{p}{q} \geq a_9 := \left(\frac{6^{-3/2}\sqrt{1019}}{9} + \frac{511}{1458}\right)^{1/3} + \frac{65}{162}\left(\frac{6^{-3/2}\sqrt{1019}}{9} + \frac{511}{1458}\right)^{-1/3} + \frac{8}{9} = 2.206\ldots.$$

We decompose as $3A_4(p,q) = h_1 + \cdots + h_7$. Here

$$h_1 = (3q^2-2)(p+2q)p^2q^3\left(6\left(\frac{p}{q}\right)^3 - 16\left(\frac{p}{q}\right)^2 + 7\left(\frac{p}{q}\right) - 2\right) \geq 0 \quad \text{if} \quad \frac{p}{q} \geq a_9,$$

$$\begin{aligned} h_2 &= (24q^2-2q)p^5 - 50q^2p^4 - 72q^4p^3 + 48q^5p^2 \\ &\geq q^5p^2\left(\frac{70}{3}\left(\frac{p}{q}\right)^3 - \frac{50}{3}\left(\frac{p}{q}\right)^2 - 72\left(\frac{p}{q}\right) + 48\right) > 0 \end{aligned}$$

since the last cubic function in p/q is increasing for $p/q \geq 2$ and equals to 24 at $p/q = 2$,

$$\begin{aligned} h_3 &= 48p^5 - (72q+48)p^4 \geq 48p^5 - 88qp^4 > 0, \\ h_4 &= 99q^3p^3 - 44q^4p^2 > 0, \\ h_5 &= (24q^2 - 6q)p^3 > 0, \\ h_6 &= (96q^3 - 24q^2)p^2 - (96q^4 + 30q^3)p > 88q^3p^2 - 106q^4p > 0, \\ h_7 &= 12q^4(pq-1) > 0. \end{aligned}$$

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