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Metric discrepancy results for geometric progressions with large ratios

Katusi FUKUYAMA · Mai YAMASHITA

Dedicated to Professor Norio Kôno on his 77th birthday

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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.

Mathematics Subject Classification (2000) Primary 11K38, 42A55, 60F15

1 Introduction

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

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

for all $0 \leq a < b < 1$, 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.

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

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

$$\overline{\lim}_{N \rightarrow \infty} \frac{ND_N\{U_k\}}{\sqrt{2N \log \log N}} = \frac{1}{2}, \quad \text{a.s.}$$

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 $n_{k+1}/n_k \geq q > 1$.

$$\frac{1}{4\sqrt{2}} \leq \overline{\lim}_{N \rightarrow \infty} \frac{ND_N\{n_k x\}}{\sqrt{2N \log \log N}} \leq \frac{1}{\sqrt{2}} \left(166 + \frac{664}{q^{1/2} - 1} \right), \quad \text{a.e.}$$

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Dhompsonsa [3] proved that the limsup equals to $\frac{1}{2}$ when $\{n_k\}$ satisfies very strong gap condition $\lim_{k \rightarrow \infty} (\log(n_{k+1}/n_k))/\log \log k = \infty$. 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 $\Sigma_\theta \geq 1/2$ such that*

$$\overline{\lim}_{N \rightarrow \infty} \frac{ND_N\{\theta^k x\}}{\sqrt{2N \log \log N}} = \Sigma_\theta, \quad a.e.$$

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.

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

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, $|p| \geq 4$ 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*

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

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

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

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

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

$$|p/q| \geq 2, \quad (3)$$

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

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

and

$$\sigma_{p/q}^2(a, b) = \tilde{V}(a, b, a, b) + 2 \sum_{k=1}^{\infty} \frac{1}{(pq)^k} \tilde{V}(\langle p^k a \rangle, \langle p^k b \rangle, \langle q^k a \rangle, \langle q^k b \rangle). \quad (4)$$

Here we list general properties that we use.

$$\tilde{V}(a, b, a', b') = \tilde{V}(a', b', a, b) = -\tilde{V}(b, a, a', b') = -\tilde{V}(a, b, b', a'), \quad (5)$$

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

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

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

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

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

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 $p = q \pmod{p-q}$, we have

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

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

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

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

for odd n , and

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

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

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

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

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

and

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

where

$$\begin{aligned} W_1 &:= X_1 + Y_1, & W_2 &:= X_2 + Y_2, & W_3 &:= X_1 + T_1, \\ W_4 &:= Z + S_q + T_2, & W_5 &:= Z + S_p + T_2, & W_6 &:= Z + T_1. \end{aligned}$$

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

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

and

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

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 $\sigma^2(a) \leq W_3(a) \leq X_1(\frac{34}{81}) + \frac{1}{2520} < \frac{222}{875} = \sigma^2(c_4)$ on $[\frac{34}{81}, c_3]$. On $[c_4, \frac{33}{81}]$, we have $\langle 16a \rangle \leq \langle 81a \rangle$ and see DX_2 is decreasing and $|DY_2(a)| \leq \frac{1}{324}$. Hence we have $DW_2(a) \leq DX_2(c_4) + \frac{1}{324} < 0$ and $\sigma^2(c_4) = W_2(c_4) \geq W_2(a) \geq \sigma^2(a)$ on $[c_4, \frac{33}{81}]$. Note that $Y_2 \leq \frac{1}{90720}$. On $[\frac{33}{81}, \frac{27}{65}]$, by $\langle 16a \rangle \geq \langle 81a \rangle$ we see that X_2 equals to a quadratic function having axis at $\frac{881}{2160}$. Hence $\sigma^2(a) \leq X_2(\frac{881}{2160}) + \frac{1}{90720} < \sigma^2(c_4)$. On $[\frac{27}{65}, \frac{34}{81}]$, by $\langle 16a \rangle < \langle 81a \rangle$, X_2 is decreasing. Hence $\sigma^2(a) \leq X_2(\frac{27}{65}) + \frac{1}{90720} < \sigma^2(c_4)$ 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 $W_3(a) \leq W_3(a_1)$. 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 $p/q \geq 9/4$. Put $\hat{A}_2(p, q) = (8q^2 - 6)p^2 + (-16q^3 + 4q)p - q^4$. We see

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

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

3.3 $[0, c_1)$ part

We consider on $[0, c_1)$. We assume $q \geq 4$, 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

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

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 $\langle q^2a \rangle = q^2a - q(q-2)/2 + 1$. 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

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

we have the third equality. The rest is proved by

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

by noting

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

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

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

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

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

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

$$\begin{aligned} & -4p^6 + (36q^3 + 4q^2 + 8q + 16)p^5 - 79q^4p^4 + 16q^5p^3 \geq (36q^3 - 2q^2)p^5 - 79q^4p^4 + 16q^5p^3 \\ & \geq \frac{71}{2}q^3p^5 - 79q^4p^4 + 16q^5p^3 = \frac{1}{2}\left(\frac{p}{q} - 2\right)\left(71\frac{p}{q} - 16\right) \geq 0, \\ & (16q^3 - 40q^2 - 20q - 16)p^4 \geq (16 - 10 - 5/4 - 1/4)q^3p^4 > 0, \\ & (12q^5 - 44q^4)p^3 \geq (12 - 11)q^5p^3 > 0, \quad 16q^5p^3 - 16q^6p^2 > 0, \quad (24q^5 + 52q^3 - 8q^2)p^2 > 0, \\ & (79q^3 - 8q^2 - 2q)p^3 - 44q^4p^2 \geq (79 - 2 - 1/8)q^3p^3 - 44q^4p^2 > 0, \\ & (16q^5 - 40q^4 - 10q^3)p - 4q^4 \geq (16 - 10 - 5/8)q^5p - 4q^4 > 0. \end{aligned}$$

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

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

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

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

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 $[c_2 - 1/p, c_2)$,

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

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

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

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

$$-2p^3 + (8q+2)p^2 + 3q^2p \leq -2p^3 + 9qp^2 + 3q^2p = pq^2 \left(-2\left(\frac{p}{q}\right)^2 + 9\left(\frac{p}{q}\right) + 3 \right) < 0$$

by $\frac{p}{q} \geq 7$ if $q \geq 4$. 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 $p \geq 9$. Hence we see the second inequality of

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

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

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

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

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

4 Even p and odd q

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

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

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

on $[c_6, c_4)$, and

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

on $[c_4, 1/2)$. Hence $W_1(a) \leq W_1(c_4) = \sigma^2(c_4)$ 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

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

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

$$(U - W_4(c_5))(4p^2 q^2 (p - q)^2 (pq - 1)) = p(p - 2q)(p(pq - 1)(p + 2q) + 4q + 2) + 4(q - 2)p^2 + 2(2p^2 - q^2) > 0.$$

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

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

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

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

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

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

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

$$\begin{aligned} h_1 &= (3q^2 - 2)(p + 2q)p^2 q^3 \left(6 \left(\frac{p}{q} \right)^3 - 16 \left(\frac{p}{q} \right)^2 + 7 \left(\frac{p}{q} \right) - 2 \right) \geq 0 \quad \text{if } \frac{p}{q} \geq a_9, \\ h_2 &= (24q^2 - 2q)p^5 - 50q^2 p^4 - 72q^4 p^3 + 48q^5 p^2 \geq q^5 p^2 \left(\frac{70}{3} \left(\frac{p}{q} \right)^3 - \frac{50}{3} \left(\frac{p}{q} \right)^2 - 72 \left(\frac{p}{q} \right) + 48 \right) > 0 \end{aligned}$$

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

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

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