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WHICH RATIONALS ARE RATIOS OF PISOT SEQUENCES?

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Dedicated to the memory of Robert Arnold Smith

ABSTRACT. A Pisot sequence is a sequence of integers defined recursively by the formula $-a_n/2 < a_{n+2}a_n - a_{n+1}^2 \leq a_n/2$. If $0 < a_0 < a_1$ then a_{n+1}/a_n converges to a limit θ. We ask whether any rational p/q other than an integer can ever occur as such a limit. For $p/q > q/2$, the answer is no. However, if $p/q < q/2$ then the question is shown to be equivalent to a stopping time problem related to the notorious $3x + 1$ problem and to a question of Mahler concerning the powers of 3/2. Although some interesting statistical properties of these stopping time problems can be established, we are forced to conclude that the question raised in the title of this paper is perhaps more intractable than it might appear.

1. **Introduction**. If x is a real number, let $N(x) = [x + \frac{1}{2}]$ denote the "nearest" integer to x. Given integers $0 < a_0 < a_1$, define the *Pisot sequence* $E(a_0, a_1)$ by $a_{n+2} = N(a_{n+1}^2/a_n)$. Pisot [11] showed that a_{n+1}/a_n converges to a limit $\theta \geq 1$ and if $\theta > 1$ then a_n/θ^n converges to $\lambda > 0$. Furthermore, if $\epsilon_n = a_n - \lambda\theta^n$, then

$$\limsup |\epsilon_n| \leq \frac{1}{2(\theta - 1)^2}. \tag{1}$$

We call θ the *ratio* of $E(a_0, a_1)$. The set E of such θ is countable and dense in $[1, \infty)$.

If $\theta > 1$ is the root of a polynomial $P(x) = x^d + c_1x^{d-1} + \ldots + c_d$ with integer coefficients, all of whose other roots lie in the unit circle then θ is in E [5]. Such θ form the set of Pisot and Salem numbers.

In [1], we conjectured that no other algebraic numbers lie in E. In particular, this conjecture would imply that the only rationals in E are the integers.

A result of [2] implies that if $p/q > q/2$ then p/q is not in E unless p/q is an integer. This also follows from Theorem 1 of this paper. Thus, for example, 3/2 is not in E.

To illustrate the situation if $p/q < q/2$, consider $\theta = 4/3$. For any integer $a_0 > 1$, define a sequence $\{a_n\}$ by $a_{n+1} = N(\theta a_n)$. That is, $\{a_n\}$ is defined by iterating the mapping $3m \to 4m$, $3m \pm 1 \to 4m \pm 1$. Then 4/3 is in E if and only if there is an $a_0 > 1$ so that in the sequence $\{a_n\}$ no two consecutive terms are congruent modulo 3 to either $(1, -1)$ or $(-1, 1)$.

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We believe that no such a_0 exists. However, Lemma 1 shows that, given any finite sequence $(e_0, \ldots, e_{k-1})$ with e_i in $\{-1, 0, 1\}$, there is a unique a_0 in $[1, 3^k]$ with $(a_0, \ldots, a_{k-1}) \equiv (e_0, \ldots, e_{k-1}) (\mathrm{mod}\ 3)$. Thus no finite set of congruence conditions can ever suffice to exclude all a_0 from consideration.

The situation is similar to that described by Mahler [10] who asked whether there is a real number $\lambda > 0$ so that the fractional parts of $\lambda(3/2)^n$ lie in $[0, 1/2]$ for all n. Our problem can be formulated in terms of $\lambda(p/q)^n$, but note that (1) implies no restriction on the fractional part of $\lambda(p/q)^n$ if $p/q < 2$. Mahler's problem leads to the iteration of the mapping $n \to [3n/2]$, i.e. $2m \to 3m$ and $2m + 1 \to 3m + 1$.

One is also reminded of the "$3x + 1$ problem" which asks about the ultimate periodicity of the mapping $2m \to m$, $2m + 1 \to 3m + 2$. Lagarias [9] discusses this and related questions. He points out the importance of the observation of Terras [12] and Everett [4] which is the analogue of our Lemma 1 for the $3x + 1$ mapping. Terras [12] has established the existence of a limiting asymptotic density for a stopping time problem associated with the $3x + 1$ problem. In our case the situation is somewhat simpler and we are able to show that the limiting distribution of our stopping time is the absorption time distribution for a certain finite transient Markov chain.

2. **A reformulation of the problem**. Throughout the paper, let $\theta = p/q$ with p and q relatively prime and $p > q > 1$. We say that $\{a_n\}$ is *eventually* a Pisot sequence if

$$- a_n/2 < a_{n+2}a_n - a_{n+1}^2 \leq a_n/2 \tag{2}$$

holds for sufficiently large n.

THEOREM 1. *Let $\{a_n\}$ be a sequence of positive integers. Define $d_n = qa_{n+1} - pa_n$. Then $\{a_n\}$ is eventually a Pisot sequence with ratio $\theta = p/q$ if and only if, for all sufficiently large n, the following hold:*

$$a_n > \frac{1}{2(\theta - 1)^2} \tag{3}$$

$$-q/2 < d_{n+1} - \theta d_n \leq q/2 \tag{4}$$

$$-b \leq d_n < b, \tag{5}$$

where $b = (q - 2)/(2(\theta - 1))$.

PROOF. The definition of d_n can be written as

$$a_{n+1} = \theta a_n + d_n/q \tag{6}$$

Using (6), we obtain the identity

$$q^2(a_{n+2}a_n - a_{n+1}^2) = a_n(q(d_{n+1} - \theta d_n) - d_n^2/a_n) \tag{7}$$

Now suppose that $\{a_n\}$ is a Pisot sequence with ratio θ. Then a_n is unbounded so (3) is obvious. By (1), d_n is a bounded sequence of integers and (2) and (7) show that

$$-q^2 < 2q(d_{n+1} - \theta d_n) - 2d_n^2/a_n \leq q^2. \tag{8}$$

In (8), all terms are integers except for $2d_n^2/a_n$ which is a null sequence of rationals. Hence (4) follows.

To prove (5), assume that (4) holds and that $d_n \geq b$. Then $d_{n+1} > \theta d_n - q/2 \geq d_n - 1$. Since these are integers, this shows $d_{n+1} \geq d_n$ and hence by induction that $\{d_n\}$ is eventually increasing. Since $\{d_n\}$ is bounded it must be eventually constant. But then a_n satisfies the difference equation $(qa_{n+2} - pa_{n+1}) - (qa_{n+1} - pa_n) = 0$ so $a_n = A\theta^n + B$ for certain constants $A \neq 0$ and B. Since θ is not an integer, a_n cannot be always an integer which is a contradiction. A similar argument rules out $d_n < -b$, establishing (5).

For the converse assume (3) through (5). Then by (3), (4) and (6), $a_{n+1} \geq a_n\theta - b/q > a_n$ so $\{a_n\}$ is strictly increasing hence unbounded. Since $q(d_{n+1} - \theta d_n)$ is an integer, (4) implies that

$$-(q^2 - 1)/2 \leq q(d_{n+1} - \theta d_n) \leq q^2/2. \tag{9}$$

Since d_n^2/a_n is a null sequence, eventually $0 \leq d_n^2/a_n < 1/2$ and then (7) and (9) imply (2). So $\{a_n\}$ is eventually a Pisot sequence, and $a_{n+1}/a_n \to \theta$ by (5) and (6).

COROLLARY 1. *If $\theta = p/q > q/2$ and θ is not an integer then θ is not the ratio of a Pisot sequence.*

PROOF. If $q = 2$ then $b = 0$ so (5) has no solutions. Hence $p/2$ is ruled out for all odd p. If $q > 2$ but $p/q > q/2$ then $b < 1$. If $\{a_n\}$ is a Pisot sequence with ratio θ then (5) shows that $d_n = 0$ eventually, but then $a_n = A\theta^n$ eventually, which is not possible as in the proof of the Theorem.

3. **A stopping time problem**. Fix $\theta = p/q < q/2$ with $q > 2$. Given any integer a_0, choose some $d_0 \equiv -pa_0 \pmod q$. Then for $n \geq 0$, define

$$a_{n+1} = (pa_n + d_n)/q \tag{10}$$

and

$$d_{n+1} \equiv -pa_{n+1} \pmod q, \tag{11}$$

where d_{n+1} is chosen to satisfy (4). Note that d_{n+1} is uniquely determined by (4) and (11). Thus, any pair (a_0, d_0) with $d_0 \equiv -pa_0 \pmod q$ determines a sequence of integers $D(a_0, d_0) = (d_0, d_1, \ldots)$ satisfying the *transition rule* (4). We call $D(a_0, d_0)$ the *orbit* of (a_0, d_0) under p/q.

Let $J = [-b, b)$. It follows easily from Theorem 1 that θ is in E if and only if there is an $a_0 > 1/(2(\theta - 1)^2)$ and a d_0 so that the complete orbit $D(a_0, d_0)$ lies in J

For each (a_0, d_0), define the stopping time

$$t(a_0, d_0) = \min\{n : d_n \in J\}. \tag{12}$$

Then $0 \leq t(a_0, d_0) \leq \infty$ and $p/q \in E$ if and only if $t(a_0, d_0) = \infty$ for some pair (a_0, d_0). We shall prove that there are almost no such pairs.

For example, if $p/q = 5/4$ then $J = [-4, 4)$. To insure $t(a_0, d_0) > 0$ we choose $d_0 \in J$ so there are two such choices for each a_0. For example, if $a_0 = 15$ then

$D(15,1) = (1,1,0,2,2,4,7,\ldots)$ and $t(15,1) = 5$. The choice $d_0 = -3$ gives $D(15,-3) = (-3,-2,-2,-3,-5,-8,-8,\ldots)$ so $t(15,-3) = 4$. For $\theta = 5/4$, the maximum stopping time for $a_0 \leq 1000$ is $t(51,1) = 24$.

REMARK. *If the interval J contains at most q integers, as it will when $p/q \geq 2 - 1/(q-1)$, then we can define a different set of sequences $\{d_n\}$ by iterating the mapping $x \to N(\theta x)$, as we mentioned in the introduction. Thus, given a_0, we form $a_{n+1} = N(\theta a_n)$ and then define $d_n \equiv -pa_n \pmod q$ with $-q/2 \leq d_n < q/2$, say. Then p/q is in E if and only if there is an $a_0 > 1/(2(\theta - 1)^2)$ such that* (4) *and* (5) *hold for all n. Although this brings out more obviously the relation to Mahler's problem and the $3x+1$ problem it does not seem as natural here since it fails if J contains more than q integers. Furthermore, if $d_0 \in J$ and $k \leq t(a_0, d_0)$, then the same initial segments $(a_0, \ldots, a_{k-1})$ and $(d_0, \ldots, d_{k-1})$ are generated by either process so the stopping time is the same in either case.*

4. **A Markov chain on the integers**. Consider a Markov chain with state space the integers and the transition from $i \to j$ permitted if and only if

$$-q/2 < j - \theta i \leq q/2. \tag{13}$$

If $c = q/(2(\theta - 1))$, then for each state outside of $[-c, c)$, each successor j satisfies $|j| > |i|$ and $\operatorname{sgn} j = \operatorname{sgn} i$ so all paths through i tend to $\pm\infty$. If $b = (q-2)/(2(\theta - 1))$ and if i is in $[-c, c)$ but not in $[-b, b)$ then each successor satisfies $|j| \geq |i|$ and $\operatorname{sgn} j = \operatorname{sgn} i$ so the only bounded paths through i are constant. Finally, if i is in $J = [-b, b)$ then there are paths which leave i and eventually return to i.

Consider the above chain restricted to J. If there are s integers in J then the transition matrix A has $a_{ij} = 1$ iff $i, j \in J$ and (13) holds. The choice of J means that A dominates the tridiagonal matrix B with $b_{ij} = 1$ iff $|i - j| \leq 1$. Since B^k is strictly positive for some k, so is A^k, and hence Perron's theorem, ([6], Chapter 13) shows that A has a strictly dominant positive eigenvalue $r(A)$. Furthermore $r(A) < q$ since all row sums of A are at most q with some strictly less than q.

If N_k denotes the number of paths $(d_0, \ldots, d_k)$ in the chain with $d_n \in J$ for all $n \leq k$, then $N_k = e^{\mathrm{tr}} A^k e$ where e is the vector with all entries 1, ([7], p. 991). Thus $N_k = 0(r(A)^k)$.

Now introduce the transition probabilities $\Pr\{i \to j\} = 1/q$ if (13) holds. Then each state is transient. For, by the above discussion, if a path leaves J it never returns. Furthermore, the probability of a path staying in J forever is $\lim (N_k/sq^k) = 0$. More precisely, if we define the absorption time distribution by

$$P(k) = \Pr\{\text{a path starting in } J \text{ first leaves } J \text{ at time } k\}. \tag{14}$$

Then

$$P(k) = p_0^{\mathrm{tr}} Q^k (I - Q) p_0, \tag{15}$$

where $p_0 = s^{-1} e$ and $Q = q^{-1} A$. Clearly

(16) $$\sum_{k=0}^{\infty} P(k) = 1.$$

This follows from $r(Q) = r(A)/q < 1$, ([8], Chapter 5).

The matrix Q defines a finite transient Markov chain and $P(k)$ is its absorption time distribution.

5. **The coding lemma**. The connection between the sequences of section 3 and the paths of the Markov chain of section 4 is given by the following simple lemma which is modeled on a result of Terras [12] and Everett [4] for the $3x + 1$ problem. If $D(a_0, d_0) = \{d_n\}$ is the orbit of (a_0, d_0) under p/q, we define

(17) $$D_k(a_0, d_0) = (d_0, d_1, \ldots, d_{k-1}).$$

LEMMA 1. *Let $(d_0, \ldots, d_{k-1})$ be any sequence satisfying* (4) *for all $n \leq k - 1$. Then there is a unique $a_0 \in [0, q^k - 1]$ such that $D_k(a_0, d_0) = (d_0, \ldots, d_{k-1})$. Furthermore, each b_0 for which $D_k(b_0, d_0) = D_k(a_0, d_0)$ is congruent modulo q^k* to a_0.

PROOF. Suppose that $D_k(a_0, d_0) = D_k(b_0, d_0)$. Iterating (6), we find that

(18) $$a_k = \theta^k a_0 + (\theta^{k-1} d_0 + \ldots + d_{k-1})/q,$$

and since this also holds for b_0, b_k we have $q^k a_k - p^k a_0 = q^k b_k - p^k b_0$. This shows that $a_0 \equiv b_0 \pmod{q^k}$. Thus, given $(d_0, \ldots, d_{k-1})$, there is at most one $a_0 \in [0, q^k - 1]$ with $D_k(a_0, d_0) = (d_0, \ldots, d_{k-1})$ so the map $(a_0, d_0) \to D_k(a_0, d_0)$ is one-one. Fixing d_0, there are q^{k-1} values of $a_0 \in [0, q^k - 1]$ with $-pa_0 \equiv d_0 \pmod q$ and the same number of sequences $(d_0, \ldots, d_{k-1})$ with first entry d_0 satisfying (3). Thus the map $(a_0, d_0) \to D_k(a_0, d_0)$ is onto and this completes the proof.

REMARKS. 1. *It is easy to give an inductive construction of the a_0 in Lemma 1.*

2. *We can extend the definition of $D(a_0, d_0)$ to allow a_0 to be a q-adic integer, $a_0 = \sum_{n=0}^{\infty} e_k q^k$ with $a \leq e_k \leq q - 1$. Simply reinterpret the formulas* (10) *and* (11). *Having done this, Lemma 1 shows that each path $\{d_n\}$ in the Markov chain with transition rule* (4) *is $D(a_0, d_0)$ for a unique q-adic integer a_0. To expand on this remark, one can imitate many of the results of Lagarias* [9] on the $3x + 1$ *mapping. An interesting difference between our maps and that one is that periodic orbits cannot occur here for integer $a_0 > 1/(2(\theta - 1)^2)$ whereas they are conjectured to be the general rule for the $3x + 1$ problem.*

THEOREM 2. *Let $N(x)$ denote the number of integers $a_0 \leq x$ which can be the initial term of a Pisot sequence with ratio p/q. Then $N(x) = 0(x^\alpha)$ where $\alpha = \log r(A)/\log q < 1$. In particular, the set of such a_0 has density zero.*

PROOF. Let k satisfy $q^k < x \leq q^{k+1}$. There are N_k sequences $(d_0, \ldots, d_k)$ satisfying (4) and (5) for $n \leq k$. Thus, by Lemma 1, there are at most N_k values of $a_0 \leq x$ with $D(a_0, d_0)$ lying in J. Hence

$$N(x) \leq N_k = 0(r(A)^k) = 0(q^{\alpha k}) = 0(x^\alpha).$$

THEOREM 3. *Let $\theta = p/q < q/2$ be fixed and let $t(a_0, d_0)$ be the stopping time defined in* (12). *Given x, let S_x be the set of pairs (a_0, d_0) with $a_0 \leq x$, d_0 in J and $d_0 \equiv -pa_0 \pmod q$. Let T_k be the set of pairs (a_0, d_0) with $t(a_0, d_0) = k$. Then*

$$\lim_{x \to \infty} \frac{\operatorname{card}(S_x \cap T_k)}{\operatorname{card}(S_x)} = P(k), \tag{19}$$

where $P(k)$ is defined by (14).

PROOF. In view of Lemma 1, the result is almost obvious. We point out only that, for fixed k and d_0 in J, the set of a_0 with $t(a_0, d_0) = k$ forms a set of congruence classes modulo q^k. If x is a multiple of q^k then the ratio in the left member of (19) is exactly $P(k)$, and when x lies between two multiples of q^k the difference is $0(x^{-1})$.

EXAMPLE. *If $\theta = 4/3$ then $J \cap \mathbb{Z} = \{-1, 0, 1\}$. We write $t(a_0) = t(a_0, d_0)$ for the unique choice of d_0 in J. The matrix A is*

$$A = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}$$

with $r(A) = 1 + \sqrt{2}$. We find that $P(k) = M_k/3^{k+1}$ where $M_0 = 0$, $M_1 = 2$ and $M_k = 2M_{k-1} + M_{k-2}$ so the distribution $P(k)$ is easily computed.

Experiments with blocks of a_0 in $[2, 100000]$ show close agreement with the theoretical distribution. The maximum of $t(a_0)$ in this range is $t(13958) = 51$. In a random sample of 100000 integers, the expected value of max $t(a_0)$ is about 56.02 so from this point of view, $t(13958)$ is not unusually large.

6. **Conclusions**. A single integer a_0 with $t(a_0, d_0) = \infty$ would suffice to show that p/q is in E. Thus the results of section 5 do not really have much to say about this question except that it may be difficult to find such an a_0. Indeed, it is hard to imagine how one would prove that $t(a_0, d_0) = \infty$ even if one were presented with the appropriate pair (a_0, d_0). In this vein, Conway [3] (see also [9]) has shown that some very similar iteration problems are recursively undecidable.

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