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Structure of the Markoff spectrum below $\sqrt{12}$

by

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Introduction. This work is a sequel to [1] and we refer there for all notation (except that we have adopted the more usual English spelling of Markoff's name). Computations were performed using the APL workspace described there, slightly updated and with some new functions added. In Section 3 of [1] we gave some results based on an algorithm for determining the extreme values of $M(A)$ for certain restrictions on the finite strings which can occur in the double-ended sequence A. The algorithm has its roots in the work of Perron [7], Satz 5, but our version appears much stronger than previous versions (cf. Cusick [3]). In this paper we will use this method to give a systematic study of the portion of the spectrum defined by sequences of 1's and 2's, i.e. the portion below $\sqrt{12}$. A subsequent paper will apply these methods in the vicinity of $\sqrt{21}$ in order to obtain an independent verification of the results of Schecker [10] that the spectrum contains all numbers greater than $\sqrt{21} = 4.58258$ and has a gap which is a neighborhood of 4.52172.

The authors's work in this area overlaps with recent work of Berstein and Freiman (see [11]). In particular, Berstein [11], Section 2.9, summarizes a computation of the division of the spectrum given here. He does not go into much detail about the determination of the optimizing sequences or the computation of numerical values, and we have noticed discrepancies in both types of result between his work and ours. An extension of the methods described here to a completely algorithmic procedure for determining the structure of the spectrum would make such results more reliable.

Foundations. The following result allows us to deal exclusively with the case in which the supremum $M(A)$ is attained.

Proposition 1 (cf. [5], Theorem 2.2; [4], Lemma 3). *If* $M(A) = a < \infty$, *then there is a sequence* A^* *such that*

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(i) *every finite substring of* A^* *occurs in* A;
(ii) $M(A^*) = M_0(A^*) = a$.

Proof. Clearly (i) implies that $M(A^*) \leqslant a$, so we need only assure that $M_0(A^*) = a$ and (i). If $M_k(A) = a$ for some k, then $A_n^* = A_{n+k}$ does the job. Otherwise, we construct a sequence $i_1, i_2, \ldots$ such that $M_{i_k}(A) \to a$. The finiteness of a gives the fact that the a_k are bounded. Hence, there are only finitely many values for a_{i_k}, and one must occur infinitely often. Let this be a_0^* and replace $i_1, i_2, \ldots$ by a subsequence for which a_i is constant. Continue in a similar fashion determining, in order, $a_{-1}^*, a_1^*, a_{-2}^*, a_2^*, \ldots$ This sequence clearly has the required properties.

Given a finite string $\langle b_i\colon i_0 \leqslant i \leqslant i_1\rangle$ with $i_0 \leqslant 0 \leqslant i_1$ we associate the collection of all A for which $a_i = b_i$ for $i_0 \leqslant i \leqslant i_1$ and for which $M(A) = M_0(A)$. The set of values of $M(A)$ for all such A will be said to be associated with the string $\langle b_{i_0}, \ldots, b_{i_1}\rangle$. Our plan is to systematically generate strings and to compute the extreme values of the associated subsets of the Markoff spectrum. In denoting strings we will omit all punctuation except that we will delimit b_0 by periods. Also, we shall not distinguish a string from its reverse. Thus, the set associated with $\langle .2. \rangle$ is initially partitioned into those associated with $\langle 1.2.1\rangle$, $\langle 1.2.2\rangle$, and $\langle 2.2.2\rangle$.

Perron's results are consequences of

Proposition 2. *Suppose* $a_i = a_{n-i}$ *for* $i = 1, \ldots, n-1$ *and let*

$$x = [A_0^-], \quad y = [A_n^+], \quad f(x) = [0, a_1, \ldots, a_{n-1}, x].$$

If $x \geqslant y$, *then*
(i) n *odd implies* $M_n(A) \leqslant y + f(y) \leqslant x + f(x) \leqslant M_0(A)$;
(ii) n *even implies* $y + f(y) \leqslant M_n(A) \leqslant M_0(A) \leqslant x + f(x)$.
Conversely, $M_n(A) \leqslant M_0(A)$ *implies* $x \geqslant y$.

Proof. Write $f(x)$ in the form $(ax+b) \div (cx+d)$ with a, b, c, d non-negative integers and $ad - bc = (-1)^n$ (Perron [8], § 6). Then $f'(x) = (-1)^n (cx+d)^{-2}$. Thus $|f'(x)| \leqslant 1$ for $x \geqslant 1$. Since $M_0(A) = x + f(y)$ and $M_n(A) = y + f(x)$, (i) would follow from $x + f(x)$ being an increasing function, and (ii) from $x - f(x)$ being increasing. Both of these follow from $|f'(x)| < 1$. The converse is similar to (ii).

Corollary (Perron [7], Satz 5). *If* A *contains the string* $\langle a_0, \ldots, a_{2i}\rangle$ *then* $M(A) \geqslant a + 1 \div a$, *where* a *is the number represented by the periodic continued fraction* $[\overline{a_0, \ldots, a_{2i}}]$.

Proof. Applying the proposition with $n = 1$, gives $M(A) \geqslant x + 1 \div x$ for any $x = [A_k^+]$ or $[A_k^-]$ in A. Now, since the given string has odd length, one of $\{x, [a_0, \ldots, a_{2i}, x]\}$ is always at least equal to a.

Examples. 1. *If* A *contains* $\langle N\rangle$, $M(A) \geqslant [\overline{N}] + 1 \div [\overline{N}] = M(\overline{N})$.

Hence $\langle \overline{N}\rangle$ is a sequence representing the minimum value of $M(A)$ for all A containing $\langle N\rangle$.

2. *The set associated with* $\langle 2.2.2\rangle$ *consists only of* $M(\overline{2})$. Write A as $\langle x2.2.2y\rangle$, then $M_0(A) \geqslant M_2(A)$ implies $y \leqslant [22x]$ and $M_0(A) \geqslant M_{-2}(A)$ implies $x \leqslant [22y]$. Thus $x \leqslant [\overline{2}]$ and $M(A) = M_0(A) \leqslant [\overline{2}] + [02, [\overline{2}]] = M(\overline{2})$. But example 1 shows $M(A) \geqslant M(\overline{2})$. This is typical of the calculation of the largest value of $M(A)$ associated with a string in those cases in which the maximum value is given by a periodic sequence ($\langle 1.2.2\rangle$, $\langle 11.2.12\rangle$, $\langle 11.2.11\rangle$, $\langle 22.2.11\rangle$, but not $\langle 12.2.12\rangle$). After showing that the maximum for $\langle 12.2.11\rangle$ contains $\langle 211222112.2.111\rangle$, this too is covered by Proposition 2. Note that (ii) gives an upper bound on the maximum value associated with a string and (i) gives a lower bound on the minimum. This may also be used in the other direction; if the maximum $M(A)$ is known to exceed m_0, then (ii) gives a lower bound on x for the maximizing sequence. Similarly (i) gives upper bounds on x for minimizing sequences.

3. *Minimum* 1.2.1. Let $x = [A_0^+]$, $y = [A_0^-]$. Then $x \geqslant y$ implies that $2x - 2 \geqslant M_0(A) \geqslant 2y - 2$. Thus, $M_0(A) \leqslant M_0(\overline{1}2\overline{1})$ implies that $y \leqslant [2\overline{1}]$. We then have $y = [211v]$, which is a decreasing function of v. $M_{-3}(A) \leqslant M_0(A)$ says $v \leqslant x$, and $x \geqslant y$ says $x \geqslant [211v]$. It follows that:

$v < [\overline{211}]$ implies $M(A) \geqslant 2[211v] - 2$, a decreasing function of v;
$v > [\overline{211}]$ implies $M(A) \geqslant v + [011v]$, an increasing function of v.
Thus $x = v = [\overline{211}]$ must provide the smallest value.

Actually, this argument could be made to show that any occurrence of $\langle 121\rangle$ in A forces $M(A) \geqslant M(\overline{211})$. This sort of result allows us to exclude certain strings in some computations (cf. example 5).

A new result. The significance of the method used here is that it allows one to *synthesize* the solution of an extremum problem. At each stage it is clear what restrictions are needed on the a_i that remain to be chosen. The full implementation of this depends on being able to express $M_n(A) \leqslant M_0(A)$ in all cases. This is accomplished by

Proposition 3. *Take* $[A_0^-] = x$, $[A_n^+] = y$ *and define* a, b, c, d *by*

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a_1 & 1 \\ 1 & 0 \end{pmatrix} \cdots \begin{pmatrix} a_{n-1} & 1 \\ 1 & 0 \end{pmatrix}.$$

Then, if $x - y \geqslant e = (b-c) \div a$ *and denoting* $f(x) = (cx+d) \div (ax+b)$, $g(x) = (bx+d) \div (ax+c)$ *we have*
(i) *for* n *odd*: $M_0(A) \geqslant x + f(x-e) \geqslant y + g(y+e) \geqslant M_n(A)$,
(ii) *for* n *even*: $x + f(x-e) \geqslant M_0(A) \geqslant M_n(A) \geqslant y + g(y+e)$.
Conversely, $M_0(A) \geqslant M_n(A)$ *implies* $x \geqslant y + e$.

Proof. The outer inequalities follow directly from $M_0(A) = x + f(y)$

and $M_n(A) = y+g(x)$. The remaining inequality in (i) follows from writing it in the form

$$ax+c+(ad-bc)\div(ax+c) \geqslant ay+b+(ad-bc)\div(ay+b)$$

and applying the fact that $z+1\div z$ is increasing for positive z to $(ax+c) \geqslant (ay+b)$. The middle inequality in (ii) also reduces to $z+1\div z$ being increasing. The symmetry induced by $a_i \to a_{n-i}$ interchanges the following pairs: $(M_0(A), M_n(A))$, (x, y), (b, c), (f, g). Thus $y-x \geqslant -e$ implies $M_n(A) \geqslant M_0(A)$; whence the converse.

COROLLARY. *If $M_0(A) \geqslant \mu$, then $ax+c \geqslant .5\big(a\mu+\sqrt{(a^2\mu^2+4)}\big)$ for n even.*

If $M_0(A) \leqslant \mu$, then $ax+c \leqslant .5\big(a\mu+\sqrt{(a^2\mu^2-4)}\big)$ for n odd.

Proposition 3 leads to the question of generating the continued fraction of $(qx+p)\div q$ from that of x. This is a special case of the general problem of relating the continued fractions of x and $(ax+b)\div(cx+d)$. This has received a fair amount of attention recently [2], [6], [9]. Our workspace contains a crude function for generating the continued fraction of a fractional linear transform of a number given by a continued fraction. A 2×2 matrix is considered to be reduced if the difference of its rows contains a positive and a negative number. Reduced matrices with positive entries represent transformations which take $(0, \infty)$ into itself with 1ϵ range. An arbitrary matrix with non-negative entries may be reduced by removing factors of $\begin{pmatrix} d & 1 \\ 1 & 0 \end{pmatrix}$ or $\begin{pmatrix} 1 & 0 \\ d & 1 \end{pmatrix}$ from the left. In the former case, d becomes a new term in the output list; in the latter case, d is added to the last term. The terms a of the input list give rise to factors $\begin{pmatrix} a & 1 \\ 1 & 0 \end{pmatrix}$ which are right multipliers of the matrix. In this procedure, the last term of the output list has the possibility of being too small, and special properties of the input list are not used. However, it seems adequate for its applications.

EXAMPLE 4. *Consider the maximum associated with* $\langle 12.2.11\rangle$. Since $[A_{-1}^-] \leqslant [A_0^+]$, the maximum must have the form $\langle y112.x\rangle$ and, by Proposition 3, $y \leqslant x-1\div 5$. $M_0(A)$ is an increasing function of both x and y. We tentatively choose each as large as possible when calculating the restriction on the other. Each possible $M_0(A)$ will give a lower bound on x or y via various applications of Proposition 3. Thus, our tentative choices may be shown to be essential after they have led to a possible optimum.

(step 1) — We take $x = [2111u]$. Then $u \leqslant [2211y]$ and $y \leqslant \big[22, \big((7u+3)\div(u+4)\big)\big]$.

(step 2) — Trying $y = [22v]$ gives $v \leqslant x-1\div 31 = \big[211, \big((34u+33)\div(25u-4)\big)\big]$. Finally,

(step 3) — $u = [22w]$ gives $w \leqslant [1122v]$,

$$v \leqslant \big[2112, \big((117w+46)\div(2w+9)\big)\big].$$

(step 4) — Taking $v = [2112t]$, we are now reduced to $\langle t211222112.2.111u\rangle$ which we have already noted to be covered by Proposition 2.

We now need to show, using the Corollary to Proposition 3, that our choices were forced. We now know that

$$M_0(A) \geqslant M_0(\overline{211122112222112}) = \mu = 3.017028\ldots$$

From the form $\langle y112.x\rangle$ we get $5x+2 \geqslant .5\big(5\mu+\sqrt{(25\mu^2+4)}\big)$ which requires that x exceed a continued fraction $[21112211\ldots]$ which justifies the assumptions about x in steps 1 and 3. Using the form $\langle y112.2.111u\rangle$ gives

$$[2211y] \geqslant [\overline{221122211122111}]$$

which justifies all assumptions about y.

Another tool. By [4], Lemma 4, every gap, (a, b), in the Markoff spectrum is characterized by certain strings. The strings occur in A iff $M(A) \geqslant b$. In particular, a is the largest value of $M(A)$ when these strings are excluded. It is a simple matter to construct such numbers. One begins by listing a sufficient number of $\langle a_i, \ldots, a_j\rangle$, with $j-i$ at least equal to the length of the longest excluded string, to include all strings which could belong to the maximum. Then, for each, one maximizes $[A_0^+]$ and $[A_0^-]$ independently subject to excluding the given strings. The one which gives the maximum $M_0(A)$ must have $M(A) = M_0(A)$. In our systematic study of the Markoff spectrum we are able to determine those strings which give values larger than an interval we are considering. Excluding these and finding the maximum can be done as sketched here. If we are not dealing with a gap in the spectrum, the quantity calculated in this way need not be the largest value in the set associated with the $\langle a_i \ldots a_j\rangle$ used in the calculation.

EXAMPLE 5. We take as known that $\min\langle 1.2.1\rangle > \max\langle 2.2.1\rangle$. Thus, 121 is to be excluded in any study within $\langle 2.2.1\rangle$. We partition $\langle 2.2.1\rangle$ into $\langle 22.2.12\rangle$, $\langle 12.2.12\rangle$, $\langle 22.2.11\rangle$ and $\langle 12.2.11\rangle$. We expect the first three to be larger than the fourth. *Excluding* $\langle 121\rangle\langle 22212\rangle\langle 12212\rangle\langle 22211\rangle$ *is equivalent to excluding* $\langle 121\rangle\langle 212\rangle\langle 2221\rangle$. *In* $\langle 12.2.11\rangle$ (the only remaining interval) *this determines a maximum of* $\langle\overline{2112.2.111221}\rangle$. However, the maximum $\langle 12.2.11\rangle$ was shown to be larger than this (it contained the string $\langle 2221\rangle$).

Expressions for endpoints. It follows from [4], Theorem 1, that the endpoints of the gaps in the Markoff spectrum have expressions which are the sum of two solutions of quadratic equations. The examples which we have already computed all have much stricter forms: either purely periodic or what we call "bridged symmetric", i.e. of the form

$$\langle x a_k \ldots a_1 . a_0 . b_1 \ldots b_{n-1} a_0 a_1 \ldots a_k x \rangle \quad \text{where} \quad b_i = b_{n-i}.$$

The periodic sequences give an M which is the square root of a rational quantity; the bridged symmetric give the root of a single quadratic equation. From [4] we note that periodic continued fractions correspond to local maximum values, and certain types are locally isolated. This will allow us to show that certain of our extreme values are isolated values of the spectrum (e.g. any periodic minimum).

The examples discussed so far all lead to periodic continued fractions. In those cases where the extreme value is of another form we need to compare the conditions arising from $M_n(A) \leqslant M_0(A)$ at various n.

Suppose

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}_{n+2k} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}_n \begin{pmatrix} p & q \\ r & s \end{pmatrix},$$

then

$$(b \div a)_{n+2k} - (b \div a)_n = \left(r a_n^2 + (s-p) a_n b_n - q b_n\right) \div (a_n a_{n+2k})$$

and

$$(c \div a)_{n+2k} - (c \div a)_n = q (ad - bc)_n \div (a_n a_{n+2k}).$$

If we also have

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}_n = \begin{pmatrix} a & b \\ c & d \end{pmatrix}_{n-2k} \begin{pmatrix} p & q \\ r & s \end{pmatrix},$$

then

$$\left(ra^2 + (s-p)ab - qb^2\right)_n = (ps - qr)\left(ra^2 + (s-p)ab - qb^2\right)_{n-2k}.$$

Since $ps - qr = 1$, it follows that

$$a_{n+2k}\left[\left((c-b) \div a\right)_{n+2k} - \left((c-b) \div a\right)_n\right] = a_{n-2k}\left[\left((c-b) \div a\right)_n - \left((c-b) \div a\right)_{n-2k}\right].$$

Once we have calculated two periods of length $2k$ we determine whether $\left((c-b) \div a\right)_n$ increases or decreases over a period. If it increases, it will continue to increase and the limit can be calculated in terms of the eigenvalues of $\begin{pmatrix} p & q \\ r & s \end{pmatrix}$. We can check if this allows a larger value for $[A_n^+]$. Similarly, if it decreases over one period, it will continue to decrease. Again we note whether a smaller value of (A_n^+) could ever be forced. In the decreasing case, the condition reduces to $M_0(A)$ exceeding M (periodic part). One should note that every spot in the period needs to be checked separately.

EXAMPLE 6. Max$\langle 12.2.12 \rangle$. We write in the form $\langle x.1y \rangle$. This gives $y \leqslant x$ and $M_0 \leqslant x + [01x]$. In particular any example with $y = x$ gives a lower bound on possible values of x. We try $x = 2211u$, i.e. $\langle u112.2.1y \rangle$, which gives

$$u \leqslant [21y] - 1 \div 5 = [2, (5y+5) \div (4y-1)].$$

We also have

$$5M_0 \leqslant (5[21y]+2) - 1 \div (5[21y]+2).$$

If we take $y = [22v]$, $u \leqslant [211, (17v+8) \div (v-1)]$ which says that u may not begin with 21 but any expression beginning with 22 is acceptable. Now we try $u = [22w]$, giving

$$w \leqslant [21y] - 1 \div 31 = [212, (69v+34) \div (10v-9)].$$

Thus $w = [2111t]$ will work, but nothing beginning with $[212\ldots]$ is possible. Assuming $w = [2111t]$ gives

$$t \leqslant [21y] - 10 \div 41 < [21y] - 1 \div 5.$$

If $t = [22\ldots]$ works, the next step will be

$$[21y] - 20 \div 599 < [21y] - 1 \div 31.$$

Thus, we are in the decreasing case. This requires that we check that

$$M_0(\overline{12221}12.2.122\overline{112221}) \geqslant M(\overline{211122}).$$

This is true. At the same time this justifies all choices made for x. It remains to show that we are forced to take $y = [22v]$. This follows from the lower bound on M_0 given by our sequence.

Tables. We list strings of 1's and 2's in a systematic order and determine maxima and minima associated with those strings. When the optimizing continued fraction is periodic we list the period beginning with a_0. In the bridged symmetric case $\langle x a_k \ldots a_1 . a_0 . b_1 \ldots b_{n-1} a_0 a_1 \ldots a_k x \rangle$ will be abbreviated by replacing $a_0 \ldots a_k x$ at the right by '...'. Where convenient we give the exact form of optimizing value of M. The numerical equivalent is rounded to 5 decimal places.

1a.	$\langle 1.2.1 \rangle$	max	$(\overline{21})$	$\sqrt{12}$	3.46410
b.	(ex.3)	min	$(\overline{211})$	$\sqrt{10}$	3.16228
2a.	$\langle 1.2.2 \rangle$	max	$(\overline{2122})$	$4\sqrt{30} \div 7$	3.12984
b.		min	$(\overline{2211})$	$\sqrt{221} \div 5$	2.97321
3.	$\langle 2.2.2 \rangle$ (ex.2)		$(\overline{2})$	$\sqrt{8}$	2.82843

Omitting $\{\langle N \rangle \mid N > 2\}$ leads to 1a as maximum; omitting $\langle 121 \rangle$ gives 2a; omitting $\langle 12 \rangle$ gives 3. Isolated points: 1b, 2a, 2b, 3.

Within $\langle 1.2.1 \rangle$ [3.16228, 3.46410]

4.	$\langle 21.2.12 \rangle$	min	$(\overline{21221})$	$\sqrt{290} \div 5$	3.40588
5a.	$\langle 11.2.12 \rangle$	max	$(\overline{212111})$	$\sqrt{1365} \div 11$	3.35872
b.		min	$(\overline{21121221})$	$\sqrt{689} \div 8$	3.28110
6.	$\langle 11.2.11 \rangle$	max	$(\overline{2111})$	$\sqrt{96} \div 3$	3.26599

Omitting only $\{\langle N\rangle \mid N > 2\}$ and $\langle 21212\rangle$ gives 5a. Omitting $\langle 2121\rangle$ gives 6. Isolated points 4, 5a, 5b.

Within $\langle 1.2.2\rangle$ [2.97321, 3.12984]

7.	$\langle 22.2.12\rangle$	min	$(\overline{22221221})$		3.11610
8a.	$\langle 12.2.12\rangle$(ex.6)	max	$(\overline{122211}2.2.1\ldots)$		3.09149
b.		min	$(\overline{221})$	$\sqrt{85}\div 3$	3.07318
9a.	$\langle 22.2.11\rangle$	max	$(\overline{222111})$	$\sqrt{3360}\div 19$	3.05082
b.		min	$(\overline{222211})$	$\sqrt{7565}\div 29$	2.99921
10.	$\langle 12.2.11\rangle$(ex.4)	max	$(\overline{21112211222112})$		3.01703

Note overlap of intervals 9 and 10. Omitting $\langle 121\rangle$ and $\langle 22212\rangle$ gives 8a. Omitting $\langle 121\rangle$ and $\langle 212\rangle$ gives 9a. Omitting $\langle 121\rangle$, $\langle 212\rangle$, $\langle 2221\rangle$ gives

11.	· (ex.5)		$(\overline{2112}.2.111\ldots)$	3.01688

This shows 7, 8b, 9a to be isolated. Since 9b is less than 3, it must also be isolated.

Within $\langle 2.2.11\rangle = [2.97321,\ 3.05082]$

12.	$\langle 22.2.111\rangle$	min	$(\overline{22221111})$	$\sqrt{229}\div 5$	3.02655
13.	$\langle 12.2.111\rangle$	min	$(\overline{211112})$	$\sqrt{1517}\div 13$	2.99605
14.	$\langle 22.2.112\rangle$	max	$(\overline{211221111111221122})$		3.00576
15.	$\langle 12.2.112\rangle$	max	$(\overline{2211})$	$\sqrt{221}\div 5$	2.97321

Note that these are the only endpoints not already computed. Also note that interval 15 reduces to a single points (cf. 2b). All values here are locally isolated. We have not computed far enough to determine if 14 is actually isolated in the spectrum.

Further computations have been performed without encountering any new type of behavior. All of the intervals associated with strings of the form $\langle a_{-3}a_{-2}1.2.1a_2a_3\rangle$ have been computed. The intervals $\langle 111.2.122\rangle$ and $\langle 111.2.121\rangle$ are the only ones which overlap. When the intervals $\langle a_{-4}111.2.12a_3\rangle$ are formed $\langle 2111.2.122\rangle$ is contained within $\langle 2111.2.121\rangle$, and there are no other overlaps. The largest interval which has not been partitioned is $\langle 111.2.111\rangle = [3.22490,\ 3.26599]$.

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