Numer. Math. 19, 195—205 (1972)

Ergodic Computations with Continued Fractions and Jacobi's Algorithm*

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Received March 26, 1971

Abstract. Ergodic computational aspects of the Jacobi algorithm, a generalization to two dimensions of the continued fraction algorithm, are considered. By means of such computations the entropy of the algorithm is estimated to be 3.5. An approximation to the invariant measure of the transformation associated with the algorithm is obtained. The computations are tested by application to the continued fraction algorithm for which both entropy and the invariant measure are known.

1. Introduction

Recently some work has been reported on the metric theory of n-dimensional continued fractions [7–10, 14]. Much of the value of these efforts depends on finding the density of the invariant measure for the associated shift. The only such density known is for the case $n=1$. The purpose of this paper, then, is to approximate the density of the invariant measure for the case $n=2$. In addition computations for the case $n=1$ are given to illustrate and check the method.

The basis of this work is the individual ergodic theorem. Let $(\Omega, \mathscr{B}, \mu)$ be a probability space and let T be a measurable transformation of Ω into itself. Such a T is said to be a measure preserving transformation (mpt) if $\mu(T^{-1}A)=\mu(A)$ for all $A \in \mathscr{B}$. T is said to be ergodic if $T^{-1}A=A$ implies $\mu(A)$ equals 0 or 1.

Theorem 1 (Ergodic Theorem). Let $(\Omega, \mathscr{B}, \mu)$ be a probability space with T an ergodic mpt. If g is an integrable function, then

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} g\left(T^k(\omega)\right) = \int_{\Omega} g(\omega)\, d\mu(\omega), \qquad \text{a.e. } [\mu]. \tag{1}$$

For a general discussion of these concepts, see Billingsley [1].

* Work partly performed under the auspices of the U.S. Atomic Energy Commission while one of the authors (M.S.W.) was a faculty participant of the Associated Western Universities at Los Alamos Scientific Laboratory. The work was also supported in part by NSF grant GP-28313 to M.S.W.

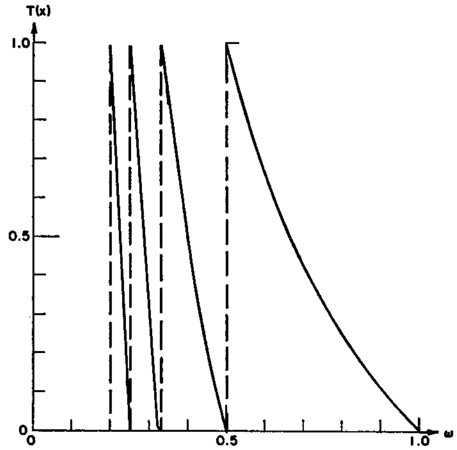

Fig. 1. Graph of the transformation $T(x) = 1/x - [1/x]$

The first transformation considered is associated with the one-dimensional continued fraction. For $x \in (0, 1)$ and [ ] denoting greatest integer, define

$$\begin{aligned} T(x) &= \frac{1}{x} - \left[\frac{1}{x}\right], \\ a_1(x) &= \left[\frac{1}{x}\right], \\ a_k(x) &= a_1\left(T^{k-1}(x)\right), \quad k \geqq 2. \end{aligned} \tag{2}$$

A graph of $T(x)$ is shown in Fig. 1. $a_1(x)$, $a_2(x)$, ... are the partial quotients in the continued fraction expansion of x. If $T^n(x) = 0$, the expansion truncates. Note that T maps (0, 1) into (0, 1). Let $\mathscr{B}$ be the Borel sets of (0, 1). It is not hard to show that T is not a mpt for Lebesgue measure λ. But with

$$\mu(A) = \frac{1}{\log 2} \int_A \frac{dx}{1+x}, \quad A \in \mathscr{B},$$

it can be shown that T is a mpt for μ and that T is ergodic for μ. Thus Theorem 1 applies. For a more complete discussion of this application see Billingsley ([1], p. 40). The measure μ or its density $\frac{d\mu}{d\lambda}(x) = \frac{1}{(\log 2)(1+x)}$ is known as the Gauss's measure. (Knuth [15] has pointed out the connection between continued fractions and Euclid's algorithm and the need for a better understanding of Euclid's algorithm, the oldest algorithm.)

The second transformation considered was introduced by Jacobi [2] and will be referred to in this paper as Jacobi's algorithm or the two-dimensional continued fraction. For $(x, y) \in (0, 1)^2$, define

$$\begin{aligned} T(x, y) &= \left(\frac{y}{x} - \left[\frac{y}{x}\right], \frac{1}{x} - \left[\frac{1}{x}\right]\right), \\ a^{(1)}(x, y) &= \left(\left[\frac{y}{x}\right], \left[\frac{1}{x}\right]\right), \\ a^{(k)}(x, y) &= a^{(1)}\left(T^{k-1}(x, y)\right), \quad k \geqq 2. \end{aligned} \tag{3}$$

The sequence of pairs of integers $a^{(1)}$, $a^{(2)}, \ldots$ are the coefficients in the two dimensional continued fraction expansion of (x, y). This expansion is obtained from the relations

$$A_k^{(n+3)} = A_k^{(n)} + a_1^{(n)} A_k^{(n+1)} + a_2^{(n)} A_k^{(n+2)}, \qquad k=0, 1, 2;\ n \geqq 0,$$

where $A_k^{(j)} = \delta_{jk}$ $(j, k = 0, 1, 2)$ and δ_{jk} is the Kronecker delta. The convergence result is:

$$x = \lim_{n\to\infty} \frac{A_1^{(n)}}{A_0^{(n)}} \quad \text{and} \quad y = \lim_{n\to\infty} \frac{A_2^{(n)}}{A_0^{(n)}}.$$

Schweiger [8, 9] has shown that there exists a unique absolutely continuous measure μ on $(0, 1)^2$ such that T is a mpt and ergodic for μ. As remarked above, the form of μ is unknown.

The main difficulty with the sort of computation undertaken in this paper is measure-theoretic. Although almost all $\omega \in \Omega$ satisfy (1), there is no known algorithm for choosing an ω satisfying (1) for a given g. For the Gauss algorithm Euler's constant γ is used, and for the Jacobi algorithm a random number generator is employed. As explained below, all transformations were done with rational arithmetic. This large integer arithmetic was carried out on the Maniac II.

2. Gauss's Measure

This section discusses the computation of an approximation to the quantity in (1) with $\Omega = (0, 1)$, $\omega = \gamma$ (Euler's constant), μ equal to Gauss's measure, and $T(\omega) = 1/\omega - [1/\omega]$. The 3561 places of γ as given by Sweeney [13] were used.

A problem which arises is to estimate the difference between

$$\frac{1}{n}\sum_{k=0}^{n-1} g(T^k x) \quad \text{and} \quad \frac{1}{n}\sum_{k=0}^{n-1} g(T^k y)$$

where y is an approximation to x. Define the cylinder of order N generated by x as

$$B_N(x) = \{y\colon a_k(y) = a_k(x),\ k = 1, \ldots, N\};$$

this cylinder is actually an interval.

Theorem 2 shows that if g is Lipshitz of order 1 one can indeed use approximates to x.

Theorem 2. Let $y \in B_N(x)$ and g satisfy $|g(t) - g(s)| \leqq C|t-s|$, where C is some fixed constant. Then

$$\left|\frac{1}{n}\sum_{k=0}^{n-1} g\left(T^k(x)\right) - \frac{1}{n}\sum_{k=0}^{n-1} g\left(T^k(y)\right)\right| \leqq \frac{C}{n} 2^{-N+n+1}, \qquad n \leqq N. \tag{4}$$

Proof. One has $\lambda\left(B_m(x)\right) \leqq 2^{-m+1}$ (see [1], p. 43). Since $y \in B_N(x)$, for $0 \leqq k \leqq N-1$, $T^k(y) \in B_{N-k}(T^k x)$, and thus

$$|T^k(y) - T^k(x)| \leqq \lambda\left(B_{N-k}(T^k(x)\right) \leqq 2^{-N+k+1}.$$

Therefore

$$\left|\frac{1}{n}\sum_{k=0}^{n-1} g(T^k x) - \frac{1}{n}\sum_{k=0}^{n-1} g(T^k y)\right| \leq \frac{C}{n}\sum_{k=0}^{n-1} |T^k(x) - T^k(y)|$$
$$\leq \frac{C\,2^{-N+1}}{n}\,\frac{2^n-1}{2-1} < \frac{C}{n}\,2^{-N+n+1}.$$

An information theory result of Rohlin [6; p. 32 of translation] gives some information about size of $B_N(x)$. Rohlin proves that the entropy of T is given by

$$h(T) = \int_0^1 \log\left|\left(\frac{1}{\omega}\right)'\right| d\mu(\omega) = \frac{\pi^2}{6\log 2} = 2.3731\ \ldots, \tag{5}$$

(where $'$ denotes differentiation) and that

$$\lim_{n\to\infty}\frac{1}{n}\log\frac{1}{\lambda(B_n(\omega))} = h(T), \qquad \text{a.e. } [\mu].$$

That is,

$$\lambda\left(B_n(\omega)\right) \sim e^{-h(T)n}, \qquad \text{a.e. } [\mu]. \tag{6}$$

It was proved by Khinchine that

$$\lim_{n\to\infty}\left(\sum_{i=1}^{n} a_i(\omega)\right)^{1/n} = K = \prod_{k=1}^{\infty}\left(1+\frac{1}{k^2+2k}\right)^{\log k/\log 2} = 2.6854\ldots, \tag{7}$$

where K is known as Khinchine's constant. This result can be deduced from Theorem 1 (see Billingsley [1; p. 45]). The computation of K in (7) has been discussed by Shanks and Wrench [11].

As a result of Theorem 2, one need only be concerned with deciding when the equation $a_i(y) = a_i(x)$ first fails, where x is the 3561 decimal digit approximation that Sweeney gives. Define x_1, x_2, so that $x_1 < y < x_2$ by subtracting and adding 1 to the last place of x. Now $1/x_2 < 1/x < 1/x_1$ and if $a_1(x_1) = a_1(x_2) = a_1$, we have $a_1 = a_1(y)$. By induction one can show $a_i(x_1) = a_i(x_2) = a_i$ implies $a_i = a_i(y)$. $a_i(x_1)$ and $a_i(x_2)$ are calculated until they differ.

The integers $a_i(x_1)$ and $a_i(x_2)$ are computed by rational arithmetic. Let $x = k/n$. It is easy to find $[1/x] = [n/k] = a_1$. Then

$$T(x) = \frac{1}{x} - \left[\frac{1}{x}\right] = \frac{n - a_1 k}{k}.$$

All $a_i(x)$ can be calculated using only $[\,\cdot\,]$ and integer multiply and subtract. It is emphasized that the expression for $T^k(x)$ as a quotient of integers is exact. When the sequence $T^k(x)$ is required, one can do a limited precision divide of the multiprecision integers. These techniques are due to Lehmer [4] and were later recommended by Shanks and Wrench [11]. Using these techniques, the first 3420 partial quotients of the continued fraction expansion of γ were found. These have been sent to the Unpublished Manuscript Tables (UMT) of the American Mathematical Society.

Two approximations connected with continued fractions were computed. First, the approximation to K gives

$$\left(\prod_{i=1}^{n} a_i(\gamma)\right)^{1/n} = 2.661277\ldots \qquad (n = 3420),$$

compared to the exact $K = 2.68$. For the second approximation, in accordance with Theorems 1 and 2 and (5), one sets $g(\omega) = \log|(1/\omega)'| = -2\log\omega$. This yielded

$$\frac{1}{3000}\sum_{k=1}^{3000} g(T^k x) = 2.351399,$$

compared to the exact $\pi^2/6\,(\log 2) = 2.37\ldots$.

It is seen from Theorem 1 and the expression for Gauss's measure that if $g(\omega) = (\log 2)(1+\omega)$,

$$\lim_{n\to\infty}\frac{1}{n}\sum_{k=0}^{n-1} g(T^k\omega) = 1 \qquad \text{a.e. } [\mu].$$

In our calculation

$$\frac{1}{3000}\sum_{k=1}^{3000} g(T^k x) = 1.000382.$$

Finally the approximation of the Gauss's measure is considered. Set

$$h(\omega) = \frac{1}{(\log 2)(1+\omega)}.$$

For a.e. ω one has

$$\lim_{n\to\infty}\frac{1}{n}\sum_{k=0}^{n-1}\chi_{[a,b]}(T^k(\omega)) = \int_a^b h(\omega)\,d\omega,$$

where $\chi_{[a,b]}$ is the characteristic function of the interval $[a, b]$. For $b-a$ small the above integral is approximately equal to $(b-a)\,h\left(\frac{a+b}{2}\right)$. This observation is used to approximate $h(\cdot)$:

$$h\left(\frac{a+b}{2}\right) \approx \frac{1}{n(b-a)}\sum_{k=0}^{n-1}\chi_{[a,b]}(T^k\omega), \qquad (n = 3000).$$

The results of the computation are summarized in Table 1 and Fig. 2. The grid selected has $b - a = 0.1$.

Table 1. The exact function $h(\omega)$ and its computed approximation given by

$$\sum_{k=0}^{3000}\chi_{[a,b]}(T^k(x))/300.$$

ω	0.05	0.15	0.25	0.35	0.45	0.55	0.65	0.75	0.85	0.95
$h(\omega)$	1.37	1.25	1.15	1.07	0.99	0.93	0.87	0.82	0.78	0.74
$\sum_{k=0}^{3000}\chi_{[a,b]}(T^k(x))/300$	1.37	1.30	1.08	1.03	1.11	0.90	0.92	0.82	0.75	0.73

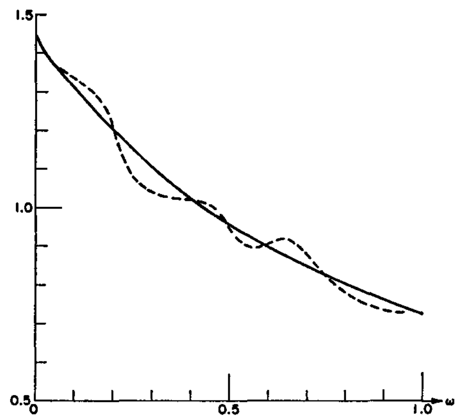

Fig. 2. Graph of the exact function $h(\omega)$ (solid) and its computed approximation (dashed)

3. Jacobi's Algorithm

In this Section the Jacobi algorithm is considered. Theorem 1 will be applied with $\Omega = (0, 1)^2$ minus an appropriate set of measure zero. $\mathscr{B}$ are the Borel subsets of Ω, and $T(x, y) = (y/x - [y/x], 1/x - [1/x])$. As was said above, the invariant measure μ is unknown and the main object is to approximate $\varrho(x, y) = d\mu/d\lambda(x, y)$ where λ is 2-dimensional Lebesgue measure.

Although Perron [5] in 1907 extended Jacobi's work, it was not until 1964 [7] that a study of the metric properties of Jacobi's algorithm was begun by Schweiger. He established that T is ergodic [8], and that there exists a unique λ-equivalent invariant measure [9]. Rohlin's formula for the entropy of T [10] is

$$h(T) = -3 \int_{(0,1)^2} \log x \ \ \varrho(x, y)\, dx\, dy \tag{8}$$

and Schweiger shows that

$$\lim_{n\to\infty} \frac{1}{n} \log \frac{1}{\lambda(B_n(x, y))} = h(T) \qquad \text{a.e. } [\mu]$$

where $B_n(x, y) = \{(u, v) : a^{(k)}(u, v) = a^{(k)}(x, y),\ k = 1, 2, \ldots, n\}$. Schweiger also shows that

$$h(T) = \lim_{n\to\infty} \frac{3}{n} \log A_0^{(n)}(\omega) \text{ for } \quad \text{a.e. } \omega. \tag{9}$$

Recently it has been proved that $\varrho(\cdot)$ satisfies a Lipshitz condition of order 1 on the set $\{(x, y) : 0 \leqq x < y\}$ and its reflection about the line $y = x$ [14].

Since the function $\sigma(n) = \sup\{\text{diam } B_n(x, y) : (x, y) \in (0, 1)^2\}$ is not known one cannot establish a theorem corresponding to Theorem 2. What is required is that for fixed n

$$\frac{1}{n} \sum_{k=0}^{n-1} \sigma(N - k - 1) \to 0 \quad \text{as} \quad N \to \infty. \tag{10}$$

Having no estimates of $\sigma(n)$, one cannot show (10).

x and y were selected by a pseudo-random number generator and the numbers are:

$$x = \frac{m}{n}, \quad y = \frac{k}{n}$$

where

$$k = \sum_{j=1}^{200} \left(5^{[2(200-j)+j]13} - [5^{[2(200-j)+1]13}/2^{43}]\right) 2^{43j}$$

$$m = \sum_{j=1}^{200} \left(5^{26(200-j)} - [5^{26(200-j)}/2^{43}]\right) 2^{43j}$$

and

$$n = 2^{8600}.$$

2589 decimal digits are required to represent k, m, and n.

The method of rational arithmetic is again used to obtain the exact values of the sequence $T^k(x, y)$. For

$$T(x, y) = \left(\frac{m}{k} - \left[\frac{m}{k}\right], \frac{n}{k} - \left[\frac{n}{k}\right]\right),$$

if one puts $a_1 = [m/k]$, $a_2 = [n/k]$, one has

$$T(x, y) = \left(\frac{m - a_1 k}{k}, \frac{n - a_2 k}{k}\right).$$

This technique can obviously be iterated to obtain $T^k(x, y)$, $k \geqq 2$.

If x and y are rational approximations to α and β, one needs something corresponding to that used to obtain the correct partial quotients for γ. The transformation $\psi(\omega, z) = (z/\omega, 1/\omega)$ takes the straight line $a\omega - bz + c = 0$ in the (ω, z) plane into the straight line $b\omega + cz + a = 0$ in the same plane. Thus if one considers a triangle containing (α, β), the image of the triangle under ψ will be a triangle containing $\psi(\alpha, \beta)$. If each corner point has the same $a^{(1)} = (a_1^{(1)}, a_2^{(1)})$ value, then $a^{(1)}(\alpha, \beta) = a^{(1)}$. This procedure is iterated to obtain $a^{(1)}(\alpha, \beta)$, $a^{(2)}(\alpha, \beta), \ldots$. By this method 3153 correct pairs of integers were found for the Jacobi expansion of the above (x, y).

An approximation to the entropy of T was found in two ways. First, by (9) the quantity:

$$h(T) \approx \frac{3}{n} \log A_0^{(n)}(\alpha, \beta) = 3.502 \ldots \qquad (n = 3156),$$

was obtained. Secondly, by analogy with Theorem 2, set $g(\alpha, \beta) = -3 \log \alpha$. The quantity

$$h(T) \approx \frac{1}{n} \sum_{k=1}^{n} g\left(T^k(x, y)\right) = 3.519 \ldots \qquad (n = 3000),$$

was obtained in this case.

It has been remarked above that $\varrho(\cdot)$ is Lipshitz order 1 except, perhaps, on the line $x = y$. To obtain an approximation of $\varrho(\cdot)$, take $R = [a, b] \times [c, d]$ to

Table 2. The approximation to $d\mu/d\lambda$ where μ is the invariant measure associated with the two-dimensional Jacobi algorithm and λ is Lebesgue measure

y \ X	0–0.1	0.1–0.2	0.2–0.3	0.3–0.4	0.4–0.5	0.5–0.6	0.6–0.7	0.7–0.8	0.8–0.9	0.9–1.0
0.9–1.0	1.13	0.83	0.80	0.57	0.57	0.73	0.80	0.90	0.93	0.63
0.8–0.9	1.00	0.80	0.97	0.50	0.50	0.67	1.03	0.63	0.40	0.60
0.7–0.8	0.73	1.07	1.17	0.80	1.00	0.93	0.53	0.50	0.53	0.63
0.6–0.7	1.23	0.90	1.20	0.87	1.30	0.77	0.67	0.90	0.60	0.83
0.5–0.6	1.23	0.93	1.40	1.23	1.13	1.17	0.83	0.57	0.87	0.63
0.4–0.5	1.27	1.23	1.33	1.47	0.83	0.63	0.77	1.00	0.67	0.57
0.3–0.4	1.53	1.33	1.20	0.77	1.07	0.93	1.00	1.10	0.97	0.67
0.2–0.3	1.70	1.67	1.70	0.80	0.90	0.77	0.90	0.67	0.77	0.90
0.1–0.2	1.73	1.33	1.43	1.20	1.20	1.10	1.47	1.23	1.03	0.83
0–0.1	2.20	1.43	1.43	1.77	1.37	1.37	1.33	1.13	1.00	1.13

be a small rectangle. Since for a.e. $(\omega, z) \in (0, 1)^2$ one has

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} \chi_R\left(T^k(\omega, z)\right) = \int_R \varrho(r, s)\, dr\, ds;$$

thus

$$\varrho\left(\frac{a+b}{2}, \frac{c+d}{2}\right) \approx \frac{1}{n(b-a)(c-d)} \sum_{k=0}^{n-1} \chi_R\left(T^k(\omega, z)\right).$$

The results of the computation are summarized in Table 2 and Fig. 3 below. The grid has $b-a=c-d=0.1$.

Fig. 3 is obtained by fitting a 50×50 grid of splines over the surface given by Table 2. Fig. 2 shows that in the one dimensional case the exact density is smoother than the computed density. From this one could conclude that a better approximation to the density in the Jacobian case could be obtained by fitting a quadratic or rational quadratic surface to the data by a least squares procedure.

4. Remarks and Conclusions

Consider the question of the number n of decimal digits of a number x which are required to yield m correct partial quotients of x. The procedure for generating partial quotients of x from a decimal representation of x correct to n decimal digits after the decimal point must stop when $\lambda(B_m) \leqq 2\cdot 10^{-n}$. Since, from (6), $\lambda(B_m) \sim e^{-h(T)m}$ one obtains the estimate $2\cdot 10^{-n} \geqq e^{-h(T)m}$ or

$$m \geqq n\,\frac{\log 10}{h(T)} = n\,\frac{6\log(10)\log(2)}{\pi^2} = n(0.9703\ldots).$$

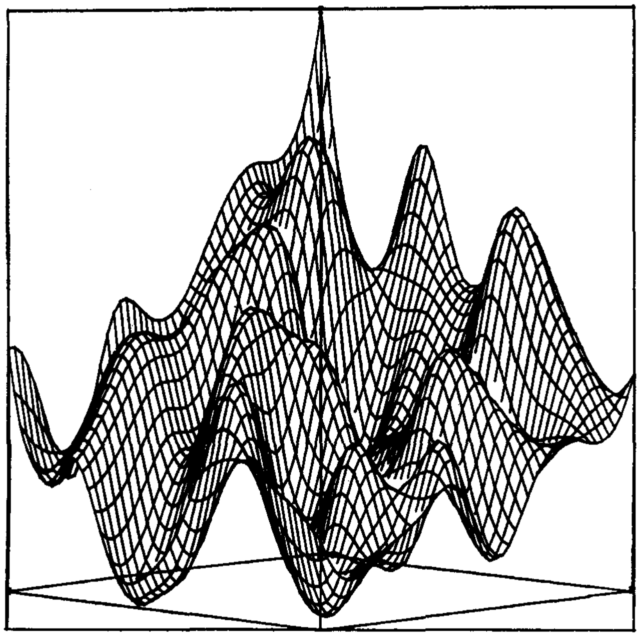

Fig. 3. Graph of the approximation to $d\mu/d\lambda$ where μ is the invariant measure associated with the two-dimensional Jacobi algorithm and λ is Lebesgue measure

For $n = 3561$, this gives an estimate of *3455* partial quotients. For γ, 3561 decimal digits actually gave *3420* partial quotients. Knuth [3] estimated that 1271 decimal digits would give over 1000 partial quotients.

An example of computation with Khinchine's constant has been pointed out [11]. However, the only mathematical example of computation for more than one dimension with the ergodic theorem the authors have found is Stein and Ulam [12]. (There are, no doubt, such computations reported in chemical or physics literature.) The transformations of Stein and Ulam were such that an estimation of the "noise" in the computation was difficult. However, calculations on both Gauss's measure and the Jacobi algorithm indicate that noise makes very little difference. Why this is so is an open and possibly very difficult problem. It would appear that a transformation which is the truncated sum of T and some uniform random variable has "approximately" the same ergodic properties.

Unfortunately our approximation of $\varrho(\cdot)$ was too rough to make a conjecture about whether or not $\varrho(\cdot)$ is continuous on the entire square.

No statistical tests were carried out with γ or (x, y). In the latter case one could compute the frequency of the digits $(0, 1)$, $(1, 1)$, etc.

It is interesting to compare the transformation $S(x, y) = (1/x - [1/x], 1/y - [1/y])$ with $T(x, y) = (y/x - [y/x], 1/x - [1/x])$. The entropy of S is double the entropy of the continued fraction transformation, so that $h(S) = \pi^2/(3 \log 2) \approx 4.75 \ldots$. In Section 3, $h(T)$ was approximated by 3.5. Thus it is seen that rate of convergence for S is significantly faster than the rate of convergence for T.

5. Note (Added in Proof)

Since the above work was completed, F. Schweiger (personal communication) has shown that $\sigma(n)$ (see (10) above) is $O(\theta^{-n})$ where θ is the unique root >1 of $x^3-x^2-1=0$. This θ is the fourth Pisot-Vijayaraghavan number (see C. L. Siegel, "Algebraic integers whose conjugates lie in the unit circle", Duke Math. J. **11**, 597–602 (1944)). His proof makes use of a paper of Paley and Ursell ("Continued fractions in several dimensions", Proc. Cambridge Philos. Soc. **26**, 127–144 (1930)). The proof of the following theorem now follows that of Theorem 2.

Theorem 3. Let $(y_1, y_2) \in B_N(x_1, x_2)$ and g satisfy

$$|g(t_1, t_2) - g(s_1, s_2)| \leq c\|(t_1, t_2) - (s_1, s_2)\|,$$

where c is some fixed constant and $\|,\|$ refers to Euclidean norm. Then

$$\left|\frac{1}{n}\sum_{k=0}^{n-1} g\big(T^k(x_1, x_2)\big) - \frac{1}{n}\sum_{k=0}^{n-1} g\big(T^k(y_1, y_2)\big)\right| = \frac{1}{n}\,O(\theta^{-N+n}).$$

M. I. Gordin (Dokl. Akad. Nauk SSSR "Exponentially fast mixing", Dokl. Akad. Nauk SSSR Tom 196 (1971), No. 6 or Soviet Math. Dokl. **12**, 331–335 (1971)) announces that $\varrho(x, y)$ in Jacobi's algorithm is discontinuous along $x=y$.

Acknowledgement. The authors express their thanks to Dr. Scott B. Guthery of Bell Telephone Laboratories and Professor John R. Kinney of Michigan State University for very helpful discussions. We are especially indebted to the Associated Western Universities for making our summer collaboration possible.

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Universitätsdruckerei H. Stürtz AG Würzburg
Printed in Germany