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On the Relaxation Time of Gauss's Continued-Fraction Map I. The Hilbert Space Approach (Koopmanism)

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It is shown that U^*, the adjoint of Koopman's isometric operator $Uf(x) = f(Tx)$ corresponding to the map $Tx = x^{-1}$ (mod 1) of the unit interval, is isomorphic to a symmetric integral operator when restricted to a Hilbert space of holomorphic functions f. This result, also obtained by Babenko in a different setting, allows us to derive new trace formulas. Using generalized Temple's inequalities, we determine the relaxation time of the above system with great accuracy. In contrast to a widespread belief, it appears to be unrelated to the entropy of the map T.

KEY WORDS: Relaxation time; continued fraction; trace formulas; Temple's inequalities

1 INTRODUCTION

Any number x in the unit interval has a continued fraction expansion. One is thus led to study the transformation T that carries x to x^{-1}(mod 1). The statistical theory of the continued fraction map T has its origin in a discovery by Gauss,[1] who, in a letter to Laplace, stated that the event $T^n x < a$ has asymptotic probability $\log_2(1+a)$ for each a in the unit interval. In modern terms, the statement is that the Lebesgue measure of the set $\{x: T^n x < a\}$ approaches

$$\frac{1}{\log 2}\int_0^a \frac{dx}{1+x} = \lim_n \text{Prob}\{T^n x < a\} \tag{1.1}$$

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where $(1+x)^{-1}$ serves as a distribution preserved under the action of T. We refer to $d\mu(x)=(1+x)^{-1}\,dx$ as Gauss's measure on $[0, 1)$. It is not clear what proof Gauss had for his assertion. Kuz'min[2] first gave a complete proof of (1.1). He also estimated the error as of the order $q^{\sqrt{n}}$, where $0<q<1$. Lévy[3] improved this to q^n, where $q \leqslant 0.68$. Szüsz[4] showed that this result can also be obtained by Kuz'min's method and found that $q \leqslant 0.485$. Finally, Wirsing,[5] using techniques from functional analysis, obtained the correct number to 20 decimal places:

$$q = 0.30366300289873265860 \tag{1.2}$$

It is not clear, though, how many of these decimals can be trusted. Wirsing's number, which is fundamental to number theory, appears to be unrelated to more familiar constants.

The solution to Gauss's problem was completed by Babenko,[6] who showed that

$$\mathrm{Prob}\{T^n x < a\} = \sum_i \lambda_i^n c_i(a) \tag{1.3}$$

where $\lambda_1 = 1$, $c_1 = \log_2(1+a)$, and $\lambda_2 = -q$. The λ_i are eigenvalues of a suitably defined symmetrical integral operator K and $|\lambda_1| \geqslant |\lambda_2| \geqslant \cdots$. Knuth[7] cites numerical results from an unpublished paper of Babenko, in particular the result $\lambda_3 = 0.1009$ and $\lambda_4 = -0.048$. While the result for λ_3 appears to be correct, the value of λ_4 must be wrong, since it violates the sum rule $\sum_i \lambda_i^2 = \mathrm{trace}\, K^2 = 1.103839654\ldots$. It is worth mentioning that Schweiger[8] has a simple rigorous upper bound,

$$q \leqslant \frac{2}{3+\sqrt{5}} \doteq 0.381966 \tag{1.4}$$

and that Waterman[9] gave a critical discussion of Kuz'min's method.

In (1.1) we emphasized the probabilistic nature of Gauss's result. Khinchin[10] and Doeblin[11] found new probabilistic results on the continued-fraction map. These results establish, among other properties, that the map T is ergodic, even strongly mixing. Kuz'min's theorem may then be rephrased by saying that the convergence encountered in the mixing process (the "approach to equilibrium") is in fact exponential: see Eq. (1.8) for a precise formulation. As a noninvertible transformation, T does not define a *K-system*. However, it can be well accommodated within the general framework of *K-systems* as an "exact transformation" in the sense of Rohlin (see, for instance, Ref. 12).

We may also look at the continued-fraction map as a dynamical system, thereby interpreting n as a discrete time variable. This then suggests we write $q = \exp(-1/\tau)$ for the constant (1.2) and to call τ the relaxation time. Only recently it was indicated that the continued-fraction map indeed arises in physical problems. Lifshitz *et al.*,[13] while investigating the Poincaré map associated with the time evolution of certain spatially homogeneous cosmologies ("Mixmaster universe"), found that it can be reduced to studying the map T. The well-known mixing properties of this map then lead to a chaotic time evolution.[14]

Let $h(T)$ denote the KS entropy of the map T. Pesin's identity claims that $h(T)$ can be expressed as a sum over all positive Liapunov exponents. This claim is known to be correct for the continued-fraction map. It then allows one to determine the entropy explicitly as

$$h(T) = \frac{1}{\log 2} \int_0^1 \frac{dx}{1+x} \log |T'(x)| = \frac{\pi^2}{6 \log 2} \tag{1.5}$$

The importance of this quantity is twofold. First, $h(T)$ is an invariant: any dynamical system isomorphic to T has the same entropy. Second, it relates to Diophantine approximation: the discrepancy between the real number $x \in (0, 1)$ and its nth approximant as a continued fraction is of the order $e^{-nh(T)}$ (see Ref. 15). This suggests we call $h(T)^{-1}$ the relaxation time of the approximation process. It seems natural to expect $h(T)^{-1}$ to coincide with the relaxation time τ of the mixing process. In fact, there is a simple example, namely the map $Tx = 2x (\text{mod } 1)$,[16] where the suggested relation, $\tau^{-1} = h(T)$, holds exactly. The relation also holds for the r-adic transformation $Tx = rx (\text{mod } 1)$, where r is a positive integer and $h(T) = \log r$. That heuristic arguments may fail is demonstrated by the continued-fraction map: While $\tau^{-1} \doteq 1.1918$, we have that $h(T) \doteq 2.3731$. Apparently, the entropy $h(T)$ and the relaxation time $\tau(T)$ are independent invariants of a map T.

Much of the quoted traditional work on the continued-fraction map relies on masure-theoretic arguments. However, two possible approaches depart from the classical path:

1. The Hilbert space approach. Here one deals with Koopman's isometric operator

$$Uf(x) = f(Tx) \tag{1.6}$$

defined on functions $f \in L^2(\mu)$, where μ is Gauss's measure on the unit interval. Actually, as it turns out, the adjoint of this operator, U^*, can be dealt with more easily.

2. The Banach space approach. Here one studies the operator

$$Lf(x) = \sum_{y \in T^{-1}x} f(y) |T'(y)|^{-1} \tag{1.7}$$

(closely related to U^*) on some Banach space of Lebesgue-integrable functions. Due to its particular structure, L will be referred to as the

Perron–Frobenius or transfer operator associated with the transformation T.

To find an appropriate setting for a formulation of Kuz'min's theorem, we need to restrict U^* (resp. L) to an invariant subspace of analytic functions. On this subspace, U^* and L become nuclear (i.e., trace-class) operators. It is then gratifying to learn that U^* and L possess the same spectrum. As usual, we order the eigenvalues λ_n according to their absolute value, i.e., $|\lambda_1| \geqslant |\lambda_2| \geqslant \cdots$, where we list each eigenvalue according to its multiplicity. Since it may be demonstrated that the inequality $|\lambda_1| > |\lambda_2|$ is strict (implying that λ_1 is a simple eigenvalue), we refer to λ_1 and λ_2 as the dominant and the subdominant eigenvalues. It is then easy to show that $\lambda_1 = 1$ and, as we proceed, it will become clear that the subdominant eigenvalue determines the relaxation, i.e., $q = |\lambda_2|$. It remains an open question whether the entropy $h(T)$ can be expressed in terms of the eigenvalues λ_n.

This paper deals with the Hilbert space approach and has to be considered a simplification and an extension of Babenko's work. In a subsequent article we will discuss the Banach space approach followed also by Wirsing in his investigations. The present paper is organized as follows. In Section 2 we relate the operator U^* to some integral operator K on $L^2(m)$, where m is a measure on R_+ given by $dm(s) = (e^s - 1)^{-1} s\, ds$; K is symmetric and nuclear. Consequently, its eigenvalues λ_n are real and summable: $\sum |\lambda_n| < \infty$. Next, we concentrate on the spectral invariants, in particular, we look at trace(K^n) and show that it may be represented as an n-fold integral over Bessel functions. Unfortunately, these integrals cannot be performed analytically, and we thus resort to a numerical treatment. In Section 3 we present results for $n = 1$ and $n = 2$.

Alternatively, we represent trace(K) and trace(K^2) as infinite sums over the fixed points of T (resp. T^2). A general proof that the trace of K^n may be written as a sum over the fixed points of T^n, hence over the obits of period n under T, is put aside until the discussion of the Perron–Frobenius operator. Section 4 is devoted to deriving first results on the eigenvalues themselves, and in Section 5 we concentrate on numerical bounds for λ_2 and λ_3 as obtained from the Ritz variational principle. To further strengthen the results, we apply new inequalities, which generalize a well-known inequality due to Temple.[18] In Section 6 we demonstrate that the functions $f(x)$ arising from $\varphi(s) \in L^2(m)$ are precisely those that belong to a certain space $H^2(\nu)$ of functions holomorphic in a half-plane in close analogy to the situation described by the Paley–Wiener theorem. Also, the introduction of $H^2(\nu)$ generalizes the concept of Hardy spaces. In Section 7 a Poisson integral formula is used to relate the scalar products in $H^2(\nu)$ and $L^2(\mu)$, which enable us to derive a new version of Kuz'min's theorem,

$$|((U^n - P_1) f, g)| \leqslant c q^n, \qquad f \in L^2(\mu), \quad g \in H^2(\nu) \tag{1.8}$$

where (f, g) denotes the scalar product in $L^2(\mu)$ and where P_1 is the projection corresponding to the dominant eigenvalue $\lambda_1 = 1$. Furthermore, $q = |\lambda_2|$, where λ_2 is subdominant and $c = \|f\| \, \|g\|_\nu$, where $\|\cdot\|_\nu$ denotes the norm in $H^2(\nu)$.

Though some of the ideas have already been employed by Wirsing and Babenko, their work particularly represents the number-theoretic point of view. Our main motivation is to stress the significance of their results for ergodic theory in general.

2. THE INTEGRAL OPERATOR K

Let $[y]$ denote the integer part of a real number y and consider the transformation $Tx = x^{-1} - [x^{-1}]$ of $x \in [0, 1]$, where it is agreed the $Tx = 0$ if $x = 0$. Then T preserves Gauss measure on $[0, 1)$ given by

$$d\mu(x) = \frac{dx}{1+x} \tag{2.1}$$

To this measure one associates the Hilbert space $L^2(\mu)$ of complex functions f on the unit interval. It is then straightforward to verify that T induces an isometry on $L^2(\mu)$ defined by $Uf(x) = f(Tx)$ and that the constant function $f(x) = 1$ serves as an eigenfunction of U with eigenvalue 1. T is strong-mixing[17] in the sense that for all $f, g \in L^2(\mu)$

$$\lim_n (U^n f, g) = (P_1 f, g) := \frac{(f, 1)(1, g)}{(1, 1)} \tag{2.2}$$

where $(\cdot, \cdot)$ denotes the scalar product in $L^2(\mu)$. The rate of convergence is expected to be arbitrarily slow, depending on the choice of f and g. An exponential rate may be achieved only if f and g are sufficiently regular functions. We aim at finding these conditions of regularity.

Our first step is to pass to the adjoint U^* given by $(Uf, g) = (f, U^*g)$; our second is to provide a simple formula for U^*:

$$U^*f(x) = \sum_{n=1}^{\infty} \frac{x+1}{(x+n)(x+n+1)} f\left(\frac{1}{x+n}\right) \tag{2.3}$$

The proof is easy and starts from

$$\int_0^1 d\mu(x)\, f(Tx)\, \overline{g(x)} = \sum_{n=1}^{\infty} \int_{(n+1)^{-1}}^{n^{-1}} d\mu(t)\, f(t^{-1} - n)\, \overline{g(t)} \tag{2.4}$$

By a change of variable, $x=t^{-1}-n$, we map the interval $(n+1)^{-1}<t\leqslant n^{-1}$ onto $[0, 1)$ so that

$$d\mu(t)=\frac{x+1}{(x+n)(z+n+1)}\,d\mu(x)$$

which gives the desired result (2.3).

Our third step is to restrict the operator U^* to an invariant subclass of functions. Here we choose generalized Laplace transforms,

$$\hat{\varphi}(x)=(x+1)\int dm(s)\,e^{-sx}\varphi(s), \qquad x\in[0, 1) \tag{2.5}$$

where m denotes a suitably chosen measure on R_+ and $\varphi\in L^2(m)$. As we go through the proof of the following theorem, we discover that there is precisely one measure (up to a constant) such that U^* induces a symmetric operator K on $L^2(m)$:

$$dm(s)=\frac{s\,ds}{e^s-1} \tag{2.6}$$

So, we might as well use this measure to formulate the final result.

Theorem 1. (1) If $f=\hat{\varphi}$ for some $\varphi\in L^2(m)$, then there exists $\psi\in L^2(m)$ such that $U^*f=\hat{\psi}$, and the following equation holds:

$$\psi(s)=\int dm(t)\,\frac{J_1(2(st)^{1/2})}{(st)^{1/2}}\,\varphi(t)=:K\varphi(s) \tag{2.7}$$

where J_1 denotes the Bessel function of order one.

(2) The correspondence $\varphi\mapsto\psi=K\varphi$ defines an integral operator K on $L^2(m)$ with continuous kernel; K is symmetric and nuclear (trace-class).

Proof. Let $f=\hat{\varphi}$. From (2.3) and (2.5)

$$(U^*f)(x)=(x+1)\sum_{n=1}^{\infty}\frac{1}{(x+n)^2}\int dm(t)\,e^{-t(x+n)^{-1}}\,\varphi(t) \tag{2.8}$$

Since $x\geqslant 0$, the integral and the sum may be interchanged. We then compute

$$\begin{aligned}\sum_{n=1}^{\infty}\frac{1}{(x+n)^2}\,e^{-t(x+n)^{-1}}&=\sum_{k=0}^{\infty}\frac{(-t)^k}{k!}\sum_{n=1}^{\infty}\frac{1}{(x+n)^{k+2}}\\&=\sum_{k=0}^{\infty}\frac{(-t)^k}{k!\,(k+1)!}\int dm(s)\,s^k e^{-sx}\\&=\int dm(s)\,\frac{J_1(2(st)^{1/2})}{(st)^{1/2}}\,e^{-sx}\end{aligned}$$

and by a simple use of Fubini's theorem,

$$U^*f(x) = (x+1) \int dm(s)\, e^{-sx} \int dm(t)\, \frac{J_1(2(st)^{1/2})}{(st)^{1/2}}\, \varphi(t)$$

which proves that $U^*f = \hat{\psi}$, where ψ is given by (2.7). It remains to prove that $\psi \in L^2(m)$. But this is automatic once we have shown that the operator K is bounded. The second part of the theorem claims much more: K is nuclear and symmetric. While symmetry is obvious, the demonstration of nuclearity requires some care. To start with, we expand the kernel in terms of Laguerre polynomials,

$$\frac{J_1(2(st)^{1/2})}{(st)^{1/2}} = \sum_{n=0}^{\infty} L_n^1(s)\, \frac{t^n e^{-t}}{(n+1)!} \tag{2.9}$$

Thus, K may be represented as

$$K\varphi = \sum_{n=0}^{\infty} (\varphi, \eta_n) e_n \tag{2.10}$$

where Y_n, $e_n \in L^2(m)$, are given by

$$e_n(s) = L_n^1(s), \qquad \eta_n(s) = \frac{s^n e^{-s}}{(n+1)!}$$

It remains to prove that $\sum \|\eta_n\|\, \|e_n\| < \infty$. The computation of $\|e_n\|$ involves a standard integral:

$$\begin{aligned}
\|e_n\|^2 &= \int dm(s)\, [L_n^1(s)]^2 \\
&= \sum_{k=1}^{\infty} \int_0^{\infty} ds\, s e^{-ks} [L_n^1(s)]^2 \\
&= \sum_{k=1}^{\infty} \frac{n+1}{k^{2n+2}} \sum_{p=0}^{n} \binom{n+1}{p} \binom{n}{p} (k-1)^{2p}
\end{aligned}$$

We use

$$\binom{n+1}{p} \leqslant 2^{n+1}$$

to obtain the bound

$$\|e_n\|^2 \leqslant (n+1) 2^{n+1} \sum_{k=1}^{\infty} \frac{(k-1)^2 + 1}{k^{2n+2}} \leqslant (n+1) 2^{n+1} \zeta(2)$$

Next, we compute the norm of η_n:

$$\|\eta_n\|^2 = \int dm(s) \left[\frac{s^n e^{-s}}{(n+1)!} \right]^2$$

$$= [(n+1)!]^{-2} \sum_{k=3}^{\infty} \int_0^{\infty} ds\, s^{2n+1} e^{-ks}$$

$$= \binom{2n+1}{n+1} (n+1)^{-1} \zeta(r, 3) \qquad (r = 2n+2)$$

where

$$\zeta(r, 3) := \sum_{k=3}^{\infty} k^{-r}$$

$$= \sum_{p=1}^{\infty} [(3p)^{-r} + (3p+1)^{-r} + (3p+2)^{-r}]$$

$$\leqslant 3 \sum_{p=1}^{\infty} (3p)^{-r} = 3^{1-r} \zeta(r)$$

We use

$$\binom{2n+1}{n+1} \leqslant 2^{2n+1} \qquad \text{and} \qquad \zeta(2n+2) \leqslant \zeta(2)$$

to obtain the bound

$$\|\eta_n\|^2 \leqslant (n+1)^{-1} \left(\frac{2}{3}\right)^{2n+1} \zeta(2)$$

and thus obtain the following result:

$$\sum_{n=0}^{\infty} \|e_n\|\, \|\eta_n\| \leqslant \frac{2}{\sqrt{3}}\, \zeta(2) \sum_{n=0}^{\infty} \left(\frac{8}{9}\right)^{n/2} < \infty$$

This proves the second part of the theorem.

Our concern will now be the operator K on $L^2(m)$. From the above theorem we conclude that K admits a spectral representation of the form

$$K\varphi = \sum_{n=1}^{\infty} \lambda_n (\varphi, \varphi_n) \varphi_n \tag{2.11}$$

where the φ_n define an orthonormal basis in $L^2(m)$. The eigenvalues λ_n are real and satisfy

1. $|\lambda_1| \geqslant |\lambda_2| \geqslant |\lambda_3| \geqslant \cdots$
2. $\sum |\lambda_n| < \infty$

The next four sections are devoted to numerical aspects of the spectrum.

3. ESTIMATES FOR tr K^n ($n=1, 2$)

The trace of a nuclear operator K on $L^2(m)$ with kernel $K(s, t)$ may be defined by the formula

$$\operatorname{tr} K = \int dm(s)\, K(s, s) \tag{3.1}$$

For the particular operator at hand we thus obtain

$$\operatorname{tr} K = \sum_{n=1}^{\infty} \lambda_n = \int_0^{\infty} ds \frac{J_1(2s)}{e^s - 1} \tag{3.2}$$

There seems to be no simple finite expression for this number, nor is the integral mentioned in any of the existing integral tables. We thus proceed to establish rigorous bounds, thereby showing that tr K is a number close to 0.75:

$$\frac{3}{4} + \frac{\pi}{e^{4\pi} - 1} \leqslant \operatorname{tr} K < \frac{3}{4} + \frac{\pi}{96} \tag{3.3}$$

The proof is based on the formula

$$J_1(2s) = \frac{2}{\pi} \int_0^{\pi/2} d\alpha \sin\alpha \sin(2s \sin\alpha) \tag{3.4}$$

By Fubini's theorem,

$$\begin{aligned}
\operatorname{tr} K &= \frac{2}{\pi} \int_0^{\pi/2} d\alpha \sin\alpha \int_0^{\infty} \frac{ds}{e^s - 1} \sin(2s \sin\alpha) \\
&= \int_0^{\pi/2} d\alpha \left[\sin\alpha \coth(2\pi \sin\alpha) - \frac{1}{2\pi} \right] \\
&= \frac{3}{4} + 2I
\end{aligned} \tag{3.5}$$

where

$$I := \int_0^{\pi/2} d\alpha \, \frac{\sin\alpha}{e^{4\pi \sin\alpha} - 1} \tag{3.6}$$

Since $s[e^s - 1]^{-1}$ is a decreasing function and $8\alpha \leqslant 4\pi \sin\alpha \leqslant 4\pi$ provided $0 \leqslant \alpha \leqslant \pi/2$, we have that

$$\frac{\pi/2}{e^{4\pi} - 1} \leqslant I \leqslant \frac{2}{\pi} \int_0^{\pi/2} d\alpha \, \frac{\alpha}{e^{8\alpha} - 1} < \frac{1}{32\pi} \int_0^\infty \frac{s\, ds}{e^s - 1} = \frac{\pi}{192} \tag{3.7}$$

which together with (3.5) yields the desired result. Of course, one may also treat the integral I using standard techniques of numerical integration. To nine decimal places, $I = 0.0105627618$, implying

$$\operatorname{tr} K = 0.7711255237 \tag{3.8}$$

Our next result states an interesting relationship between tr K and the fixed points under the continued-fraction map. Consider the following continued fractions:

$$x_n = \frac{1}{n+} \frac{1}{n+} \frac{1}{n+} \cdots \qquad (n \in N) \tag{3.9}$$

Obviously, $x_n \in [0, 1)$ and any nonzero solution of $Tx = x$ is of this form.

Theorem 2.

$$\operatorname{tr} K = \sum_{n=1}^{\infty} (1 + x_n^{-2})^{-1}$$

The proof is based on the integral

$$\int_0^\infty ds \, J_1(2s) \, e^{-ns} = \frac{1}{2} [1 - n(n^2 + 4)^{-1/2}] \tag{3.10}$$

and on the fact that x_n is the positive solution of the quadratic equation $x(x + n) = 1$, i.e.,

$$2x_n = (n^2 + 4)^{1/2} - n$$

$$2x_n^{-1} = (n^2 + 4)^{1/2} + n$$

$$\frac{2x_n}{x_n + x_n^{-1}} = 1 - n(n^2 + 4)^{-1/2}$$

Summing both sides of (3.10) over $n \in N$, we obtain the desired result.

The representation of $\operatorname{tr} K$ in terms of fixed points does not come unexpectedly. It is a consequence of quite general (known) arguments for dynamical systems, as will be discussed later. It may be worthwhile to remark that the convergence of the sum appearing in Theorem 2 is rather slow: asymptotically, the sum behaves like $\sum n^{-2}$, implying

$$\operatorname{tr} K = \sum_{n=1}^{N} (1 + x_n^{-2})^{-1} + O\left(\frac{1}{N}\right) \tag{3.11}$$

which shows that this representation is not well-suited for a numerical computation.

Continuing, we may study the next quantity of interest, the trace of K^2:

$$\operatorname{tr} K^2 = \sum_{n=1}^{\infty} \lambda_n^2 = \int dm(s) \int dm(t)\, K(s, t)\, K(t, s) \tag{3.12}$$

Due to (2.6), this trace is represented by the following integral:

$$\operatorname{tr} K^2 = \int_0^\infty \int_0^\infty ds\, dt \frac{J_1(2(st)^{1/2})^2}{(e^s - 1)(e^t - 1)} \tag{3.13}$$

Here, the problem is harder: it seems difficult both to derive sharp bounds and to compute this number using numerical integration.

Of course, from the obvious bound $J_1(2(st)^{1/2})^2 \leqslant st$ we easily obtain $\operatorname{tr} K^2 \leqslant \zeta(2)^2 = \pi^4/36$. However, this upper bound overestimates the integral by a factor greater than 2. There is another more promising approach; namely, we write

$$\operatorname{tr} K^2 = \sum_{n,m=1}^{\infty} \int_0^\infty \int_0^\infty ds\, dt\, e^{-ns-mt} J_1(2(st)^{1/2})^2 \tag{3.14}$$

With help of tables, the integrals can now be performed and we obtain $\operatorname{tr} K^2$ as a double sum in the form

$$\operatorname{tr} K^2 = \sum_{n,m=1}^{\infty} h\left(\frac{1}{nm}\right) \tag{3.15}$$

letting

$$2h(x) + 1 = (1 + 2x)(1 + 4x)^{-1/2} \tag{3.16}$$

With x restricted to the interval $(0, 1]$ we have that $0 < h(x) < x^2$. This shows that the sum (3.16) is indeed convergent, though slowly. The function $h(x)$ has a number of peculiar represention. One of them is

$$h(x) = \frac{1}{4}\left[(1+4x)^{1/2} + (1+4x)^{-1/2} - 2\right] \tag{3.17}$$

Using an identity among binomial coefficients,

$$\frac{1}{4}\left[\binom{1/2}{k} + \binom{-1/2}{k}\right] = (-4)^{-k}\binom{2k-2}{k-2} \tag{3.18}$$

we obtain another representation,

$$h(x) = \sum_{k=2}^{\infty}\binom{2k-2}{k-2}(-x)^k \tag{3.19}$$

though this expansion is valid only for $|x| < 1/4$. To effectively compute $\operatorname{tr} K^2$, we split the sum (3.15) into three partial sums, that is, we write

$$\operatorname{tr} K^2 = S_1 + 2S_2 + S_3 \tag{3.20}$$

where

$$S_1 = \sum_{n=1}^{N-1}\sum_{m=1}^{N-1} h\left(\frac{1}{nm}\right)$$

$$S_2 = \sum_{n=N}^{\infty}\sum_{m=1}^{N-1} h\left(\frac{1}{nm}\right) = \sum_{n=1}^{N-1}\sum_{m=N}^{\infty} h\left(\frac{1}{nm}\right)$$

$$S_3 = \sum_{n=N}^{\infty}\sum_{m=N}^{\infty} h\left(\frac{1}{nm}\right)$$

If $N > 4$, we may use (3.19) to rewrite S_2 and S_3:

$$S_2 = \sum_{k=2}^{M-1}(-1)^k\binom{2k-2}{k-2}\zeta(k, N)\sum_{n=1}^{N-1} n^{-k} + R_{M,N}$$

$$S_3 = \sum_{k=2}^{M-1}(-1)^k\binom{2k-2}{k-2}\zeta(k, N)^2 + R'_{M,N}$$

where

$$\zeta(k, N) = \sum_{n=N}^{\infty} n^{-k}$$

The remainder terms are

$$R_{M,N} = \sum_{k=M}^{\infty} (-1)^k \binom{2k-2}{k-2} \zeta(k, N) \sum_{n=1}^{N-1} n^{-k}$$

$$R'_{m,N} = \sum_{k=M}^{\infty} (-1)^k \binom{2k-2}{k-2} \zeta(k, N)^2$$

These have to be kept small. We use

$$\zeta(k, N) < N^{1-k}\zeta(k), \qquad \binom{2k-2}{k-2} < 4^k, \qquad \sum_{1}^{N-1} n^{-k} < \zeta(k), \qquad \zeta(k) < 2$$

to obtain the following estimates:

$$|R_{M,N}| < 4N^2(N-4)^{-1}(4/N)^M$$

$$|R'_{M,N}| < 4N^4(N^2-4)^{-1}(4/N^2)^M$$

For instance, $|R_{20,20}| < 10^{-12}$ and $|R'_{20,20}| < 10^{-37}$, which seems sufficient. The problem in thus reduced to efficiently computing $\zeta(k, N)$ for $2 \leqslant k < M$. This is a relatively simple task provided one takes advantage of the Euler summation formula. The result of this numerical exercise is an approximate value for the trace of K^2,

$$\operatorname{tr} K^2 \doteq 1.103839654 \tag{3.21}$$

which, we claim, is correct of ten decimal places.

Remember that $\operatorname{tr} K$ has a remarkable representation in terms of fixed points (Theorem 2). We now claim that $\operatorname{tr} K^2$ may be represented as a sum over continued fractions $x \in [0, 1)$ of period $\leqslant 2$, i.e., fixed points of T^2. Consider the fractions

$$x_{m,n} = \frac{1}{m+} \frac{1}{n+} \frac{1}{m+} \frac{1}{n+} \cdots \qquad (m, \; n \in N) \tag{3.22}$$

so that $Tx_{m,n} = x_{n,m}$. It is not hard to check that any solution of $T^2 x = x$ is of the form (3.22) and hence solves the quadratic equation $mx(x+n) = n$ such that

$$x_{m,n} = \left(\frac{n^2}{4} + \frac{n}{m}\right)^{1/2} - \frac{n}{2} \tag{3.23}$$

Theorem 3:

$$\operatorname{tr} K^2 = \sum_{n,m=1}^{\infty} [(x_{m,n} x_{n,m})^{-2} - 1]^{-1}$$

Proof. If $a=x_{m,n}x_{n,m}$, then a is merely a function of the product mn:

$$a=\tfrac{1}{4}[(mn+4)^{1/2}-(n)^{1/2}]^2$$
$$a^{-1}=\tfrac{1}{4}[(mn+4)^{1/2}+(mn)^{1/2}]^2$$

Since $a^{-1}-a=(mn)^{1/2}(mn+4)^{1/2}$,

$$(a^{-2}-1)^{-1}=a(a^{-1}-a)^{-1}=h(1/mn) \tag{3.24}$$

where

$$h(x)=\tfrac{1}{4}[(1+4x)^{1/4}-(1+4x)^{-1/4}]^2 \tag{3.25}$$

Comparison with (3.17) shows that $h(x)$ coincides with our previously defined function as it was used in the representation (3.15) of $\operatorname{tr} K^2$. The asserted equality, $\operatorname{tr} K^2=\sum(a^{-2}-1)^{-1}$, is just another way of writing (3.15).

In general, the trace of K^n, the nth power of the operator K, may be represented as a sum over all solutions x to the equation $T^n x=x$, as will be shown in a subsequent paper. On the other hand, $\operatorname{tr} K^n$ may also be expressed as an n-fold integral over some n-fold product of Bessel functions. The alleged relationship between these integrals and sums over continued fractions of period n (prime period $\leqslant n$) is rather striking.

4. FIRST RESULTS ON THE SPECTRUM

With all this numerical work, what have we learned about the dominant eigenvalue λ_1, and about λ_2? In Section 2, we argued that the constant function on $[0, 1)$ is an eigenvector of U corresponding to the eigenvalue 1, $U1=1$. This implies $U^*1=1$, since U is an isometry on $L^2(\mu)$. Is there a corresponding eigenvector of K in $L^2(m)$? To answer this, we write the constant function as a generalized Laplace transform, $1=(x+1)\int dm(s)\,e^{-sx}\varphi(s)$, where $\varphi(s)=s^{-1}(1-e^{-s})$. For φ to describe a legitimate eigenvector of K, it is crucial to observe that $\varphi\in L^2(m)$. A simple computation shows that $\|\varphi\|^2=\log 2$. Hence, the normalized function

$$\varphi_1(s)=(\log 2)^{-1/2}s^{-1}(1-e^{-s}) \tag{4.1}$$

is a unit vector in $L^2(m)$ for which $K\varphi_1=\varphi_1$. We have tacitly assumed that $\lambda_1=1$, i.e., 1 is the dominant eigenvalue of the operator K. But this assertion can be proved: $\lambda_n=1$ implies that $\operatorname{tr} K^2\geqslant n$, since the eigenvalues are ordered according to their absolute value. However, this lower bound contradicts (3.21) unless $n=1$.

Let us introduce the following partial sums:

$$s_n = \sum_{k \geqslant n} \lambda_k \tag{4.2}$$

$$r_n = \sum_{k \geqslant n} \lambda_k^2 \tag{4.3}$$

From (3.8) and (3.21),

$$s_2 = \operatorname{tr} K - 1 \doteq -0.228874 \tag{4.4}$$

$$r_2 = \operatorname{tr} K^2 - 1 \doteq 0.103840 \tag{4.5}$$

We have thus discovered that there exist negative eigenvalues. Actually, we can state more:

Lemma. $\inf \lambda_n = \lambda_2 < 0$.

Proof. Because K is symmetric, $\inf \lambda_n \leqslant (\varphi, K\varphi)$ for any $\varphi \in L^2(m)$ such that $\|\varphi\| = 1$. To start with, we choose $\varphi_0(s) = 1 - e^{-s}$. We then project φ_0 onto the orthogonal complement of φ_1 and normalize to obtain φ. It is easy to check that

$$(\varphi, K\varphi) = \frac{(\varphi_0, K\varphi_0) - |(\varphi_0, \varphi_1)|^2}{\|\varphi_0\|^2 - |(\varphi_0, \varphi_1)|^2} \tag{4.6}$$

The expression to the right involves only integrals of known types:

$$(\varphi_0, K\varphi_0) = \int_0^\infty \int_0^\infty ds\, dt\, s^{1/2} t\, e^{-s-t} J_1(2(st)^{1/2}) = \tfrac{1}{4}$$

$$(\log 2)^{1/2} (\varphi_0, \varphi_1) = \int_0^\infty ds\, e^{-s}(1 - e^{-s}) = \tfrac{1}{2}$$

$$\|\varphi_0\|^2 = \int_0^\infty ds\, s e^{-s}(1 - e^{-s}) = \tfrac{3}{4}$$

Hence $\inf \lambda_n \leqslant -a$, where

$$a = \frac{1 - \log 2}{3 \log 2 - 1} \doteq 0.2843 \tag{4.7}$$

Since $\lim \lambda_n = 0$, there exists some $m \geqslant 2$ such that $\lambda_m = \inf \lambda_n$. Argue as before to find that $r_2 \geqslant (m-1)|\lambda_m|^2 \geqslant (m-1)a^2$, which contradicts (4.5) unless $m = 2$.

As a side result, we obtain the following bounds:

$$a \leqslant -\lambda_2 \leqslant r_2^{1/2} \tag{4.8}$$

Numerically, $0.2843 \leqslant -\lambda_2 \leqslant 0.3222$. Of course, our choice of φ_0 is not optimal, since was dictated by simplicity. With a little more labor (see next section) we can sharpen the bounds to show that $\lambda_2 \doteq 0.303663$, where all six digits are significant. Granted this result, we are left with

$$s_3 \doteq 0.074789, \qquad r_3 \doteq 0.011629 \tag{4.9}$$

We also find that $\lambda_3 \doteq 0.1009$ to four significant digits, so that

$$s_4 \doteq -0.0261, \qquad r_4 \doteq 0.00145$$

It is conspicuous that the first four partial sums of the eigenvalues, $s_1,..., s_4$, alternate in sign. We take this as an indication of a general fact and conjecture that $(-1)^n s_n < 0$ for all n. Assuming this to be true, we may conclude that the eigenvalues themselves alternate in sign: $(-1)^n \lambda_n < 0$. We also expect that the λ_n drop to zero at an exponential rate, i.e., $0 < -\lambda_{n+1}/\lambda_n < 1/3$. Now, $\lambda = 0$ cannot be an eigenvalue, since

$$\int dm(r)\,(st)^{-1/2}\,J_1(2(st)^{1/2})\,\varphi(t) = 0$$

implies that $(e^t - 1)^{-1}\, t\varphi(t) = 0$ by the invertibility of the Hankel transformation.

5. HIGH-PRECISION BOUNDS FOR λ_n $(n = 2, 3)$

The space of interest will now be the subspace $H \subset L^2(m)$ orthogonal to the dominant eigenfunction φ_1. Let A denote the restriction of the operator K to H. We appeal to the variational principle

$$\lambda_2 = \inf(A\varphi, \varphi)/\|\varphi\|^2, \qquad \lambda_m = \sup(A\varphi, \varphi)/\|\varphi\|^2 \tag{5.1}$$

where the infimum (resp. supremum) is taken with respect to $0 \neq \varphi \in H$ and where $m \geqslant 3$ is defined such that $\lambda_m = \max \lambda_{n \geqslant 3}$. At the end we will show that $m = 3$. We then choose trial functions $\varphi = \varphi_0 - (\varphi_0, \varphi_1)\varphi_1$,

$$\varphi_0(s) = (e^s - 1)(e^{-rs} + ce^{-ps}) \tag{5.2}$$

where we wish to optimize the constants r, p, and c (all real) subject to the restrictions $\frac{1}{2} < r < p$. Our choice (5.2) is motivated by the observation that the Schwarz constants

$$\alpha_n = (A^n\varphi, \varphi), \qquad n = 0, 1, 2, 3 \tag{5.3}$$

can be evaluated at ease writing

$$\alpha_n = F_n(r, r) + 2cF_n(r, p) + c^2 F_n(p, p)$$

where

$$F_n(r, p) = G_n(r, p) - [(r + r^2)(p + p^2) \log 2]^{-1}$$

and

$$\begin{aligned}
G_0(r, p) &= (r + p - 1)^{-2} - (r + p)^{-2} \\
G_1(r, p) &= (1 + rp)^{-2} \\
G_2(r, p) &= \sum_{n=1}^{\infty} (r + p + nrp)^{-2} \\
G_3(r, p) &= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} [rp + (mr + 1)(np + 1)]^{-2}
\end{aligned} \tag{5.4}$$

I. Let us first address the problem of obtaining accurate bounds for λ_2. Here we adopt the following values:

$$r = 1.158183, \qquad p = 2.24343, \qquad c = -0.12439203 \tag{5.5}$$

The numbers have been chosen because then the quotient α_1/α_0 is close to its minimal value. In fact, we find

$$\lambda_2 \leqslant \alpha_1/\alpha_0 \doteq -0.3036556 \tag{5.6}$$

Let us adopt the following terminology. A bound is said to be of nth order if it is an expression in terms of α_k, $k \leqslant n$. In connection with these bounds it is convenient to introduce nth-order functions of $n-1$ arguments:

$$\begin{aligned}
\beta_1 &= \frac{\alpha_1}{\alpha_0} \\
\beta_2(x) &= \frac{\alpha_2 - x\alpha_1}{\alpha_1 - x\alpha_0} \\
\beta_3(x, y) &= \frac{\alpha_3 - (x + y)\alpha_2 + xy\alpha_1}{\alpha_2 - (x + y)\alpha_1 + xy\alpha_0} \\
&\vdots
\end{aligned} \tag{5.7}$$

The inequality (5.6) provides us with a first-order bound: $\lambda_2 \leqslant \beta_1$. Second-order bounds may be derived if we possess additional information about the location of eigenvalues. Suppose that for certain constants a and b and all $n \geqslant 3$

$$\beta_1 < a \leqslant \lambda_n < b \tag{5.8}$$

These conditions imply that $(A-\lambda_2)(A-b) \leqslant 0 \leqslant (A-\lambda_2)(A-a)$, and taking scalar products $(\varphi, ..., \varphi)$ we conclude that

$$\beta_2(a) \leqslant \lambda_2 \leqslant \beta_2(b) \tag{5.9}$$

which are second-order bounds due to Temple.[18] It remains to find a and b. From (5.6) and (3.21) we obtain the numerical bound $\sum \lambda^2_{n \geqslant 3} \leqslant 0.011622$. Hence, the condition (5.8) is met if $-a = b = 0.1079$. Insertion in (5.9) yields

$$-0.3036671 \leqslant \lambda_2 \leqslant -0.3036610 \tag{5.10}$$

Continuing, we derive third-order bounds from

$$(A-\lambda_2)(A-a)(A-b) \leqslant 0 \leqslant (A-\lambda_2)(A-x)^2$$

Again, we take scalar products to obtain

$$\beta_3(a, b) \leqslant \lambda_2 \leqslant \inf_x \beta_3(x, x) \tag{5.11}$$

Notice that $\alpha_2 - (a+b)\alpha_1 + ab\alpha_0 > 0$ has been used to get the lower bound. This inequality, being a consequence of $\beta_2(a) < b$ and $\beta_1 < a$, follows from (5.6), (5.8), and (5.9). The evaluation of (5.11) yields

$$-0.3036641 \leqslant \lambda_2 \leqslant -0.3036629 \tag{5.12}$$

II. Let us now turn to the problem of obtaining bounds for λ_m. Here we adopt the values

$$r = 1.2133, \qquad p = 1.2899, \qquad c = -1.21425 \tag{5.13}$$

which are close to the location of the maximum of α_1/α_0 in parameter space.

As a first-order bound, we thus get

$$\lambda_m \geqslant \beta_1 \doteq 0.10072 \tag{5.14}$$

This in particular proves that $m = 3$, since

$$0.012 > r_3 \geqslant (m-2)\,|\lambda_m|^2 > (m-2)0.01$$

from (4.9) and (5.14). Let a and b be numbers such that for all $n \geqslant 4$

$$a \leqslant \lambda_2 < \lambda_n \leqslant b < \beta_1 \tag{5.15}$$

Then, arguing as before, we obtain second-order bounds,

$$\beta_2(a) \leqslant \lambda_3 \leqslant \beta_2(b) \tag{5.16}$$

How do we choose a and b? The inequalities (5.12) permit us to choose $a = -0.3036641$, and from (5.14) and $\sum \lambda^2{}_{n \geqslant 3} \leqslant 0.011633$ we get $\sum \lambda^2_{n \geqslant 4} \leqslant 0.0014885$. Hence, (5.15) is satisfied if $b = 0.038581$. Insertion in (5.16) yields

$$0.10076 \leqslant \lambda_3 \leqslant 0.10096 \tag{5.17}$$

Finally, we may employ the following third-order bounds:

$$\sup_x \beta_3(x, x) \leqslant \lambda_3 \leqslant \beta_3(a, b) \tag{5.18}$$

to obtain

$$0.10088 \leqslant \lambda_3 \leqslant 0.10094 \tag{5.19}$$

III. Having derived accurate bounds for λ_3, we are ready for a minor improvement over our results regarding λ_2. In (5.11) we may now take $a = -0.038581$ and $b = 0.10094$ knowing that the conditions (5.8) are satisfied. With this modification we get

$$-0.30366327 \leqslant \lambda_2 \leqslant -0.30366299 \tag{5.20}$$

The numerical values r_i, $i = 1, 2, 3$, show that the three eigenvalues λ_1, λ_2, and λ_3 are all simple.

6. THE SPACE $H^2(\nu)$

In Section 2, we defined the generalized Laplace transform of $\varphi \in L^2(m)$ as

$$\hat{\varphi}(z) = (1 + z) \int dm(s)\, e^{-sz} \varphi(s)$$

Though z was restricted to the interval $[0, 1)$, $\hat{\varphi}$ can be extended to a function of a complex variable holomorphic in the half-plane $D = \{z = x + iy \mid x > -\frac{1}{2}\}$. A simple calculation, using the Plancherel theorem, then shows that

$$\int dm(s)\, |\varphi(s)|^2 = \frac{1}{\pi} \int_{-1/2}^{0} dx \int_{-\infty}^{\infty} dy \left| \frac{\hat{\varphi}(z)}{1 + z} \right|^2 \tag{6.1}$$

This equality suggests we introduce the following measure on D.

$$d\nu(z)=\begin{cases}\dfrac{1}{\pi}\dfrac{dx\,dy}{(1+x)^2+y^2}, & -\frac{1}{2}<x<0\\ 0, & x>0\end{cases} \tag{6.2}$$

Furthermore, let $H^2(\nu)$ denote the space of all functions $f(z)$ holomorphic in D such that $|(1+z)^{-1}f(z)|$ is bounded in any of the half-planes $x>-\frac{1}{2}+\varepsilon$ $(\varepsilon>0)$ and

$$\|f\|_\nu^2 := \int d\nu(z)\, |f(z)|^2 < \infty \tag{6.3}$$

Then the map $\varphi \mapsto \hat{\varphi}$ is an isometry from $L^2(m)$ to $H^2(\nu)$. By invoking the Paley–Wiener theorem, one shows that the map is onto. Thus, we regard $L^2(m)$ and $H^2(\nu)$ as the "same" space. We also regard $H^2(\nu)$ as being densely embedded in $L^2(\mu)$, where μ is Gauss measure. All told, $H^2(\nu)$ is an invariant subspace for U^*, the adjoint of U is an operator on $L^2(\mu)$, and the spectrum of U^*, when restricted to $H^2(\nu)$, is that of the operator K on $L^2(m)$. By construction, $H^2(\nu)$ consists of complex functions holomorphic in D with restricted growth near the boundary ∂D, and, in that respect, our construction is rather similar to the introduction of Hardy spaces over half-planes.

We wish to stress that $H^2(\nu)$ is not invariant under U. In fact, if $0 \neq f \in H^2(\nu)$, the function Uf is no longer analytic, but is discontinuous at almost all points $(1/n)$ $(n \in N)$, $U^2 f$ is discontinuous at almost all points

$$\frac{1}{n+\frac{1}{m}} \qquad (n, m \in N)$$

and so on. As $n \to \infty$, $U^n f$ eventually becomes a function discontinuous at almost all rational points in $[0, 1)$.

To avoid confusion, we will write $\hat{K}$ in place of U^* whenever U^* is regarded as an operator on $H^2(\nu)$. This notation is suggestive, since the isomorphism $L^2(m) \to H^2(\nu)$, $\varphi \mapsto \hat{\varphi}$, carries the operator K (see Theorem 1) into $\hat{K}$.

7. A POISSON INTEGRAL FORMULA

We now focus on the relationship between $L^2(\mu)$ and $H^2(\nu)$, i.e., we look for a relation between their scalar products. To establish such a relation, we use the Poisson integral formula usually stated for the disc.[19]

It may also be stated for the half-plane $x>0$ using a conformal mapping argument[20]:

$$F(z)=\frac{1}{\pi}\int_{-\infty}^{\infty} ds\, \mathrm{Re}\left[\frac{1}{z-is}\right] F(is) \tag{7.1}$$

Here, one asumes that $F(z)$ is holomorphic and bounded for $x>0$. Define

$$F(z)=f(z+t)\,\overline{g(\bar{z}+t)}$$

where $f, g\in H^2(\nu)$ and $t>-\frac{1}{2}$, and apply (7.1). Then put $z=x+1$, $t=x$, and $s=y$, assuming $x>-\frac{1}{2}$. Integrating both sides over $-\frac{1}{2}<x\leqslant 0$, we have shown the following:

$$(f, g)=\int d\nu(z)\, f(z)\, \overline{g(\bar{z})} \tag{7.2}$$

The expression to the left is the scalar product in $L^2(\mu)$, whereas the scalar product in $H^2(\nu)$ is

$$(f, g)_\nu=\int d\nu(z)\, f(z)\, \overline{g(z)}$$

Obviously, if $g(x)=1$, the two expressions give the same result:

$$(f, 1)_\nu=(f, 1)=\int_0^1 \frac{dt}{1+t} f(t) \tag{7.3}$$

Without danger of confusion, we therefore do not distinguish between the projection P_1 in $L^2(\mu)$ and the corresponding projection in $H^2(\nu)$, i.e., we write

$$(P_1 f, g)_\nu=(P_1 f, g)=\frac{(f, 1)(1, g)}{(1, 1)} \tag{7.4}$$

for all $f, g\in H^2(\nu)$. From

$$\left|\int d\nu(z)\, g(z)\, \overline{g(\bar{z})}\right|^2 \leqslant \int d\nu(z)\, |g(z)|^2 \int d\nu(z)\, |g(\bar{z})|^2$$

$$\int d\nu(z)\, |g(\bar{z})|^2=\int d\nu(z)\, |g(z)|^2$$

[$d\nu(z)$ is symmetric under $y\mapsto -y$!] we infer that

$$\|g\| \leqslant \|g\|_\nu \tag{7.5}$$

Mixing relates to the asymptotic behavior of $(U^n f, g)$. The rate of convergence can be estimated by first writing

$$((U^n - P_1)f, g) = (f, (U^{*n} - P_1)g) = (f, (U^* - P_1)^n g)$$

so that

$$|((U^n - P_1)f, g)| \leqslant \|f\| \, \|(U^* - P_1)^n g\|$$

Though $f \in L^2(\mu)$ may be arbitrary, we shall assume that $g \in H^2(v)$. Hence, $(U^* - P_1)^n g \in H^2(v)$ and

$$\|(U^* - P_1)^n g\| \leqslant \|(\hat{K} - P_1)^n g\|_v$$

by virtue of (7.5). The spectral radius of $\hat{K} - P_1$ is $|\lambda_2|$ and thus $\|(\hat{K} - P_1)^n g\|_v \leqslant |\lambda_2| \, \|g\|_v$. Hence, there is the following version of Kuz'min's theorem.

Theorem 4. For $f \in L^2(\mu)$ and $g \in H^2(v) \subset L^2(\mu)$, $|((U^n - P_1)f, g)| \leqslant cq^n$, with constants $c = \|f\| \, \|g\|_v$ and $q = |\lambda_2|$.

For this formulation, we have chosen one particular space of analytic functions. As it turns out, there are many versions of Kuz'min's theorem, each using some Banach space of analytic functions different from $H^2(v)$. This will be discussed in a subsequent paper when we focus on the Perron–Frobenius operator. Our goal is then to show that the eigenvalues λ_i remain the same.

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