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Finite Approximation for the Frobenius-Perron Operator. A Solution to Ulam's Conjecture*

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1. INTRODUCTION

Let τ be a function from [0, 1] into [0, 1] and let g be any meaningful physical measurement. For practical reasons, one would ask when does

$$\lim_{n\to\infty} (1/n) \sum_{k=0}^{n-1} g(\tau^k(x)) \tag{1.1}$$

exist, how does it depend on $x \in [0, 1]$, and how is the limit in (1.1) calculated if it exists?

A possible application of the above mathematical formulation is as follows [9]. An oil well drilling bit has a convex cutting tip which can pivot at high speed on the drive shaft of the drill. During operation the drill will hit and bounce off the substance being cut and recontact the surface at a different point on the tip. In order to design bits which are effectively more durable, one asks what the relative hitting frequency is for different parts of the bits surface and how the frequency distribution can be found if it exists.

A straightforward numerical way to calculate the limit in (1.1) is suggested directly by the formula (1.1) itself. Surprisingly, however, computer round-off error can completely dominate the calculation and make the implementation impossible. In this paper we give a rigorous numerical procedure, based on the Birkhoff and von Neumann ergodic theorems, which can be implemented on a computer with negligible round-off error problems. It shows how the original infinite-dimensional operator can be approximated by a finite-dimensional operator (even though the original operator is not compact). It gives, also, a solution to a published conjecture of Ulam [8, p. 75] concerning a finite approximation for the Frobenius–Perron operator (see

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Section 2). In Section 2, we use a technique introduced by Lasota and Yorke [5] to provide the theoretical background for the numerical method. In Section 3, results of computer implementation of the method are described.

2. Main Theorem

Let $X = [0, 1]$ and τ be a transformation from X into itself. The mapping $\tau: X \to X$ is not assumed to be one-to-one. For $A \subset [0, 1]$ write $\tau^{-1}(A)$ for $\{x: \tau(x) \in A\}$. We consider the average amount of time $\tau^n(x)$ spends in a set $S \subset [0, 1]$. The number of times $\tau^n(x)$ is in S for n between 0 and N is

$$\sum_{n=0}^{N} \chi_S(\tau^n(x))$$

where χ_S is the characteristic function of S, ($= 1$ on S and $= 0$ off S). The "average time" spent in S may be defined to be

$$\lim_{N\to\infty} (1/N) \sum_{n=0}^{N-1} \chi_S(\tau^n(x))$$

when this limit exists. This limit is the special case of (1.1) where $g = \chi_S$. We will say f is a *density of x for τ* if

$$\lim_{N\to\infty} (1/N) \sum_{n=0}^{N-1} \chi_S(\tau^n(x)) \qquad \text{exists and equals} \int_S f(x)\, dx \tag{2.1}$$

for every measurable set S. Notice that

$$\int_0^1 f(x)\, dx = 1$$

since $\chi_{[0,1]}(\tau^k(x)) = 1$ for all k. Frequently f is "almost" independent of x; that is, f is the density of x for τ for almost all x. The Birkhoff ergordic theorem [3, p. 18] gives a condition for f to be independent of x. First we recall some definitions. A measure μ is an *absolutely continuous measure* if and only if there is an L_1-function $f: x \to [0, \infty)$ for which $\mu(S) = \int_S f(x)\, dx$ for every Lebesgue measurable set $S \subset X$. The density in (2.1) or the corresponding measure $\mu(s) = \int_S f(x)\, dx$ for any measurable set $S \subset X$ is called *invariant* (under τ) if $\mu(\tau^{-1}(A)) = \mu(A)$ for every measurable set A. The Birkhoff ergordic theorem permits f in (1.1) to be any bounded integrable function on [0, 1]. It says that if there exists an invariant density and the density is unique, then the limit (1.1) exists for almost all x and in fact

$$\lim_{N\to\infty} (1/N) \sum_{n=0}^{N-1} g(\tau^n(x)) = \int_0^1 g(x) f(x)\, dx \tag{2.2}$$

for almost all x, that is, except for x in a set N with $\mu(N) = 0$. Therefore, if one can find the absolutely continuous invariant measure μ for τ, then the problem of finding the limit in (1.1) is transformed into computing $\int_X g\, d\mu$. To find the absolutely continuous invariant measure μ for τ, let $g = \chi_S$ in (2.2) so that

$$\mu(S) = \int_{[0,1]} \chi_S f(x)\, dx = \lim_{n\to\infty} (1/n) \sum_{k=0}^{n-1} \chi_S(\tau^k(x))$$

for almost every x in $[0, 1]$. Hence, one might choose almost any x in $[0, 1]$ and calculate the average time for iterations $\tau^k(x)$ to recur in S. But the following example shows that numerical round-off errors can completely dominate the calculation, making invalid the use of a computer in this approach.

EXAMPLE 2.1. For a positive integer k, define τ on $[0, 1]$ by $\tau(x) = 2kx \pmod 1$.

This is the simplest nontrivial example of ergodic theory. Here the Lebesgue measure is the only absolutely continuous invariant measure (Halmos [3, p. 6]). But for this τ, any $x \geqslant 2^{-k}$ stored in a binary system of n bits will lead to $\tau^m(x) = 0$ for all $m \geqslant n + k$. Thus, any subset of $[0, 1]$ containing 0 will have measure 1 and others have measure 0. This obviously is not an absolutely continuous measure.

This example's difficulties are generated by the property of the number 2, but other general functions τ give similar difficulties. The following approach is based on the von Neumann ergodic theorem. For this method round-off errors are not significant in practice.

Denote by $(L_1, \|\cdot\|)$ the space of all integrable functions defined on the interval $[0, 1]$. Lebesgue measure on $[0, 1]$ will be denoted by m. Let $\tau: [0, 1] \to [0, 1]$ be a *nonsingular* measurable transformation, i.e., for any measurable subset of A with $m(A) = 0$, we have $m(\tau^{-1}(A)) = 0$. Rechard [7] introduced the transformation P_τ of L_1 into itself defined by the formula

$$(P_\tau f)(x) = (d/dx) \int_{\tau^{-1}([0,x])} f(s)\, ds.$$

This is known as the Frobenius–Perron operator and is defined when τ is nonsingular. We study P_τ here because if there exists $f \in L_1$ with $P_\tau f = f$ then the measure $\mu = \int f\, dm$ is invariant under τ. Thus, to calculate invariant measures for τ, we may calculate instead the fixed points of the Frobenius–Perron operator. More precisely, we need $P_\tau f = f$ almost everywhere (with respect to Lebesgue measure). From now on we will sometimes omit mention of such sets of Lebesgue measure 0.

A transformation τ: $[0, 1] \to R$ will be called *piecewise* C^2, if there exists a partition $0 = b_0 < b_1 < \cdots < b_p = 1$ of the unit interval such that for each integer k ($k = 1,..., p$) the restriction τ_k of τ to the open interval (b_{k-1}, b_k) is a C^2-function which can be extended to the closed interval $[b_{k-1}, b_k]$ as a C^2-function. τ need not be continuous at the point b_k.

Let the unit interval $[0, 1]$ be divided into n equal subintervals $I_1, I_2,..., I_n$, with $I_i = [a_{i-1}, a_i]$ and $m(I_i) = 1/n = l$ for $i = 1,..., n$. Define P_{ij} as the fraction of interval I_j which is mapped into interval I_i by τ, i.e.,

$$P_{ij} = m(I_i \cap \tau^{-1}(I_j))/m(I_i). \tag{2.3}$$

Let Δ_n be the n-dimensional linear subspace of L_1 which is the finite element space generated by $\{\chi_i\}_{i=1,...,n}$ where χ_i denotes the characteristic function for the interval I_i. Define $P_n(\tau)$: $\Delta_n \to \Delta_n$ by

$$P_n(\tau)\,\chi_i = \sum_{j=1}^{n} P_{ij}\chi_j\,. \tag{2.4}$$

We shall often write P_n for $P_n(\tau)$ when no clarification is needed. Ulam conjectured [8, p. 75] that the sequence of fixed points f_n of P_n should converge to a fixed point of P_τ as $n \to \infty$ when P_τ has a unique fixed point (up to linear independence). The following theorem gives a positive answer to this conjecture.

THEOREM 1. *Let* τ: $[0, 1] \to [0, 1]$ *be a piecewise* C^2*-function with* $M = \inf |\tau'| > 2$. *Suppose* P_τ *has a unique fixed point. Then, for any positive integer* n, P_n *has a fixed point* f_n *in* Δ_n *with* $\|f_n\| = 1$ *and* $\{f_n\}$ *converges to the fixed point of* P_τ.

Remark. In Theorem 1 we suppose P_τ has a *unique* fixed point (up to linear independence) which is usually the case in practice. In [2], Li and Yorke give a sufficient condition for the uniqueness of this kind of fixed point. If the fixed point of P_τ is not unique, then the closure of the set of fixed points of P_τ is always a convex hull of a finite set. The proof of Theorem 1 actually shows, even if the fixed point of P_τ is not unique, that there exists a relatively compact set C of fixed points of P_τ such that $d(f_n, \bar{C}) \to 0$ in L_1. So, for large n, every f_n approximates an absolutely continuous invariant measure of τ.

The following corollary shows that we can also obtain fixed points indirectly when $2 \geqslant M > 1$. Notice

$$P_{\tau^i} = (P_\tau)^i.$$

COROLLARY OF THEOREM 1. *Assume $M > 1$. Suppose P_τ has a unique fixed point. Let k be an integer such that $M^k > 2$. Let $\phi = \tau^k$ and f_n be a fixed point of $P_n(\phi)$. Let $g_n = (1/k) \sum_{i=0}^{k-1} P_{\tau^i} f_n$. Then $\{g_n\}$ converges in L_1 to the fixed point of P_τ.*

Proof. Since P_{τ^i} is continuous for all i, by Theorem 1, $g_n \to g = (1/k) \sum_{i=0}^{k-1} P_{\tau^i} f$ in L_1 as $n \to \infty$. Therefore,

$$P_\tau g = (1/k) \sum_{i=1}^{k} (P_\tau)^i f = (1/k) \sum_{i=0}^{k} (P_\tau)^i f = g. \quad \blacksquare$$

Before proving Theorem 1, we prove a sequence of lemmas. The following lemma indicates P_τ is invariant on some compact subset of Δ_n.

LEMMA 2.1. *Let $\Delta_n^1 = \{\sum_{i=1}^n a_i \chi_i : a_i \geqslant 0$ and $\sum_{i=1}^n a_i = 1\}$. Then P_n maps Δ_n^1 to a subset of Δ_n^1.*

Proof. Let $f = \sum_{i=1}^n a_i \chi_i$. Then $f \in \Delta_n^1$ and

$$P_n f = P_n \left(\sum_{i=1}^n a_i \chi_i \right) = \sum_{i=1}^n a_i (P_n \chi_i) = \sum_{j=1}^n \left(\sum_{i=1}^n a_i P_{ij} \right) \chi_i .$$

But,

$$\sum_{j=1}^n P_{ij} = \sum_{j=1}^n \frac{m(I_i \cap \tau^{-1}(I_j))}{m(I_i)} = 1 \qquad \text{for all } i = 1,..., n. \tag{2.5}$$

Hence,

$$\sum_{j=1}^n \left(\sum_{i=1}^n a_i P_{ij} \right) = \sum_{i=1}^n a_i \left(\sum_{j=1}^n P_{ij} \right) = \sum_{i=1}^n a_i = 1.$$

Therefore, $P_n f \in \Delta_n^1$. $\blacksquare$

Since $P_n(\Delta_n^1) \subset \Delta_n^1$ is a compact convex set there exists, by the Brouwer fixed point theorem, a point $g_n \in \Delta_n^1$ for which $P_n g_n = g_n$. Let $f_n = n g_n$. Then $f_n \in \Delta_n$ and $\|f_n\| = 1$ for all n. To prove $\{f_n\}$ converges, we first show some relations between P_n and P_τ by introducing the operator Q_n.

DEFINITION 2.1. For $f \in L_1$, and for every positive integer n we define $Q_n: L_1 \to \Delta_n$ by

$$Q_n f = \sum_{i=1}^n c_i \chi_i \qquad \text{where} \quad c_i = \frac{1}{m(I_i)} \int_{I_i} f(s)\, ds$$

LEMMA 2.2. *For $f \in L_1$, the sequence $Q_n f$ converges in L_1 to f as $n \to \infty$.*

Proof. Since $f \in L_1$, for any $\epsilon > 0$ there exists a continuous function g such that $\| g - f \| < \epsilon/3$. Since g is continuous in $[0, 1]$, g is uniformly continuous. We may choose N large enough such that for $n > N$, we have $| g(x_1) - g(x_2)| < \epsilon/3$ for all x_1, x_2 in I_i, $i = 1,..., n$. It follows that,

$$\begin{aligned}\int_{I_i} |(Q_n g)(s) - g(s)|\, ds &= \int_{I_i} \left| (1/m(I_i)) \int_{I_i} g(s')\, ds' - g(s) \right| ds \\ &\leqslant \int_{I_i} (1/m(I_i)) \left(\int_{I_i} | g(s') - g(s)|\, ds' \right) ds \\ &\leqslant m(I_i) \times \epsilon/2.\end{aligned}$$

Hence,

$$\| Q_n g - g \| = \int_0^1 | Q_n g - g | = \sum_{i=1}^{n} \int_{I_i} | Q_n g - g | < \epsilon/3.$$

On the other hand, for $f \geqslant 0$

$$\begin{aligned}\int_0^1 Q_n f &= \int_0^1 \sum_{i=1}^{n} \left((1/m(I_i)) \int_{I_i} f(s)\, ds \right) \chi_i(s')\, ds' \\ &= \sum_{i=1}^{n} \int_{I_i} f(s)\, ds = \int_0^1 f.\end{aligned}$$

Therefore, $\| Q_n \| = 1$ and hence,

$$\begin{aligned}\| Q_n f - f \| &\leqslant \| Q_n f - Q_n g \| + \| Q_n g - g \| + \| g - f \| \\ &< \epsilon/3 + \epsilon/3 + \epsilon/3 = \epsilon. \quad \blacksquare\end{aligned}$$

The following lemma gives the key relation between P_n and P_τ.

LEMMA 2.3. *For f in Δ_n we have $P_n f = Q_n P_\tau f$.*

Proof. We only need to show $P_n \chi_i = Q_n P_\tau \chi_i$ for $1 \leqslant i \leqslant n$. Since

$$(P_\tau \chi_i)(x) = (d/dx) \int_{\tau^{-1}([0,x])} \chi_i(s)\, ds$$

we have

$$\begin{aligned}Q_n(P_\tau \chi_i) &= \sum_{j=1}^{n} \left[\frac{1}{m(I_j)} \int_{I_j} \left(\frac{d}{dx} \int_{\tau^{-1}([0,x])} \chi_i(s)\, ds \right) dx \right] \chi_j \\ &= \sum_{j=1}^{n} \left[\frac{1}{m(I_j)} \int_{\tau^{-1}(I_j)} \chi_i(s)\, ds \right] \chi_j \\ &= \sum_{j=1}^{n} \frac{m(I_i \cap \tau^{-1}(I_j))}{m(I_i)} \chi_j = \sum_{j=1}^{n} P_{ij} \chi_j = P_n \chi_i .\end{aligned}$$

By direct application of Lemmas 2.2, and 2.3 we have the following.

LEMMA 2.4. *For f in Δ_n, the sequence $P_n f$ converges to $P_\tau f$ in L_1 as $n \to \infty$.*

We now show the convergence of $\{f_n\}$. We will use the technique introduced by Lasota and Yorke [5]. They indicated in their paper (see the following lemma) that the Frobenius–Perron operator P_τ under consideration has the property of occasionally "shrinking" the variation of the function. In Lemma 2.6 we show P_n also has this property by first showing that the operator Q_n always shrinks the variation of the function.

DEFINITION 2.2. For $f \in L_1$, we use $V_a{}^b f$ as well as $V_{[a,b]} f$ to denote the variation of f over the closed interval $[a, b]$.

LEMMA 2.5 (Lasota–Yorke [5]). *Let $0 = b_0 < b_1 < \cdots < b_q = 1$ be the partition of $[0, 1]$ for which the restriction τ_j of τ to the interval (b_{j-1}, b_j) is a C^2-function for every $1 \leqslant j \leqslant q$. Let $\psi_j = \tau_j^{-1}$, $\sigma_j(x) = |\psi_j'(x)|$, $h = \min_{1 \leqslant j \leqslant p} (d_j - d_{j-1})$, and $k = \max |\sigma_j'|/\min(\sigma_j)$. Suppose $\| \tau' \| > 2$. Then, for $f \in L_1$*

$$V_0{}^1 P_\tau f \leqslant \alpha \|f\| + \beta V_0{}^1 f$$

where $\alpha = K + h^{-1}$ and $\beta = 2(\inf |\tau'|)^{-1} < 1$.

LEMMA 2.6. *If $f \in L_1$, $V_0{}^1 Q_n f \leqslant V_0{}^1 f$.*

Proof. Let $c_i = (1/l) \int_{I_i} f$ then

$$V_0{}^1 Q_n f = V_0{}^1 \left(\sum_{i=1}^{n} c_i \chi_i \right) = \sum_{i=1}^{n} (1/l) \left| \int_{I_i} f - \int_{I_{i+1}} f \right|.$$

For every $1 \leqslant i \leqslant n$, there exist m_i and M_i in $[a_{i-1}, a_i]$ such that

$$f(m_i) \leqslant (1/l) \int_{I_i} f \leqslant f(M_i).$$

For simplicity we assume $m_i \leqslant M_i$ for all i, the other cases being almost identical. There are two cases to consider, first

$$\frac{1}{l} \int_{I_i} f < \frac{1}{l} \int_{I_{i+1}} f.$$

and second, the same equation with the inequality reversed. For case 1

$$\left| \frac{1}{l} \int_{I_i} f - \frac{1}{l} \int_{I_i} f \right| \leqslant |f(m_i) - f(M_{i+1})|$$
$$\leqslant |f(m_i) - f(M_i)| + |f(M_i) - f(m_{i+1})| + |f(m_{i+1}) - f(M_{i+1})|,$$

While for case 2,

$$\left|\frac{1}{l}\int_{I_i} f - \frac{1}{l}\int_{I_{i+1}} f\right| \leqslant |f(M_i) - f(m_{i+1})|.$$

Hence, in either case, we have

$$\begin{aligned} V_0^1 Q_n f &\leqslant \sum_{i=1}^{n} (|f(m_i) - f(M_i)| + |f(M_i) - f(m_{i+1})| + |f(m_{i+1}) - f(M_{i+1})|) \\ &\leqslant V_0^1 f. \quad \blacksquare \end{aligned}$$

LEMMA 2.7. *The sequence* $\{V_0^1 f_n\}$ *is bounded.*

Proof. By Lemma 2.3, $f_n = P_n f_n = Q_n P_\tau f_n$ for all n, hence by Lemma 2.6,

$$\begin{aligned} V_0^1 f_n &= V_0^1 Q_n P_\tau f_n \leqslant V_0^1 P_\tau f_n \\ &\leqslant (K + h^{-1}) + \beta V_0^1 f_n \qquad \text{(by Lemma 2.5).} \end{aligned}$$

Since $V_0^1 f_n < \infty$, we have $V_0^1 f_n \leqslant (K + h^{-1})/(1 - \beta)$. $\blacksquare$

Proof of Theorem 1. It follows from Lemma 2.7 and Helly's theorem [6], that the set $C = \{f_n : n = 1, 2,...\}$ is relatively compact. Let $\{f_{n_i}\}$ be any convergent subsequence of C and let $f = \lim_{i\to\infty} f_{n_i}$. Then

$$\begin{aligned} \|f - P_\tau f\| \leqslant \|f - f_{n_i}\| &+ \|f_{n_i} - Q_{n_i} P_\tau f_{n_i}\| \\ &+ \|Q_{n_i} P_\tau f_{n_i} - Q_{n_i} P_\tau f\| + \|Q_{n_i} P_\tau f - P_\tau f\|. \end{aligned}$$

Taking into account that f_{n_i} is a fixed point of P_{n_i}, Lemma 2.2 implies that the right-hand side of above inequality tends to zero when n_i tends to infinity. Hence, $f = P_\tau f$. Therefore, any convergent subsequence of C converges to a fixed point of P_τ. By assumption, P_τ has a unique fixed point, hence, $\lim_{n\to\infty} f_n = f$. $\blacksquare$

3. COMPUTATIONAL RESULTS

Consider the simple transformation of the form:

$$\begin{aligned} \tau(x) &= 2x & 0 \leqslant x \leqslant \tfrac{1}{2} \\ \tau(x) &= (2 - a) + (a - 1)x & \tfrac{1}{2} \leqslant x \leqslant 1 \end{aligned}$$

where $0 < a < \frac{1}{2}$. In [8, p. 75] Ulam pointed out that it was not known even in this simple case whether the corresponding Frobenius–Perron operator has an invariant function. Existence was established in [5]. In this section, we discuss the computational results for this example using the method we introduced in Section 2. Then we compare them with the results using the iterative approach for trying to find the invariant measures.

As in Section 2, we divide [0, 1] into n equal subintervals $I_i = [a_{i-1}, a_i]$ and $m(I_i) = 1/n = l$ for $i = 1,..., n$ and define P_{ij} and P_n as in (2.3) and (2.4). We may denote P_n by the matrix $\pi_n = (P_{ij})$.

Remark. From (2.3) and (2.4), the matrix π_n has the following properties:

$$P_{ij} \geqslant 0 \qquad \text{for all} \quad 1 \leqslant i, j \leqslant n. \tag{3.1}$$

The sum of each row is equal to 1. (3.2)

Matrices satisfying (3.1) and (3.2) are known as *stochastic matrices* [1, 4]. There exist several ways to calculate the fixed points of stochastic matrices. The most efficient one is to use quadratic programming to minimize $| x\pi_n - x |^2$ with the constraints

$$x_i \geqslant 0 \qquad \text{and} \qquad \sum_{i=1}^{n} x_i = 1.$$

Other methods are also rather fast for cases we investigated, usually $n \leqslant 30$.

For $a = \frac{1}{4}$ and n even the computation result indicates that the fixed points f_n of P_n with $\|f_n\| = 1$ equal to f when $n \geqslant 4$ where

$$\begin{aligned} f(x) &= 0, && \text{for} \quad 0 \leqslant x < \tfrac{1}{4} \\ &= 1, && \text{for} \quad \tfrac{1}{4} \leqslant x < \tfrac{1}{2} \\ &= 1.5, && \text{for} \quad \tfrac{1}{2} \leqslant x \leqslant 1. \end{aligned}$$

It is easily verified that, indeed, $P_\tau f = f$. So, f is not only a fixed point of P_n with $n > 4$ but also of P_τ and the method gives exact results in this case.

In addition to the convergence difficulties described in Section 2, the straightforward iteration method using (2.2) converges at best slowly. We compare the iteration method using 10,000 iterates for $a = \frac{1}{4}$. We choose 10,000 iterations because it takes about the same execution time (about 1 second on the Univac 1106) as the above computation for $n = 20$. For the invariant measure, the intervals (.25, .30), (.30, .35),..., (.45, .50) all have measure .050. But using 10,000 iterations we get one estimate as high as .058 and one estimate as low as .044. We may use a heuristic estimate to explain the slow convergence. Suppose the measure of an interval J is p using the invariant measure. Heuristically we now consider a sequence x_n of independent random points each of whose probability for lying in J is p. The expected number of x_n, $n = 1,..., N$, lying in J is Np and the standard deviation is $(p(1-p)N)^{1/2}$. If we want the standard deviation to be less than 1% of Np then

$$(p(1-p)N)^{1/2}/Np = .01$$

and $N = 10^4(1-p)p$. For $p = .050$, $N \simeq 200{,}000$. Hence for an estimate for p to be likely to be between $.99p$ and $1.01p$ we must use about 200,000 iterates.

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