

An Elementary Approach to Rigorous Approximation of Invariant Measures*

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Abstract. We describe a framework in which it is possible to develop and implement algorithms for the approximation of invariant measures of dynamical systems with a given bound on the error of the approximation. Our approach is based on a general statement on the approximation of fixed points for operators between normed vector spaces, allowing an explicit estimation of the error. We show the flexibility of our approach by applying it to piecewise expanding maps and to maps with indifferent fixed points. We show how the required estimations can be implemented to compute invariant densities up to a given error in the L^1 or L^∞ distance. We also show how to use this to compute an estimation with certified error for the entropy of those systems. We show how several related computational and numerical issues can be solved to obtain working implementations and experimental results on some one dimensional maps.

Key words. approximation of invariant measure, transfer operator, fixed point approximation, Lyapunov exponent, interval arithmetics

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1. Introduction.

Overview. Several important features of the statistical behavior of a dynamical system are “encoded” in invariant measures, and in particular in the so-called *physical invariant measures*. These measures represent the statistical behavior of a large set of initial conditions. Having quantitative information on these measures can give information on the statistical behavior for the long time evolution of the system.

The problem of the existence and properties of such invariant measures has become a central area of research in the modern theory of dynamical systems. For the most part the results are abstract and give no quantitative precise information on the measure. This is a significant limitation in applications and strongly motivates the search for algorithms which are able to compute quantitative information on the physical measure.

The problem of approximating some interesting invariant measure of dynamical systems has been quite widely studied in the literature. Some algorithms are proved to converge to the real invariant measure (up to errors in some given metrics) in some classes of systems.

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Sometimes asymptotical estimates on the rate of convergence are provided (see, e.g., [10, 11, 8, 9, 5, 27, 13]), but results giving an explicit (rigorous) bound on the error are relatively few (see e.g., [25, 3, 22, 28, 19]).

Most of the known results thus do not provide a rigorous bound on the error which is made in the approximation. In this way, the result of a single (finite) computation such as those we can perform on everyday computers does not have a precise mathematical meaning. If we implement an approach providing such explicit bounds, the results of suitable, careful computations can be interpreted as rigorously (computer-aided) proved statements on the behavior of the observed system.

In this paper we describe an approach which is able to provide algorithms to approximate interesting invariant measures with a precise bound on the error and its practical implementation. The approach is quite general and is based on a quantitative statement on the stability of fixed points of operators under suitable approximations. In our approach we focus on the estimations which are important in computing fixed points (rather than the whole spectral picture, as in [22]) in a way that we can keep our estimations as sharp as possible, trying also to use as much as possible the information that can be recovered by a suitable (and computable) finite dimensional approximation of the problem. The practical implementation of the method and the necessary precise estimates are described here at various levels of generality, arriving at a complete implementation for a class of piecewise expanding maps and a class of maps with an indifferent fixed point. We perform the estimates for the computation of the invariant measure up to small errors in the L^1 norm in these cases, and also with small errors in the L^∞ norm for a class of piecewise expanding maps with higher regularity. We also present some real computer experiments, performing the rigorous computation on interval maps, and our solution to the nontrivial computational/numeric issues that arise.

We end by remarking that general, abstract results on the computability of invariant measures are given in [15] (see also [14]). In these papers some negative results are also shown. Indeed, *there are examples of computable¹ systems without any computable invariant measure*. This shows some subtlety in the general problem of computing the invariant measure up to a given error.

Plan of the paper. In section 3 we show a general result regarding the approximation of fixed points for linear operators between normed spaces. In this result fixed points are approximated by extracting and exploiting as much information as possible from the approximating operator. This general statement is suitable for application to the Ulam approximation method and other discretizations. In section 4 we show how this can be done, and we show an algorithm for the approximation of invariant measures up to small errors in the L^1 norm for the case of piecewise expanding maps (with bounded derivative).

In section 6 we show how, in suitably regular systems, we can use a similar construction to compute the invariant measure, up to small errors in the L^∞ norm.

In section 7 we show how to apply the approach to a class of maps with indifferent fixed points.

In section 8 we show how to implement the algorithms in practice. In particular, we have

¹“Computable” here means that the dynamics can be approximated at any accuracy by an algorithm; see, e.g., [15] for a precise definition.

to show a way to rapidly compute the steady state of a large Markov chain up to a prescribed error. We also discuss several other computational and programming issues, explaining how we have implemented the algorithm to perform real rigorous computations on some examples of piecewise expanding maps.

In section 9, as an application we show a rigorous estimation of the entropy (by the Lyapunov exponent) of such maps. These estimations can be used as a benchmark for the validation of statistical methods to compute entropy from time series.

In section 10 we show the result of some experiments. Here the invariant measure is computed up to an error of less than 1% with respect to the L^1 distance, while in section 11 we show an experiment in the L^∞ framework.

2. Invariant measures and transfer operator. Let X be a metric space, $T : X \mapsto X$ a Borel measurable map, and μ a T -invariant Borel probability measure. An invariant measure is a Borel probability measure μ on X such that for each measurable set A it holds that $\mu(A) = \mu(T^{-1}(A))$.

A set A is called T -invariant if $T^{-1}(A) = A \pmod{0}$. The system (X, T, μ) is said to be ergodic if each T -invariant set has total or null measure. In such systems the well-known Birkhoff ergodic theorem says that for any $f \in L^1(X, \mu)$ it holds that

$$(2.1) \quad \lim_{n \rightarrow \infty} \frac{S_n^f(x)}{n} = \int f \, d\mu$$

for μ almost each x , where $S_n^f = f + f \circ T + \dots + f \circ T^{n-1}$.

We say that a point x belongs to the basin of an invariant measure μ if (2.1) holds at x for each bounded continuous f . In case X is a manifold (possibly with a boundary), a physical measure is an invariant measure whose basin has positive Lebesgue measure (for more details and a general survey see [29]).

The transfer operator. Let us consider the space $SM(X)$ of Borel measures with sign on X . A function T between metric spaces naturally induces a function $L : SM(X) \rightarrow SM(X)$ which is linear and is called the transfer operator (associated to T). Let us define L : if $\mu \in SM(X)$, then $L[\mu]$ is such that

$$L[\mu](A) = \mu(T^{-1}(A)).$$

Measures which are invariant for T are fixed points of L ; hence the computation of invariant measures can be done by computing the fixed points of this operator (restricted to a suitable Banach subspace where the interesting invariant measure is supposed to be). The most applied and studied strategy is to find a finite dimensional approximation for L reducing the problem to the computation of the corresponding relevant eigenvectors of a finite matrix (some examples are in sections 4 and 6.2). An approach to estimating the distance between a fixed point of a discretization and a fixed point for the real operator can be based on quantitative spectral stability results given in [18]. The method requires some estimation (see [22]) which cannot be trivially done in a rigorous way in a reasonable time. The approach we explain below requires simpler assumptions and estimations; moreover a portion of the required estimations will be done by the computer.

3. A general statement on the approximation of fixed points. Let us consider a restriction of the transfer operator to an invariant normed subspace (often a Banach space of measures having some regularity) $\mathcal{B} \subseteq SM(X)$, and let us denote its norm as $\|\cdot\|_{\mathcal{B}}$. Let us still denote the restricted transfer operator by $L: \mathcal{B} \rightarrow \mathcal{B}$. Suppose it is possible to approximate L in a suitable way by another operator L_{δ} for which we can calculate fixed points and other properties. We suppose $\delta \in \mathbb{R}$ is a parameter measuring the accuracy of the approximation (e.g., the size of a grid).

Our extent is to exploit as much as possible the information contained in L_{δ} to approximate fixed points of L . Let us hence suppose that $f, f_{\delta} \in \mathcal{B}$ are fixed points, respectively, of L and L_{δ} .

Theorem 3.1. *Suppose that*

- (a) $\|L_{\delta}f - Lf\|_{\mathcal{B}} < \infty$,
- (b) $\exists N$ such that $\|L_{\delta}^N(f_{\delta} - f)\|_{\mathcal{B}} \leq \frac{1}{2}\|f_{\delta} - f\|_{\mathcal{B}}$, and
- (c) L_{δ}^i is continuous on \mathcal{B} ; $\exists C_i$ s.t. for all $g \in \mathcal{B}$, $\|L_{\delta}^i g\|_{\mathcal{B}} \leq C_i \|g\|_{\mathcal{B}}$.

Then

$$(3.1) \quad \|f_{\delta} - f\|_{\mathcal{B}} \leq 2\|L_{\delta}f - Lf\|_{\mathcal{B}} \sum_{i \in [0, N-1]} C_i.$$

Remark 3.2. *We remark that the estimation for the error computed in (3.1) is an estimation which contains quantities coming from the three items (a), (b), and (c). To use the theorem we have to estimate the relevant quantities in each of these items. In the applications of the theorem we present in the following, (a) will be estimated a priori by the same way the approximating operator is defined and related to the quality of the approximation. The size of $\|L_{\delta}f - Lf\|_{\mathcal{B}}$ will be small if the approximation is good in some sense.*

The quantities N and C_i related to items (b) and (c) can be computed from the behavior of the iterates of the approximating operator; this can be done by the computer while running the algorithm. Hence these will be a posteriori estimations. In our applications, the required N will be calculated from a description of L_{δ} , which will be a finite rank operator. As $(L_{\delta} - L)f$ belongs to the space V of zero total mass measures ($V = \{\mu \text{ s.t. } \mu(X) = 0\}$), N can be estimated by computing the norm of iterates of L_{δ} restricted to V (see section 4.1 for more details). Since the contraction speed of the zero average space is related to the speed of decay of correlations, this can be seen as a “finite resolution decay of correlation estimation.” This replaces some a priori estimations on the decay of correlation of the real system which are needed in some other approaches. Note that (b) also means that there is no “projection” of f on other fixed points of L_{δ} aside from f_{δ} .

We also remark that the assumptions required on the operators L, L_{δ} are quite weak; in particular, they are not required to satisfy some particular Lasota–Yorke (LY) inequality.

Proof of Theorem 3.1. The proof is a direct computation from the assumptions

$$\begin{aligned} \|f_{\delta} - f\|_{\mathcal{B}} &\leq \|L_{\delta}^N f_{\delta} - L^N f\|_{\mathcal{B}} \\ &\leq \|L_{\delta}^N f_{\delta} - L_{\delta}^N f\|_{\mathcal{B}} + \|L_{\delta}^N f - L^N f\|_{\mathcal{B}} \\ &\leq \|L_{\delta}^N(f_{\delta} - f)\|_{\mathcal{B}} + \|L_{\delta}^N f - L^N f\|_{\mathcal{B}} \\ &\leq \frac{1}{2}\|f_{\delta} - f\|_{\mathcal{B}} + \|L_{\delta}^N f - L^N f\|_{\mathcal{B}} \end{aligned}$$

(applying item (b)). Hence

$$\|f_\delta - f\|_{\mathcal{B}} \leq 2\|L_\delta^N f - L^N f\|_{\mathcal{B}},$$

but

$$L_\delta^N - L^N = \sum_{k=1}^N L_\delta^{N-k} (L_\delta - L) L^{k-1};$$

hence

$$\begin{aligned} (L_\delta^N - L^N)f &= \sum_{k=1}^N L_\delta^{N-k} (L_\delta - L) L^{k-1} f \\ &= \sum_{k=1}^N L_\delta^{N-k} (L_\delta - L) f \end{aligned}$$

by item (c); hence

$$\begin{aligned} \|(L^N - L_\delta^N)f\|_{\mathcal{B}} &\leq \sum_{k=1}^N C_{N-k} \|(L_\delta - L)f\|_{\mathcal{B}} \\ &\leq \|(L_\delta - L)f\|_{\mathcal{B}} \sum_{i \in [0, N-1]} C_i \end{aligned}$$

by item (a); and then

$$\|f_\delta - f\|_{\mathcal{B}} \leq 2\|(L_\delta - L)f\|_{\mathcal{B}} \sum_{i \in [0, N-1]} C_i. \quad \blacksquare$$

Remark 3.3. We remark that by the above proof, the factor 2 in (3.1) can be reduced as near as wanted to 1 by putting at item (b) a factor smaller than $\frac{1}{2}$. Moreover, the coefficients C_i can be replaced by the operator norm of L_δ^i restricted to V .

4. Estimation with L^1 norm and Ulam method. We now give an example of application of the above general result to the approximation of invariant measures of dynamical systems up to small errors in the L^1 norm with the Ulam method, going into more detail for this case. Let us briefly recall the basic notions about the Ulam method. Let us suppose now that X is a manifold with boundary. In the *Ulam discretization* method the space X is discretized by a partition I_δ (with k elements), and the system is approximated by a (finite state) Markov chain with transition probabilities

$$(4.1) \quad P_{ij} = m(T^{-1}(I_j) \cap I_i) / m(I_i)$$

(where m is the normalized Lebesgue measure on X) and a corresponding finite dimensional operator L_δ (L_δ depends on the whole chosen partition, but to simplify notation we will indicate it with a parameter δ related to the size of the elements of the partition). We remark that, in this way, to L_δ corresponds a matrix $P_k = (P_{ij})$.

We remark that L_δ can be seen in the following way: let F_δ be the σ -algebra associated to the partition I_δ ; then

$$(4.2) \quad L_\delta(f) = \mathbf{E}(L(\mathbf{E}(f|F_\delta))|F_\delta)$$

(see also [22, notes 9–10] for some more explanations). Taking finer and finer partitions, in certain systems the finite dimensional model converges to the real one and its natural invariant measure to the physical measure of the original system; see, e.g., [5, 12, 13, 22].

In the remaining part of this section we explain how to apply Theorem 3.1 to have an explicit estimation for the approximation error in a more concrete case: L^1 estimations with Ulam discretization. Hence we suppose that

- L_δ is the Ulam approximation of L as defined above,
- $\mathcal{B} = L^1(X)$,² and
- there is an estimation for the regularity of f compatible with the approximation procedure (to have the estimation needed at item (a) of Theorem 3.1).

As an example to explain this latter point, the norm $\|f\|_{\mathcal{B}'}$ can be estimated (in some space \mathcal{B}' of regular measures), and there is an estimation for the norm $\|L_\delta - L\|_{\mathcal{B}' \rightarrow L^1}$ (where $\|\cdot\|_{\mathcal{B}' \rightarrow L^1}$ is the operator norm, as an operator $\mathcal{B}' \rightarrow L^1$).

In this way, the estimate required at item (a) of Theorem 3.1 can be given as

$$(4.3) \quad \|L_\delta f - Lf\|_{L^1} \leq \|L_\delta - L\|_{\mathcal{B}' \rightarrow L^1} \|f\|_{\mathcal{B}'},$$

and we could bound the final error as

$$\|f_\delta - f\|_{L^1} \leq 2 \sum_0^{N-1} C_i \|L_\delta - L\|_{\mathcal{B}' \rightarrow L^1} \|f\|_{\mathcal{B}'}$$

The estimation of $\|f\|_{\mathcal{B}'}$ is possible, for example, when L satisfies an LY inequality (see, e.g., [1, 21, 16] and Theorem 5.2) of the type

$$(4.4) \quad \|L^n g\|_{\mathcal{B}'} \leq \lambda^n \|g\|_{\mathcal{B}'} + B \|g\|_{L^1},$$

implying $\|f\|_{\mathcal{B}'} \leq B$.

Hence, considering these remarks, in certain classes of examples the estimations needed to apply Theorem 3.1 can be implemented in a sequence of steps we outline below, and which will be described in more detail in the following sections.

- I1. A suitable estimation for the regularity of f can be provided by the coefficients of the LY inequality (see also section 5.0.1) or by other techniques, such as invariant cones (see section 7).
- I2. An approximation inequality can be provided to satisfy item (a) of Theorem 3.1; for example, $\|L_\delta - L\|_{\mathcal{B}' \rightarrow L^1}$ is estimated a priori by the method of approximation (see section 5.0.2).

²To be more precise, we suppose \mathcal{B} to be the space of absolutely continuous measures on X . We will informally identify a measure of this kind with its density.

I3. The integer N relative to item (b) in Theorem 3.1 can be estimated by the matrix P_k relative to L_δ (see section 4.1).

I4. Since $\mathcal{B} = L^1(X)$ and we consider the Ulam approximation, $C_i = 1$ (see section 5.0.3).

Now let us discuss more precisely item I3, which is central in this approach and whose discussion is general. We discuss the other items in section 5, with precise estimations related to a particular family of cases: the piecewise expanding maps.

4.1. About item I3. To compute N we consider $V = \{\mu \in \mathcal{B} | \mu(X) = 0\}$ and $\|L_\delta^n|_V\|_{L^1 \rightarrow L^1}$. Since $f - f_\delta \in V$, if we prove

$$\|L_\delta^n|_V\|_{L^1 \rightarrow L^1} < \frac{1}{2},$$

we imply item (b) of Theorem 3.1. In the Ulam approximation, L_δ is a finite rank operator; hence, once we fix a basis, this is given by a matrix.

For the sake of simplicity we will suppose that all sets I_j have the same measure: $m(I_j) = 1/k$. This will simplify some notation.

The natural basis $\{f_1, \dots, f_k\}$ to consider is the set of characteristic functions of the sets in the partition I_δ . If $I_\delta = \{I_1, \dots, I_k\}$, then $f_i = \frac{1}{\delta} 1_{I_i}$; after the choice of this basis, the set of linear combinations of such characteristic functions can be identified with \mathbb{R}^k . By a slight abuse of notation we will also indicate by V the set of zero average vectors in \mathbb{R}^k .

To determine N we have to consider the matrix $P_k|_V$ associated to the action of L_δ on the space of zero mean vectors with respect to this basis and compute its operator norm $\|P_k|_V\|_1$ where³

$$\|P_k|_V\|_1 = \sup_{|v|_1=1} |P(v)|_1.$$

By (4.2) the behavior of L_δ and its relation with P_k is described by

$$f \xrightarrow{\mathbf{E}|_{F_\delta \circ I^{-1}}} v \xrightarrow{P_k} v' \xrightarrow{I} f' = L_\delta(f),$$

where $I: \mathbb{R}^k \rightarrow L^1$ is the trivial identification of a vector in \mathbb{R}^k with a piecewise constant function given by the choice of the basis. This implies that

$$\|L_\delta\|_{L^1 \rightarrow L^1} \leq \|P_k\|_1.$$

Indeed, if $f \in L^1$, $\|\mathbf{E}(f|F_\delta)\|_{L^1} \leq \|f\|_{L^1}$ and I is trivially an isometry.

Note that if $\int f dm = 0$, then $\int E(f|F_\delta) dm = 0$ and conversely, and hence

$$\|L_\delta|_V\|_{L^1} \leq \|P_k|_{I^{-1}(V)}\|_1.$$

Since each vector is represented by a suitable step function, then $\|L_\delta|_V\|_{L^1} = \|P_k|_{I^{-1}(V)}\|_1$.

The matrix corresponding to L_δ^N is P_k^N . Then

$$\|L_\delta^N|_V\|_{L^1} = \|P_k^N|_{I^{-1}(V)}\|_1.$$

Summarizing, we can have an estimation of $\|L_\delta^N|_V\|_{L^1 \rightarrow L^1}$ by computing a matrix $\tilde{P}_{k,V}^N$ approximating $P_k|_{I^{-1}(V)}$ and $\|\tilde{P}_{k,V}^N\|_1$.

³ $|\cdot|_1$ will denote the L^1 norm on \mathbb{R}^n .

The algorithm will hence compute $\|\tilde{P}_{k,V}^j\|_1$ for each integer $j > 0$, computing $\tilde{P}_{k,V}^j$ iteratively from $\tilde{P}_{k,V}^{j-1}$, until it finds some j for which it can deduce $\|P_k^N|_{I^{-1}(V)}\|_1 < \frac{1}{2}$. This j will be output as the N required in item (b) of Theorem 3.1.

4.2. The algorithm. We now informally present the general algorithm which arises from the previous considerations for the approximation of invariant measures by our fixed point stability result. More details on the implementation, in particular cases, are given for each step in the following subsections.

Algorithm 4.1. *The algorithm works as follows:*

1. *Input the map and the partition.*
2. *Compute the matrix \tilde{P}_k approximating L_δ and the corresponding approximated fixed point \tilde{f}_δ up to some required approximation ϵ_1 .*
3. *Compute ΔL , an estimation for $\|L_\delta f - Lf\|_{L^1}$ up to some error ϵ_2 .*
4. *Compute N such that item (b) of Theorem 3.1 is verified as described in item I3 above.*
5. *If all computations end successfully, output \tilde{f}_δ .*

All that was mentioned previously allows us to state the following proposition.

Proposition 4.2. *$I^{-1}(\tilde{f}_\delta)$ is an approximation of one invariant measure in \mathcal{B} , up to an error ϵ given by*

$$\epsilon \leq \epsilon_1 + 2N(\Delta L + \epsilon_2)$$

in the L^1 norm.

Of course, it is possible that some computation will not stop or that the approximation error estimated above is not satisfactory. In this case the algorithm will be started again with a finer partition. With some a priori estimate on N , it is possible to prove that in certain cases the computations will stop and the error will go to zero as $\delta \rightarrow 0$ (and even estimate the rate of convergence); see section 5.1.

5. The piecewise expanding case. We now go into more detail, showing how the previously explained algorithm works in a concrete but nontrivial family of cases, where all the required computations and estimations can be done.

Let

$$\|\mu\| = \sup_{\phi \in C^1, |\phi|_\infty=1} |\mu(\phi')|.$$

This is related to bounded variation⁴: If $\|\mu\| < \infty$, then μ is absolutely continuous with respect to Lebesgue measure with BV density (see [23]).

In this case $X = [0, 1]$, $\mathcal{B}' = \{\mu, \|\mu\| < \infty\}$. The dynamics we will consider are defined by a map satisfying the following requirements.

Definition 5.1. *We will call a nonsingular function $T : ([0, 1], m) \rightarrow ([0, 1], m)$ piecewise expanding if*

⁴Recall that the variation of a function g is defined as

$$\text{var}(g) = \sup_{(x_i) \in \text{Finite subdivisions of } [0, 1]} \sum_{i \leq n} |g(x_i) - g(x_{i+1})|.$$

- there is a finite set of points $d_1 = 0, d_2, \dots, d_n = 1$ such that, for each i , $T|_{(d_i, d_{i+1})}$ is C^2 and $\int_{[0,1]} \frac{|T''|}{(T')^2} dx < \infty$; and
- $\inf_{x \in [0,1]} |T'(x)| > 2$ on the set where it is defined.

We remark that usually the definition of piecewise expanding map is weaker; in particular, it is supposed that $\inf_{x \in [0,1]} |D_x T| > 1$ for some iterate. In concrete examples it can be supposed that the derivative is bigger than 2 by considering some iterate of T (the physical measure of the iterate is the same).

We suppose that the map is computable in the sense that we can compute the probabilities P_{ij} defined in (4.1) up to any given accuracy. This is the case, for example, if the map has branches which are given by analytic functions with computable coefficients.

Piecewise expanding maps have a finite set of ergodic absolutely continuous invariant measures with bounded variation density. If the map is topologically mixing, such an invariant measure is unique.

Such densities are also fixed points of the (Perron–Frobenius) operator⁵ $L : L^1[0, 1] \rightarrow L^1[0, 1]$ defined by

$$[Lf](x) = \sum_{y \in T^{-1}(x)} \frac{f(y)}{|T'(y)|}.$$

We now explain how to face all the points raised in the concrete implementation of Algorithm 4.1.

5.0.1. About Item I1. In this section we obtain an explicit estimation of the coefficients of the LY inequality for piecewise expanding maps. We follow the approach of [23], trying to optimize the size of the constants.

Theorem 5.2. *If T is piecewise expanding as above and μ is a measure on $[0, 1]$, then*

$$\|L\mu\| \leq \frac{2}{\inf T'} \|\mu\| + \frac{2}{\min(d_i - d_{i+1})} \mu(1) + 2\mu \left(\left| \frac{T''}{(T')^2} \right| \right).$$

Proof. Note that

$$L\mu(\phi') = \sum_{Z \in \{(d_i, d_{i+1}) | i \in (1, \dots, n-1)\}} L\mu(\phi' \chi_Z)$$

since $L\mu$ gives zero weight to the points d_i ($L\mu$ is absolutely continuous).

For each such Z define ϕ_Z to be linear and such that $\phi_Z = \phi$ on ∂Z ; then define $\psi_Z = \phi - \phi_Z$ on Z , and extend it to $[0, 1]$ by setting it to zero outside Z . This is a continuous function. Moreover, for each $x \in Z$

$$|\phi'_Z|_\infty \leq \frac{2|\phi|_\infty}{\min(d_i - d_{i+1})}.$$

Thus

$$|L\mu(\phi')| = \left| \sum_Z \mu(\psi'_Z \circ T \chi_{T^{-1}(Z)}) + \mu(\phi'_Z \circ T \chi_{T^{-1}(Z)}) \right|.$$

⁵Note that this operator corresponds to the above defined transfer operator, but it acts on densities instead of measures.

Now note that, on Z , $\psi'_Z \circ T = \left(\frac{\psi_Z \circ T}{T'}\right)' + \frac{(\psi_Z \circ T)T''}{(T')^2}$; then

$$\begin{aligned} |L\mu(\phi')| &\leq \left| \sum_Z \mu \left(\left(\frac{\psi_Z \circ T}{T'} \right)' \chi_{T^{-1}(Z)} \right) \right| + \left| \sum_Z \mu \left(\frac{(\psi_Z \circ T)T''}{(T')^2} \chi_{T^{-1}(Z)} \right) \right| \\ &\quad + \frac{2|\phi|_\infty}{\min(d_i - d_{i+1})} \mu(1) \\ &\leq \left| \mu \left(\left(\frac{\psi_Z \circ T}{T'} \right)' \right) \right| + 2|\phi|_\infty \mu \left(\left| \frac{T''}{(T')^2} \right| \right) + \frac{2|\phi|_\infty}{\min(d_i - d_{i+1})} \mu(1). \end{aligned}$$

$\sum_Z \frac{\psi_Z \circ T}{T'}$ is not C^1 , but it can be approximated as best as wanted by a C^1 function ψ_ϵ such that $|\psi_\epsilon - \sum_Z \frac{\psi_Z \circ T}{T'}|_\infty$ and $\mu(|\psi_\epsilon - \sum_Z \frac{\psi_Z \circ T}{T'}|)$ are as small as wanted. Hence

$$\left| \mu \left(\left(\frac{\psi_Z \circ T}{T'} \right)' \right) \right| \leq \|\mu\| \left| \frac{\psi_Z \circ T}{T'} \right|_\infty \leq \|\mu\| \frac{2}{\inf T'} |\phi|_\infty$$

and

$$\begin{aligned} |L\mu(\phi')| &\leq \|\mu\| \frac{2}{\inf T'} |\phi|_\infty + 2|\phi|_\infty \mu \left(\left| \frac{T''}{(T')^2} \right| \right) + \frac{2|\phi|_\infty}{\min(d_i - d_{i+1})} \mu(1), \\ \|L\mu\| &\leq \frac{2}{\inf T'} \|\mu\| + \frac{2}{\min(d_i - d_{i+1})} \mu(1) + 2\mu \left(\left| \frac{T''}{(T')^2} \right| \right). \quad \blacksquare \end{aligned}$$

Remark 5.3. We remark that from the above statement it is easy to extract

$$\|L\mu\| \leq \frac{2}{\inf T'} \|\mu\| + \left(\frac{2}{\min(d_i - d_{i+1})} + 2 \left| \frac{T''}{(T')^2} \right|_\infty \right) |\mu|_1,$$

where

$$|\mu|_1 = \sup_{|\phi|_\infty=1} |\mu(\phi)|$$

coincides with the L^1 norm for a density of μ .

Remark 5.4. From now on, the following notation is going to be used throughout the paper:

$$(5.1) \quad \lambda := \frac{1}{\inf T'}, \quad B' := \frac{2}{\min(d_i - d_{i+1})} + 2 \left| \frac{T''}{(T')^2} \right|_\infty.$$

These constants play a central role in our treatment, and B' is the biggest obstruction in getting good estimates for the rigorous error. We also remark that if T is continuous, the estimate for B' given above can be improved.

We remark that once an inequality of the form

$$\|Lg\|_{\mathcal{B}'} \leq 2\lambda \|g\|_{\mathcal{B}'} + B' \|g\|_{\mathcal{B}}$$

is established (with $2\lambda < 1$), then, iterating, we have

$$\|L^n g\|_{\mathcal{B}'} \leq 2^n \lambda^n \|Lg\|_{\mathcal{B}'} + \frac{1}{1 - 2\lambda} B' \|g\|_{\mathcal{B}},$$

obtaining the inequality in the form required at (4.4) and the coefficient

$$B = \frac{1}{1 - 2\lambda} B',$$

which bounds $\|f\|$ from above, in our algorithm.

5.0.2. About item I2. As outlined before, on the interval $[0, 1]$ we consider a partition made of intervals having length δ . As remarked in item I2, we need an estimate of the quality of approximation by Ulam discretization.

Lemma 5.5. *For piecewise expanding maps, if L_δ is given by the Ulam discretization as explained before and $f \in BV[0, 1]$ is a fixed point of L , we have that*

$$\|Lf - L_\delta f\|_{L^1} \leq 2\delta \|f\|.$$

Proof. Recalling that $Lf = f$, it holds that

$$\|(L - L_\delta)f\|_{L^1} \leq \|\mathbf{E}(L(\mathbf{E}(f|\mathcal{F}_\delta)|\mathcal{F}_\delta)) - \mathbf{E}(Lf|\mathcal{F}_\delta)\|_{L^1} + \|\mathbf{E}(f|\mathcal{F}_\delta) - f\|_{L^1},$$

but

$$\mathbf{E}(L(\mathbf{E}(f|\mathcal{F}_\delta)|\mathcal{F}_\delta)) - \mathbf{E}(Lf|\mathcal{F}_\delta) = \mathbf{E}[L(\mathbf{E}(f|\mathcal{F}_\delta) - f)|\mathcal{F}_\delta].$$

Since both L and the conditional expectation are L^1 contractions,

$$\|(L - L_\delta)f\|_{L^1} \leq 2\|\mathbf{E}(f|\mathcal{F}_\delta) - f\|_{L^1}.$$

It is not difficult to see that for $f \in \mathcal{B}'$, there holds

$$\|\mathbf{E}(f|\mathcal{F}_\delta) - f\|_{L^1} \leq \delta \cdot \|f\|.$$

Indeed, from the definition of the norm we can see that $\|f\| \geq \sum_i |\sup_{I_i}(f) - \inf_{I_i}(f)|$, where I_i are the various intervals composing \mathcal{F} .

By this, since $\sup_{I_i}(f) \geq \mathbf{E}(f|I_i) \geq \inf_{I_i}(f)$, it follows that $\int_{I_i} |\mathbf{E}(f|\mathcal{F}_\delta) - f| \leq \delta |\sup_{I_i}(f) - \inf_{I_i}(f)|$, and the above equation follows.

By this

$$\|(L - L_\delta)f\|_{L^1} \leq 2\delta \|f\|. \quad \blacksquare$$

Remark 5.6. *This gives the estimate which is needed at item 3 of Algorithm 4.1. We have that, when f is an invariant measure, the inequality implies (see (4.3))*

$$\|Lf - L_\delta f\|_{L^1} \leq \frac{2}{k} B.$$

5.0.3. About item I4. It is easy to see that if L_δ is given by the Ulam method,

$$\|L_\delta f\|_{L^1} \leq \|f\|_{L^1};$$

indeed, $\|Lf\|_{L^1} \leq \|f\|_{L^1}$ and $\|\mathbf{E}(f|\mathcal{F}_\delta)\|_{L^1} \leq \|f\|_{L^1}$, as seen in section 4.1, and L_δ comes from the composition of such functions.

5.1. The algorithm works. We show that the described algorithm can provide an estimate of the invariant measure with an error as small as wanted if the size of the grid δ is chosen small enough.

Theorem 5.7. *It is possible to compute the invariant measure of a topologically mixing piecewise expanding map at any precision with our algorithm.*

Proof. Since L and L_δ satisfy the same LY inequality and $\|L - L_\delta\|_{BV \rightarrow L^1} \rightarrow 0$ as $\delta \rightarrow 0$, by [22, Proposition 3.1; Lemma 6.1] the spectral gap of L combined with the stability of the spectral picture implies that there are $A, \lambda \in \mathbb{R}, \lambda < 1$, independent of δ , such that for δ small enough L_δ satisfies $\|L_\delta^n|_V\|_{BV \rightarrow BV} \leq A\lambda^n$.

Since $\|\mathbf{E}(g|\mathcal{F}_\delta)\|_1 \geq 2\delta^{-1}\|\mathbf{E}(g|\mathcal{F}_\delta)\|$, this implies

$$\|L_\delta^n\|_{L^1 \rightarrow L^1} \leq 2\delta^{-1}\|L_\delta^n\|_{BV \rightarrow BV} \leq 2\delta^{-1}A\lambda^n.$$

Hence if $n \geq \frac{\log(4A)^{-1}\delta}{\log \lambda}$, $\|L_\delta^n\|_{L^1 \rightarrow L^1} \leq \frac{1}{2}$. And the algorithm stops. Moreover, by Proposition 4.2 and Remark 5.6 we have that up to multiplying constants, the error will be of the order $O(\delta \log \delta^{-1})$ and can be made as small as wanted as $\delta \rightarrow 0$. ■

Remark 5.8. *We remark that the above proof gives a rate of approximation of the order $O(\delta \log \delta^{-1})$; this is indeed the optimal rate of approximation for the Ulam approximation for piecewise expanding maps, as proved in [5].*

6. Higher regularity and L^∞ estimations. In this section we explain an implementation of the general strategy to compute invariant measures with a rigorous error with respect to the L^∞ norm in the case of expanding maps having C^2 regularity. A similar problem was faced in [3] and outlined in [22] using the Keller–Liverani spectral stability result [18].

The general strategy in this case is, as before, applying Theorem 3.1 with the L^∞ norm as $\|\cdot\|_{\mathcal{B}}$. This is possible by replacing the usual Ulam approximation with a more regular discretization, projecting on a partition of unity made of piecewise linear hat functions (see section 6.2) and proving for this approximation scheme an “approximation inequality” like in item I2 of section 4 (see Theorem 6.6). The remaining necessary estimation on the regularity of the fixed point (such as in item I1) is done again by a suitable LY inequality (see Lemma 6.4).

To estimate N and the numbers C_i we use a “a posteriori” estimate, done by the computer, by estimating the norm of the discretized operator restricted to the space of zero average discretized measures; by definition

$$C_i := \max_{\|v\|_\infty=1, v \in V} \|L_\delta^i v\|_\infty.$$

We denote $S = \{v \mid \|v\|_\infty = 1, v \in V\}$; this is a convex set with vertices the points $e_i - e_j$ as i and j vary between 1 and k ; since the norm is a convex function, it attains its maximum on one of the extremes of S . The extremes of S are $2 \cdot \text{Bin}(k, 2)$, where by Bin we mean the binomial coefficient; since we are looking for an estimate from above, we can observe that $\|L_\delta^i(e_i - e_j)\|_\infty \leq \|L_\delta^i(e_i - e_1)\|_\infty + \|L_\delta^i(e_j - e_1)\|_\infty$. Therefore, $\|L_\delta^i|_V\|_\infty \leq 2 \cdot \max_i \|L_\delta^i(e_i - e_1)\|_\infty$.

In the next subsections we specify the estimates which are needed to implement this strategy. We write explicitly only the arguments that differ substantially from the theory developed above and sketch the arguments that can be deduced from the former sections.

6.1. Higher regularity: The general framework. In this section we consider expanding maps of S^1 ; note that expanding Markov maps of the interval can be treated in a similar way.

Definition 6.1. Let $\tau : S^1 \rightarrow S^1$ be a measurable transformation, $\tau \in C^2(S^1, S^1)$; we say that τ is an expanding map of the circle if $|\tau'(x)| \geq \lambda > 1$ for every $x \in S^1$.

Such maps have a Lipschitz invariant density (see, e.g., [23]). Let us see how to find it with our approach.

In this section we will denote by $\|\cdot\|_\infty$ the supremum norm on the interval, and $\|\cdot\|_{Lip} := \|\cdot\|_\infty + Lip(\cdot)$, where $Lip(\cdot)$ is the Lipschitz constant of an observable. We also denote by $C^{Lip}(I)$ the set of Lipschitz functions over the interval. Below, we will denote the operator norm $\|\cdot\|_{L^\infty \rightarrow L^\infty}$ with $\|\cdot\|_\infty$.

Since τ satisfies an LY inequality of the form $\text{var}(L^n g) \leq \lambda^n \text{var}(g) + B\|g\|_1$, Lemma 3.1 and section 3.1 of [3] give us the following.

Remark 6.2. The L^∞ operator norm of L^n can be bounded by

$$\|L^n\|_\infty \leq M := B + 1.$$

Remark 6.3. For Markov maps of the interval, such an LY inequality is proved in [23], with coefficients

$$\lambda \leq 1/\inf |\tau'|, \quad B \leq \frac{1}{1-\lambda} \cdot \left\| \frac{T''}{T'^2} \right\|_\infty.$$

Fix now $k \geq k_0$ such that $\alpha = M\lambda^k < 1$. Let $T := \tau^k$, and let L be (by abuse of notation) the transfer operator associated to T ; Lemma 3.3 of [3] proves the following.

Lemma 6.4. The transfer operator $L : C^{Lip}(I) \rightarrow C^{Lip}(I)$ satisfies the following LY inequality:

$$Lip(Lg) \leq \alpha Lip(g) + B_1 \|g\|_\infty,$$

where $B_1 := Lip(L1)$ (the transfer operator applied to the characteristic function of the unit interval). For every $n \geq 1$ we have

$$\|L^n g\|_{Lip} \leq \alpha^n \|g\|_{Lip} + M \left(1 + \frac{B_1}{1-\alpha} \right) \|g\|_\infty.$$

Suppose $\{I_i\}$ is a partition of S^1 such that $T|_{I_i}$ is invertible, and denote by T_i^{-1} the inverse. As a first remark, we give an estimate for B_1 :

$$\begin{aligned} |L1(x) - L1(y)| &= \left| \sum_{i=1}^l \frac{1(T_i^{-1}(x))}{T'(T_i^{-1}(x))} - \sum_{i=1}^l \frac{1(T_i^{-1}(y))}{T'(T_i^{-1}(y))} \right| \\ &\leq \sum_{i=1}^l \left| \frac{1(T_i^{-1}(x)) - 1(T_i^{-1}(y))}{T'(T_i^{-1}(x))} \right| + \sum_{i=1}^l \left| \frac{1(T_i^{-1}(y))}{T'(T_i^{-1}(x))} - \frac{1(T_i^{-1}(y))}{T'(T_i^{-1}(y))} \right| \\ &\leq l \cdot \left\| \frac{T''}{(T')^2} \right\|_\infty |x - y|. \end{aligned}$$

Therefore, $B_1 \leq l \cdot \|T''/(T')^2\|_\infty$.

If $f \in C^{Lip}$ is the fixed point of L , from the variation LY inequality, we have

$$\|f\|_\infty \leq \|f\|_{BV} \leq B + 1.$$

6.2. Higher regularity: The approximation strategy. We define now a discretization of the operator L , projecting on finite dimensional subspace of densities with higher regularity with respect to the standard Ulam one. This permits us to get an estimate in the $\|\cdot\|_\infty$ norm for the approximation error.

Theorem 6.5. *Let P be a partition a_0, \dots, a_n of S^1 in k homogeneous intervals; let $\{\phi_i\}$ be the family of functions given by*

$$\phi_i(x) = \begin{cases} k \cdot (x - a_{i-1}), & x \in [a_{i-1}, a_i], \\ -k \cdot (x - a_{i+1}), & x \in [a_i, a_{i+1}], \\ 0, & x \in [a_{i-1}, a_{i+1}]^c, \end{cases}$$

where by definition $a_{-1} := a_n$. The finite dimensional “projection”⁶

$$\pi(f)(x) = \sum_j \frac{\int_{S^1} f \phi_j}{\int_{S^1} \phi_j} \cdot \phi_j(x)$$

has the following properties:

1. $Lip(\pi(f)) \leq Lip(f)$;
2. $\|\pi(f)\|_\infty \leq \|f\|_\infty$;
3. $\|\pi(f) - f\|_\infty \leq Lip(f)/k$.

Proof. Item 1 is true since

$$Lip(\pi(f)) = \frac{k}{|x_j - x_i|} \cdot \max_{i,j} \left| \int_{x_{j-1}}^{x_{j+1}} (f(x) - f(x + (x_j - x_i))) \phi_j(x) dx \right| \leq Lip(f).$$

Item 2 is true since

$$|\pi(f)(x)| = \left| \sum_i \frac{1}{\int_{S^1} \phi_i} \int_{S^1} f \phi_i dy \phi_i(x) \right| \leq \|f\|_\infty \left| \sum_i \phi_i(x) \right| \leq \|f\|_\infty.$$

Item 3 is true since

$$\begin{aligned} |\pi(f)(x) - f(x)| &\leq \sum_i \frac{1}{\int_{S^1} \phi_i} \int_{S^1} Lip(f) |y - x| \phi_i(y) dy \cdot |\phi_i(x)| \\ &\leq Lip(f) \cdot \frac{1}{k}. \quad \blacksquare \end{aligned}$$

From Lemma 6.4 and the properties of π we have the following theorem.

Theorem 6.6. *If f is a fixed point of L , then*

$$\|(L - \pi L \pi)f\|_\infty \leq \frac{2}{k}(1 + M)Lip(f).$$

Proof.

$$\|(L - \pi L \pi)f\|_\infty \leq \|f - \pi f\|_\infty + \|\pi(L - L\pi)f\|_\infty,$$

⁶We warn the reader that this is not a formal projection in the sense that π is not necessarily equal to π^2 .

and, from the fact that $\|L\|_\infty < M$ we have the thesis. \blacksquare

Now we have all the ingredients to apply Theorem 3.1 and our algorithm, but for a different norm.

Computing $L\phi_i$ rigorously can be an expensive task; we can avoid computing it directly. Instead of computing $L_k := \pi L \pi$, we can compute a suitable approximation \tilde{L}_k . This operator is obtained by projecting on $\{\phi_j\}$ the functions

$$\tilde{L}\phi_i(x) = \frac{1}{T'(a_i)}\phi_i\left(a_i + \frac{1}{T'(a_i)}(y - T(a_i))\right),$$

i.e., studying the operator obtained by taking on each interval $[a_{i-1}, a_{i+1}]$ the linearization \tilde{T} of the map T . A simple computation shows that

$$\begin{aligned} & \|L_k\phi_i - \tilde{L}_k\phi_i\|_\infty \\ & \leq \left\| \frac{\phi_i(T^{-1}(x))}{|T'(T^{-1}(x))|} - \frac{\phi_i(T^{-1}(x))}{|T'(x_i)|} \right\|_\infty + \left\| \frac{\phi_i(T^{-1}(x))}{|T'(x_i)|} - \frac{\phi_i(\tilde{T}^{-1}(x))}{|T'(x_i)|} \right\|_\infty \\ & \leq \frac{4}{k^2} \cdot \left\| \frac{T''}{(T')^2} \right\|_\infty. \end{aligned}$$

Remark 6.7. Note that

$$\|Lf - \tilde{L}_k f\|_\infty \leq \|Lf - L_k f\|_\infty + \|L_k f - \tilde{L}_k f\|_\infty.$$

Let \tilde{v}_k be the eigenvector computed using the operator \tilde{L}_k . We can now express the rigorous error using Theorem 3.1 and the fact that the $\|L_k^i\|_\infty < M$ for every i (by Remark 6.2):

$$\begin{aligned} \|f - \tilde{v}_k\|_\infty & \leq \frac{2}{k} \cdot N \cdot \sum_0^{N-1} C_i \cdot (\|L - L_k\|_\infty + \|L_k - \tilde{L}_k\|_\infty) \|f\|_\infty \\ & \leq \frac{2}{k} \cdot N \cdot \sum_0^{N-1} C_i \left(2(M+1)M \left(1 + \frac{B_1}{1-\alpha} \right) + \frac{4}{k} \left\| \frac{T''}{(T')^2} \right\|_\infty \right) \cdot (B+1). \end{aligned}$$

7. Maps with indifferent fixed points. In the literature, the computation of the invariant measures for such types of maps has been discussed from different points of view (see, e.g., [4, 15, 27]). In particular, two approaches have been proposed:

- reduction of the problem to a piecewise expanding induced system [4];
- direct application of a discretization method [27].

No explicit implementations are provided. So it is not clear what method could be really suitable for the purpose. We implement a direct discretization, following the general strategy described in our paper.

We also compute the entropy of an example of such systems. In [7] it is shown that statistical estimators converge slowly for these systems, further motivating the rigorous calculation of the entropy for such systems.

Let $0 < \alpha < 1$, and let us consider a map $T : [0, 1] \rightarrow [0, 1]$ of the following type:

1. $T(0) = 0$, and there is a point $d \in (0, 1)$ s.t. $T : [0, d] \xrightarrow{\text{onto}} [0, 1)$, $T : [d, 1] \xrightarrow{\text{onto}} [0, 1]$.
2. Each branch of T is increasing and convex and can be extended to a C^1 function; $T' > 1$ for all $x \in (0, d) \cup (d, 1)$ and $T'(0) = 1$.
3. There is a constant $C \in (0, \infty)$ such that

$$(7.1) \quad T(x) \geq x + Cx^{1+\alpha}.$$

This kind of maps are now well known to have an absolutely continuous invariant measure f which is decreasing and unbounded; moreover, they have slow (polynomial) decay of correlation.

To apply our strategy we need an estimate for the regularity of f (see item I1 in section 4). A useful estimate can be found in [27, Proposition 1.1, Theorem 1, equation 3]; see also [24].

Proposition 7.1. *Let us consider the transfer operator L associated to T and the following cone of decreasing functions:*

$$C_A = \left\{ g \in L^1 \mid g \geq 0, g \text{ decreasing}, \int_0^1 g \, dm = 1, \int_0^x g \, dm \leq Ax^{1-\alpha} \right\}.$$

Let $A_* = ((1-\alpha)Cd^{2+\alpha})^{-1}$; if $A \geq A_*$, then $L(C_A) \subseteq C_A$. Moreover, the unique invariant density f of T is in C_{A_*} .

We remark [27, Lemma 2.1] that if $f \in C_A$, then $f(x) \leq Ax^{-\alpha}$.

7.1. Application of our strategy: Items (a), (b), and (c). Let us show the a priori estimation which is needed to start our strategy: item (a).

Let $g \in C_A$. Let π be the Ulam projection with δ size intervals $\pi(g) = \mathbf{E}(g|\mathcal{F}_\delta)$, and let $x_0 = \tilde{n}\delta \in I$, with \tilde{n} a small integer, and $g = g_{<x_0} + g_{>x_0}$, where $g_{<x_0} = g \mathbf{1}_{[0, x_0]}$ and $g_{>x_0} = g \mathbf{1}_{[x_0, 1]}$.

Now

- $\|g_{>x_0} - \pi g_{>x_0}\|_1 \leq \delta \operatorname{var}(g_{>x_0}) \leq \delta Ax_0^{-\alpha}$,
- $\|g_{<x_0} - \pi g_{<x_0}\|_1 \leq \|g_{<x_0}\|_1 \leq Ax_0^{1-\alpha}$;

hence

$$\|g - \pi g\|_1 \leq \delta Ax_0^{-\alpha} + Ax_0^{1-\alpha}.$$

We can take $x_0 = \delta$ and obtain

$$\|g - \pi g\|_1 \leq 2A\delta^{1-\alpha}.$$

Now let $f \in C_{A_*}$ be the invariant density. Note that since L and π are L^1 contractions, for what is said above, $\|Lf - L\pi f\|_1 \leq \|f - \pi f\|_1 \leq 2A_*\delta^{1-\alpha}$. Now,

$$\begin{aligned} \|f - \pi L\pi f\|_1 &\leq \|f - \pi Lf + \pi Lf - \pi L\pi f\|_1 \\ &\leq \|f - \pi f\|_1 + \|Lf - L\pi f\|_1 \\ &\leq 4A_*\delta^{1-\alpha}. \end{aligned}$$

This gives the estimation needed at item (a) of Theorem 3.1.

About items (b) and (c), since we are approximating in L^1 , the discussion is the same as that shown in sections 4.1 and 5.0.3; thus $C_i \leq 1$.

Remark 7.2. *In this approach we considered a discretization which is made starting from a uniform grid of size δ . Since the density and its regularity are not uniform at all (having an asymptote in the origin), a smarter grid to consider could be nonuniform, with larger cells far from the origin and smaller cells near the origin. This adaptive design of the grid, providing more resolution where we expect less regularity, may reduce the total number of cells considered and the computation time; see, for example, [27], where a better rate of approximation is proved for the Ulam method with these adaptive grids.*

8. Implementing the algorithm. In this section we explain the details of the implementation of our algorithm and some related numerical issues. The main points are the computation of a rigorous approximation of the related Markov chain and a fast method to rigorously approximate its steady state. We include some implementation and numerical supplementary remarks, which can be skipped on a first reading.

8.1. Computing the Ulam approximation. To compute the matrix of the Ulam approximation, we have developed an algorithm that computes, with a rigorous algorithm, the entries of a matrix \tilde{P}_k which approximates P_k . Now let us see how our algorithm computes a matrix \tilde{P}'_k which is a preliminary to obtaining \tilde{P}_k . Our algorithm computes each entry and the error associated to each entry in a way that the maximum of all these errors is bounded by a certain quantity ε . To compute the entries P'_{ij} of the matrix, consider each interval I_i of the partition, and consider two main cases: if T is monotone on I_i , we can follow Algorithm 1; if T has a discontinuity in I_i , we use Algorithm 2. In the algorithms ν is an input constant which is used to control the error on the coefficients.

Algorithm 1 Computing \tilde{P}'_{ij} if T is monotone on I_i .

Set $\tilde{P}'_{ij} = 0$

Partition I_i into m intervals $I_{i,k}$ for $k = 0, \dots, m - 1$

for $k = 0 \rightarrow m$ **do**

 Compute $T(I_{i,k})$

if $T(I_{i,k}) \subset I_j$, **then** add $m(I_{i,k})$ to the coefficient \tilde{P}'_{ij}

if $T(I_{i,k}) \subset (I_j)^C$, **then** discard $I_{i,k}$

if $T(I_{i,k}) \cap I_j \neq \emptyset$ and $T(I_{i,k}) \cap (I_j)^C \neq \emptyset$ and $m(I_{i,k}) > \nu$, **then** divide $I_{i,k}$ into m intervals, and iterate the procedure

if $T(I_{i,k}) \cap I_j \neq \emptyset$ and $T(I_{i,k}) \cap (I_j)^C \neq \emptyset$ and $m(I_{i,k}) < \nu$, **then** add $m(I_{i,k})$ to ε_{ij} , the error on the coefficient \tilde{P}'_{ij} , and discard $I_{i,k}$

The maximum of all the ε_{ij} is very important for all of our estimates; we denote it by ε .

We denote the matrix containing the computed coefficients by \tilde{P}'_k to distinguish it from P_k , the actual matrix of the Ulam discretization. Please note that \tilde{P}'_k is not a stochastic matrix, and we will need a stochastic matrix in what follows. We perturb its entries to modify it and

Algorithm 2 Computing \tilde{P}'_{ij} if T has a discontinuity in I_i

Set $\tilde{P}'_{ij} = 0$

Partition I_i in m intervals $I_{i,k}$ for $k = 1, \dots, m$

for $k = 0 \rightarrow m$ **do**

if $I_{i,k}$ does not contain a discontinuity **then** apply Algorithm 1 to $I_{i,k}$

if $I_{i,k}$ contains the discontinuity and $m(I_{i,k}) > \nu$ **then** divide $I_{i,k}$ in m intervals and iterate the procedure

if $I_{i,k}$ contains the discontinuity and $m(I_{i,k}) < \nu$ **then** add $m(I_{i,k})$ to ε_{ij} , the error on the coefficient \tilde{P}'_{ij}

obtain a stochastic matrix by computing the sum of the elements for each row, subtracting this number by 1, and spreading the result uniformly on each of the nonzero elements of the row, obtaining a new “markovized” matrix \tilde{P}_k .

Let ε be the maximum of the errors $|\tilde{P}'_{ij} - P_{ij}|$, and let nnz_i be the number of nonzero elements of the row. We have that for each row i the sum of its entries differs from 1 by at most $\text{nnz}_i \cdot \varepsilon$. So, if we spread the result uniformly on each of the nonzero elements of the row, we have a new matrix \tilde{P}_k such that

$$|\tilde{P}_{ij} - P_{ij}| < 2 \cdot \varepsilon.$$

Let $\text{NNZ} = \max_i \text{nnz}_i$; then, the matrix \tilde{P}_k is such that

$$\|P_k - \tilde{P}_k\|_1 < 2 \cdot \text{NNZ} \cdot \varepsilon.$$

The matrix \tilde{P}_k is the matrix we are going to work with, and the “markovization” process ensures that the biggest eigenvalue of \tilde{P}_k is 1. Please note that, thanks to Theorem 3.1, we have a rigorous estimate of the L^1 -distance between the eigenvectors of \tilde{P}_k and P_k , as we explain below.

Remark 8.1. *Due to the form of (4.1), we can bound the maximum number of nonzeros per row: $\text{NNZ} \leq \sup |T'| + 4$.*

8.2. Computing the L^∞ approximation. As explained in section 6.2, we compute an approximation \tilde{Q}_k to the matrix Q_k associated to the operator \tilde{L}_k linearizing the dynamics in correspondence to the nodes a_0, \dots, a_n of the discretization. This permits us to express $\tilde{L}_k \phi_i$ in closed form and compute explicit formulas for the coefficients (finding the primitives). Using the iRRAM library [26], we computed these coefficients so that all the digits represented in the `double` type are rigorously checked. Therefore, the error in the computation of the matrix \tilde{Q}_k in the higher regularity case is due to the truncation involved in the markovization process:

$$\|\tilde{Q}_k - Q_k\|_\infty < 2^{-50} = \varepsilon.$$

8.3. Computing rigorously the steady state vector and the error.

Remark 8.2. *Our algorithm and our software work for maps which are topologically transitive. This implies transitivity in the Markov chain approximating them. Indeed, let I_i and*

$\overset{\circ}{I}_j$ be the interior of two intervals of the partition; since the map is topologically transitive and the derivative is bounded away from zero, there exists an N_{ij} such that $T^{N_{ij}}(\overset{\circ}{I}_i) \cap \overset{\circ}{I}_j \neq \emptyset$, and this intersection is a union of intervals with nonzero measure. Therefore, if we call \tilde{N} the maximum of all these N_{ij} , the matrix $P_k^{\tilde{N}}$ has strictly positive entries, and therefore the matrix P_k represents an irreducible Markov chain. By the Perron–Frobenius theorem this implies that the steady state of the Markov chain is unique.

We want to find the steady state of the irreducible Markov matrix \tilde{P}_k . To do so we use the power iteration method; given any initial condition b_0 , if we set

$$b_{l+1} = b_l \cdot \tilde{P}_k,$$

we have that b_l converges to the steady state; we want to bound the numerical error of this operation from above.

In the following section we will denote by $\|\cdot\|_F$ either the 1-norm or the ∞ -norm, depending on which framework are we working in (the F stands for finite dimensional).

We build an enclosure for the eigenvector using an idea from the proof of the Perron–Frobenius theorem [1, Theorem 1.1]: a Markov matrix A (aperiodic, irreducible) contracts the simplex Λ of vectors v having 1-norm 1.

This simplex is given by the convex combinations of the vectors e_1, \dots, e_k of the base; therefore, if we denote by Diam_F the diameter in the distance induced by the norm F , we have

$$\begin{aligned} \text{Diam}_F(A^l \Lambda) &\leq \max_{i,j} \|A^l(e_i - e_j)\|_F \leq \max_{i,j} \|A^l(e_1 - e_j)\|_F + \|A^l(e_1 - e_i)\|_F \\ &\leq 2 \max_i \|A^l(e_1 - e_i)\|_F. \end{aligned}$$

Fixing an input threshold ε_{num} , we iterate the vectors $\{e_1 - e_j\}$ with $j = 2, \dots, n$ and look at their F -norm until we find an l such that $\text{Diam}_F(A^l \Lambda) < \varepsilon_{num}$. Therefore, for any initial condition b_0 , iterating it l times, we get a vector contained in $A^l(\Lambda)$ whose numerical error is enclosed by ε_{num} .

Numerical Remark 1. We refer the reader to [17] for the following inequality about roundoff error in matrix vector multiplication, which we used to rigorously compute N and N_ε (as usual, k is the size of the partition):

$$\|\text{float}(Av) - Av\|_F \leq \gamma_k \cdot \|A\|_F \|v\|_F,$$

where, if u is the machine precision,

$$\gamma_k = \frac{ku}{1 - ku}.$$

Please note that $\|A\|_1 = 1, \|v\|_1 \leq 2$ in the Ulam case and that, since our matrix is sparse, we can substitute k by NNZ in the computation of the above constant.

8.4. Estimation of the rigorous error for the invariant measure. The main issue that remains to be solved is the computation of the number of iterations N needed for the Ulam approximation L_δ to contract to $1/2$ the space of average 0 vectors as explained in section 4.1.

In some way, we already assessed this question while we were computing the iterations of the simplex; the vectors $e_1 - e_j$ with $j = 1, \dots, k$ are a base for the space of average 0 vectors, so, while rigorously computing the eigenvector, we can also compute the number of iterations needed to contract the simplex. We have to be careful since we do not know the matrix P_k of the Ulam approximation L_δ explicitly; we know only its approximation \tilde{P}_k .

Indeed (see section 4.1),

$$\|L_\delta^j|_V\|_1 \leq \|(P_k^j - \tilde{P}_k^j + \tilde{P}_k^j)|_V\|_1 \leq \|(P_k^j - \tilde{P}_k^j)|_V\|_1 + \|\tilde{P}_k^j|_V\|_1.$$

We can estimate the second summand as

$$\begin{aligned} \|P_k^j - \tilde{P}_k^j|_V\|_1 &\leq \sum_{i=1}^j \|P_k^{j-i}|_V\|_1 \cdot \|P_k - \tilde{P}_k|_V\|_1 \cdot \|\tilde{P}_k^{i-1}|_V\|_1 \\ &\leq 2 \cdot j \cdot \text{NNZ} \cdot \varepsilon, \end{aligned}$$

since $\|P_k - \tilde{P}_k|_V\|_1 < 2 \cdot \text{NNZ} \cdot \varepsilon$, $\|P_k^j|_V\|_1 \leq 1$, and $\|\tilde{P}_k^h|_V\|_1 \leq 1$ for every j, h . Therefore,

$$\|P_k^j|_V\|_1 \leq 2 \cdot j \cdot \text{NNZ} \cdot \varepsilon + \|\tilde{P}_k^j|_V\|_1.$$

Following the same line of thought, we have, in the higher regularity case, that

$$\|Q_k^j|_V\|_\infty \leq 2 \cdot j \cdot M^2 \left(\varepsilon + \frac{4}{k^2} \cdot \left\| \frac{T''}{(T')^2} \right\|_\infty \right) + \|\tilde{Q}_k^j|_V\|_\infty.$$

These two inequalities are very important for us, since they tell us that if ε and j are small enough, we can estimate the number N of iterates needed for P_k (resp., Q_k) to contract the space V by the number of iterates needed by the matrix \tilde{P}_k .

Numerical Remark 2. *If ε and k are big, after some iterations the approximation error could hide the contraction of \tilde{P}_k . Therefore, it is important to compute \tilde{P}_k with a small ε .*

In the following we denote by f the fixed point of L , by v_k the fixed point of P_k (resp., Q_k), by v_ε the fixed point of \tilde{P}_k (resp., \tilde{Q}_k), and by \tilde{v} the numerical approximation of v_ε . We recall now the sources of error in our computation to clarify the last step of our algorithm:

1. $\|f - v_k\|_F$, the discretization error, coming from the (Ulam or higher regularity) discretization of the transfer operator, whose final form was estimated in Remarks 5.6 and 6.7;
2. $\|v_k - v_\varepsilon\|_F$, the approximation error; since we cannot compute exactly the matrix P_k , we have to approximate it by computing a matrix \tilde{P}_k ;
3. $\|v_\varepsilon - \tilde{v}\|_F$, the numerical error in the computation of the eigenvector, which was estimated in subsection 8.3,

Then

$$\|f - \tilde{v}\|_F \leq \|f - v_k\|_F + \|v_k - v_\varepsilon\|_F + \|v_\varepsilon - \tilde{v}\|_F.$$

The last thing we need to compute to get our rigorous estimate is a bound for the approximation error, item 2. We computed the number of iterates N_ε ⁷ needed for \tilde{P}_k to contract to 1/2 the space of average 0 vectors; then by using Theorem 3.1 we have that

$$\|v_k - v_\varepsilon\|_1 \leq 2N_\varepsilon \|P_k - \tilde{P}_k\|_1 \|v_k\|_1 \leq 4N_\varepsilon \cdot \text{NNZ} \cdot \varepsilon.$$

In the L^∞ case, the same reasoning leads to

$$\|v_k - v_\varepsilon\|_\infty \leq 2N \|Q_k - \tilde{Q}_k\|_\infty \|v_\varepsilon\|_\infty \leq 2N \cdot \varepsilon \cdot \|v_\varepsilon\|_\infty.$$

Remark 8.3. *In this inequality we used N instead of N_ε . This is not a misprint but is due to the fact that we have no a priori estimate of $\|v_k\|_\infty$ since we are using the piecewise linear approximation. To solve this issue we use Theorem 3.1 with Q_k as L_δ and \tilde{Q}_k as L , respectively.*

Finally, we have that, if f is the invariant measure and \tilde{v} is the computed vector, using the estimate in Remark 5.6, the rigorous error is

$$\|f - \tilde{v}\|_1 \leq 2N \frac{2B}{k} + 4N_\varepsilon \cdot \text{NNZ} \cdot \varepsilon + \varepsilon_{num}.$$

In the ∞ case, summing up all the inequalities, we get an explicit formula for the error

$$\begin{aligned} \|f - \tilde{v}\|_\infty \leq & \frac{2}{k} \cdot N \cdot M \left(\frac{4}{k} \left\| \frac{T''}{(T')^2} \right\|_\infty + 2(M+1)M \left(1 + \frac{B_1}{1-\alpha} \right) \right) \cdot (B+1) \\ & + 2N \cdot M^2 \left(\varepsilon + \frac{4}{k^2} \left\| \frac{T''}{(T')^2} \right\|_\infty \right) (\|\tilde{v}\|_\infty + \varepsilon_{num}) + \varepsilon_{num}, \end{aligned}$$

where N is computed with respect to $\|\cdot\|_\infty$.

9. Rigorous computation of the Lyapunov exponent and entropy. The rigorous computation of the invariant density allows a rigorous estimation of the Lyapunov exponent of the system. This estimation can be used as a benchmark for the validation of statistical methods to compute entropy from time series. We remark that, for the experimental validation of these methods, to understand how fast they converge to the real value of the entropy an exact estimate for the value is needed. We give a method which can produce such an estimate on interesting systems where an exact estimate of the entropy is not possible. This can also be applied to systems not having a Markov structure, where the convergence of statistical, symbolic methods may be slow (see, e.g., [7]). We remark that our approach gives statements on the entropy, which can be considered as real mathematical theorems with a computer-aided proof.

The Lyapunov exponent at a point x , denoted by $\lambda(x)$, of a one dimensional map is defined by

$$L_{exp}(x) = \lim_{n \rightarrow +\infty} \frac{1}{n} \sum_{i=0}^n \log((T^i)'(x));$$

⁷Please note that, if ε is small, $N_\varepsilon = N$ is expected. In the program we compute the two values independently, even if in general $N_\varepsilon \leq N$.

by the Birkhoff ergodic theorem, we have that, relative to an ergodic invariant measure μ , for μ -a.e. x we have that

$$L_{exp}(x) = \int_0^1 \log(|T'|) d\mu = L_{exp}.$$

Our algorithm permits us to compute the density of an invariant measure with a rigorous error bound. Suppose \tilde{v} is the computed approximation for the invariant density, considered as a piecewise constant function; by Young's inequality we have that

$$\left| \int_0^1 \log(|T'(x)|) f(x) dx - \int_0^1 \log(|T'(x)|) \tilde{v}(x) dx \right| \leq \max_{x \in [0,1]} (\log |T'(x)|) \|f - \tilde{v}\|_1.$$

Therefore, to compute the Lyapunov exponent, the only thing we have to do is compute with a (relatively) small numerical error the integral

$$\int_0^1 \log(|T'(x)|) \tilde{v} dx.$$

10. Numerical experiments (L^1 case). In this section we show the output of some complete experiments we performed, using the programs described above.

The code is now in a hybrid state: the routines that generate the matrix are written using the BOOST library and the iRRAM and can run on almost any computer, while the enclosure method for the certified computation of the eigenvector requires a number of matrix-vector products proportional to the size of the partition; in our examples the size of the partition is $2^{20} \approx 10^6$. This forced us to implement and run our programs in a parallel HPC environment, using the library PETSc and running them on the CINECA Cluster SP6. See 91104_01.zip [local/web 120KB] for the code for the programs.

In every component where the maps are continuous, the maps are polynomials. So, we can use exact arithmetics (rationals) to compute the matrix \tilde{P}_k . Please note that the discontinuity points are irrational; this is taken care of as we explained in section 8.1.

To ease the reading of the tables of the data, here is a rapid summary of the different quantities involved with reference to where they appear in the paper.

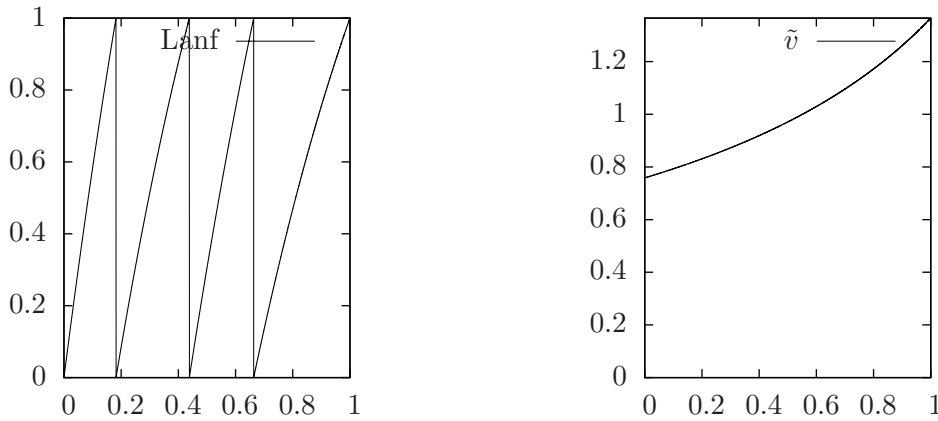
Inputs		Outputs	
λ	LY inequality Remark 5.4	N_ε	iterates of $\tilde{P}_k _V$
B'	LY inequality Remark 5.4	N	iterates of $P_k _V$
B	Bound for $\ f\ _{BV}$ section 4	l	iterates for the enclosure
ε	error on the matrix section 8.1	ε_{rig}	computed rigorous error
ε_{num}	numerical error section 8.3	L_{exp}	computed Lyapunov exponent

10.1. The Lanford map. For our first numerical experiment we chose one of the maps investigated in [20]. The map $T : [0, 1] \rightarrow [0, 1]$ is given by

$$T : x \mapsto 2x + \frac{1}{2}x(1-x) \pmod{1}.$$

What seems to be a good approximation of the invariant measure of the map is plotted in Figure 1 of the cited article. Since this map does not comply with the hypothesis of our article, i.e., there are some points where $1 < |D_x T| \leq 2$, we study the map $T^2 := T \circ T$. Clearly, the invariant measures for T and T^2 coincide.

In Figure 1(a) you can see a plot of this map, and in Figure 1(b) you can see the plot of density of the the invariant measure we obtain through our method.



(a) The second iterate of the Lanford map

(b) The invariant measure for the Lanford map

Figure 1. Lanford's example.

The following are the data (input and outputs) of our algorithm.

Inputs		Outputs	
λ	$4/3\sqrt{17}$	N_ε	17
B'	≤ 7.019	N	18
B	19.88	l	25
ε	$\leq 3 \cdot 10^{-11}$	ε_{rig}	0.0016
ε_{num}	≤ 0.0001	L_{exp}	1.315 ± 0.003

10.2. A map without the Markov property. The map $T : [0, 1] \rightarrow [0, 1]$ given by

$$(10.1) \quad T(x) = \frac{17}{5}x \bmod 1,$$

whose graph is plotted in Figure 2(a). This map does not enjoy the Markov property: since $(17/5)^k$ is never an integer, the orbit of 1 is dense.

The density of the invariant measure we obtain through our method is plotted in Figure 2(b).

Below are some of the data (input and outputs) of our algorithm; please note that in this case we know the exact value of the Lyapunov exponent.

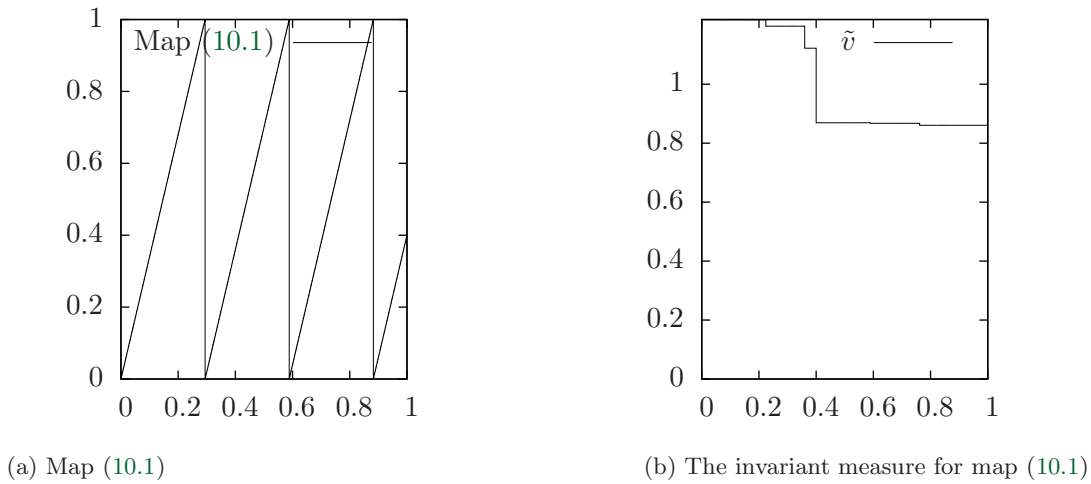


Figure 2. Example (10.1).

Inputs		Outputs	
λ	5/17	N_ε	13
B'	< 17	N	14
B	41.47	l	20
ε	$\leq 1.75 \cdot 10^{-10}$	ε_{rig}	0.0026
ε_{num}	≤ 0.0001	L_{exp}	$\ln(17) - \ln(5)$

10.3. A nonlinear version. We study the map $T : [0, 1] \rightarrow [0, 1]$ given by

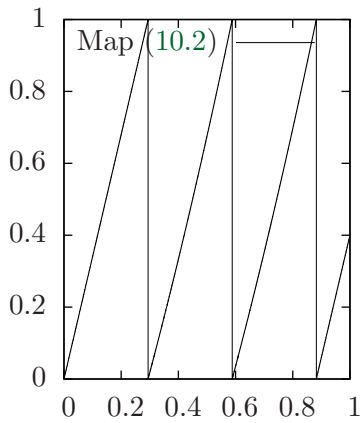
$$(10.2) \quad T(x) = \begin{cases} \frac{17}{5}x, & 0 \leq x \leq \frac{5}{17}, \\ \frac{34}{25}(x - \frac{5}{17})^2 + 3(x - \frac{5}{17}), & \frac{5}{17} < x \leq \frac{10}{17}, \\ \frac{34}{25}(x - \frac{10}{17})^2 + 3(x - \frac{10}{17}), & \frac{10}{17} < x \leq \frac{15}{17}, \\ \frac{17}{5}(x - \frac{15}{17}), & \frac{15}{17} < x \leq 1, \end{cases}$$

whose graph is plotted in Figure 3(a). This map is similar to map (10.1), but it is nonlinear in the two intervals $[5/17, 10/17]$ and $[10/17, 15/17]$, where it is defined by two branches of a polynomial of degree 2.

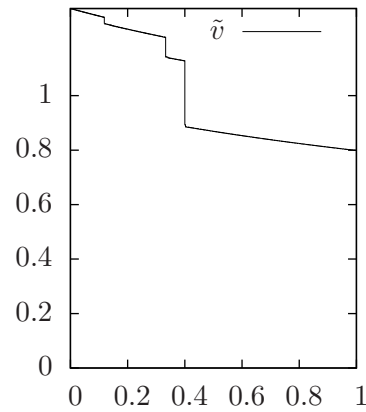
The density of the invariant measure we obtain through our method is plotted in Figure 3(b). Please note that near 0.337 and 0.403 there are two small “staircase steps” which are visible only zooming the graph.

Below are some of the data (input and outputs) of our algorithm.

Inputs		Outputs	
λ	1/3	N_ε	14
B'	< 18.22	N	15
B	54.69	l	21
ε	$\leq 2.19 \cdot 10^{-11}$	ε_{rig}	0.004
ε_{num}	≤ 0.0001	L_{exp}	1.219 ± 0.004



(a) Map (10.2)



(b) The invariant measure for map (10.2)

Figure 3. Example (10.2).

10.4. A Manneville–Pomeau map. In this section we compute a density with small error in the L^1 norm, using the estimates developed in section 7.

The numerical part is essentially the same as that used to compute the invariant measure in the L^1 case; the only big difference resides in the fact that to compute the Ulam approximation we used an algorithm based on an interval Newton root-finding algorithm instead of using the exhaustion algorithm.

The example we have studied is

$$(10.3) \quad T(x) = x + x^{1+\frac{1}{8}} \pmod{1},$$

whose graph is plotted in Figure 4(a), using a discretization in 1048576 elements.

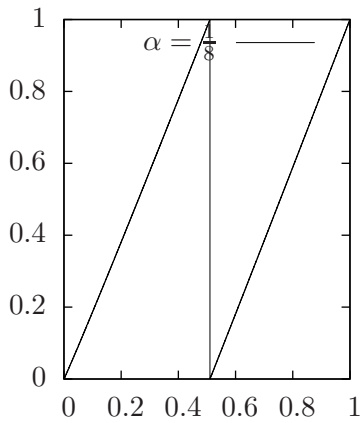
The density of the invariant measure is plotted in Figure 4(b).

Inputs		Outputs	
α	0.125	N_ε	49
A_*	≤ 4.58	N	50
ε_{num}	≤ 0.001	l	88
d	$[0.52039, 0.52040]$	ε_{rig}	0.006
ε	$\leq 2.1 \cdot 10^{-15}$	L_{exp}	0.685 ± 0.005

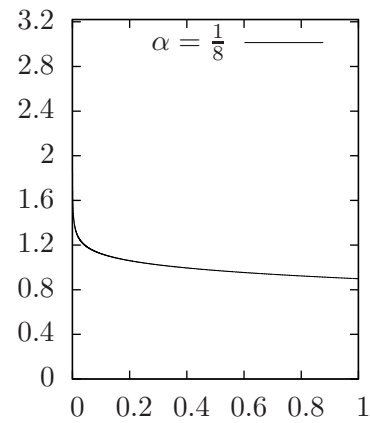
11. Numerical experiments (L^∞ case). In this section we compute a density with small error in the L^∞ norm, using the estimates developed in sections 6.1 and 6.2 and using the methods explained in the subsections 8.2, 8.3, and 8.4.

11.1. A Markov perturbation of $4 \cdot x \pmod{1}$. The example we have studied is

$$(11.1) \quad T(x) = 4x + 0.01 \cdot \sin(8\pi x) \pmod{1},$$



(a) Map (10.3)



(b) The invariant measure for map (10.3)

Figure 4. Example (10.3).

whose graph is plotted in Figure 5(a) using a discretization in 131072 elements.

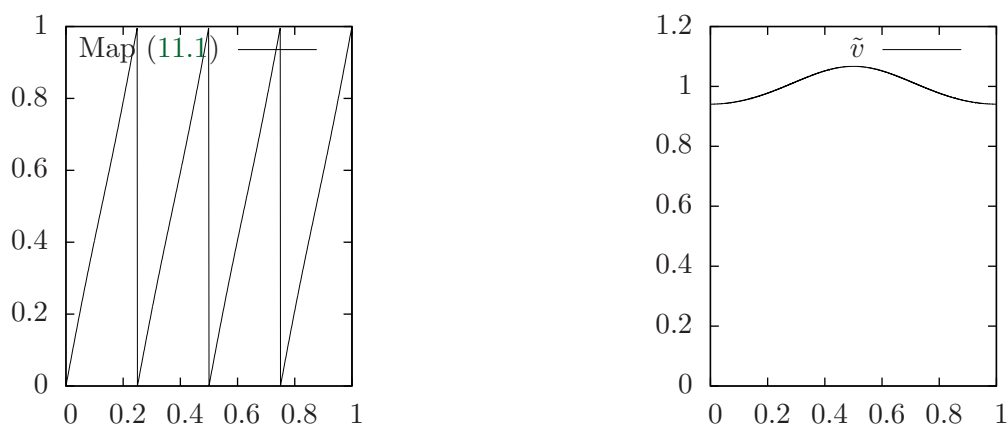
The density of the invariant measure is plotted in Figure 5(b).

Inputs		Outputs	
λ	0.27	N_ε	1
B	≤ 0.62	N	1
B_1	< 1.8	C_1	0.49
M	1.62	l	10
α	≤ 0.44	ε_{rig}	0.0014
ε_{num}	≤ 0.0000001	L_{exp}	1.386 ± 0.002
$(4\ T''/(T')^2\ _\infty)/k^2$	$\leq 4 \cdot 10^{-10}$		

12. Conclusion and directions. We have seen a quite general strategy for obtaining rigorous computation of invariant measures by a fixed point stability statement. We showed theoretical and practical details of the strategy implementation on some classes of one dimensional maps.

We remark that since the estimate for the error is a posteriori and is applied to the discretized operator, the algorithm can also work in systems where the spectral gap is not present (e.g., the indifferent fixed point systems). What is needed is an approximation estimation to satisfy item (a) of Theorem 3.1 and the discretized system to contract the zero average vectors fast enough to make the error small.

The next examples where it is natural to try the strategy are multidimensional piecewise hyperbolic systems. Typically here there will be no absolutely continuous invariant measure but measures having fractal support. Some (quite complicated) functional analytic framework (see, e.g., [16, 2]) was proved to give nice spectral properties, but an actual implementation seems to be computationally too complex. Here probably the use of suitable



(a) Map (11.1)

(b) The invariant measure for map (11.1)

Figure 5. Example (11.1).

simplified anisotropic norms will be useful, but the implementation must be able to avoid the problems arising from the bigger dimension of the space.

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