Chapter 4
Graph Theoretic Methods and Markov Models of Dynamical Transport

The topic of this chapter stems from the idea that Frobenius–Perron operators can be understood as if they were infinitely large stochastic matrices acting on an infinite-dimensional linear space. Furthermore, there are finite rank (corresponding to finite sized matrices) representations that can give excellent results. Such is the story of compact operators, and this leads not only to better understanding of the operator, but most importantly also to computable methods for carrying forward a practical basis for numerics on digital computers.

We use what may be called the Ulam–Galerkin method—a specialized case of the Galerkin method [199]—to approximate the (perhaps stochastic) Frobenius–Perron operator (3.44). In this chapter, we flesh out the discussion mentioned earlier that the approximate action of dynamical system on density looks like a directed graph, and that Ulam’s method is a form of Galerkin’s method. To hopefully offer some insight, we again refer the reader to the caricature partitioning of the action of the Henon mapping in Fig. 1.1.

The approximation by Galerkin’s method is based on the projection of the infinite-dimensional linear space \(L^1(M)\) with basis functions,

\[
\{\phi_i(x)\}_{i=1}^{\infty} \subset L^1(M),
\]

onto a finite-dimensional linear subspace with a subset of the basis functions,

\[
\Delta_N = \text{span}\{\phi_i(x)\}_{i=1}^{N}.
\]

For the Galerkin method, the projection

\[
\Pi_N : L^1(M) \to \Delta_N
\]

maps an operator from the infinite-dimensional space to an operator of finite rank, an \(N \times N\)

---

A compact operator is defined in the field of functional analysis in terms of having an atomic spectrum [8]. Compact operators are most easily described in a Hilbert space [189] (a complete inner product space) as these are the operators that are the closure of operators of finite rank. In other words, their action is “well approximated” by matrices, and approximated in the appropriate sense.
matrix, by using the inner product,\textsuperscript{34}

\[ P_{i,j} = (P_{F_\nu}(\phi_i),\phi_j) = \int_M P_{F_\nu}(\phi_i(x))\phi_j(x)\,dx. \quad (4.4) \]

The advantage of such a projection is that the action of the Markov operator which is initially a transfer operator in infinite dimensions reduces approximately to a Markov matrix on a finite-dimensional vector space. Such is the usual goal of Galerkin’s method in PDEs, and similarly it is used here in the setting of transfer operators.

Historically, Ulam’s conjecture was proposed by S. Ulam \[305\] in a broad collection of interesting open problems from applied mathematics, including the problem of approximating Frobenius–Perron operators. His conjecture has been essentially proved as cited below, but referred to both,

**Ulam’s Conjecture (see [305]).**

1. A finite rank approximation of the Frobenius–Perron operator by Eq. (4.6); and

2. the conjecture that the dominant eigenvector (corresponding to eigenvalue equal to 1 as is necessary for stochastic matrices) weakly approximates\textsuperscript{35} the invariant distribution of the Frobenius–Perron operator.

Ulam did not write his conjecture in the formal language of a Galerkin projection, (4.1)–(4.4), but due to the equivalence to such, we will use the phrase \textit{Ulam–Galerkin matrix} to refer to any projection of the Frobenius–Perron operator by an inner product as in Eq. (4.4), not necessarily including the infinite time limit part of the conjecture regarding steady state, item 2.

**Ulam’s method** is often used to describe the process of using Ulam’s conjecture, by developing what we call here the Ulam–Galerkin matrix, and then using the dominant eigenvector of this stochastic matrix to estimate the invariant density. Sometimes, however, the phrase Ulam’s method is used to simply describe what we call here the developing of the Ulam–Galerkin matrix. Some discussion of computational aspects of the Ulam–Galerkin matrix and the Ulam method can be found in Appendix A. As we will see, the one-step action of the transfer of the operator is well approximated by Ulam–Galerkin matrices. The analysis to describe the approximation of the one-step action is much simpler than that of the infinite limit referred to in the Ulam method, and other issues such as decomposition of the space into almost-invariant sets is naturally approximated as well by the short time representation. Also, in a special case the approximation is in fact exact, as discussed in Section 4.4. This exact representation may occur when the \textit{dynamical system is Markov}.

Ulam’s conjecture \[305\] has been proven in the special case of one-dimensional maps by methods of bounded variation \[199\]. In higher-dimensional dynamical systems, a rigorous footing of Ulam’s conjecture is incomplete, except for special cases \[49, 100, 101, 116, 118, 119\], and it remains an active area of research. We should also point out recent

\textsuperscript{34}Our use of the inner product structure requires the further assumption that the density functions are in the Hilbert space \(L^2(M)\) rather than just the Banach space \(L^1(M)\), which uses the embedding \(L^2(M) \hookrightarrow L^1(M)\), provided \(M\) is of finite measure.

\textsuperscript{35}Weak approximation by functions may be defined as convergence of the functions under the integral relative to test functions. That is, if \(\{f_n\}_{n=1}^\infty \in L^1(M)\), it is defined that \(f_n \to f^*\) if \(\lim_{n \to \infty} \int_M |f^*(x) - f_n(x)|h(x)\,dx = 0\) for all \(h \in L^\infty(M)\), which is referred to as the test function space.
developments in a nonuniformly expanding setting [234]. Nonetheless in practice it is easy and common to simply proceed to use the dominant eigenvector of the stochastic matrix and then to refer to it as an approximation of the invariant density. See Section 4.2, and compare to Fig. 1.1.

### 4.1 Finite-Rank Approximation of the Frobenius–Perron Operator

The quality of the Ulam–Galerkin approximation is discussed in several references, as is the convergence of Ulam’s method [117, 116, 57, 100, 170, 49, 34]. It is straightforward to cast Ulam’s method as Galerkin’s method with a special choice of basis functions, as follows. For Ulam’s method, the basis functions are chosen to be a family of characteristic functions:

\[
\phi_i(x) = \chi_{B_i}(x) = 1 \text{ for } x \in B_i \text{ and zero otherwise.} \tag{4.5}
\]

Generally, \(B_i\) is chosen to be a simple tiling of the region of interest in the phase space, meaning some region covering a stable invariant set such as an attractor. For convenience, \(B_i\) may be chosen as a simple covering of rectangle boxes, but we have also had success in using triangular tessellations using software packages often affiliated with PDE-based finite element methods technology. In the deterministic case, using the inner product (4.4) the matrix approximation of the Frobenius–Perron operator has the form

\[
P_{i,j} = \frac{m(B_i \cap F^{-1}(B_j))}{m(B_i)}, \tag{4.6}
\]

where \(m\) denotes the normalized Lebesgue measure on \(M\) and \(\{B_i\}_{i=1}^N\) is a finite family of connected sets with nonempty and disjoint interiors that covers \(M\). That is, \(M = \bigcup_{i=1}^N B_i\), and indexed in terms of nested refinements [305]. These \(P_{i,j}\) can be interpreted as the ratio of the fraction of the box \(B_i\) that will be mapped inside the box \(B_j\) after one iteration of a map to the measure of \(B_i\).

Note that one may consider this matrix approximation of the Frobenius–Perron operator as a finite Markov chain, where the partition set \(\{B_i\}_{i=1}^N\) represents a set of “states” and \(P_{ij}\) characterizes transition probabilities between states. It is well known that the matrix \(P\) in (4.6) is stochastic and has a left eigenvector with the eigenvalue one. Simply put, this eigenvector characterizes the equilibrium distribution of the Frobenius–Perron operator. In fact, it can be proven [50] that if the partition \(\{B_i\}_{i=1}^N\) is a Markov partition, then the (unique) left eigenvector of the matrix \(P\) defines a good approximation of the equilibrium distribution, a statement that will be made precise in the next subsection. This leads to a straightforward way to understand the approximation theory for the generic non-Markov case, by approximation using Markov representations. Definition of the phrase Markov partition will be the subject of Section 4.2.

However, first we note a more readily computable experimental perspective to stand in for Eq. (4.6), essentially by a Monte Carlo sampling.
**Remark 4.1.** A key observation is that the kernel form of the operator in Eq. (3.44) allows us to generally approximate the action of the operator with test orbits as follows. If we only have a test orbit \( \{x_j\}_{j=1}^N \), which is actually the main interest of this work, the Lebesgue measure can be approximated by

\[
P_{i,j} \approx \frac{\#(\{x_k | x_k \in B_i \text{ and } F(x_k) \in B_j\})}{\#(\{x_k \in B_i\})}.
\]

(4.7)

This statement can be made precise in terms of quality of the approximation and number of sample points by Monte Carlo sampling theory for integration of the inner product, Eq. (4.4). See Section A.1.1 and the demo in Appendix A for a MATLAB implementation of this orbit sampling method of developing an Ulam–Galerkin matrix.

See Fig. 4.1 for a graphical description of the situation of the approximations described in the previous paragraphs. Compare this to Fig. 4.2, which is developed using Eq. (4.7) in the case of a Henon map, and a rather coarse partition for the sake of illustration. Then recording the relative transition numbers according to Eq. (4.6) as estimated by Eq. (4.7) leads to stochastic matrices as presented by the transition matrix shown in Fig. 1.1. See Figs. 4.2 and 4.3 for illustrations of the set oriented methods reflected by the Ulam–Galerkin approach in realistic systems, the Henon map, and the flow of the Gulf, respectively.

**Figure 4.1.** An Ulam–Galerkin method approximation of the Frobenius–Perron operator is described by the action of a graph, as estimated by Eq. (4.7). Here we see a box \( i \) that maps roughly across \( j \), \( j + 1 \), and \( j + 2 \). As such a graph \( G_A \) generated by matrix \( A \) would have an edge between vertex \( i \) and each of \( j \), \( j + 1 \), and \( j + 2 \). The matrix \( A \) is formally described by the inner product, Eq. (4.4), where the basis functions are chosen to be characteristic functions \( \chi_k(x) \) supported over each of the boxes in the covering, including \( j \), \( j + 1 \), \( j + 2 \), and \( i \). As shown, the \( T(j) \) does not cover the \( i \) boxes in a way that allows a Markov partition, and thus the lost measure causes the finite rank to be only an approximation.
4.2 The Markov Partition: How It Relates to the Frobenius–Perron Operator

Generically, most dynamical systems are not Markov, meaning that they do not admit a Markov partition, and most partitions for such systems will not be Markov partitions. But when we do have such, then the corresponding Frobenius–Perron operator can be exactly represented by an operator of finite rank. We will give the necessary technical details and interpretations here. In the next section, we will show how this perspective of Markov partitions can be used to formulate a notion of approximation in the non-Markov case. Thus, as we will see, besides having an important role in a symbolic dynamics (from topological dynamics) of a dynamical system where the concept of a generating partition of the symbols is significantly simplified when there is a Markov partition, in measurable dynamics Markov partitions allow for a greatly simplified finite rank description of the Frobenius–Perron operator. Hence the computation of relevant statistical measures is greatly simplified.
Figure 4.3. The Ulam–Galerkin approximation of the Frobenius–Perron starts with the study of evolution of an ensemble of initial conditions from a single cell. Here a (rather large for artistic reasons) box $B_i$ in a flow developed from an oceanographic model of the fluid flow in the Gulf reveals how a single square progressively becomes swept in the Gulf Stream. The useful time scale is one that reveals some nontrivial dynamic evolution, stretching across several image cells, but not so long that a loss of correlation may occur. Compare this image to a similar image developed for the Henon mapping, Figs. 4.1 and 4.2, and stochastic matrix estimates in Eqs. (4.6) and (4.7). The operator in its simplest terms is a “set oriented method” in that how points in sets map to other sets is recorded and this is used as an approximation of the action of the dynamical system on points. Compare this figure showing a covering of boxes $B_i$ which will be used to estimate the action of the Henon map dynamical system in those cells $B_i$ in which the attractor is embedded (yellow). Compare this covering to the action of a Henon mapping so estimated and shown in Fig. 1.1. The underlying estimates of the stochastic matrix are summarized by the computations shown in Eqs. (4.6) and (4.7). Compare to a similar presentation in the Duffing oscillator, Fig. 1.16.

4.2.1 More Explicitly, Why a Markov Partition?

To simplify analysis of a dynamical system, we often study a topologically equivalent system using symbol dynamics, representing trajectories by infinite length sequences using a finite number of symbols. (An example of this idea is that we often write real numbers as sequences of digits, a finite collection of symbols.) Symbolic dynamics will be discussed in some detail in the next chapter.

To represent the state space of a dynamical system with a finite number of symbols, we must partition the space into a finite number of elements and assign a symbol to each one. In probability theory, the term “Markov” denotes a finite memory property. In other words the probability of each outcome conditioned on all previous history is equal to conditioning on only the current state; no previous history is necessary. The same idea has been adapted to dynamical systems theory to denote a partitioning of the state space so that all of the past information in the symbol sequence is contained in the current symbol, giving rise to the idea of a Markov transformation.
4.2.2 Markov Property of One-Dimensional Transformations

In the special but important case that a transformation of the interval is Markov, the symbol dynamic is simply presented as a finite directed graph. A Markov transformation in \( \mathbb{R}^1 \) is defined as follows [50].

**Definition 4.1.** Let \( I = [c, d] \) and let \( \tau : I \to I \). Let \( \mathcal{P} \) be a partition of \( I \) given by the points \( c = c_0 < c_1 < \cdots < c_p = d \). For \( i = 1, \ldots, p \), let \( I_i = (c_{i-1}, c_i) \) and denote the restriction of \( \tau \) to \( I_i \) by \( \tau_i \). If \( \tau_i \) is a homeomorphism from \( I_i \) onto a union of intervals of \( \mathcal{P} \), then \( \tau \) is said to be Markov. The partition \( \mathcal{P} \) is said to be a Markov partition with respect to the function \( \tau \).

**Example 4.1 (one-dimensional example).** Map 1, (Fig. 4.4(a)) is a Markov map with the associated partition \( \{I_1, I_2, I_3, I_4\} \). The symbol dynamics are captured by the transition graph (Fig. 4.4(b)). Although map 2 (Fig. 4.4(c)) is piecewise linear and is logically partitioned by the same intervals as map 1, the partition is not Markov because interval \( I_2 \) does not map onto (in the mathematical sense) a union of any of the intervals of the partition. However, we are not able to say that map 2 is not Markov. There may be some other partition that satisfies the Markov condition [38].

![Figure 4.4](image)

**Figure 4.4.** (a) A Markov map with partition shown. (b) The transition graph for map a. (c) The partition is not Markov because the image of \( I_2 \) is not equal to a union of intervals of the partition.

4.2.3 Markov Property in Higher Dimensions

**Definition 4.2.** A topological partition of a topological space \( (M, \tau) \) is a finite collection \( \mathcal{P} = \{P_1, P_2, \ldots, P_r\} \) of disjoint open sets whose closures cover \( M \) in the sense that \( M = \overline{P_1} \cup \cdots \cup \overline{P_r} \).

**Definition 4.3.** A topological space \( (M, \tau) \) is a set \( M \) together with the set of subsets \( \tau \subset 2^M \) that are defined to be open; as such \( \tau \) must include the empty set \( \emptyset \) and all of \( M \), and \( \tau \) must be closed under arbitrary unions and finite intersections [233].

Any topological partitioning of the state space will create symbol dynamics for the map. In the special case where the partition is Markov, the symbol dynamics capture the essential dynamics of the original system.

\[ 2^M \] denotes the “power-set” of \( M \), meaning it is the set of all subsets.
Definition 4.4. Given a metric space $M$ and a map $f: M \to M$, a Markov partition of $M$ is a topological partition of $M$ into rectangles $\{R_1, \ldots, R_m\}$ such that whenever $x \in R_i$ and $f(x) \in R_j$, then $f[W^u(x) \cap R_i] \supset W_u[f(x)] \cap R_j$ and $f[W^s(x) \cap R_i] \subset W_s[f(x)] \cap R_j$ [46, 44].

In simplified terms, this definition says that whenever an image rectangle intersects a partition element, the image must stretch completely across that element in the expanding directions and must be inside that partition element in the contracting direction (see Fig. 4.5) [38].

Figure 4.5. In the unstable (expanding) direction, the image rectangle must stretch completely across any of the partition rectangles that it intersects.

4.2.4 Generating Partition

It is important to use a “good” partition so that the resulting symbolic dynamics of orbits through the partition well represents the dynamical system. If the partition is Markov, then goodness is most easily ensured. However, a broader notion, called generating partition, may be necessary to capture the dynamics. A Markov partition is generating, but the converse is not generally true. See [271, 39] for a thorough discussion of the role of partitions in representing dynamical systems.

Definition 4.5. Given a topological space $(M, \tau)$ (Definition 4.3) and a topological partition, $\mathcal{P} = \{P_1, P_2, \ldots, P_r\}$ is a topological generating partition for a mapping $T: M \to M$ if

$$\tau = \vee_{i=0}^{\infty} T^{-i} \mathcal{P}$$

(4.8)

(or require $\tau = \vee_{i=-\infty}^{\infty} T^{-i} \mathcal{P}$, for invertible dynamical systems).

As usual, $T^{-i}$ denotes the $i$th preimage (possibly with many branches), but it is the $i$th composition of the inverse map if the map is invertible. This definition is in terms of the join of partitions, which is defined recursively.
Definition 4.6. The join of two partitions, \( P \) and \( P' \), is defined as

\[
P \vee P' = \{ P_k \cap P'_l : 0 \leq k \leq |P| - 1, 0 \leq l \leq |P'| - 1 \}.
\]  

(4.9)

Thus terms such as \( T^{-i} P \) in the definition of the generating partition are joined with other iterates of the original partition, \( T^{-j} P \). The idea of a generating partition is that this process of joining many iterates of open sets creates collections of open sets. Proceeding infinitely in this manner creates infinitely many open sets, and the question is whether all of the open sets in the topology are generated.

If, furthermore, a measure space is assumed \((M, \mathcal{A}, \mu)\), where \( \mathcal{A} \) is defined as the Borel sigma algebra of sets which are \( \mu \)-measurable, then the question a generating partition becomes as follows.

Definition 4.7. Given a measure space \((M, \mathcal{A}, \mu)\), then a topological partition \( \mathcal{P} = \{ P_1, P_2, \ldots, P_r \} \) of measurable sets is a measurable generating partition for a mapping \( T : M \rightarrow M \) if

\[
\mathcal{A} = \vee_{i=0}^{\infty} T^{-i} \mathcal{P}
\]  

(4.10)

(or require \( \tau = \vee_{i=-\infty}^{\infty} T^{-i} \mathcal{P} \), for invertible dynamical systems). We require that all the measurable sets are generated.

Example 4.2 (two-dimensional example—toral automorphism). The cat map, defined by

\[
x = (Ax) \mod 1,
\]  

(4.11)

where

\[
A = \begin{bmatrix} 2 & 1 \\ 1 & 1 \end{bmatrix},
\]  

(4.12)

yields a map from the unit square onto itself. This map is said to be on the toral space \( T^2 \) because the \( \mod 1 \) operation causes the coordinate \( 1 + z \) to be equivalent to \( z \). A Markov partition for this map is shown in Fig. 4.6. The cat map is part of a larger class of functions called toral Anosov diffeomorphisms, and [267] provides a detailed description of how to construct Markov partitions for this class of maps [38].

Figure 4.6. The cat map is a toral automorphism. (a) The operation of the linear map on the unit square. (b) Under the mod operation, the image is exactly the unit square. (c) Tessellation by rectangles \( R_1 \) and \( R_2 \) forms an infinite partition on \( R^2 \). However, since the map is defined on the toral space \( T^2 \), only two rectangles are required to cover the space. The filled gray boxes illustrate that \( R_1 \) and \( R_2 \) are mapped completely across a union of rectangles.
**Chapter 4. Graph Theory and Markov Models of Transport**

**Example 4.3 (generating partition of the Henon map).** Consider again the Henon map, \( T(x,y) = (1 - ax^2 + y, bx) \), \((a,b) = (1.4,0.3)\), the prototypical diffeomorphism of the plane with the famous strange attractor. See Fig. 6.31 in which a piecewise linear curve \( C \) produced as connecting tangencies of stable and unstable manifolds, according to the well-regarded conjecture [70, 142], produces what is apparently a generating partition but not a Markov partition. See also the generating partition discussion of the Ikeda map (9.87) in Example 9.3 shown in Fig. 9.8.

**4.3 The Approximate Action of Dynamical System on Density Looks Like a Directed Graph: Ulam’s Method Is a Form of Galerkin’s Method**

The title of this section says that the approximate action of dynamical system on a density looks like a directed graph: Ulam’s method is a form of Galerkin’s method. This is a perspective in which we already discussed the theory of Galerkin’s method in Section 4.1. In fact, as stated above, when the dynamical system is Markov and using the Markov partition and the corresponding basis functions which are supported over the elements of that Markov partition, the action of the dynamical system is exactly represented by a directed graph. In this case, the inner product form (4.4) becomes exactly (4.6), resulting in a stochastic matrix \( A \) whose action and steady state are both discussed by the Frobenius–Perron theorem. In this section, we will summarize these statements more carefully, but first we motivate with the following examples.

**Example 4.4 (finite rank transfer operator of a one-dimensional transformation).** The map shown in Fig. 4.4(a) was already discussed to be a Markov map in the interval, with a Markov partition \( \{I_1, I_2, I_3, I_4\} \) as shown, and according to the definition of Markov partition shown in Fig. 4.4.

In this piecewise linear case, it is easy to directly integrate the Galerkin method (4.4) integrals when choosing the basis functions to be one of each of the four characteristic functions, \( \{ \chi_{I_1}(x), \chi_{I_2}(x), \chi_{I_3}(x), \chi_{I_4}(x) \} \). Let

\[
\phi_i(x) = \chi_{I_i}(x), \quad i = 1, 2, 3, 4. \tag{4.13}
\]

For the sake of example, we will explicitly write one such integral here. From the drawing, writing the function in Fig. 4.4(a) explicitly, for simplicity assuming the uniform partition shown,

\[
I_i = [i-1, i], \quad i = 1, 2, 3, 4, \tag{4.14}
\]

and that

\[
\bigcup_{i=1}^4 \overline{I_i} = [0,4], \tag{4.15}
\]

then \( F : [0,4] \to [0,4] \) may be written

\[
F(x) = \begin{cases} 
3x & \text{if } x < 1 \\
-x + 4 & \text{if } 1 \leq x < 2 \\
2x - 2 & \text{if } 2 \leq x < 3 \\
-4x + 16 & \text{else } x \geq 3 
\end{cases}. \tag{4.16}
\]

---

A characteristic function, also called an indicator function, takes on the value 1 inside the argument set, \( \chi_A(x) : M \to [0,1], \chi_A(x) = \text{if } (x \in A,1,0) \).
4.3. Action on Densities as a Directed Graph

Now we may write and evaluate the inner product (4.4) to derive each of the elements of the $4 \times 4$ matrix $A$ which describes the relative movement of ensemble density with each iteration of the map. Substitution into Eq. (4.4) gives

$$P_{i,j} = \langle P_F(\phi_i),\phi_j \rangle = \int_{x=0}^{4} P_F(x) \chi_j(x) dx, \quad i,j = 1,2,3,4. \quad (4.17)$$

Continuing to produce $A$ requires $16 = 4^2$ such integrations for each $\chi_i(x), \chi_j(x)$ basis function pairing, but in this simplified case where we have piecewise linear functions, we will illustrate with just one pairing, $i = 1$ and $j = 2$, to produce $P_{1,2}$ using the basis functions $\chi_1(x)$ and $\chi_2(x)$ in the Galerkin method’s inner product computation,

$$P_{1,2} = \int_{x=0}^{4} P_F(\chi_1(x)) \chi_2(x) dx,$$
$$= \int_{x=1}^{2} P_F(\chi_1(x)) dx, \quad (4.18)$$

by considering the nonzero support of $\chi_2(x)$. Evaluating the Frobenius–Perron image of the initial density $\chi_1(x)$ for the integration by referring to the definition and specializing to this example,

$$P_F[\chi_1(x)] = \sum_{y \in F^{-1}(x)} \frac{\chi_1(x)}{|\det D_y F|} = \frac{1}{3} \chi_1(x). \quad (4.19)$$

Again we recall the region of nonzero support required to be considered in evaluating the integral in Eq. (4.18). In this region, colored as shown in Fig. 4.7, each $x$ has exactly one preimage, still in $I_1$, and thus, $|\det D_y F| = 3$ there. Hence continuing,

$$P_{1,2} = \int_{x=1}^{2} \frac{1}{3} \chi_1(x) dx = \frac{1}{3}. \quad (4.20)$$

![Figure 4.7](image.png)

**Figure 4.7.** The Markov map shown in Fig. 4.4(a) is again shown here, but the yellow region here is shaded to highlight the set which is active when computing the integrations necessary to produce the matrix element $P_{1,2}$ as described in (4.13) to (4.20).
Similarly repeating this computation in kind for each $i, j$ pairing results in the rest of the transition matrix:

$$
A = \begin{bmatrix}
\frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & \frac{1}{2} & \frac{1}{2} \\
\frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4}
\end{bmatrix}.
$$

(4.21)

As a side note, observe that when computing $P_F[\chi_i(x)]$, there is a potential for multiple preimages, but then considering the inner product $\langle P_F(\phi_i), \phi_j \rangle$ means that we will always select exactly one of those branches since the other function in the inner product, $\chi_j(x)$, selects just one branch and no more. This follows from the fact that we have specialized to characteristic functions supported over the elements of a Markov partition; thus we implicitly rely on the monotonicity which follows the required homeomorphism for each leg.

Thus the transfer operator becomes an operator of finite rank in terms of Galerkin’s method with finitely many terms. Furthermore, the approximation is exact when a Markov partition and associated basis functions are used. The resulting $A$ may be interpreted as a transfer matrix, for which it is easy to check that all row sums are 1,

$$
\sum_j P_{i,j} = 1 \quad \forall j.
$$

(4.22)

As such, it is a stochastic matrix. Correspondingly, this generates a weighted directed graph for a representing Markov process, as shown in Fig. 4.4(b).

It is general that matrices produced in this way have positive elements, and they will be stochastic matrices when the Markov partition property exists and is used. As such, the theory of Frobenius–Perron matrices applies and specializes to stochastic matrices. Some elements of this theory will be reviewed in the next section, but we will illustrate a main idea continuing with the example of Fig. 4.4(a). That is, the dominant eigenvalue equals 1, and uniquely if the dynamical system is ergodic or correspondingly the resulting matrix is irreducible. The dominant eigenvector corresponds to the steady state, and therefore associates to the steady state measure.

**Example 4.5 (steady state of a finite rank transfer operator).** Continuing with Example 4.4 from Fig. 4.4(a), we compute the steady state distribution. The steady state distribution of the Markov process, Fig. 4.4(b), can be shown from the Frobenius–Perron theory of positive matrices (see Section 4.3.3) to equal the eigenvector of the transition matrix corresponding to the largest eigenvalue, which is 1. This eigenvector of matrix (4.21) is

$$
v = \frac{1}{\sqrt{226}} \begin{bmatrix} 3 \\ 3 \\ 12 \\ 8 \end{bmatrix}.
$$

(4.23)

---

38 Without using the existing Markov partition, or if one does not exist, then a stochastic matrix does not result, but it may be “almost” stochastic in that row sums are almost 1, reflecting some leak of measure in the representation, while not reflecting the reality of the dynamical system.

39 Contrast that phrase to “Frobenius–Perron operators” already discussed here. While the names of these mathematicians associated with the operator are found ordered both ways in the literature, we will take here a common convention that FP denotes the operators, and PF denotes the finite rank situation and the related linear algebra.
4.3. Action on Densities as a Directed Graph

Figure 4.8. Steady state of the system in Fig. 4.4(a,b) and Fig. 4.7 and defined by Eq. (4.16) was noted to be Markov, and as such the corresponding stochastic matrix from the Ulam–Galerkin method gives the dominant eigenvector Eq. (4.23). (Top) The map shown again to help match the regions of the partition relevant for the states in the density. Note that each piecewise linear section of the map matches piecewise constant sections of the invariant density. (Bottom) The histogram for a $10^5$ iterate test orbit agrees quite well with the density predicted by the eigenvector (4.23).

Now this eigenvector represents the steady state distribution of ensembles of initial conditions over long times, where each partition element of the Markov partition should see a relative number of points land in them, according to the relative proportions of this vector. To punctuate this point, we illustrate the histogram from a long orbit of $10^5$ iterates in Fig. 4.8. Note that by showing the histogram of a long orbit, rather than the histogram produced by an ensemble of many initial conditions, we have again appealed to the notion that time averages and spatial averages can be exchanged. Such correspondence is the premise of the Birkhoff ergodic theorem, which is valid since this example is an ergodic system. The resulting matrix is irreducible and the system is Markov. Thus the finite rank representation exactly describes the steady state measure.
4.3.1 Graph Theory, Reducible Matrices

A broader theme of this book is the analysis of global transport, which can be defined in terms of a partition to discuss how ensembles may propagate from one element of the partition to others. The discrete counterpart of this discussion for a directed graph also corresponds to notions of partitions of a graph into subgraphs, as discussed here.

In this section we briefly review some basic concepts of reducible matrices and corresponding relationships to the graph induced by the matrices due to discrete approximations of a Frobenius–Perron operator. In particular, we introduce the question of how to discover a permutation of the transition matrix (4.7) that reveals the basin structure of a dynamical system revealed to us in the form of a test orbit segment \( \{x_j\}_{j=1}^N \).

A graph \( G_A \) associated to a matrix \( A \) consists of a set of vertices \( V \) and a set of edges \( E \subset V \times V \). The entry \( P_{ij} \) is nonzero when there exists an edge \( (i, j) \in E \) that connects the vertices \( i \) and \( j \).

As we will describe, borrowing a term from the recent activity in complex networks, it is also useful to consider structure within a graph. First we have components, and then generalizing that we have communities. If a disjoint collection \( \{S_i\}_{i=1}^k \) of subsets \( S_i \subset V \) consists of vertices such that there is a higher density of edges within each \( S_i \) than between them, then we say roughly that \( \{S_i\}_{i=1}^k \) forms a community structure for \( G_A \) [238, 239].

For the discussion of this section, it is only necessary to consider the sign of the entries of a transition matrix \( A \), or perhaps of a stochastic matrix \( A \). We shall define

\[
B = \text{sign}(A),
\]

which when \( A \) is a nonnegative matrix, \( B_{i,j} = 0 \) or \( 1 \), and comparing to the directed graph \( G_A = (E, V) \) generated by \( A \) implies that there is an edge from \( j \) to \( i \),

\[
B_{i,j} = \begin{cases} 
1 & \text{if } j \rightarrow i \\
0 & \text{else}
\end{cases}.
\]

Such is called an adjacency matrix when it encodes just possible transitions without weights. That is, a one-step path is on an edge from a vertex labeled \( j \) to vertex labeled \( i \).

When the graph represents the action of the Frobenius–Perron operator from a dynamical system, a one-step path means that there exists a direct transfer from mode \( \phi_j(x) \) to \( \phi_i(x) \) when those modes are characteristic functions. This in turn implies existence of at least a one-step orbit of the dynamical system between the cells when basis functions are characteristic functions. If an \( n \)-step path in the graph is possible, this does not imply that an \( n \)-step orbit through the corresponding cells covering the phase space of the dynamical system is possible. Instead, the correct statement is that an epsilon-chain pseudo-orbit\(^{40}\) is possible, but perhaps not a true orbit segment.

An essential question then is if a given path\(^{41}\) in the graph is possible, which has significance to the distribution of measure in the corresponding Markov chain? A few issues relevant to transition matrices are captured by the following language.

\(^{40}\) An epsilon-chain pseudo-orbit is a sequence of points, \( \{x_i\} \), such that \( \|T(x_i) - x_{i+1}\| \leq \epsilon \) for each \( i \), and this specializes to a true orbit if \( \epsilon = 0 \). There are theorems from the shadowing literature [45, 46], especially for hyperbolic systems, that describe that near an epsilon chain there may be true orbits. In the context used here, however, those true orbits may not pass through the boxes corresponding to a particular refinement.

\(^{41}\) An \( n \)-step path from vertex \( i \) to vertex \( j \) is the existence of \( n \) edges in order “end-to-end” (stated roughly to mean the obvious that each edge ends at a vertex where the next begins) beginning at \( i \) and ending at \( j \).
4.3. Action on Densities as a Directed Graph

Figure 4.9. A path in the graph corresponding to the transfer matrix produced from orbits in a dynamical system may not imply an orbit in the dynamical system passing through the same corresponding boxes, but rather an epsilon-chain pseudo-orbit. Here the graph has an orbit from boxes labeled \( i \to j \to k \), but \( x \in i \), \( T(x) \in j \), and perhaps \( T^2(x) \in k + 1 \), but perhaps there is an \( x' \) such that \( T(x') \in k \).

Definition 4.8. A square matrix \( A_{n \times n} \) is called primitive if there exists a (time) \( k \) such that \([A_{n \times n}]^k_{i,j} > 0\) for all \( i, j \).

Remark 4.2. A sufficient condition for a matrix to be a primitive matrix is for the matrix to be a nonnegative, irreducible matrix with a positive element on the main diagonal.

The primitive property may be interpreted as follows. Since a direct path between \( j \) to \( i \) exists if and only if \( P_{i,j} > 0 \), and \( P^2 \) describes the two-step action of the graph, then a two-step path exists between \( j \) to \( i \) if and only if \( P^2_{i,j} > 0 \). In these terms, the primitive property demands that there is a time \( k \) when there is a path from everywhere to everywhere else in the graph. Conversely, if there is an \( i,j \) pair such that \( P^k_{i,j} = 0 \) for all times \( k \), then as a graph structure, the two vertices must occupy different components of the graph. “Component” then describes much the same information as primitiveness for the corresponding graph.

Definition 4.9. A component of a graph \( G \) is a subgraph \( G' \) of \( G \) such that between every pair of vertices, there is a path between every vertex in the subgraph. A graph is called connected if it consists of exactly one component.

As an example, we see in Fig. 4.10 that the component including \( i \), \( i + 1 \), and \( j \) is apparently not connected to the component including vertices \( k \), \( k + 1 \). As such, the adjacency matrix \( A \) which generates this graph cannot be primitive.

Let \( I = \{1, \ldots, N\} \) be an index set. For our specific application to the transition matrix \( P \) generated by the Ulam–Galerkin method, we define the set of vertices \( V = \{v_i\}_{i \in I} \) to label the original boxes \( \{B_i\}_{i \in I} \) used to generate the matrix \( P \), and define the edges to be the set of ordered pairs of integers \( E = \{(i,j) : i, j \in I\} \) which label the vertices as their starting and ending points.
Another concept which is useful in the discussion of partitioning a graph into dynamically relevant components is to ask if the graph is reducible.

**Definition 4.10.** A graph is said to be **reducible** if there exists a subset $I_o \subset I$ such that there are no edges $(i, j)$ for $i \in I_o$ and $j \in I \setminus I_o$; otherwise, it is said to be **irreducible** [22, 306].

This condition implies that the graph is irreducible if and only if there exists only one connected component of a graph, which is $G_P$ itself. In terms of the transition matrix $P$, $G_P$ is reducible if and only if there exists a subset $I_o \subset I$ such that $P_{ij} = 0$ whenever $i \in I_o$ and $j \in I \setminus I_o$. Furthermore, $P$ is said to be a reducible matrix if and only if there exists some permutation matrix $S$ such that the result of the similarity transformation

$$ R = S^{-1}PS $$

is block upper triangular:

$$ R = \begin{pmatrix} R_{1,1} & R_{1,2} \\ 0 & R_{2,2} \end{pmatrix}. $$

This means that $G_P$ has a decomposition into a partition,

$$ V = V_1 \cup V_2, $$

such that $V_1$ connects with $V_1$ and $V_2$, but $V_2$ connects only with itself. When $R_{1,2} = 0$, $P$ is said to be **completely reducible** [306],

$$ R = \begin{pmatrix} R_{1,1} & 0 \\ 0 & R_{2,2} \end{pmatrix}. $$

**Figure 4.10.** A segment of a larger directed graph. We see that a one-step walk from vertex $i$ to $i + 1$ is possible but a walk to $j$ from $i$ requires two steps. No walk from the component containing vertices $i, i + 1, and j$ to the $k, k + 1$ component is possible, at least along the edges shown.
4.3. Action on Densities as a Directed Graph

Figure 4.11. The matrix in this figure is reducible. However, the members of the original transition matrix before sorting are placed haphazardly. After using a diagonalizing similarity transformation (4.26) to the form (4.29) (when it exists), then the block-diagonal form is revealed. The corresponding graph description of the same is seen in Fig. 4.12.

An instructive observation when relating these concepts back to dynamical systems is that in the case that $G_P$ is generated from a bistable dynamical system as from Example 7.1, the transition matrix $A$ will be completely reducible. Therefore, $R_{1,1}$ and $R_{2,2}$ correspond to the two basins of attractions of the system. The off-diagonal elements $R_{1,2}$ and $R_{2,1}$ give information regarding transport between these partition elements if there are any nonzero off-diagonal elements. Also, in a general multistable dynamical systems the transition matrix $A$ has a similarity transformation into a block (upper) triangular form—emphasizing many components which may not communicate with each other.

A key point relevant to the theme of this writing is that most (randomly or arbitrarily realized) indexing of the configuration resulting from an Ulam–Galerkin matrix makes it difficult to observe even simple structures, like community structure or reducibility, of the graph and the corresponding transition matrix. That is, the indexing that may come from a sensible and suitable covering of a phase space by rectangles, or perhaps of triangles, will not generally be expected to directly reveal a useful structure in the associated Ulam–Galerkin matrix. The goal is then to reveal reducibility or at least community structure when it is there. Figs. 4.11 and 4.12 illustrate the kind of graph that results from a bistable system coming from a bistable system, when usefully sorting to reveal the structure. Notice that there are two disjoint components that do not communicate with each other. Corre-
Chapter 4. Graph Theory and Markov Models of Transport

Figure 4.12. Graph representation of the adjacency matrices shown in Fig. 4.11.

spondingly this informs that the bistable system has two basins that do not communicate with each other. A more difficult problem of sorting a transition matrix comes from the scenario when there may be some off-diagonal elements even in a suitable sorting, as would arise when there may be some “leaking” or small transport between two basins which may no longer be invariant sets, but rather simply almost invariant.

In Figs. 5.3(a) and 5.3(b) we show an example of a transition matrix for a 30-vertex random community-structured graph with three communities whose members are placed haphazardly, but after a proper permutation this matrix is transformed into an “almost” block-diagonal form. This is the sort of Ulam–Galerkin matrix which would be expected from a bistable dynamical system. Figs. 5.4(a) and 5.4(b) illustrate the associated graph of the matrix in the above example. Before sorting the vertices into three separate communities, the graph looks like a random graph that has no community structure. However, after sorting, the community structure of the graph becomes obvious. This is central to the problem of this topic, to find the sorting that reveals the useful partition illustrative of transport.

There are several techniques for finding an appropriate permutation if the matrix is reducible. In the language of graph theory, we would like to discover all connected components of a graph. The betweenness methods in [239] and the local method in [9] are examples of numerous methods as reviewed in [72, 239] that can be successfully used to uncover various kinds of community structures.

Remark 4.3. Lack of reducibility of a graph relates to the measure theoretic concept of ergodicity (Definition 3.7), and the topological dynamical concept of transitivity (see Definition 6.1), in that when the graph representation is sufficient, they all describe the reduction of the system either into noncommunicating components, or not in the case of the complement.
Remark 4.4. An essential question is whether the represented dynamical system is well coarse grained by the graph and the action of the matrices. The question can be settled in terms of discussion of those dynamical systems which are exactly represented by a coarse grain, which are those called Markov dynamical systems, and then the density of these. When a coarse-grained representation is used, the associated transition matrix may reveal some off-diagonal elements when sorted, suggesting some transitivity in the dynamical system, but this could just arise as the error of the coarse-grain estimation.

4.3.2 Convergence Rates, the Power Method, and Stochastic Matrices

Analysis of the result of iterating a matrix is very instructive regarding the long time behavior of the transfer operators, and the matrix discussion is a simplifying discussion. It is a well-known feature in matrix theory that certain matrices are composed such that large powers tend to point arbitrary vectors toward the dominant eigenvector. This feature is the heart of the power method in numerical analysis [296] which has become crucial in computing eigenvalues and eigenvectors of very large matrices—too large to consider a computation directly by the characteristic polynomial det(A − λI) = 0. This discussion is meant to give some geometric notion of the action of the Ulam–Galerkin matrices in the vector spaces upon which they act.

We will begin this discussion with a simple illustrative example.

Example 4.6 (power method). Let

$$A = \begin{bmatrix}
\frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & \frac{1}{2} & \frac{1}{2} \\
\frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4}
\end{bmatrix}, \quad (4.30)$$

which is again a matrix from the Ulam–Galerkin method example (4.21), derived from Fig. 4.4(a). Here we discuss it simply in terms of its matrix properties. Checking

$$A \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad (4.31)$$

confirms that $\lambda = 1$ is a right eigenvalue with a corresponding right eigenvector, $v = [1,1,1,1]'$, (the prime symbol denotes transpose), in the usual definition of an eigenvalue/eigenvector pair,

$$Av = \lambda v. \quad (4.32)$$

Likewise, a substitution,

$$\begin{bmatrix} 1,1,4,\frac{8}{3} \end{bmatrix} A = \begin{bmatrix} 1,1,4,\frac{8}{3} \end{bmatrix}, \quad (4.33)$$

which as an instance of the left eigenvalue/eigenvector equation,

$$uA = \tau u, \quad (4.34)$$

wherein $\tau = 1$ is a left eigenvalue with corresponding left eigenvector, $u = [1,1,4,\frac{8}{3}]$. 

These particular eigenvalue/eigenvector pairs have special significance. It is easy to check that \( A \) row sums to 1,
\[
\sum_{j} P_{i,j} \quad \forall i,
\] (4.35)
which defines \( A \) to be a stochastic matrix with probabilistic implications to be defined later in this section. In particular, the left side of Eq. (4.31) may be directly interpreted as a row-by-row summation, and matching the right side of the equation means that the result must be 1. Thus, we are able to summarize.

**Remark 4.5.** \((\lambda = 1, v = [1, 1, 1, 1]')\) will be a right eigenvector/eigenvector pair if and only if \( A \) is row-wise stochastic.

That \((\tau = 1, u = [1, 1, 4, \frac{8}{3}])\) is a left eigenvalue/eigenvector pair may be derived from the characteristic polynomial,
\[
\det(A' - \tau I) = 0. \tag{4.36}
\]
That we may directly solve this 4th degree polynomial, with up to four roots due to the fundamental theorem of algebra, is possible primarily because the matrix is small. In principle these roots may be found directly by a direct computation akin to the quadratic formula [201], or at least by numerical root solvers. However, numerically approaching the spectrum of large matrices is feasible only through the power method cited in many texts in numerical analysis [296]. Furthermore, specifically considering the power method in this simple case allows us an easy presentation of the behavior of the evolution of the corresponding Markov chain, as we shall see.

Consider an arbitrary vector \( w \in E^n \), where \( E^n \) denotes the vector space which serves as the domain of \( A \), which in this case we generally choose to be \( \mathbb{R}^n \). By arbitrary we generally mean almost any. A full measure of those “good” vectors \( w \) shall suffice, and those which are not good shall become clear momentarily. Let \( A \) act on \( w \) from the left,
\[
wA = (c_1 u_1 + c_2 u_2 + \cdots + c_n u_n) A, \tag{4.37}
\]
where we have written as if we have a canonical situation in which there is a spanning set of \( n \)-eigenvectors \( \{u_i\}_{i=1}^n \), but all we require is that
- one eigenvalue is unique and largest, and
- the subspace corresponding to the rest of the spectrum may be more degenerate.

Of course in general there can be both algebraic and geometric multiplicities, but for now, for sake of presentation we describe the simplest situation of unique eigenvectors, and further assume that the corresponding eigenvalues are such that one eigenvector is unique and largest:
\[
\tau_1 > \tau_i \quad \forall i > 1. \tag{4.38}
\]
By linearity of \( A \), and further by resorting to the definition of a left eigenvector for each of the \( u_i \), Eq. (4.37) becomes
\[
wA = c_1 A u_1 A + c_2 u_2 A + \cdots + c_n u_n A = c_1 \tau_1 u_1 + c_2 \tau_2 u_2 + \cdots + c_n \tau_n u_n. \tag{4.39}
\]
4.3. Action on Densities as a Directed Graph

Then proceeding similarly, applying $A^m$ times, we get,

$$w A^m = c_1 \tau_1^m u_1 + c_2 \tau_2^m u_2 + \cdots + c_n \tau_n^m u_n.$$  

(4.40)

Therefore, we see roughly that

$$\tau_1 > \tau_i \implies \tau_1^m \gg \tau_i^m$$  

(4.41)

for large $m$, from which follows

$$w A^m \approx c_1 \tau_1^m u_1.$$  

(4.42)

This says that repeated application of the matrix rotates arbitrary vectors toward the dominant ($u_1$) direction.

The general power method from numerical analysis does not proceed in this way alone because, while it may be true that $\tau_1^m \gg \tau_i^m$, for large $m$ both (all) of these numbers become large, and the computation becomes impractical on a computer. In general it is better to renormalize at each application of $A$ step, at each step in the following form. Let $s_0$ be chosen arbitrarily as was stated in Eq. (4.37), but then

$$s_{k+1} = \frac{s_k A}{\|s_k A\|},$$  

(4.43)

stated in terms of left multiplication of left eigenvectors and where $\|w_k A\|$ is a renormalization factor at each step in terms of a vector norm. Similar arguments to those stated in Eqs. (4.37)–(4.42) can be adjusted to show that

$$s_k \to w_1$$  

as $k \to \infty$.

(4.44)

in the vector norm, $\|s_k - w_1\| \to 0$. The general statement is that a subsequence of $s_k$ converges to $w_1$ because a general scenario is that the eigenvalue largest in magnitude may be complex. Rotations upon application of $A$ may occur, complicating discussion of convergence. This will not be an issue for our specific problem of interest, which involves Frobenius–Perron matrices and in particular stochastic matrices, since such matrices have a positive real eigenvalue, as we will expound upon below.

The three most common vector norms we will be interested in here are

1. $\|v\|_1 = \sum_{i=1}^n |v_i|$, the sum of the absolute values of the entries of a vector $v$,

2. $\|v\|_2 = \sqrt{\sum_{i=1}^n v_i^2} = \sqrt{v^T v}$, the Euclidean norm, and

3. $\|v\|_\infty = \max_{i=1,2,...,n} |v_i|$, the infinity norm, also known as the max norm,

in terms of an $n \times 1$ column vector. We shall discuss the power method in terms of the Euclidean norm $\|\cdot\|_2$. Further, by similar arguments, the (left) spectral radius follows from the Raleigh quotient

$$\frac{s_k A s_k^T}{s_k s_k^T} \to \tau_1$$  

as $k \to \infty$.  

(4.45)

42. The notation “$\gg$” denotes “exceedingly larger than,” which can be defined formally by the statement $\tau_1^m \gg \tau_i^m \equiv \lim_{m \to \infty} \frac{\tau_i^m}{\tau_1^m} = 0$.

43. The spectral radius is the largest eigenvalue in complex modulus.
Also from the discussion of the power method, we get an idea regarding the rate of convergence. Again we start with

\[
wA = c_1 Au_1 + c_2 u_2 A + \cdots + c_n u_n A = c_1 \tau_1 \left( u_1 + \frac{c_2}{c_1} \frac{\tau_2}{\tau_1} u_2 + \cdots + \frac{c_n}{c_1} \frac{\tau_n}{\tau_1} u_n \right),
\]

(4.46)

from which

\[
wA^n = c_1 \tau_1^n \left( u_1 + \frac{c_2}{c_1} \left( \frac{\tau_2}{\tau_1} \right)^n u_2 + o\left( \left( \frac{\tau_2}{\tau_1} \right)^n \right) \right).
\]

(4.47)

Thus follows geometric convergence as,

\[
r = \left| \frac{\lambda_2}{\lambda_1} \right|.
\]

(4.48)

See a geometric presentation of the power method in Fig. 4.13. Really, the only part of the terms after the first two are that they form \( \text{proj}_\perp[w,\text{span}(u_1,u_2)] \), where \( \text{proj}_\perp[w,\text{span}(u_1,u_2)] \) denotes the orthogonal projection of \( w \) onto the subspace spanned by \( u_1 \) and \( u_2 \), meaning \( w = c_1 u_1 + c_2 u_2 \). The details of the multiplicities and degeneracies of that main subspace are irrelevant to our discussion since we are interested in Frobenius–Perron matrices. See a caricature representation of the power method in Fig. 4.13 and its spectrum in Fig. 4.14.

![Figure 4.13. Geometric representation of the power method representation of Eqs. (4.46) and (4.47).](image)

Note that usually this discussion of the power method is carried out regarding right eigenvectors in the numerical analysis literature, which we adapted here for our interest in row-stochastic matrices. In particular, in the case of a stochastic matrix when \( \tau_1 = 1 \), then the renormalization step will not be zero, and the convergence rate will be geometric with rate \( r = |\lambda_2| \). While the expectation of the projection of Frobenius–Perron operators may be
4.3. Action on Densities as a Directed Graph

![Diagram of the spectrum of stochastic matrices in the complex plane.](image)

Figure 4.14. Spectrum of the stochastic matrices in the complex plane. We expect the dominant eigenvalue to be $\lambda_1 = 1$, and the second eigenvalue, $|\lambda_2| < \lambda_1$, to describe the geometric convergence of the power method according to Eqs. (4.47) and (4.48), $r = |\frac{\lambda_2}{\lambda_1}|$.

a row-stochastic matrix, with projection errors (due to truncation of the would-be infinite set of basis functions) and computational errors due to finite precision in the computers, typically the computation behaves as if $\tau \approx 1$ as if there were a small mass leak. There will be more on this leak issue in Section 4.3.4 (see Eq. (4.58)).

4.3.3 Frobenius–Perron Theory of Nonnegative Matrices

There are several important and succinct statements that can be proven regarding stochastic matrices, since they are nonnegative. There are many useful statements which are part of the Frobenius–Perron theory, but we will highlight only a few here—those that are most relevant to the stochastic matrices which result from Ulam–Galerkin’s projection of Frobenius–Perron operators. These matrices are nonnegative. As such, they have special properties that complement the description in the previous subsection, regarding the (non)possibility of multiplicity and complex value of the largest eigenvalue.

Where the previous section on the power method was meant to give the geometry of the action of an Ulam–Galerkin matrix, this section should be considered complementary since it is meant to give some algebraic information regarding the same action. We will start by stating a particular form of the Frobenius–Perron theorem, following the necessary definitions to interpret it, and then examples. We omit the proofs of this theorem since it is standard from matrix theory; refer to [13]. To interpret this theorem, we state the following definitions with brief examples.

**Definition 4.11.** An $n \times n$ square matrix $A_{n \times n}$ is called a positive matrix if $A_{n \times n} > 0$, meaning that each and every term in the matrix is nonnegative, $[A_{n \times n}]_{i,j} > 0$ for all $i, j$. 
We present the definition in terms of square matrices since we are interested only in spectral properties. However, the theory of positive matrices is more broadly interesting.

**Definition 4.12.** An $n \times n$ square matrix $A_{n \times n}$ is called a **nonnegative matrix** if $A_{n \times n} \geq 0$, meaning that each and every term in the matrix is positive, $[A_{n \times n}]_{i,j} \geq 0$ for all $i,j$.

**Example 4.7 (positive and nonnegative matrices).** Inspecting

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}, B = \begin{pmatrix} 1 & 2 & 0 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}, C = \begin{pmatrix} 1 & -1 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}, D = \begin{pmatrix} 1 & 2 & 3 & 3.1 \\ 4 & 5 & 6 & 6.2 \\ 7 & 8 & 9 & 9.2 \end{pmatrix},$$

$a_{i,j}$

$A$ is a positive matrix, but $B$ is nonnegative because of the single nonzero entry. $C$ is neither because of the single negative entry, and $D$ is not considered in the discussion of positivity since it is nonsquare and therefore irrelevant when discussing spectral properties.

**Remark 4.6.** A nonnegative matrix has a unique positive and real dominant eigenvalue due to the Frobenius–Perron theory. Therefore, the power method proceeds as described in Eqs. (4.37)–(4.42) without the possible complications regarding multiplicities either geometric or algebraic when discussing convergence and convergence rate.

**Remark 4.7.** A stochastic matrix is nonnegative. We have already noted that $\tau_1 = 1$ is an eigenvalue since it corresponds to the definition that the matrix must row sum to 1. Further, any larger eigenvalue would correspond to a larger row sum, so it must be largest. Therefore, by the Frobenius–Perron theory, this is the unique largest eigenvalue of a stochastic matrix.

**Theorem 4.1 (see [13]).** If $A_{n \times n}$ is nonnegative and irreducible, then the following hold:

1. The spectrum of eigenvalues of $A_{n \times n}$ includes one real positive eigenvalue which is uniquely the largest in absolute value—meaning that it is the only eigenvalue on the outermost spectral circle. See Fig. 4.14.

2. The eigenvector corresponding to that eigenvalue has entries which are all positive real numbers.

3. Further, the largest eigenvalue $\lambda$ is algebraically unique, meaning that it is a simple root of the characteristic polynomial, $\det(A - \lambda) = 0$.

### 4.3.4 Stochastic Matrices

It is easy to see that a stochastic matrix is a Frobenius–Perron matrix.

**Definition 4.13.** A (row) **stochastic matrix** is a square matrix $A_{n \times n}$ such that

1. each row sums to 1, $\sum_{j=1}^{n} A_{i,j} = 1$ for all $i = 1,2,\ldots,n$, and

2. $0 \leq A_{i,j} \leq 1$ for all $i,j = 1,2,\ldots,n$.

$D$ has no eigenvalues, but there is a related discussion of the singular spectrum through the SVD decomposition.
4.3. Action on Densities as a Directed Graph

A convenient way to state the row-sums-to-1 property is through a matrix natural norm.

**Definition 4.14.** Given a square matrix $A_{n \times n}$, its **matrix natural norm** is defined as

$$
\| A_{n \times n} \| = \sup_{v} \frac{\| A v \|}{\| v \|} = \sup_{w : \| w \|=1} \| A w \|,
$$

which is also often called an induced norm since the matrix norm is induced (inherited) by the vector norm $\| \cdot \| : E \to \mathbb{R}^+$, where $E$ is the vector space domain of $A_{n \times n}$. Often $E = \mathbb{R}^n$.

In terms of the popular matrix norms listed in Section 4.3.2, the matrix natural norms are especially conveniently computed:

1. $\| A \|_1$ is the matrix 1-norm induced by the vector 1-norm, $\| A \|_1 = \max_{i=1,...,n} \sum_{j=1}^{n} |A_{i,j}|$, which is the maximum row sum.

2. $\| A \|_\infty$ is the matrix infinity-norm induced by the vector sup-norm, $\| A \|_\infty = \max_{j=1,...,n} \sum_{i=1}^{n} |A_{i,j}|$, which is the maximum column sum.

3. However, $\| A \|_2$ is conveniently but not as conveniently computed as $\| A \|_2 = \sqrt{\rho(A'A)}$, where $\rho(A'A)$ is the spectral radius of $A'A$.

In this notation, a stochastic matrix must satisfy the properties

$$
\| A \|_1 = 1, \quad 0 \leq A_{i,j} \leq 1 \quad \forall i, j.
$$

The purpose of defining a stochastic matrix in such a manner is that it may be interpreted as reflecting the transition probabilities of a finite state Markov chain, which is a special case of a discrete time stochastic process.

**Definition 4.15.** A **discrete time stochastic process** is a sequence of random variables, $X_1, X_2, X_3, \ldots$.

**Definition 4.16.** A **Markov chain** is a discrete time stochastic process of random variables, $X_1, X_2, X_3, \ldots$ such that the conditional probability of each next state is independent of the prior history,

$$
P(X_{m+1} = x | X_1 = x_1, X_2 = x_2, \ldots, X_m = x_m) = P(X_{m+1} = x | X_m = x_m),
$$

where $P(\cdot)$ denotes the probability of the enunciated state of the random variable.

In each of these, we have referred to the concept of random variable; see Definition 3.3.

We may consider the random variable as a measurement device that returns a real number, or the random experiment in our language, for a given subset of $\Omega$. Recall that
for a measure space \((\Omega, \mathcal{F}, \mu)\), a measure \(\mu\) is called a probability measure if \(\mu : \mathcal{F} \rightarrow [0, 1]\) and \(\mu(\Omega) = 1\); hence a measure space \((\Omega, \mathcal{F}, \mu)\) will also be accordingly referred to as a probability space. With a probabilistic viewpoint in mind, the random variable tells us that the probability to observe a measurement outcome in some set \(A \in \mathcal{B}(\mathbb{R})\) based on a probability measure \(\mu\) is precisely \(\mu(X^{-1}(A))\), which makes sense only if \(X\) is measurable.

When the state space is a finite set, \(\Omega = \{x_1, x_2, \ldots, x_n\}\) or simply write \(\Omega = \{1, 2, \ldots, n\}\), we have a **finite state Markov chain**, from which the set of all transition probabilities in Eq. (4.52) form a finite-sized table of possibilities, which may be recorded in a matrix:

\[
P_{i,j} = P(X_{m+1} = x_j | X_m = x_i) \forall i, j \in 1, 2, \ldots, n. \tag{4.53}
\]

To draw the connection to our larger theme, in some sense any Ulam–Galerkin method is simply an accounting of these probabilities for transitions between states identified by energy in each mode, as represented by a given chosen basis function. When a full (countable) basis set is used, then the resulting “matrix” would be infinite, but the truncation involved in Galerkin’s method corresponds to ignoring the “less important states,” to be discussed further shortly. Generally, this ignoring of less important states leads to a leak of measure in the states.

Further, evaluation of probability of events is a measure of the relative volume of a state in the set of outcomes. That is, given a probability space \((\Omega, \mathcal{F}, \mu)\), then formally the assignment of probability to an event \(\omega \in \Omega\) corresponds to a measure which may be described by integration,

\[
P(\cdot) : \Omega \rightarrow [0, 1],
\]

\[
P(B) = \int_{\Omega} \chi_B(x)d\mu(x) = \int_B d\mu(x), \tag{4.55}
\]

in terms of the indicator function \(\chi_B(x)\) of a Borel set \(B\). Here we follow a conventional abuse of notation so that \(P(B)\) is technically equivalent to \(P(\{\omega \in \Omega : X(\omega) \in B\})\), where in the above case the random variable \(X\) is \(\chi_B\).

That a finite state Markov chain results in a stochastic matrix is a direct consequence of independence,

\[
P(X_{m+1} = x_j) = \sum_{i=1}^{n} P(X_{m+1} = x_j | X_m = x_i)P(x_i) = 1 \forall j \in 1, 2, \ldots, n, \tag{4.56}
\]

simply because the union of all the states forms the full set of possibilities which is the full probability:

\[
\Omega = \bigcup_{j=1}^{n} B_j. \tag{4.57}
\]

Here is where we see the consequence of truncation in the Galerkin method in regard to leak of measure in terms of the probabilities. If Eq. (4.56) is a finite, and the true state space is infinite, but a small fraction of the states account for the majority of the probability,
then we may write

\[ P(x_j) = \sum_{i=1}^{n} P(X_{m+1} = x_j | X_m = x_i) < \sim 1 = \sum_{i=1}^{\infty} P(X_{m+1} = x_j | X_m = x_i) \]

\[ = \sum_{i=1}^{n} P(X_{m+1} = x_j | X_m = x_i) + \sum_{i=n}^{\infty} P(X_{m+1} = x_j | X_m = x_i), \tag{4.58} \]

when

\[ \sum_{i=n}^{\infty} P(X_{m+1} = x_j | X_m = x_i) \ll 1, \tag{4.59} \]

which will happen when

\[ \bigcup_{j=1}^{n} B_j \] is a proper subset of \( \Omega \), \tag{4.60}

but measures most of the set. Formally, the way to extend the notions of finite state Markov chains even to uncountable state chains is through Harris chains [156]. We already noted in Section 4.2 how the Markov property of a map results in the Galerkin method yielding a finite truncation Ulam–Galerkin matrix, which we now describe as representing the transitions of a finite state Markov chain.

We now revert to a discussion of uniqueness of dominant states, in terms of matrix issues such as reducible matrices, primitive matrices, and the relationship to the dynamical systems analogue of the dominant state(s) to (unique) ergodicity.

### 4.4 Exact Representations Are Dense, and the Ulam–Galerkin Method

We close the chapter with presentations of some results from [19] of how Markov maps are dense. In this manner, analysis of approximation of the matrix approximations of the Frobenius–Perron operator can be developed. The error in an approximation of the infinite-dimensional operator can be described in two ways. The more common way is by discussion of an approximation due to finite truncation of the series in the Galerkin method, Eq. (4.4). A lesser known but also useful description of the same question is as follows. Each finite series approximation can be understood as an exact presentation of another map, a map which is Markov on exactly the finite partition used. As such, the approximation can be analyzed by a description of how far the approximating Markov map is from the non-Markov map under description. Finally, the expectation is that there is always a nearby Markov map for such a description. The concept we will discuss in this section is that Markov maps are expected to be dense in the space of maps, and therefore an error analysis of a finite truncation can be considered by the nearby map where the representation is exact. We can prove this statement at least for a certain class of systems. The results
here are drawn from our work [19], where the fuller details of the brief presentation here can be found.

Consider a family of chaotic skew tent maps. The skew tent map is a two-parameter, piecewise linear, unimodal map of the interval. We show that these maps are Markov for a dense set of parameters and we find the exact probability density function (PDF) for any of these maps.

**Remark 4.8.** The central concept to this approach is the following: It is well known [50] that when a sequence of transformations has a uniform limit \( F \) and the corresponding sequence of invariant PDFs has a weak limit, then that invariant PDF must be \( F \) invariant.

As a case in point [19], we show for a family of skew tent maps that not only does a suitable sequence of convergent sequences exist, but also that these can be constructed entirely within the family of skew tent maps. Furthermore, such a sequence can be found among the set of Markov transformations, for which PDFs are easily and exactly calculated. While the theorems in the following sections assume the family of one-dimensional transformations, we will discuss extensions to higher dimensions at the end of the chapter.

Before we begin the main theme of this section, note that the discussion requires sharpening our analysis so that the underlying topology is clearer as to what we mean by dense as well as in what sense functions and invariant densities may converge.

### 4.4.1 Background Analysis and Topology

In discussing convergence, there is an implication of an underlying topology with respect to which the convergence may be defined. Analysis [270], topology [233], and functional analysis [189, 8] are the background fields here, and of course these are major areas of mathematics for which there are many excellent textbooks; we have just listed some of our favorites for each. For a quick start relevant to this discussion we can recommend [23]. This becomes an appropriate place to sketch in brief details the different kinds of convergence relevant here, for the sake of completeness of our discussion. We avoid an overly structured presentation of this would-be deep branch into extensive and interesting mathematics, which undoubtedly would require a large volume. For a complete introduction we recommend one of the cited texts. When discussing convergence of sequences of functions, a uniform limit is a “stronger” form of convergence than simply convergence, which is often used as the short form for the synonymous pointwise convergence. Therefore, we define both, and in terms of sequences of functions. Given a sequence of functions \( \{f_n(x)\}_{n=0}^{\infty} \) for each \( f_n : D \to R \) defined on a domain \( x \in D \) and range \( R \), \( f_n \) converges (pointwise) to \( f \) if each and every sequence of values \( f_n(x) \in R \) (you get values by plugging \( x \) into each \( f_n \)) converges to a value which we shall label \( f(x) \) one for each \( x \). Stated formally, \( y_n = f_n(x) \) is a sequence of numbers that converge \( y_n \to y \equiv f(x) \) if for every \( \epsilon > 0 \) there exists \( N(x) > 0 \) such that \( \|y - y_n\| < \epsilon \) if \( n > N \), which is in terms of the metric topology of \( \| \cdot \| \) on the range space \( y_n \in R \). Note that as stated there is allowed an \( \epsilon > 0 \) for each \( x \), and thus pointwise, \( \epsilon(x) \) implies \( N \) is a function of \( x \), \( N(x) > 0 \).

In terms of uniform convergence, the change relative to pointwise convergence is when we identify that there exists an \( N > 0 \) to discuss pointwise convergence, but that \( N \) may be found independently of \( x \). \( N \) is not a function of \( x \) but still allows the convergence throughout the domain and range. A primary theorem regarding the notion of uniform convergence is that a sequence of continuous functions that converge uniformly must have