Constructing Markov State Models of Reduced Complexity from Agent-Based Simulation Data

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Abstract

Agent-based models usually are very complex so that models of reduced complexity are needed, not only to see the wood for the trees but also to allow the application of advanced analytic methods. We show how to construct so-called Markov state models that approximate the original Markov process by a Markov chain on a small finite state space and represent well the longest time scales of the original model. More specifically, a Markov state model is defined as a Markov chain whose state space consists of sets of population states near which the sample paths of the original Markov process reside for a long time and whose transition rates between these macrostates are given by the aggregate statistics of jumps between those sets of population states. An advantage of this approach in the context of complex models with large state spaces is that the macrostates as well as transition probabilities can be estimated on the basis of simulated short-term trajectory data.

1 Introduction

Agent-based models (ABMs) study systems of boundedly rational, interacting economic agents by means of computer simulations. The basic idea is that the microscopic behavior of the agents is specified via individual rules of behavior and the dynamical evolution of the whole system as well as related macroscopic quantities is iteratively determined by the computer. ABMs have many desired features that traditional economic models are lacking. However, their high complexity makes them difficult to understand and analyze. Up to now, there are few approaches that go beyond traditional "look and see" analyses.

In this context, we present the *Markov state modelling* approach to the construction of Markov models of reduced complexity. This approach originates from the study of large bio-molecules [e.g., 1–3]. Bio-molecules undergo statistically rare transitions between different conformations, where in a conformation the large-scale geometric structure of the bio-molecule is understood to be

conserved while on smaller scales it may well change, e.g., rotate, oscillate or fluctuate. A similar situation is given in economics where the system of interest is often characterized by punctuated equilibrium dynamics [e.g., 4, 5], that is, its sample paths exhibit long periods of stasis near one population state which are infrequently interrupted by switching events after which the sample paths stay close to a different population state, again for a long time. In the economic context, the subsets of state space in which the sample paths of the dynamical system reside for a long time might be interpreted as conventions or norms.

The basic idea of a Markov state model is to consider each conformation, convention, or, more generally, each subset of state space in which the sample paths reside for a long time, as a *macrostate* of a Markov chain which approximates the original Markov process. The transition rates between the macrostates are given by the aggregate statistics of jumps. An advantage of this approach for complex models with large state spaces is that the macrostates and the transition probabilities between the macrostates can be estimated from simulated short-term trajectory data. Moreover, it has been shown that such Markov state models have good approximation properties if punctuated equilibrium dynamics characterize the system of interest.

In what follows, we give an introductory overview of how to construct interpretable Markov models from agent-based models either directly from the rules of the game or simulated trajectory data (Sections 2 and 3). Subsequently, we discuss the limitation that the approach relies on the original process to be reversible and give an outlook for further research in this direction (Section 4).

2 Markov Representation of Agent-Based Models

Throughout what follows, let $(X_k)_{k\in\mathbb{N}}$ be the irreducible discrete-time Markov chain that represents an agent-based model of interest and that has been constructed either from simulation data or derived by analytical arguments. We denote by $Z = \{1, \cdots, l\}$ a finite, but possibly large state space of the chain, by $P = (p_{xy})_{x,y\in Z}$ its transition matrix and by μ its unique stationary distribution. We assume that (X_k) is *reversible*, that is, it fulfills

$$\mu(x)p_{xy} = \mu(y)p_{yx}. \tag{1}$$

For illustration, we consider the following stochastic evolutionary game as a simple "toy" agent-based model that will serve as a paradigm throughout the paper. Let us consider a population of n agents that are randomly matched to play the 2×2 pure coordination game with payoff matrix A given by

	1	2
1	a, a	$0, 0$
2	$0, 0$	b, b

where $a, b > 0$. This game allows an interpretation of the strategies in terms of currencies, e.g., strategy 1 represents "silver" and strategy 2 "gold". At times $t = k\delta$, where $\delta = 1/n, k \in \mathbb{N}$, exactly one agent is randomly drawn (with equal probability for all players) to reconsider her strategy choice. We assume statistical independence between successive draws. More specifically, we assume that revising agents use the *best response with mutations* (BRM) revision protocol at *mutation rate* $\varepsilon > 0$ [6] to update their strategy choice as follows: with probability $(1 - \varepsilon)$ he chooses a best response $b \in B(x)$ to the current population state, while with probability ε he chooses a strategy $s \in S$ at random (uniform distribution). The strategy updating process can be represented as a birth-and-death chain on the state space $Z = \{0, 1/n, 2/n, \cdots, 1\}$ where $x \in Z$ represents the proportion of players in the population playing strategy 1 [for details see 7]. Birth-and-death chains can easily be shown to be irreducible and reversible. Figure 1 gives an impression of characteristic sample paths for a resulting evolutionary process with parameters $a = b = 1, n = 11, \varepsilon = .3$.

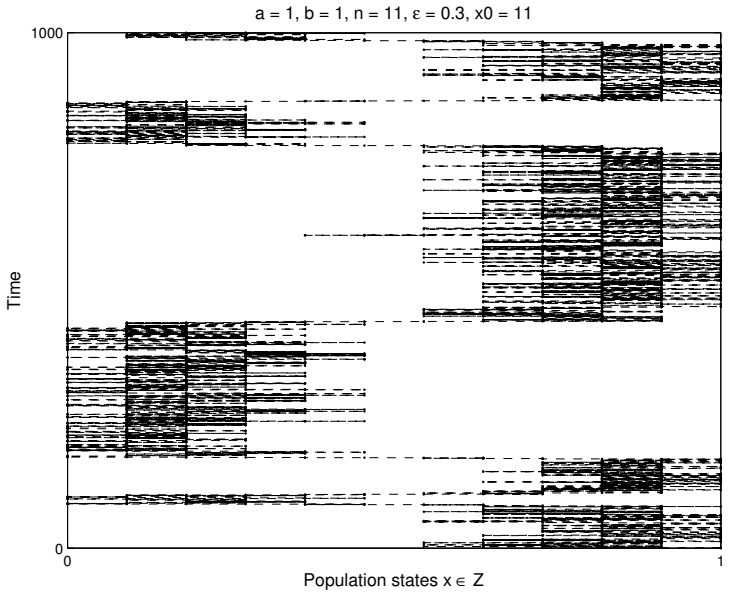

Figure 1: Typical sample path of the number of players holding strategy 1 in the evolutionary game defined by the currency game and the BRM revision protocol ($a = b = 1$, $n = 11$, $\varepsilon = .3$).

For a discussion on formal representations of ABM as Markov chains see, e.g., Tesfatsion [8]. In the case the transition probabilities may be not be explicitly available, in which case the transition matrix can be estimated from simulation data, e.g. using maximum likelihood estimation or Bayesian inference [e.g., 9], taking into account the reversibility constraint (1).

3 Towards Markov State Models

The basic idea of a Markov state models is to approximate the original Markov process by a Markov chain on a small finite state space. Thus, more formally, our goal is to construct a Markov chain $(\hat{X}_k)_{k\in\mathbb{N}}$ on the state space $\hat{Z} = \{1, \cdots, m\}$ with m considerably smaller than l such that $(\hat{X}_k)$ captures the essential dynamics of the original Markov chain (X_k). In general, each of the macrostates $i \in \hat{Z}$ corresponds to a subset of states $C_i \subset Z$, where we assume that the C_i's are pairwise disjoint. The C_i's are called *core sets*. Roughly speaking, the idea is to cluster the state space into core sets that may or may not partition the state space, but that represent the punctuated equilibrium dynamics in that

(i) the core sets carry most of the total statistical weight of the invariant distribution μ of the original Markov chain and

(ii) the process resides inside each core set for a long time (relative to the typical time scale of the original chain).

In the context of molecular dynamics, for example, these core sets represent the possible conformations of a bio-molecule; in an economic context, we might think of core sets as possible conventions or norms.

In Section 3.1, we first consider the special case in which the core sets $C_1, \cdots, C_m$ partition the state space Z, that is,

$$C_i \cap C_j = \emptyset \text{ for } i \neq j \quad \text{and} \quad \bigcup_{j=1}^{m} C_j = Z. \tag{2}$$

Using this special case, we demonstrate formally the basic idea of the Markov state modeling approach. Subsequently, in Section 3.2, we explain how to generalize the special case, and how to identify suitable core sets representing the represent the essential equilibria of the system.

3.1 Full Partition Markov State Models

In the special case in which the core sets partition the state space Z, each macrostate i directly represents the subset C_i and we can define the reduced chain $(\hat{X}_k)$ with transition matrix $\hat{P} = (\hat{p}_{ij})$ by

$$\hat{p}_{ij} = \mathbb{P}[\tilde{X}_1 = j \mid \tilde{X}_0 = i], \tag{3}$$

where $(\tilde{X}_k)_{k\in\mathbb{N}}$ is the discrete-time process on $\hat{Z}$ that describes the dynamics of (X_k) between the sets $C_1, \cdots, C_m$, i.e.,

$$\tilde{X}_k = i \Leftrightarrow X_k \in C_i. \tag{4}$$

Note that we have to differentiate between $(\hat{X}_k)$ and $(\tilde{X}_k)$ because $(\tilde{X}_k)$ is in general not Markovian [10]. However, we still want to approximate (X_k) by a Markov chain which is why we consider $(\hat{X}_k)$.

Example. We consider the introductory example from Section 2 again, the Markov chain representation of the 2×2 coordination game on the state space $Z = \{0, 1/n, 2/n, \cdots, 1\}$, with states $x \in Z$ respresenting the fraction of agents adopting strategy 1. The sample path shown in Figure 1 shows the characteristic punctuated equilibrium behavior, i.e., the sample path usually stays either near the population state $x = 0$ or $x = 1$ for a long time while it switches infrequently to the other population state. In the specific case of the currency game under BRM dynamics with parameters $a = b = 1, n = 11, \varepsilon = .3$, a reasonable partition of the set of population states into subsets such that there are only rare switches between them (see Figure 1) is $A = \{0, \cdots, 5/11\}$, $B = \{6/11, \cdots, 1\}$. The resulting matrix $\hat{P}$ is given by (rounded to four digits)

$$\hat{P} = \begin{pmatrix} .9989 & .0011 \\ .0011 & .9989 \end{pmatrix}. \tag{5}$$

Best-approximation property of the full partition model In order to appreciate the approximation of the orgiginal model by the coarse-grained chain $(\hat{X}_k)$ it is helpful to analyse the relation between the transition probabilities p_{xy} and $\hat{p}_{ij}$. To this end, suppose that the original chain starts in equilibrium, $X_0 \sim \mu$. Now, the transition probability $\hat{p}_{ij}$ in (3) can be recast as

$$\hat{p}_{ij} = \frac{\sum_{x,j} p_{xy} \chi_{C_i}(y) \chi_{C_j}(x) \mu(x)}{\sum_x \chi_{C_i}(x) \mu(x)}, \tag{6}$$

where $\chi_C \colon Z \to \{0, 1\}$ denotes the indicator function of a set $C \subset Z$, and the notation $\mathbb{P}_\mu$ indicates that X_0 is distributed according to μ.

Let us assume that the indicator functions $\chi_{C_1}, \ldots, \chi_{C_m}$ form a partition of unity, i.e., $\sum_i \chi_{C_i}(x) = 1$, which is the case if the $C_1, \ldots, C_m$ partition our state space Z. The last equation can then be interpreted as the orthogonal projection onto the span of the functions $\chi_{C_1}, \ldots, \chi_{C_m}$ with respect to the μ-weighted scalar product

$$\langle v, w \rangle_\mu = \sum_{x \in Z} v(x) w(x) \mu(x) \tag{7}$$

on $\mathbb{R}^l$. A compact way to write (6) thus is

$$\hat{p}_{ij} = \frac{\langle P \chi_{C_i}, \chi_{C_j} \rangle_\mu}{\langle \chi_{C_i}, \chi_{C_i} \rangle \mu}, \tag{8}$$

which shows that the corresponding transition matrix $\hat{P} = (\hat{p}_{ij})_{i,j \in \hat{Z}}$ is in fact the orthogonal projection of $P = (p_{xy})_{x,y \in Z}$ onto $\mathrm{span}\{\chi_{C_1}, \ldots, \chi_{C_m}\}$, understood as a linear subspace of $\mathbb{R}^l$ endowed with the weighted scalar product μ.

By being an orthogonal projection, $\hat{P}$ is the best approximation of P onto the space spanned by the indicator functions on the core sets $C_1, \ldots, C_m$ in the sense of least squares where the weighting with the invariant measure μ arises naturally as a consequence of the fact that the Markov chain is initialized in its stationary distribution so as to make the macroscopic transition probabilities time-independent. The projected transition matrix $\hat{P}$ is a stochastic matrix and inherits many important properties of the original transition matrix P:

1. If P is irreducible and aperiodic, then so is $\hat{P}$.
2. $\hat{P}$ has a unique invariant distribution $\hat{\mu}$:

$$\hat{\mu}(i) = \mu(C_i)\,, \quad i \in \hat{Z}. \tag{9}$$

3. If P is reversible with respect to μ, then $\hat{P}$ is reversible with respect to $\hat{\mu}$.

A further advantage of (8) is that it tells us that, given a long realization of the original Markov chain (X_t) of length T, the expression

$$\hat{p}_{ij}^{(T)} = \frac{\sum_{t=1}^{T} \chi_{C_i}(X_t)\chi_{C_j}(X_{t+1})}{\sum_{t=1}^{T}(\chi_{C_i}(X_t))^2} \tag{10}$$

is an unbiased estimator of the macroscopic transition probabilities $\hat{p}_{ij}$. By the assumption that μ is unique and Z is finite, the law of large numbers implies that $\hat{p}_{ij}^{(T)}$ converges almost surely to $\hat{p}_{ij}$ as $T \to \infty$ for every initial value $X_0 = x_0$.

3.2 Core Set Markov State Models

The case of a full partition of state space demonstrates the basic idea of Markov state models as a coarse-grained Markov chain that can be obtained by projection onto suitable ansatz functions. In the general case, however, the sets $C_1, \cdots, C_m$ do not necessarily partition the state space Z; thus, the approach has to be modified since already the definition of the process $\tilde{X}$ in Eq. (4) is not well defined anymore.

In order to construct a reduced Markov chain that best approximates our original Markov chain in this case, the idea is to replace the set of indictator functions by a clever "mollification", forming a partition of unity and having support outside the sets $C_1, \ldots, C_m$. One such choice is the set of probabilistic ansatz functions $\{q_1, \ldots, q_m\}$, so-called *committor functions*, defined by

$$q_i(x) = \mathbb{P}_{\delta_x}(\tau^0_{C_i} < \tau^0_{C\setminus C_i}), \tag{11}$$

where $C = \cup_i C_i$, δ_x is the point mass on x, and $\tau^k_A = \inf\{k' \geq k | X_{k'} \in A\}$ denotes the k-th *hitting time* for $k \geq 0$. In words, the committor function $q_i : Z \to [0,1]$ is the function that gives for a state $x \in Z$ the probability that the Markov chain (X_k) will visit the set C_i first rather than $C \setminus C_i$. By construction, each q_i is equal to one on C_i, equal to zero on the other sets C_j, $j \neq i$, and interpolates between these values outside the sets $C_1, \ldots, C_m$. Moreover, since (X_t) is irreducible and positive recurrent (by Z being finite), the process terminates after finite time with probability one by hitting one of the sets C_i, independently of the initial condition $X_0 = x$, and as a consequence the q_i sum up to one and form a partition of unity.

Best-approximation property of the core set model The analysis that is carried out in Sarich [10] shows that the reduced Markov chain on $\hat{Z}$ can be defined in terms of the *quasi*-transition matrix $\hat{P}W^{-1}$, where the matrices $\hat{P} = (\hat{p}_{ij})_{i,j\in\hat{Z}}$ and $W = (w_{ij})_{i,j\in\hat{Z}}$ are given by

$$\hat{p}_{jk} = \frac{\langle Pq_j, q_k\rangle_\mu}{\hat{\mu}(j)}, \qquad w_{ij} = \frac{\langle q_i, q_j\rangle_\mu}{\hat{\mu}(i)}, \tag{12}$$

where $\hat{\mu}(j) = \sum_{i\in Z} \mu(i)q_j(i)$.

In this general case, each macrostate $i \in \hat{Z}$ is associated with the respective committor function q_i on the core set C_i and can thus be interpreted as representing the affiliation with set C_i. Note that while the definition of the quasi-transition matrix of our Markov state model by $\hat{P}W^{-1}$ might not seem intuitively obvious, it reduces to the matrix $\hat{P}$ defined in Eq. (3) in the case of a full partition of state space.

We call $\hat{P}W^{-1}$ a quasi-transition matrix since $\hat{P}W^{-1}$ is not always a stochastic matrix (even though P and W are). We only know that its rows sum up to one since this is the case for both $\hat{P}$ and W, and thus also for W^{-1} as well as $\hat{P}W^{-1}$. In the example given here as well as in the examples studied in Hallier [7] the entries of $\hat{P}W^{-1}$ are also non-negative, but in general the entries can be negative as has been pointed out in Sarich [10].

It is possible to show, however, that $\hat{\mu}$ is the unique ergodic stationary distribution of $(\hat{X}_k)$. Unlike in the case of a full state space partition, the matrix $\hat{P}W^{-1}$ does not trivially inherit all properties of the original chain, such as irreducibility, aperiodicity and reversibility; but $(\hat{X}_k)$ is reversible with respect to $\hat{\mu}$ if $\hat{P}$ and W^{-1} commute.

Despite the apparent lack of structure preservation, the sparse core set approximation shows excellent spectral approximation properties, in that the dominant eigenvalues of the original chain are generally well approximated. The latter implies that the projected transition matrix can be used to accurately estimate transition rates between the core sets as well as mean residence times, and hence residence times and rates for the punctuated equilibria.

Example. We consider again the currency game under BRM dynamics. Let $C_1 = \{0\}$ and $C_2 = \{1\}$. The resulting Markov state model is thus a Markov chain on the state space $\hat{Z} = 1, 2$ where state $i \in \hat{Z}$ refers to the committor function q_i, $i = 1, 2$. The matrices $\hat{P}$ and W are given by

$$\hat{P} = \begin{pmatrix} .9327 & .0673 \\ .0673 & .9327 \end{pmatrix}, \tag{13}$$

$$W = \begin{pmatrix} .9333 & .0667 \\ .0667 & .9333 \end{pmatrix}. \tag{14}$$

We can thus calculate

$$\hat{P}W^{-1} = \begin{pmatrix} .9993 & .0007 \\ .0007 & .9993 \end{pmatrix}, \tag{15}$$

$$W^{-1}\hat{P} = \begin{pmatrix} .9993 & .0007 \\ .0007 & .9993 \end{pmatrix}. \tag{16}$$

Thus, $\hat{P}W^{-1}$ is a stochastic matrix and $\hat{P}W^{-1} = W^{-1}\hat{P}$. The Markov chain $(\hat{X}_t)_{t\in\mathbb{T}}$ representing the core set Markov state model is thus reversible with stationary distribution $\hat{\mu} = (.5, .5)$.

Estimation of the core set model parameters In order to arrive at an estimator for $\hat{p}_{ij}$ as well as w_{ij} notice that it can be shown that

$$\hat{p}_{ij} = \mathbb{P}(\tau_{C_j}^{k+1} < \tau_{C\setminus C_j}^{k+1} \mid \tilde{X}_k = i), \tag{17}$$

$$w_{ij} = \mathbb{P}(\tau_{C_j}^{k} < \tau_{C\setminus C_j}^{k} \mid \tilde{X}_k = i), \tag{18}$$

where $(\tilde{X}_k)$ is the *milestoning process* defined by

$$\tilde{X}_k = i \Leftrightarrow X_{\sigma(k)} = i, \text{ where } \sigma(k) = \max\{t \leq k \mid X_t \in C\}. \tag{19}$$

Equation (19) means that the milestoning process remains in state i as long as the original Markov chain (X_k) last visited core set i (see Figure 2). Thus, in words, $W(i,j)$ for $j \neq i$ gives the probability that the Markov chain next hits C_j while being in a state in $Z \setminus C$ at some time k and last came from core set C_i, where $C = \cup_{j=1}^{m} C_j$. Similarly, $\hat{P}(i,j)$ gives the probability that the next core set hit is C_j conditional on having hit the core set C_i last at some time k.

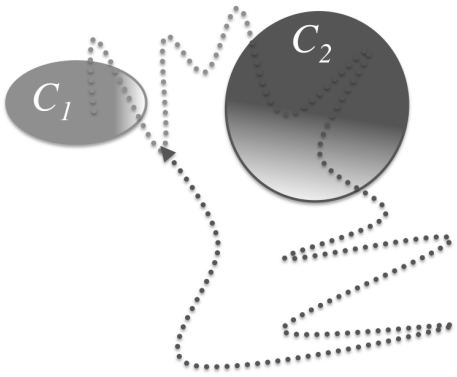

Figure 2: Illustration of the milestoning process for two core sets C_1 and C_2.

Consequently, both matrices W and $\hat{P}$ can be estimated from trajectory data in the following way: given a realization $(x_0, \cdots, x_K)$ of (X_k) of length K, we can estimate

$$w_{ij}^{*,K} = \begin{cases} \frac{R_{ij}^K}{r_i^K} & \text{if } j \neq i, \\ 1 - \sum_{j\neq i} w_{ij}^{*,K} & \text{otherwise,} \end{cases} \tag{20}$$

$$\hat{p}_{ij}^{*,K} = \frac{R_{ij}^{+,K}}{r_i^K}, \tag{21}$$

where R_{ij}^K denotes the number of times where the chain came from core set C_i, is in a state in $Z \setminus C$ and hits C_j next, r_i^K is the total number of time steps

the trajectory was in i; that is, $\tilde{X}_k = i$, and $R_{ij}^{+,K}$ denotes the number of times where the chain came from core set C_i and hit C_j next.

Identification of core sets While we outlined above how to construct Markov state models given core sets $C_1, \cdots, C_m$, the question remains of how to actually identify suitable core sets. One approach is to use the results on the relationship between the approximation quality and the projection error. For full partition models, the projection error is as small as possible if the dominant right eigenvectors of the transfer matrix P are as constant as possible on the sets of the partition. This relationship has been exploited by approaches that partition state space by clustering algorithms [as has, for example, been done in the molecular dynamics context by 11]. Similarly, in terms of core set Markov state models, finding core sets $C_1, \cdots, C_m$ so that the projection error is as small as possible can be interpreted as a fuzzy clustering problem [10, 12].

If the original model has a noise parameter that determines the punctuated equilibrium behavior, we might also use the information given by its stationary distribution to identify possible core sets. More specifically, if the system under investigation depends on a noise parameter $\varepsilon > 0$ in such a way that for smaller ε the punctuated equilibrium behavior increases, that is, for smaller ε the sample paths of the process stay even longer in certain subsets of the population state space and the switches between such subsets get more rare – just as in our example – we can identify the set $C = \cup_{i=1}^{m} C_i$ by comparing the stationary distribution μ^* of the system with noise level ε^* with its propagated distribution $\mu^* P^\theta$ under a decreased noise level $\varepsilon < \varepsilon^*$ for a chosen timescale $\theta > 0$. Note that the distributions $\mu^* P^\theta$ of μ^* converge to the stationary distribution μ associated with the stochastic evolutionary game at the lower noise level ε. Moreover, both stationary distributions μ and μ^* have the same form in the sense of local minima and maxima, but the stationary distribution μ^* with increased noise intensity is less peaked. Now, the basic idea of the identification strategy is that a population state x belongs to the core set region C if it gets more attractive in the model with the decreased noise parameter ε, i.e., if

$$\mu^*(x) < \left(\mu^* P^\theta\right)(x). \tag{22}$$

Example. In our example with parameters $a = 1$, $b = 1$, $\varepsilon^* = .3$, $\varepsilon = .15$, $n = 11$, this identification approach leads to the set $C = \{0, 1/11, 10/11, 1\}$ for all $\theta \in \mathbb{T}$, which suggests the core sets $C_1 = \{0, 1/11\}$ and $C_2 = \{10/11, 1\}$, see also Figure 3. The analysis of the approximation error in Hallier [7] shows that these core sets lead to the Markov state model with the best approximation quality.

As in this example, the clustering of C into core sets is usually straightforward as the core sets are dynamically well separated. An advantage of the just sketched approach is that the necessary quantities can be estimated from trajectory data as well. Thus, it allows for a simulation-based approach to the construction of Markov state models. For more details, see Hallier [7].

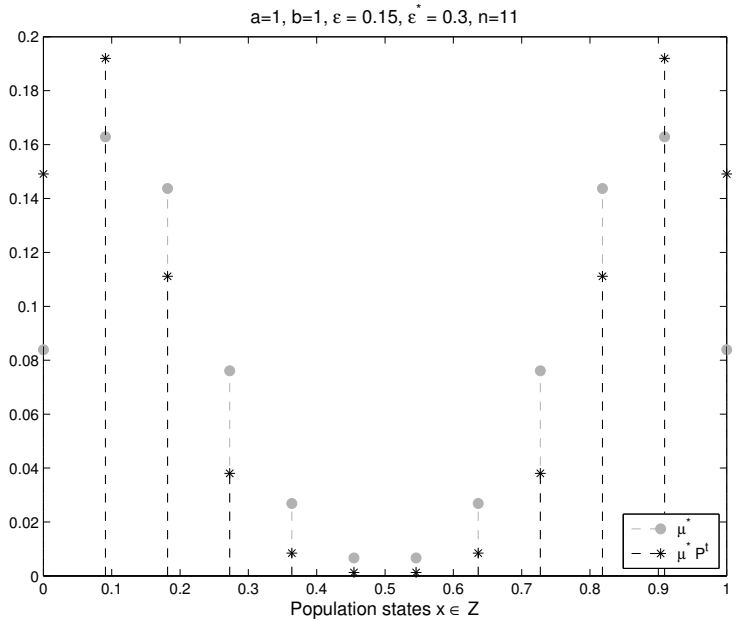

Figure 3: Weights of the stationary distribution μ^* for the stochastic evolutionary game of our running example with parameters $a = 1, b = 1, \varepsilon^* = .3, n = 11$ and its propagation $\mu^* P^\theta$ under the stochastic evolutionary game with parameters $a = 1, b = 1, \varepsilon = .15, n = 11, t = 10/11$.

4 Discussion and Outlook

We presented the Markov state modeling approach to extract the aggregated long term dynamics of reversible Markov chains. The approach is especially interesting for large, complex models in order to see the wood for the trees. In essence, Markov state models approximate the original Markov chain on a reduced state space. The macrostates as well as transition probabilities between them can be estimated on the basis of short-term trajectory data. Apparent advantages of a reduced state space are that it is easier to compute eigenvalues and eigenvectors as well as other properties such as waiting times.

One limitation is, however, that the approach and its analysis depends on the original Markov chain that represents, e.g., an agent-based model of interest, to be reversible. This is the case for simple example we presented. In general, it will be difficult to say whether it is reasonable to assume that an agent-based model results in a reversible Markov chain. One reason for this difficulty is that, if we estimate the transition matrix from simulated trajectory data, it does not need to fulfill the detailed balance equation, even if the underlying Markov chain is reversible [13, 14]. In the context of molecular dynamics, however, it was possible to derive approximative models that can be proven to be reversible although the original model is not. An example is the diffusion model, which

represents an approximation to the Langevin model in the limit of high friction [see, e.g., 3, Chapter 2 and references therein]. As a future research question, it seems worthwhile to explore whether similar results can be obtained for agent-based models; that is, whether there are approximations of certain agent-based models that can be shown to be reversible.

Beyond that, we would like an approach that applies also to non-reversible Markov dynamics. Notice that it is not difficult to derive a construction of a matrix representation of the core set Markov state models for given core sets in the case of non-reversible Markov chains [see, e.g., 12, 15]. However, we neither have results with respect to their approximation quality nor an approach to the identification of core sets for non-reversible Markov chains. One fundamental problem is that the eigenvalues and eigenvectors of the transfer matrices corresponding to non-reversible Markov chains need not be real anymore. In this case, the interpretation of the spectral information is unclear. Up to now, there are few approaches that apply also to non-reversible Markov chains [16]. A graph-theoretical framework for constructing reversible surrogates of non-reversible dynamics, based on a cycle decomposition of the underlying Markov chain, has been suggested in Banisch [17], however the applicability to agent-based models is yet open.

The construction of Markov state models for general agent-based models is therefore an open problem and will be a topic of future research.

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