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# Uncertainty quantification for Markov chain models

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Transition probabilities serve to parameterize Markov chains and control their evolution and associated decisions and controls. Uncertainties in these parameters can be associated with inherent fluctuations in the medium through which a chain evolves, or with insufficient data such that the inferential value of the chain is jeopardized. The behavior of Markov chains associated with such uncertainties is described using a probabilistic model for the transition matrices. The principle of maximum entropy is used to characterize the probability measure of the transition rates. The formalism is demonstrated on a Markov chain describing the spread of disease, and a number of quantities of interest, pertaining to different aspects of decision-making, are investigated. © *2012 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4757645]

**Markov chains are attractive models widely used for dynamical systems whose transition between different states through time is considered to be random. Finite-state discrete-time Markov chains are the subject of the work in this paper. The time evolution of the state probabilities from a time instance to the next is determined by the transition rates that collectively constitute the transition matrix. These transition rates can be estimated as deterministic model parameters using such criteria as least squares, maximum likelihood, maximum a-posteriori (MAP), and maximum entropy (MaxEnt). However, it is too restricting to postulate, even in a time-homogeneous Markov chain, that these transition rates should remain constant over time. Moreover, the data used in these estimation procedures are inevitably incomplete and thus insufficient to synthesize sufficiently detailed underlying behavior. Finally, divergence of underlying dynamics from a Markovian model could manifest itself in an apparent variability in the transition rates. These observations motivate our work in estimating the transition rates as random parameters. To this end, we rely on the maximum entropy principle to synthesize a probability measure on the set of transition matrices. The resulting probabilistic representation will assist decision makers by supporting them with quantified confidence on the consequences of their decisions.**

## I. INTRODUCTION

Markov chains are ubiquitous in modeling phenomena that exhibit random fluctuations while evolving in time. Their value lies in their simplicity, both of interpretation and implementation. Indeed, the mere justification of finite memory with constant structure allows the postulation of a Markovian model from which consistent sample paths for futures of the system can be realized. Decision processes associated with this behavior can also be readily formalized yielding elegant analytical insight. These Markovian models are typically parameterized by their initial state and the probabilities of transition between states. These so-called transition probabilities are usually estimated from the evolution of the Markov chain observed along a number of sample paths. Given the dichotomy between the simplicity of Markovian models, and the highly complex natural, man-made, and social phenomena to which they have been adapted, a framework for assessing the uncertainty in associated mode-based inferences is essential. One can contemplate two constructions of Markov chains that provide different perspectives on these uncertainties. The first construction maintains the belief that a Markov model is a suitable description of the underlying motives such as physical or social processes. In this case, uncertainty is attributed to lack of knowledge (due perhaps to insufficient observations) of the true values of transition probabilities, which are themselves treated as random. An ensemble of Markov chains is thus obtained, that is in one-to-one correspondence with the ensemble of transition matrices. The second construction recognizes that a Markov model is merely a convenient representation of the processes of interest, and develops adaptation strategies as information is acquired. Accordingly, the transition matrix of the Markov chain is permitted to vary in time, effectively, refitting a new Markov chain. Clearly, in this construction, the amount of data available to re-fit a Markov chain is more limited than in the first construction, and uncertainty in the estimated transition probability can be significant. In this paper, we will refer to these two constructions as the time-invariant and to the time-variant models, respectively. We present a methodology for ascertaining the uncertainty in transition probabilities of Markov chains, and demonstrate its value in quantifying the uncertainty in the predicted steady-state dynamics and associated decisions.

Without loss of generality, we will focus our attention on finite-state discrete-time Markov chains. The time evolution of the state probabilities from a time instance to the next is determined by the entries of the transition matrix which describe the transition rates between two states of the chain. These transition rates are usually estimated as deterministic

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model parameters using least squares, maximum likelihood, most a-posteriori, or MaxEnt arguments. Within the confines of probability theory, our objective, then, is to characterize a probability measure for the transition matrix that is consistent, in some sense, with mathematical constraints and available evidence.

Authors in Ref. 1 constructed a Markov chain based on the concept of imprecise probabilities. They formed the credal sets for the probability mass function and the transition probabilities, whose extreme points were used in estimating upper and lower bounds on the expected behavior of the Markov chain, yielding results similar to the classical Perron-Frobenius theorem (Ref. 2) on the asymptotic behavior of the associated Markov chains. No probabilistic characterization of the state distributions of the Markov chain were introduced, a factor that distinguishes it from our formulation. Alternatively, authors in Refs. 3 and 4 investigated the dynamics of Markov chains under parametric perturbations of transition matrices. This approach is, however, restrictive in that the mathematical form of the parametric perturbation together with the number and range of the parameters should be manually specified. In our formulation, the variability in the transition matrices follows from imposing the maximum entropy principle where only summary statistics based on observation are exploited and other subjective assumption may not pollute the estimation.

A different approach proposed in the literature is based on characterizing a support domain for random transition matrices (RTM). In Ref. 5, the authors characterized this domain by considering first the deterministic maximum likelihood estimate of the transition matrix. They then formed a set of transition matrices whose members have likelihoods that are within a prescribed range with respect to the maximum likelihood. They also proposed a similar construction by considering those transition probabilities that are within a Kullback-Leibler distance with respect to a given prior transition probability. These proposed support regions are subsequently used in the control of the Markov decision processes. This approach, however, does not permit the probabilistic characterization of the fluctuations in Markov Chain's behavior, hence the limitation in its inferential value.

Our approach involves characterizing a probability measure over the set of all mathematically admissible transition matrices, constraining them to be valid stochastic matrices. We estimate this measure using the MaxEnt principle given the information on the mean values and possibly higher moments. We make use of no other assumptions in the estimation procedure. With a MaxEnt RTM available, a Markov chain can be constructed in two different ways, describing two distinct behaviors. In the first one, referred to as Markov chain with time-invariant RTM, a single sample of the random transition matrix is assumed to govern the Markov chain's time evolution. In the second implementation, referred to as Markov chain with time-variant RTM, at each time step, a new independent sample is drawn from the RTM based on which the Markov chain makes a one-step transition. The second variation is also referred to as Markov chains in random environment.[6–11]

Markovian dynamics has proven particularly useful to problems in social dynamics where the complexity of interactions between individual agents emphasizes the importance of a statistical approach (Refs. 12–17). In these situations, complex interactions at the agent scale could give rise to emergent dynamics that is not well-characterized with a Markov model. The method developed in the present paper can be used in these cases to assess the statistical proximity of a given situation to Markovian behavior. The present work also provides foundation for applying probabilistic dynamical models to problems of social dynamics, under current conditions of immersed sensing and computing.

The paper is structured as follows. After motivating, our research using a simple numerical example, we describe the mathematical settings based on which a Markov chain is constructed with a RTM. Two different settings are discussed for the time-invariant and time-variant implementations. Next, we present the MaxEnt formulation used to construct the probability measure of the RTM based on the observed values for the mean and standard deviation of transition rates. As illustration, the implementation of the MaxEnt RTM is demonstrated on a simplified model of infection dynamics, where the implications of the uncertainty representation of the Markov chain model on ensuing decision processes are discussed.

## II. MOTIVATION

The stochastic behavior described through Markovian dynamics is typically attributed to white noise disturbances which, when closely viewed within a multiscale context, could be further explained by subscale interactions. It is thus the effect of these unmodeled physics, or more generally causal relationships, which is captured by the random evolution of a Markov chain. As indicated above, additional uncertainties accrue in the process of calibrating the transitions of these chains from finite samples. While standard approaches to analyzing Markovian behavior aggregates the effect of these uncertainties, their segregation provides a path towards addressing each of them appropriately.

First, and through a simple numerical example, we seek to emphasize the significance of representing and propagating uncertainty in transition matrices. Consider a single dynamical system with three possible states and the corresponding transition matrix known to be

$$P = \begin{bmatrix} 0.92 & 0.04 & 0.04 \\ 0.58 & 0.24 & 0.18 \\ 0.23 & 0.23 & 0.54 \end{bmatrix}. \tag{1}$$

We argue that one cannot deterministically recover the true transition matrix by observing a single realization or even a few realizations from a Markov chain. To do so, we generate 200 sample trajectories, each of length 1000, based on the known transition matrix. We then deterministically estimate the transition matrix entries for each trajectory, using transition frequencies. That is, the deterministic transition rate of the $k$-th trajectory, $p_{ij}^k$, is calculated by

$$\bar{p}_{ij}^k = \frac{c_{ij}^k}{\sum_j c_{ij}^k}, \tag{2}$$

where $c_{ij}^k$ denotes the number of transitions from state $i$ to state $j$ in the $k$-th trajectory recorded over a given time window. We expect that as the size of the time window increases, the bias in 200 estimates of the transition matrix decreases. However, limited resources often impede the long time observation of a chain. This will result in considerable errors in predicting the "exact" transition matrix, even in the rare cases that such underlying matrix uniquely exists.

In order to investigate the impacts of limited observation on the predicted quantities of interest (QoI), we consider a set of time windows with different sizes, ranging from 20 to 1000. For each fixed time window size, we estimate the asymptotic distributions for each of the 200 trajectories. This asymptotic distribution, indicated by $\hat{\boldsymbol{\pi}}$, is our QoI, which is known to satisfy, for a given transition matrix $P$

$$\hat{\boldsymbol{\pi}} = \hat{\boldsymbol{\pi}} P. \tag{3}$$

Fig. 1 shows the standard deviation in the 200 estimated QoI versus the size of observation window, where significant scatter in the estimated QoI can be observed. One can, therefore, conclude that the transition matrix estimation based on observation data involves inevitable variability and error, hence the motivation for treating these matrices as random.

## III. CONSTRUCTION OF UNCERTAIN MARKOV CHAINS

As indicated above, probabilistic transition matrices can be motivated by either time-invariant or time-variant systems. The mathematical setting for these two implementations is discussed next, in the context of finite-state discrete-time Markov chains. Consider the probability triple $(\mathcal{S}, \mathcal{F}_S, \boldsymbol{\pi})$, where $\mathcal{S} = \{1, \cdots, n\}$ is the sample space (finite set of states), $\mathcal{F}_S$ is a $\sigma$-algebra on $\mathcal{S}$, and $\boldsymbol{\pi} = [\pi_1, \cdots, \pi_n]$ is the probability measure (probability mass function) on $(\mathcal{S}, \mathcal{F}_S)$, which is referred to as the state distribution. Let $\boldsymbol{X} = \{X^1, X^2, \cdots\}$ denote the states that the Markov chain resides in at different times, with $X^t \in \mathcal{S},\ t = 1, 2, \cdots$. Let $P^t$ denote the transition matrix at time $t$ of this chain with its $ij$-th component, $p_{ij}^t$, defined by

$$p_{ij}^t = \Pr(X^{t+1} = j | X^t = i)\,. \tag{4}$$

Transition matrices, also referred to as stochastic matrices, are square matrix with non-negative components satisfying $\sum_{j=1}^n p_{ij}^t = 1,\ \forall i \in \mathcal{S}$. The dynamics of the state distributions $\{\boldsymbol{\pi}^t\}$ is assumed to be governed by the following finite-memory equation:

$$\boldsymbol{\pi}^{t+1} = \boldsymbol{\pi}^t P. \tag{5}$$

The set of admissible probability measures on the set $\mathcal{S}$, denoted by $\Pi$ and the set of admissible transition matrices, denoted by $\mathcal{P}$, can be formed as follows:

$$\begin{aligned}\Pi &= \left\{ \boldsymbol{\pi} \in \mathbb{R}^{1\times n} \,\middle|\, \sum_{i=1}^n \pi_i = 1, \pi_i \in [0,1] \right\},\\ \mathcal{P} &= \left\{ P \in \mathbb{R}^{n\times n} \,\middle|\, \sum_{j=1}^n [P]_{ij} = 1\ \forall i \in \mathcal{S}, p_{ij} \in [0,1] \right\}.\end{aligned} \tag{6}$$

### A. Time-invariant RTM

Consider $(\Omega_0, \mathcal{F}_\Omega, \mu)$ with $\Omega_0 = \mathcal{P}$. The RTM, denoted by $P(\omega)$, is a $\mathcal{P}$-valued random matrix whose $ij$-th component determines the transition probabilities from state $i$ to state $j$ for $\omega \in \Omega_0$. A realization of time-invariant Markov chain is constructed with a single transition matrix sampled at $\omega_s$ from the probability measure of $P(\omega)$ and is denoted by $\boldsymbol{X}_s$. The dynamics of this chain is governed by the transition matrix whose $ij$-th component is defined as

$$[P(\omega_s)]_{ij} = \Pr(X_s^{t+1} = j | X_s^t = i, \omega = \omega_s) \quad \forall t. \tag{7}$$

Associated with the sample Markov chains constructed based on $P(\omega_s)$, there exists a stationary distribution $\hat{\boldsymbol{\pi}}_s^{TI}$ which is its left eigenvector, i.e.,

$$\hat{\boldsymbol{\pi}}_s^{TI} = \hat{\boldsymbol{\pi}}_s^{TI} P(\omega_s). \tag{8}$$

Using sufficient samples of the RTM, one can estimate the pdf of the stationary distribution $\hat{\boldsymbol{\pi}}^{TI}(\omega)$ which will predict the asymptotic behavior of the Markov chain by

$$\hat{\boldsymbol{\pi}}^{TI}(\omega) = \hat{\boldsymbol{\pi}}^{TI}(\omega) P(\omega) \quad \mu - \text{a.s.} \tag{9}$$

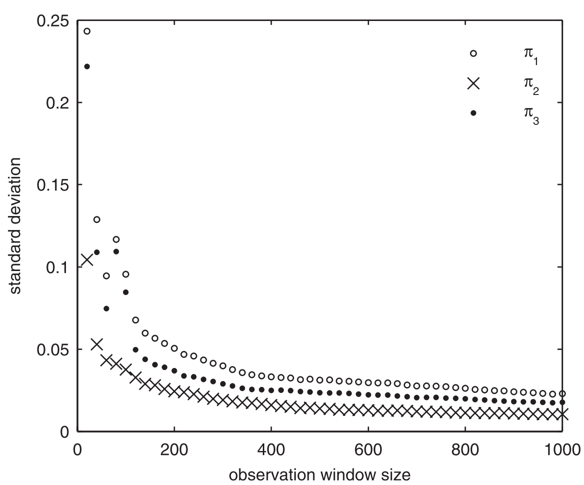


FIG. 1. The standard deviation in the 200 estimates of asymptotic distributions (taken to be the QoI) versus the length of the observation window—in each time window, 200 QoIs are estimated based on the 200 sampled trajectories.

### B. Time-variant RTM

In this section, we present the mathematical setting for the time-variant RTM implementation (Refs. 6 and 18). Consider the probability triple $(\Omega_0, \mathcal{F}_\Omega, \mu)$ defined in Sec. III A.

We define the product probability triple $(\boldsymbol{\Omega}, \mathbb{B}, \boldsymbol{\mu})$ where its elements are given by

$$\begin{aligned} \boldsymbol{\Omega} &= \{ [\omega_1, \omega_2, \ldots] : \omega_t \in \boldsymbol{\Omega}_0, \ \forall t \in \mathbb{N}^+ \}, \\ \mathbb{B} &= \mathcal{F}_\Omega \times \mathcal{F}_\Omega \times \cdots, \\ \boldsymbol{\mu} &= \mu \times \mu \times \cdots. \end{aligned} \tag{10}$$

Let the mapping $P_t : \Omega \to \mathcal{P}$ be the $t$-th transition matrix, defined as $P_t(\omega) = \omega_t$. In other words, one deals with a set of independent random transition matrices $\{P_1(\omega), P_2(\omega), \cdots\}$ each with identical probability measure $\mu$. The $ij$-th component of the $\mathcal{P}$-valued random matrix $P_t(\omega)$ is denoted by $[P_t(\omega)]_{ij}$ and governs the transition probabilities from state $i$ to state $j$ in one step in the random environment $\omega_t$. Therefore, if the chain starts off at position $x_1$ the probability that it will visit $x_1, x_2, \cdots, x_T$ at times $1, 2, \ldots, T$ is given by

$$\begin{aligned} &P^{\omega}_{x_1}[X_1 = x_1, X_2 = x_2, \cdots, X_T = x_T] \\ &\quad = \mathbb{1}_{x_1}(x)[P_1(\omega)]_{x_1 x_2}[P_2(\omega)]_{x_2 x_3} \cdots [P_{T-1}(\omega)]_{x_{T-1} x_T}, \end{aligned} \tag{11}$$

where $\mathbb{1}_{x_1}$ is the indicator function for state $x_1$.

A Markov chain in random environment is then defined as a sequence of probability measures $\{\boldsymbol{\pi}^t \in \Pi : t \in \mathbb{N}^+\}$ that are generated by the RTM $P_t(\omega)$ according to the following definition

$$\boldsymbol{\pi}^{t+1}(\omega) = \boldsymbol{\pi}^t(\omega) P_t(\omega) \quad \boldsymbol{\mu} - \text{a.s.} \tag{12}$$

## IV. MaxEnt FORMULATION

We seek to characterize the probability measure on the support of random matrices, $\mathcal{P}$, using MaxEnt principle. We assume the rows of the RTM to be statistically independent from each other. This assumption implies that the change in the transition pattern outgoing from node $i$ has no impact on the transition pattern outgoing from node $j$. Therefore, in this exposition, for the sake of notation brevity, we formulate the uncertainty representation for a given row of a transition matrix, called a *transition row* hereinafter. To this end, let the random vector $\boldsymbol{r}(\omega) := [r_1(\omega), \cdots, r_n(\omega)]$ denote a particular transition row of the RTM.

Our MaxEnt formalism for the estimation of probability measure for the multivariate $\boldsymbol{r}(\omega)$ relies on two classes of available information; (1) the support for the probability measure, and (2) the statistical moments of $\boldsymbol{r}(\omega)$ obtained from data. With regards to availability of the statistical moments, we consider two different cases in this work. The first case corresponds to situations where only the mean values of the entries of $\boldsymbol{r}(\omega)$ are available from the observation data, whereas the second case corresponds to the situations where we also include the second statistical moments. In what follows, we will elaborate on the implications of each case on the corresponding MaxEnt probability measure and, henceforth, on the Markov chain behavior.

Let $[\overline{m}_1, \cdots, \overline{m}_n]$ denote the mean values for $\boldsymbol{r}(\omega)$. These mean values can be calculated using the transition records (i.e., using Eq. (2)). The sole use of mean values may fail to provide enough information about the variability of the transition probabilities. Using two conceptual cases, we will justify the need for including second moments, in addition to mean values, in the MaxEnt formulation.

First, consider a Markov chain which is observed for a long time period. Let us further assume that this observation time period consists of a number of time windows of smaller size close to the characteristic time scale of the system. In general, the mean transition probabilities estimated based on one time window may differ from those calculated in another window. By incorporating the second order statistics of the observation data obtained from different time windows, one can account for the level of the inter-window fluctuations around the mean value.

Second, consider a dynamical system that is composed of multiple heterogeneous constituents. Let us assume that the overall behavior of the system is to be represented by a single Markov chain and only certain types of the constituents are to be observed. In order to capture variability in the transition frequencies from one type to another, a robust parameter estimator needs to accommodate the second order statistics, hence the justification for including standard deviation in the MaxEnt estimation.

In summary, one can think of the total observation data to be decomposed into patches; temporal patches in the first case, and categorical patches in the second one. To account for the variabilities, we calculate the standard deviation, based on the temporal or categorical patches, for the transition probabilities on the row $\boldsymbol{r}$ and denote them by $[s_1, \cdots, s_n]$.

Having the information on the mean values and standard deviations, our objective is to characterize the MaxEnt probability measure knowing that the random multivariate $\boldsymbol{r}(\omega)$ takes values in $\Pi$. Let $f_r(r_1, \cdots, r_n)$ denote a joint probability density function for the multivariate $\boldsymbol{r}(\omega)$. Given the one-sum constraint, we can relate the $n$-th component of the multivariate to other components using

$$r_n(\omega) = 1 - \sum_{i=1}^{n-1} r_i(\omega) \quad \mu - \text{a.s.} \tag{13}$$

In other words, in each random row, there are indeed $n - 1$ independent components, and thus, we consider an $(n - 1)$-dimensional multivariate denoted by $\boldsymbol{r}'(\omega) = [r_1(\omega), \cdots, r_{n-1}(\omega)]$ to represent the random row. Therefore, we can fully characterize the uncertainty in the $n$-dimensional random row by the lower dimensional joint pdf $f_{r'}(r_1, \cdots, r_{n-1})$ together with the relation in Eq. (13).

*Definition [MaxEnt jpdf]*. Let $f_{r'}(r_1, \cdots, r_{n-1})$ denote a joint pdf on $n - 1$ components of the transition row $\boldsymbol{r}'(\omega)$. The MaxEnt joint density function, $f^*_{r'}(\boldsymbol{r}')$, among the family of the joint probability distribution, is the one given by

$$f^*_{r'}(\boldsymbol{r}') = \arg\max_{f_{r'}} - \int_{V'} f_{r'}(\boldsymbol{r}') \ln f_{r'}(\boldsymbol{r}') d\boldsymbol{r}', \tag{14}$$

$$\begin{aligned} \text{s.t.} \quad & \int_{V'} f_{r'}(\boldsymbol{r}') d\boldsymbol{r}' = 1, \\ & \int_{V'} r_i f_{r'}(\boldsymbol{r}') d\boldsymbol{r}' = \overline{m}_i \qquad i = 1, \ldots, n-1, \\ & \int_{V'} r_i^2 f_{r'}(\boldsymbol{r}') d\boldsymbol{r}' = s_i^2 + \overline{m}_i^2 \qquad i = 1, \ldots, n-1, \end{aligned} \tag{15}$$

where the support $V'$ is characterized by

$$V' = \left\{ \boldsymbol{r}' \subset \mathbb{R}^{n-1} \,\middle|\, \sum_{i=1}^{n-1} r'_i \leq 1,\, \boldsymbol{r}' \geq 0 \right\}. \quad (16)$$

A solution to Eqs. (14) and (15) is obtained by solving the following optimization problem:

$$\sup_{\mu,\boldsymbol{\lambda},\boldsymbol{\eta}} \inf_{f_{r'}} \mathcal{L}(f_{r'}, \mu, \boldsymbol{\lambda}, \boldsymbol{\eta}), \quad (17)$$

where $\mathcal{L}()$ is the associated Lagrangian, $\mu, \boldsymbol{\lambda} \in \mathbb{R}^{n-1}$, and $\boldsymbol{\eta} \in \mathbb{R}^{n-1}$ are the Lagrange multipliers associated, respectively, with the first, the second, and the third of Eqs. (15).

For the case where only knowledge of mean values are used, the last constraint in the Eqs. (15) is not used. The MaxEnt distribution $f^*$ in this case is of the form:

$$f^*_{r'}(\boldsymbol{r}') = e^{(\mu-1)} \exp\left[\sum_{i=1}^{n-1} \lambda_i r_i\right] \mathbb{1}_{V'}(\boldsymbol{r}'), \quad (18)$$

where $1_{V'}$ is the indicator function for $V'$. If the standard deviations are also included the MaxEnt solution will instead have the following form:

$$f^*_{r'}(\boldsymbol{r}') = e^{(\mu-1)} \exp\left[\sum_{i=1}^{n-1} \lambda_i r_i + \sum_{i=1}^{n-1} \eta_i r_i^2\right] \mathbb{1}_{V'}(\boldsymbol{r}'). \quad (19)$$

The solution of the dual Lagrangian problem involves solving $2n-1$ equations for $2n-1$ Lagrange multipliers. We resort to numerical integration in order to calculate the multiple integrals due to the difficulty imposed by the support $V'$.

## V. NUMERICAL EXAMPLE

We now present a numerical example that illustrates the behavior of Markov chains with a RTM. We consider the Swiss HIV cohort study[19] where the progression of HIV-infected subjects at the greatest risk of developing the Mycobacterium avium complex (MAC) infection is studied. The progression is considered to involve transitions between three states categorized by CD4-cell count ranges (with and without AIDS). The transitions between these three states are observed between 1993 and 1995 in 6-month intervals. Based on the observed transition records, the average transition matrix is found to be

$$P = \begin{bmatrix} 0.92 & 0.04 & 0.04 \\ 0.58 & 0.24 & 0.18 \\ 0.23 & 0.23 & 0.54 \end{bmatrix}. \quad (20)$$

The diagram representing the Markov chain showing the mean values is depicted in Fig. 2. In the MaxEnt estimation based on mean values and standard deviations, we artificially induce standard deviations for these transition rates by assuming a constant coefficient of variation of 30% for all nine transition rates.

Three MaxEnt joint pdf's were then independently obtained for the rows of the RTM. Figs. 3 and 4 depict the MaxEnt joint pdf for the two independent random components

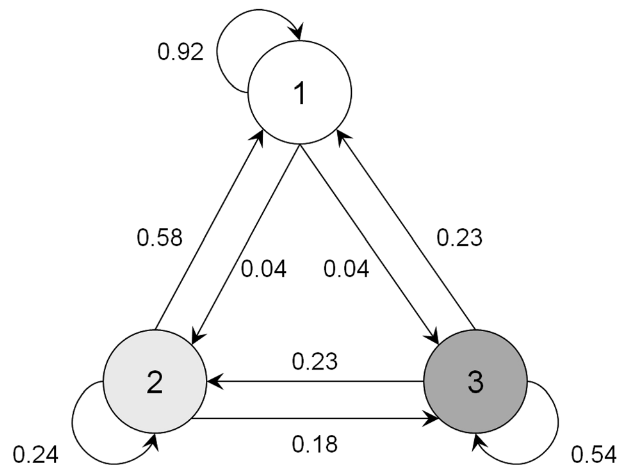


FIG. 2. The 3-state Markov chain modeling the HIV progression; states are identified by the CD4-cell count ranges. Shown on the edges are the observed transition frequencies between the corresponding states, which are taken to be the mean transition probabilities in the MaxEnt estimation.

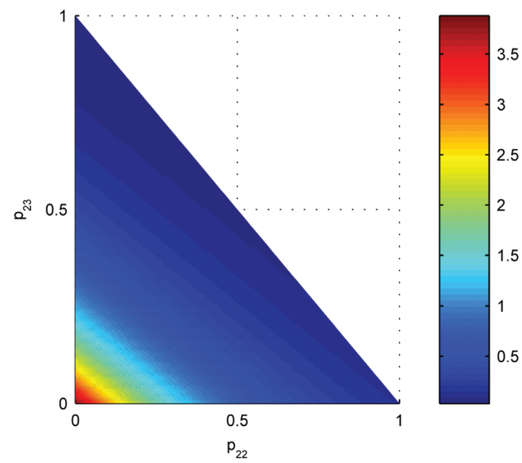


FIG. 3. The joint pdf for $p_{22}$ and $p_{23}$ computed by MaxEnt RTM estimation with mean values. The mean values are $\bar{p}_{22} = 0.24$ and $\bar{p}_{23} = 0.18$.

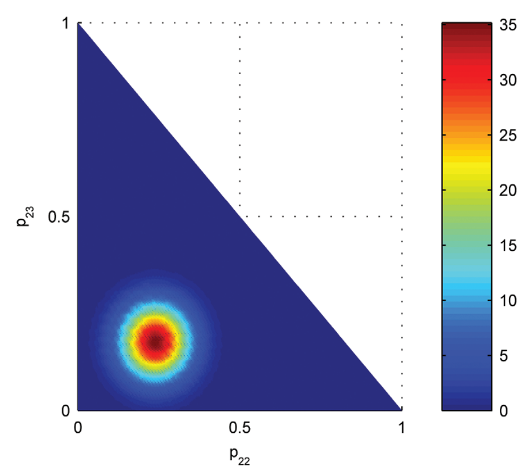


FIG. 4. The joint pdf for $p_{22}$ and $p_{23}$ computed by MaxEnt RTM estimation with mean values and standard deviations. The same mean values with 30% coefficient of variation are considered.

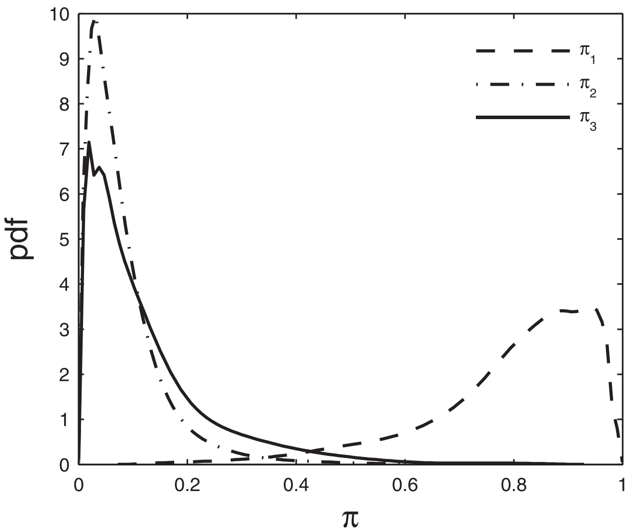


FIG. 5. Stationary distribution for the three cell count states, $\pi_1^\infty, \pi_2^\infty, \pi_3^\infty$ in time-invariant Markov chain using MaxEnt RTM estimation with mean values.

on the second row, i.e., for the transition rates outgoing state 2, and respectively, correspond to the MaxEnt formulation with only mean values and that with mean values and standard deviations. It is of worth noting that the inclusion of the standard deviation has resulted in a joint density function that is more concentrated around the associated mean value.

We next investigate the impact of the uncertainty representation of transition rates on the behavior of the Markov chain. We first focus on the time-invariant implementation and quantify the uncertainty in the stationary or asymptotic state distribution as a major QoI. Figs. 5 and 6 show the variability in these QoI where, as expected, less scatter is observed when second order statistics is included in the MaxEnt density estimation.

The uncertainty in the time evolution of the state distributions is studied next. Specifically, we focus on the dynamics of the state distribution corresponding to state 2, denoted

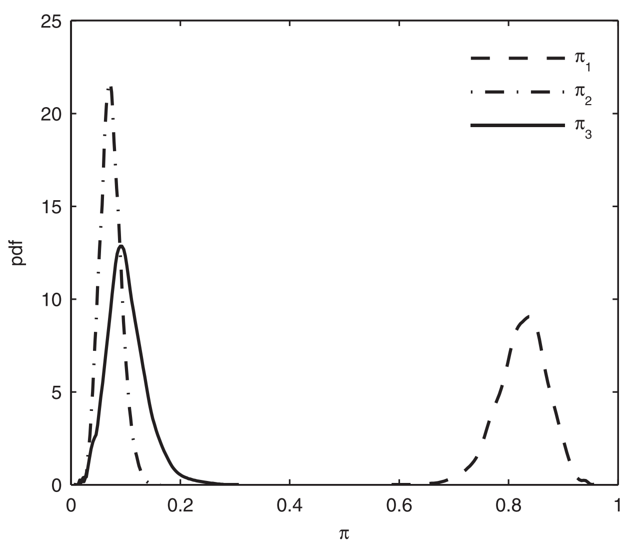


FIG. 6. Stationary distribution for the three cell count states, $\pi_1^\infty, \pi_2^\infty, \pi_3^\infty$ in time-invariant Markov chain using MaxEnt RTM estimation with mean values and standard deviation.

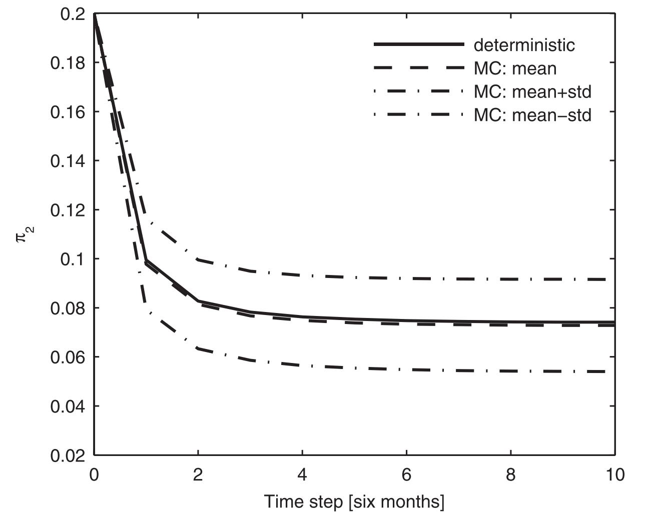


FIG. 7. The scatter in the random progression path in a time-invariant Markov chain using MaxEnt RTM estimation with mean values and standard deviation.

by $\{\pi_2^t\}$, when the initial state distribution is assumed to $\boldsymbol{\pi}^0 = [0.7\ 0.2\ 0.1]$. We study this dynamics in a time-invariant and time-variant construction of Markov chain using the MaxEnt RTM. Fig. 7 compares the resulting random trajectory in a time-invariant construction with the deterministic trajectory obtained based on the average transition matrix. On the other hand, Fig. 8 refers to the time-variant chain where at each time step an independent realization of the random transition matrix is used. An ensemble of 400 Markov chains with time-variant RTM is considered based on which the scatter in the state distribution $\pi_2$ shown in the figure is calculated. As the chain marches through time and consequently traces of initial conditions fade away, one can expect the variability in these state distributions to depend on a finite-length stretch in the pseudo-stationary regime of the probabilistic trajectory. Thus, the probabilistic descriptors, such as pdf's, in this pseudo-stationary region are expected not to differ significantly from one time step to another; a fact that is evident in Fig. 8.

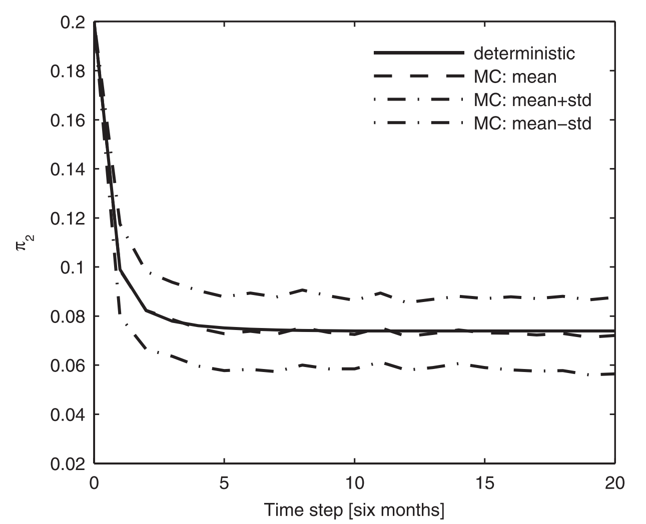


FIG. 8. The scatter in the random progression path in a time-variant Markov chain using MaxEnt RTM estimation with mean values and standard deviation.

Besides the stationary state distribution, another important decision-supporting variable is the probability that a system transits from a specific state to another in a given number of steps. This variable for the transition from state $i$ to state $j$ in exactly $m$ steps is given by $p_{ij}^{(m)} = [P^m]_{ij}$, i.e., the $ij$-th component of matrix $P^m$. In the time-invariant RTM implementation, we have

$$p_{ij}^{(m)(TI)}(\omega) = [P(\omega)^m]_{ij} \quad \mu - \text{a.s.}, \tag{21}$$

whereas for the time-variant case we have

$$p_{ij}^{(m)(TV)}(\boldsymbol{\omega}_{1m}) = [P_1(\omega)P_2(\omega)\cdots P_m(\omega)]_{ij} \quad \boldsymbol{\mu} - \text{a.s.}, \tag{22}$$

where $\boldsymbol{\omega}_{1m} = [\omega_1, \cdots, \omega_m]$. Fig. 9 depicts the pdf of transition probability from a lowest cell count state (state 1) to next cell count state (state 2) in 10 steps in a time-invariant implementation. Since, we are dealing with the product of a number of independent identically distributed random matrices with their common mean value equal to the average matrix of Eq. (20), the average of the estimated random QoI is expected to coincide with the QoI obtained from the deterministic model with the average matrix. This is clearly verified in the figure.

Next, we consider the uncertainty quantification of another important decision variable called the first passage time, which is the time it takes the dynamical system to reach a particular state starting from different initial states. In our example, let $\boldsymbol{t}_3 = [t_{13}\ t_{23}]^T$ denote the expected first passage times to state 3, from states 1 and 2, which is given by

$$\begin{aligned} \boldsymbol{t}_3 &= (I + Q + Q^2 + Q^3 + \cdots)\mathbf{1} \\ &= (I - Q)^{-1}\mathbf{1}, \end{aligned} \tag{23}$$

where $\mathbf{1} = [1\ 1]^T$ and

$$Q = \begin{bmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{bmatrix}. \tag{24}$$

For time-invariant and time-variant RTM implementation, we have

$$\begin{aligned} \boldsymbol{t}_3^{TI}(\omega) &= (I - Q(\omega))^{-1}\mathbf{1} \qquad \mu - \text{a.s.}, \\ \boldsymbol{t}_3^{TV}(\boldsymbol{\omega}_{1m}) &= [I + Q_1(\omega) + Q_1(\omega)Q_2(\omega) + \cdots \\ &\quad + \underbrace{Q_1(\omega)\cdots Q_m(\omega)}_{\text{m times}}]\,\mathbf{1} \quad \text{as } m \to \infty \quad \boldsymbol{\mu} - \text{a.s.}, \end{aligned} \tag{25}$$

where $Q_t(\omega)$ is constructed from the random transition matrix $P_t(\omega)$ according to Eq. (24). Fig. 10 shows the pdf of the expected first passage time from the lowest cell count to the highest cell count for the time-invariant case. The nonlinear form of this QoI induces the discrepancy between the average value of the random QoI and the QoI obtained from the deterministic model that is apparent in the figure.

In order to further emphasize the significant impact of the uncertainty treatment of the Markov chains on policy making, a resource allocation problem for this disease progression example is considered. Let us assume that two types of medical services, denoted by $\alpha_1$ and $\alpha_2$, are available to enhance the conditions of the populations in states 1 and 2. The policy maker is then concerned with the optimal allocation of each medical service according to the following optimization problem

$$\begin{aligned} &[\alpha_1^*, \alpha_2^*] = \arg \max_{[\alpha_1,\alpha_2]} \sum_{i=1}^{2} G_i(\alpha_1, \alpha_2) - \sum_{i=1}^{2} C_i(\alpha_i), \\ &\quad \text{s.t.} \quad \underline{\alpha_i} \le \alpha_i \le \overline{\alpha_i} \qquad i = 1, 2, \\ &\quad 12\alpha_1 + \alpha_2 = B, \end{aligned} \tag{26}$$

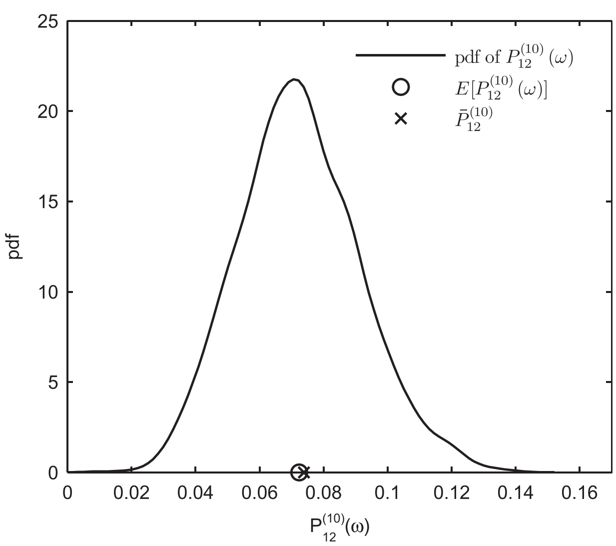


FIG. 9. The pdf of the probability that the system starting in state 1 will be at state 2 in exactly 10 steps. Circle marker refers to the average value of this random quantity of interest. Cross marker refers to the same quantity of interest obtained by the deterministic transition matrix. Time-invariant RTM implementation is used.

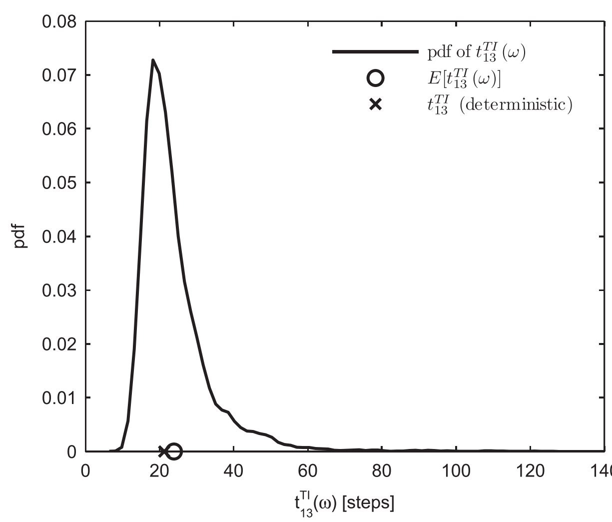


FIG. 10. The pdf of the expected first passage time from state lowest cell count state to the highest one. Circle marker refers to the average value of this random quantity. Cross marker refers to the same quantity of interest obtained by the deterministic transition matrix. Time-invariant RTM implementation is used.

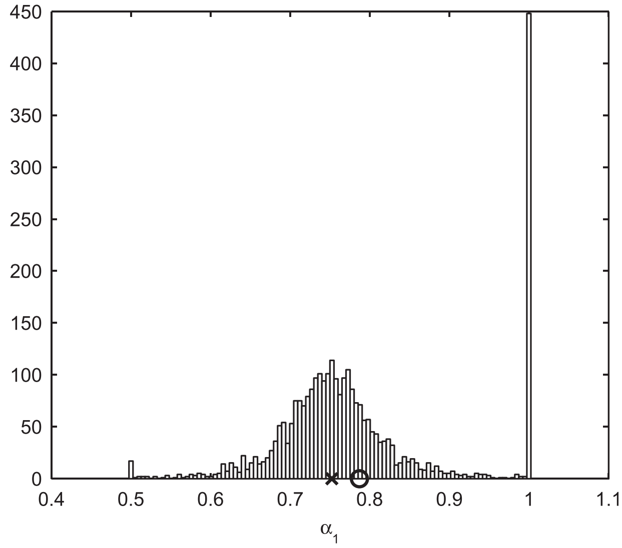


FIG. 11. The histogram of the random optimal allocation of service $\alpha_1$ obtained by 3000 samples of the MaxEnt RTM. Circle marker refers to the average value of this random quantity. Cross marker refers to the optimal allocation obtained by using the deterministic transition model. Time-invariant RTM implementation is used.

where $\underline{\alpha_1} = 0.5$, $\overline{\alpha_1} = 1$, $\underline{\alpha_2} = 5$, $\overline{\alpha_2} = 12$ are the bounds on the two types of medical service. The total budget to be invested on the services is assumed to be $B = 12$. The objective is to maximize the utility minus the implementation costs. The utility, which is a measure of acceptable health conditions, is assumed to be the sum of mean first time passage to the third state, i.e., $\boldsymbol{G} = [G_1\ G_2]^T = \boldsymbol{t}_3$. The implementation cost for each service is assumed to be given by $C_1(\alpha_1) = \exp(\alpha_1)$ and $C_2(\alpha_2) = 0.0001\exp(\alpha_2)$. Let us assume that the implementation of these medical services will impact the disease progression by changing the transition rates in the $Q$ matrix (Eq. (24)) according to

$$Q = \begin{bmatrix} p_{11}(1+\alpha_1/100) & p_{12}(1-\alpha_1/50) \\ p_{21}(1+\alpha_2/100) & p_{22}(1+\alpha_2/100) \end{bmatrix}. \tag{27}$$

We seek to investigate the implication of the random treatment of the transition rates on the optimal resource allocation for a time-invariant disease progression. To this end, we solve the optimal resource allocation problem (Eqs. (26)) for the average transition matrix and also for 3000 samples obtained from the MaxEnt probability measure of the RTM. The histogram of Fig. 11 shows the variability in the optimal allocation of medical service 1 resulting from the 3000 samples. As can be seen, there is a wide scatter in the optimal allocation. More importantly, the random model provides the policy makers with a point estimate (i.e., a mean value) that is profoundly different from the one obtained by the deterministic model. This further accentuates the significance of uncertainty quantification in decision making procedures.

## VI. CONCLUSION

We explore the characterization, construction, and consequences to decision-making associated with uncertainty in the transition rates of Markov chains. This uncertainty reflects a conspiracy between complex dynamics, that limits the validity of the Markovian assumption, and data paucity, that limits the evidential value of deterministically calibrated transition probabilities. By separating the randomness inherent in Markovian dynamics from these extrinsic uncertainties, mitigation strategies can be adapted, analytically and through feedback, to optimize the utility of available information.

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[1]G. Cooman, F. Hermand, and E. Quaeghebeur, "Imprecise Markov chains and their limit behavior," Prob. Eng. Inform. Sci. **23**, 597–635 (2009).
[2]D. Luenberger, *Introduction to Dynamic Systems: Theory, Models, and Applications* (Wiley, New York, 1979).
[3]B. Li and J. Si, "Robust optimality for discounted infinite-horizon Markov decision processes with uncertain transition matrices," IEEE Trans. Autom. Control **53**(9), 2112–2116 (2008).
[4]M. Abbad and J.-A. Filar, "Perturbation and stability theory for Markov control problems," IEEE Trans. Autom. Control **37**(9), 1415–1420 (1992).
[5]A. Nilim and L. El Ghaoui, "Robust control of Markov decision processes with uncertain transition matrices," Oper. Res. **53**, 780–798 (2005).
[6]R. Cogburn, "The ergodic theory of Markov chains in random environments," Z. Wahrscheinlichkeitstheor. Verwandte Geb. **66**, 109–128 (1984).
[7]S. Orey, "Markov chains with stochastically stationary transition probabilities," Ann. Probab. **19**(3), 907–928 (1991).
[8]R. Cogburn, "On the central limit theorem for Markov chains in random environments," Ann. Probab. **19**(2), 587–604 (1991).
[9]G. Lu and A. Mukherjea, "Invariant measures and Markov chains with random transition probabilities," Probab. Math. Stat. **17**(1), 115–138 (1997).
[10]O. Stenflo, "Markov chains in random environment and random iterated function systems," Trans. Am. Math. Soc. **383**(9), 3548–3562 (2001).
[11]J. Lasserre, "Invariant probabilities for Markov chains on a metric space," Stat. Probab. Lett. **34**, 259–265 (1997).
[12]R. McGinnis, "A stochastic model of social mobility," Am. Sociol. Rev. **33**(5), 712–722 (1968).
[13]J. Berger, T. Conner, and W. McKeown, "Evaluations and the formation and maintenance of performance expectations," Hum. Relat. **22**(6), 481–502 (1969).
[14]S. Spilerman, "The analysis of mobility processes by the introduction of independent variables into a Markov chain," Am. Sociol. Rev. **37**(3), 277–294 (1972).
[15]B. Singer and S. Spilerman, "The representation of social processes by Markov models," Am. J. Sociol. **82**(1), 1–54 (1976).
[16]Y. Zou, V. Fonoberov, M. Fonoberova, I. Mezic, and I. Kevrekidis, "Model reduction for agent-based social simulation: Coarse-graining a civil violence model," Phys. Rev. E **85**(6), 066106 (2012).
[17]Y. Zou, P. Torrens, R. Ghanem, and I. Kevrekidis, "Accelerating agent-based computation of complex urban systems," Int. J. Geograph. Inf. Sci. **26**, 1917–1937 (2012).
[18]Y. Takahashi, "Markov chains with random transition matrices," Kodai Math. Semin. Rep. **21**, 426–447 (1969).
[19]B. Ledergerber, J. von Overbeck, M. Egger, and R. Luthy, "The Swiss HIV Cohort Study: Rationale, organization and selected baseline characteristics," Soz. Praventivmed. **39**(6), 387–394 (1994).