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Bivariate Markov Processes and Their Estimation

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Abstract

A bivariate Markov process comprises a pair of random processes which are *jointly* Markov. One of the two processes in that pair is observable while the other plays the role of an underlying process. We are interested in three classes of bivariate Markov processes. In the first and major class of interest, the underlying and observable processes are continuous-time with finite alphabet; in the second class, they are discrete-time with finite alphabet; and in the third class, the underlying process is continuous-time with uncountably infinite alphabet, and the observable process is continuous-time with countably or uncountably infinite alphabet. We refer to processes in the first two classes as bivariate Markov chains. Important examples of continuous-time bivariate Markov chains include the Markov modulated Poisson process, and the batch Markovian arrival process. A hidden Markov model with finite alphabet is an example of a discrete-time bivariate Markov chain. In the third class we have diffusion processes observed in Brownian motion, and diffusion processes modulating the rate of

a Poisson process. Bivariate Markov processes play central roles in the theory and applications of estimation, control, queuing, biomedical engineering, and reliability. We review properties of bivariate Markov processes, recursive estimation of their statistics, and recursive and iterative parameter estimation.

1

Introduction

A bivariate Markov process comprises a pair of random processes which are *jointly Markov*. One of the two processes is observable, while the other plays the role of an underlying process. The underlying process affects the statistical properties of the observable process. Usually, the observable process is not Markov, but the underlying process is often conveniently chosen to be Markov. The theory of bivariate Markov processes does not require either process to be Markov.

The family of bivariate Markov processes is very rich, and has produced powerful models in many applications. Perhaps the most familiar bivariate Markov process stems from the hidden Markov model, see, e.g., [13, 40]. The underlying process of a hidden Markov model is a discrete-time finite-state Markov chain, and the observable process comprises a collection of conditionally independent random variables, e.g., normal, given the underlying Markov chain. Together, the two processes form a bivariate Markov process. Another example follows from the Markov modulated Poisson process, see, e.g., [43, 78, 93]. Here, the underlying process is a continuous-time finite-state Markov chain, and the observable process is conditionally Poisson given the underlying Markov chain. A generalization of this process is given by a Poisson

process whose rate is modulated by an underlying diffusion process, see, e.g., [16, 103, 120]. As a final example, we mention the bivariate Markov process formed by an underlying diffusion process, and the same process observed in Brownian motion. Here the underlying process is a continuous-time continuous-alphabet Markov process. Bivariate Markov processes play central roles in the theory and applications of estimation, control, queuing, economics, biomedical engineering, and reliability.

In general, each of the two process components of a bivariate Markov process may be discrete-time or continuous-time, with finite, countably infinite, or uncountably infinite alphabet. We shall focus on three classes of bivariate Markov processes. In the first class, the pair of processes comprising the bivariate Markov process are continuous-time with finite alphabet; in the second class, they are discrete-time with finite alphabet; and in the third class, both processes are continuous-time with a diffusion underlying process and an observable process with a countably or uncountably infinite alphabet. Our primary focus in this paper will be on the first class of processes, which we refer to as *continuous-time bivariate Markov chains* or simply as *bivariate Markov chains*. We shall refer to processes from the second class as *discrete-time bivariate Markov chains*. The processes in the third class are assumed to be diffusion processes observed in Brownian motion, in a counting process, or in a mixture of Brownian motion and a counting process. Some of the results reported here for finite alphabet processes, apply to bivariate Markov processes with countably infinite alphabet, by resorting to modulo arithmetic.

The theory of *univariate* Markov processes applies to bivariate Markov processes. Excellent sources for that theory may be found in Doob [31], Breiman [15] and Todorovic [109]. Application of the theory of univariate Markov processes to bivariate Markov processes, with the observable and underlying processes playing different roles, is not straightforward. Research on various forms of bivariate Markov processes has been ongoing for more than four decades. The research has focused on two main interrelated estimation problems, namely, parameter and signal estimation. In parameter estimation, the maximum likelihood approach has dominated the field. Here, identifiability

of the parameter of the bivariate Markov process was studied; iterative estimation approaches in the form of the expectation-maximization (EM) algorithm were developed; and consistency and asymptotic normality were proven for parameter estimation of some bivariate Markov chains. Application of the EM approach requires minimum mean square error recursive estimation of several statistics of the bivariate Markov chain. In particular, estimation of the number of jumps from one state to another, and the total sojourn time of the process in each state, in a given interval, are required. In other applications, estimation of the state of the underlying process is of primary interest.

In this paper we present some of the fundamentals of the theory of bivariate Markov processes, and review the various parameter and signal estimation approaches. Our goals are to provide a comprehensive introduction to bivariate Markov chains, along with the details of the various estimation algorithms. While proofs are generally omitted, an interested reader should be able to implement the estimation algorithms for bivariate Markov chains straight out of this paper. Most of the material in this paper should be accessible to the signal processing community. It requires some familiarity with Markov chains and the intricacies of the theory of hidden Markov models. The discussion on diffusion processes requires some further knowledge in nonlinear estimation theory.

Our presentation in Sections 1 to 7 focuses on continuous-time bivariate Markov chains with a finite or countably infinite number of states. In Section 8 we discuss finite alphabet discrete-time bivariate Markov chains. In Section 9 we consider a bivariate Markov chain observed through Brownian motion. In Section 10, we provide a glimpse into the fascinating topic of bivariate Markov processes with underlying diffusion processes. Several applications are discussed in Section 11, and some concluding remarks are given in Section 12.

2

Preliminaries

The theory of continuous-time univariate Markov chains applies to continuous-time bivariate Markov chains. In this section we review that theory, and state the results as they specialize to continuous-time bivariate Markov chains. The latter is the main class of processes reviewed in this paper. Our presentation in this section follows Todorovic [109], and Breiman [15]. We also provide in this section several important examples of bivariate Markov processes, and discuss their interrelations. We conclude this section by reviewing a result due to Van Loan [110], which has turned out to be quite useful in recursive estimation of the statistics and parameter of the bivariate Markov chain.

Throughout this paper, we use capital letters to denote random variables and lower case letters to denote their realizations. We also use the generic notation $P(\cdot)$ for a probability measure and $p(\cdot)$ for a density. We indicate that a matrix A has non-negative elements by writing $A \geq 0$. This notation should not be interpreted as A being positive semi-definite. Similarly, $A > 0$ indicates that all elements of A are positive.

2.1 Continuous-time Markov Chains

Let $Z = \{Z(t), t \geq 0\}$ denote a continuous-time bivariate Markov chain, which takes values in a countable state space $\mathbb{Z}$, and is defined on a given probability space. The bivariate Markov chain comprises a pair of random processes, say $Z = (X, S)$, which are *jointly* Markov. For the given probability measure P, any positive integer n, any sequence of time instants $t_0 < t_1 < \cdots < t_n$, and any sequence of states $z_0, z_1, \ldots, z_n$ in $\mathbb{Z}$,

$$\begin{aligned} P(Z(t_n) &= z_n \,|\, Z(t_{n-1}) = z_{n-1}, Z(t_{n-2}) = z_{n-2}, \ldots, Z(t_0) = z_0) \\ &= P(Z(t_n) = z_n \,|\, Z(t_{n-1}) = z_{n-1}). \end{aligned} \tag{2.1}$$

The right hand side (rhs) of (2.1) represents the *transition probability* of the bivariate Markov chain. When this transition probability depends only on $t_n - t_{n-1}$, but not on t_{n-1}, the process is said to be *homogeneous*. Homogeneity of the bivariate Markov chain is assumed throughout this paper. The transition probability of a homogeneous bivariate Markov chain is given by $P(Z(t) = z_1 \,|\, Z(0) = z_0)$ for any $t \geq 0$ and any $z_1, z_0 \in \mathbb{Z}$. We also assume that the bivariate Markov chain is *irreducible*. This means that the probability of reaching each state from any other state at some time $t > 0$ is positive. For a continuous-time Markov chain, $P(Z(t) = z_1 \,|\, Z(0) = z_0)$, $z_1 \neq z_0$, is either positive or zero for all $t > 0$ [51, Theorem 6.10.11].

The process $X = \{X(t), t \geq 0\}$ of the bivariate Markov chain is designated as the observable process, and $S = \{S(t), t \geq 0\}$ is designated as the underlying process of the bivariate Markov chain. In general, neither X nor S need be Markov. A jump of the bivariate Markov chain Z may be due to a jump of X, a jump of S, or a simultaneous jump of X and S. The state space of X is denoted by $\mathbb{X}$, the state space of S is denoted by $\mathbb{S}$, and the state space of the bivariate Markov chain is $\mathbb{Z} = \mathbb{X} \times \mathbb{S}$. Most of the presentation in this paper focuses on bivariate Markov chains which take values in a finite state space $\mathbb{Z}$ for which we assume, without loss of generality, that $\mathbb{X} = \{1, \ldots, d\}$ for some finite d, and that $\mathbb{S} = \{1, \ldots, r\}$ for some finite r. Countable state spaces, however, are encountered in some applications and hence we shall try to keep the discussion general whenever possible.

2.1.1 Infinitesimal Generator

The *transition matrix* of a homogeneous bivariate Markov chain comprises the matrix of transition probabilities of the form $P(Z(t) = (b, j) \mid Z(0) = (a, i))$ for all (a, i) and (b, j) in $\mathbb{Z}$ and any $t \geq 0$. We denote this matrix by P_t. We assume that $P_0 = I$, where I denotes an identity matrix, and that the elements of P_t are continuous at $t = 0$, that is,

$$\lim_{t \downarrow 0} P_t = I. \tag{2.2}$$

Such P_t is called a *standard* transition matrix. Clearly, P_t is a stochastic matrix, i.e., it has non-negative entries and each row sums up to one. Furthermore, P_t satisfies the *Chapman-Kolmogorov equations* given by $P_{t+\tau} = P_t P_\tau$ for $t, \tau \geq 0$. Using these equations, one can determine the transition probabilities of the process at any time $t > 0$, from the transition probabilities in any small neighborhood of $t = 0$. Thus, global properties of P_t, and consequently of the Markov chain, are determined from local properties of P_t in the neighborhood of $t = 0$. We are particularly interested in continuity and differentiability of P_t at $t = 0$. We mention, without going into details, that the family $\{P_t, t \geq 0\}$ constitutes a *semigroup* [109, Eq. 8.37].

Continuity of P_t at $t = 0$ implies that the bivariate Markov chain is continuous in probability, that is, for any $t \geq 0$ and $\epsilon > 0$,

$$\lim_{\tau \to t} P(|Z(\tau) - Z(t)| > \epsilon) = 0 \tag{2.3}$$

for any initial distribution. This result has several important measure theoretic implications such as the process being separable and measurable on every compact interval [109, Section 8.5]. Roughly speaking, separability means that probabilities of events of the continuous-time process in a given time interval, may be calculated over a dense countable set of time instants in that interval. Furthermore, continuity in probability of the process implies that the process has a stochastically equivalent version with right-continuous sample paths. Thus, references to the process may be considered as references to its stochastically equivalent version, and both are denoted indistinguishably as the original process Z. Another important consequence of the continuity of the transition matrix P_t, and its Chapman-Kolmogorov equations, is

that the entries of P_t are uniformly continuous on $[0,\infty)$ for all pairs of states (a,i) and (b,j) in $\mathbb{Z}$ [109, Corollary 8.3.1].

The transition matrix P_t is differentiable at $t=0$ [109, Propositions 8.3.2–8.3.3]. The derivative of P_t at $t=0$ is the infinitesimal *generator* of the bivariate Markov chain, which is denoted here by G. We have,

$$G = \lim_{t \downarrow 0} \frac{1}{t}(P_t - I). \tag{2.4}$$

Suppose that the states $\{(a,i) \in \mathbb{Z}\}$ of the bivariate Markov chain are ordered lexicographically, and let the $((a,i),(b,j))$ element of G be denoted by $g_{ab}(ij)$. The generator $G = \{g_{ab}(ij)\}$ has the following properties:

(i) $-\infty \le g_{aa}(ii) \le 0$,
(ii) $0 \le g_{ab}(ij) < \infty$ whenever $(a,i) \ne (b,j)$,
(iii) $\sum_{b,j} g_{ab}(ij) \le 0$ for all $(a,i) \in \mathbb{Z}$ with equality if

$$\sup_{(a,i)} \{-g_{aa}(ii)\} < \infty. \tag{2.5}$$

Thus, the generator G has non-positive main diagonal elements, non-negative off-diagonal elements, and each of its rows sums to zero if (2.5) is satisfied. Under this condition, which is assumed throughout this paper, we have the following intuitively pleasing interpretation of the generator [15, p. 333]. For sufficiently small t,

$$\begin{aligned} &P(Z(t) = (b,j) \,|\, Z(0) = (a,i)) \\ &\qquad = \begin{cases} g_{ab}(ij)t + o(t), & (a,i) \ne (b,j) \\ 1 + g_{aa}(ii)t + o(t), & (a,i) = (b,j). \end{cases} \end{aligned} \tag{2.6}$$

Moreover, under (2.5), the semigroup $\{P_t, t \ge 0\}$ is differentiable for all $t \ge 0$, and $\{P_t, t \ge 0\}$ satisfies *Kolmogorov's forward and backward equations*,

$$\begin{aligned} \frac{dP_t}{dt} &= P_t G \\ \frac{dP_t}{dt} &= G P_t, \end{aligned} \tag{2.7}$$

respectively, subject to $P_0 = I$ [109, Proposition 8.3.4]. The unique solution of either equation in (2.7) is given by

$$P_t = e^{Gt}. \tag{2.8}$$

2.1.2 Sample Paths

As we have seen, the Markov chain has a stochastically equivalent separable version with right-continuous, piecewise constant sample paths or trajectories. Each jump of the process corresponds to a state transition, and the process remains in each state for a random duration of time, called the *sojourn time*. When the chain enters a state z, and $\Delta\tau$ denotes the sojourn time of the chain in that state, then $\Delta\tau$ is exponentially distributed [109, Lemma 8.7.1],

$$P(\Delta\tau > t \,|\, Z(0) = z) = e^{-\lambda(z)t}, \quad t \geq 0, \tag{2.9}$$

with some rate $0 \leq \lambda(z) \leq \infty$. When $\lambda(z) = 0$, the chain remains in z forever, and z is an *absorbing* state. When $\lambda(z) = \infty$, $P(\Delta\tau = 0 \,|\, Z(0) = z) = 1$, and the chain exits the state z as soon as it enters it. In that case, z is said to be an *instantaneous* state. When $0 < \lambda(z) < \infty$, $P(0 < \Delta\tau < \infty \,|\, Z(0) = z) = 1$, and the state z is considered *stable*.

The separable right-continuous version of the Markov chain cannot have instantaneous states. Hence, if τ_n denotes the time of the nth jump of the process, then starting from any state z [59, p. 263],

$$\tau_\infty = \lim_{n\to\infty} \tau_n = \infty \quad a.s. \tag{2.10}$$

In that case, we say that the process does not terminate. If, starting from any state z, $P(\tau_\infty < \infty) > 0$, then the chain may jump infinitely many times on the finite interval $[0, \tau_\infty)$, in which case, it is said to be *explosive*.

A Markov chain is called *regular* if it satisfies (2.10). Clearly, any finite-state Markov chain is regular [25, Proposition 1.12]. Recall that the expected value of the exponentially distributed sojourn time in a given state, say z, is $1/\lambda(z)$. A Markov chain is regular, or non-explosive, if and only if the expected value of τ_∞, starting from any

state z, satisfies [109, Proposition 8.7.2]

$$\sum_{n=1}^{\infty} \frac{1}{\lambda(Z(\tau_n))} = \infty, \quad a.s. \tag{2.11}$$

This condition is satisfied when $\sup_{z\in\mathbb{Z}} \lambda(z) < \infty$ [15, Corollary 15.44], [109, Eq. 8.7.12].

2.1.3 Pure Jump Processes

A regular bivariate Markov chain is a *pure jump* process. Such a process is also called *Markov jump process*, or càdlàg, which is a French abbreviation for "right-continuous with left limit." All sample paths of a Markov jump process are right-continuous, piecewise constant functions, with a *finite* number of jumps in any finite interval. A Markov jump process Z can be written as [59, Eq. 9.27]

$$Z(t) = Z(0) + \sum_{n=1}^{\infty} \zeta_n I(\tau_n \leq t) \tag{2.12}$$

where τ_n is the time of the nth jump, $\zeta_n = Z(\tau_n) - Z(\tau_n-) = Z(\tau_n) - Z(\tau_{n-1})$ denotes the size of the nth jump of Z in its two components, and $I(\tau_n \leq t)$ is an indicator function which equals one when $\tau_n \leq t$ and zero otherwise. Given $Z(\tau_{n-1}) = z$, the *sojourn time* $\Delta\tau_n = \tau_n - \tau_{n-1}$ of the process in state z, and the jump ζ_n at time τ_n, are independent random variables, and both are independent of the entire past $\{Z(t), t < \tau_{n-1}\}$ of the process [109, Lemma 8.7.2]. Each of the random variables $\{\Delta\tau_n, \zeta_n\}$ has its own conditional distribution, where the conditional distribution of the sojourn time $\Delta\tau_n$, given $Z(\tau_{n-1}) = z$, is exponential with a non-negative finite rate $\lambda(z)$.

A Markov jump process may be envisioned as a process that starts in some state z_0 at some given time, stays in that state for t_1 seconds, where t_1 is a realization of an exponentially distributed random variable with parameter $\lambda(z_0)$, then jumps to another state $z_1 \neq z_0$ according to some transition probability, stays there for an exponentially distributed duration with parameter $\lambda(z_1)$, and so on. The process may be seen as an amalgam of a discrete-time Markov chain, say $\{U_n, n = 0, 1, 2, \ldots\}$, and an independent non-homogeneous Poisson process with a rate of

$\lambda(U_n)$ at the nth jump. In this analogy, the jumps of the continuous-time Markov chain are consistent with the jumps of $\{U_n\}$, and its sojourn time in U_n is the sojourn time of the Poisson process whose rate is $\lambda(U_n)$.

The rate $\lambda(z)$ of the conditional exponential distribution of the sojourn time of the bivariate Markov chain in state $z = (a, i)$ is given by $-g_{aa}(ii)$. The probability that the chain jumps to (b, j) from (a, i) is given by $-g_{ab}(ij)/g_{aa}(ii)$ [15, p. 333], [51, Claim 6.9.13–4]. Thus, the Markov chain is regular if (2.5) is satisfied. This assumption is made throughout the paper, and hence, all bivariate Markov chains in this paper are regular.

The stationary distribution of an irreducible bivariate Markov chain with semigroup $\{P_t\}$ and corresponding generator G satisfies $\pi = \pi P_t$, or equivalently, $\pi G = \mathbf{0}$ where $\mathbf{0}$ is an all zero matrix of appropriate dimensions [51, Claim 6.9.20].

2.1.4 Strong Markov Property

We next discuss two rather important properties of a continuous-time Markov chain. A non-negative random variable τ^*, which may take the value ∞, is called a *stopping time* for the Markov chain Z, if for every $t \geq 0$, the occurrence of the event $\{\tau^* \leq t\}$ can be determined from $\{Z(\tau), \tau \leq t\}$. In other words, τ^* is a stopping time of Z if the event $\{\tau^* \leq t\}$ is in the σ-field $\mathcal{F}_t$ generated by $\{Z(\tau), \tau \leq t\}$. The jump points of a Markov jump process Z are stopping times w.r.t. $\mathcal{F}_t$ [15, Proposition 15.27]. A Markov chain Z possesses the *strong Markov property* if for every stopping time τ^*, every $t > 0$, every initial state in $z \in \mathbb{Z}$, and any state $z_1 \in \mathbb{Z}$ [15, Definition 15.17],

$$\begin{aligned} &P(Z(\tau^* + t) = z_1 \,|\, Z(\tau^*) = z, \{Z(\tau), \tau < \tau^*\}) \\ &\quad = P(Z(t) = z_1 \,|\, Z(0) = z). \end{aligned} \tag{2.13}$$

A Markov jump process Z is strong Markov [15, Proposition 15.25]. A stopping time for a Markov process is called a *Markov time*.

Recall that τ_n denotes the time of the nth jump of the bivariate Markov chain Z, and $\Delta\tau_n$ denotes the sojourn time of the chain in state $Z(\tau_{n-1})$, for $n = 1, 2, \ldots$, where $\tau_0 = 0$. Define $\Delta\tau_0 = 0$. Recall also that

$\{\tau_n\}$ are stopping times for Z. The sequence $\{(\Delta\tau_k, Z(\tau_k)), k = 0, 1, \ldots\}$ forms a *Markov renewal process* [109, Proposition 8.7.1]. That is, the sequence satisfies for $n \geq 1$,

$$\begin{aligned} &P(\Delta\tau_n \leq t, Z(\tau_n) = j \,|\, (\Delta\tau_k, Z(\tau_k)), k = 0, 1, \ldots, n-1) \\ &\quad = P(\Delta\tau_n \leq t, Z(\tau_n) = j \,|\, Z(\tau_{n-1})) \\ &\quad = P(\Delta\tau_1 \leq t, Z(\tau_1) = j \,|\, Z(0)). \end{aligned} \tag{2.14}$$

A comprehensive review of Markov renewal theory may be found in [25]. The last two results will play a central role in Section 3 where we develop the likelihood function of the observable process of the bivariate Markov chain.

2.1.5 Bivariate Markov Chains with Varying Order G_{aa}

It is convenient to order the states $\{(a, i)\}$ of the bivariate Markov chain lexicographically, and to organize the generator as a block matrix $G = \{G_{ab}; a, b \in \mathbb{X}\}$ where each $G_{ab} = \{g_{ab}(ij); i, j \in \mathbb{S}\}$. When $\mathbb{S}$ contains r states, the order of G_{ab} is r for any $a, b \in \mathbb{X}$. A somewhat more general bivariate Markov chain may be defined, by allowing the matrices $\{G_{aa}, a \in \mathbb{X}\}$ to have varying orders. We denote the order of G_{aa} by r_a. This condition implies that each observable state is associated with a varying number of underlying states. In that case, the matrices $\{G_{ab}, b \neq a\}$ are rectangular rather than square matrices. Such bivariate Markov chains occur naturally in some applications as we shall see in Sections 2.2.1 and 3.6. This model is also of interest in ion-channel current analysis [27]. The two models can be treated in a similar manner, and most of the results obtained for one model apply to the other. To keep the notation simple, we shall proceed with the bivariate Markov chain for which $r_a = r$ for all a's, and comment on the alternative model when the results disagree. One such case is concerned with conditions for the underlying chain S to be Markov. When $r_a = r$, the underlying chain is Markov, if and only if $\sum_b G_{ab} = Q$ for all $a \in \mathbb{X}$ and some matrix Q [6]. In that case, Q is the generator of the underlying Markov chain. A similar condition can be given for the observable chain X to be Markov. Clearly, this result does not hold for the model with varying r_a.

2.1.6 Properties of G_{aa}

Throughout this paper, we assume that G and $\{G_{aa}\}$ are *irreducible*. Rather than give the formal definition of an irreducible matrix [63, Section 10.7], we quote the following result. A square matrix is irreducible if and only if its associated directed graph is strongly connected [63, Theorem 1, p. 529]. For the matrix G_{aa}, for example, this means that for any two states, say $i, j \in \mathbb{S}$, there exists a sequence of intermediate states $k_1, k_2, \ldots, k_n$ such that

$$g_{aa}(i,k_1) \cdot g_{aa}(k_1,k_2) \cdots g_{aa}(k_{n-1},k_n) \cdot g_{aa}(k_n,j) \neq 0. \tag{2.15}$$

Irreducibility of a matrix depends only on the arrangement of the zero entries within the matrix, and not on the magnitudes or signs of the remaining entries. A matrix with all non-zero entries is always irreducible. A Markov chain is irreducible if and only if its generator is irreducible [51, Problem 6.15.15].

Properties of G_{aa} are important for establishing the likelihood function of the observable process of the bivariate Markov chain. Several properties were studied in [39]. By definition, the matrix G_{aa} is *diagonally dominant*, that is, for each $i \in \mathbb{S}$,

$$|g_{aa}(ii)| \geq \sum_{j=1, j\neq i}^{r} g_{aa}(ij). \tag{2.16}$$

Irreducibility of G implies that at least one element in one of the submatrices $\{G_{ab}, b \in \mathbb{X}; b \neq a\}$ must be positive. Furthermore, $g_{aa}(ii) < 0$ for every $i \in \mathbb{S}$. Thus, (2.16) must hold with strict inequality for at least one $i \in \mathbb{S}$. Together with irreducibility of G_{aa}, this implies that G_{aa} is nonsingular, [63, Theorem 1, p. 375]. Furthermore, from [63, Theorem 3, p. 531], the matrix $-G_{aa}$ is an *M-matrix*. This means that $-G_{aa}$ is a *monotone* matrix with non-positive off-diagonal elements. A monotone matrix is a nonsingular matrix where all elements of its inverse are non-negative. In fact, from [39, Corollary 1], $-G_{aa}^{-1} > 0$. From [63, p. 532, Exercise 3], all eigenvalues of G_{aa} have negative real parts. We also have that the matrix exponential $e^{G_{aa}t} > 0$ for all $t > 0$ [39, Lemma 1]. In summary, under the assumption that G and G_{aa} are irreducible, G_{aa} is non-singular, $-G_{aa}^{-1} > 0$, all eigenvalues of G_{aa} have negative real parts, and $e^{G_{aa}t} > 0$ for all $t > 0$.

2.2 Examples of Bivariate Markov Chains

In this section we specialize the continuous-time bivariate Markov chain, and show that several commonly used stochastic models are in fact finite-state bivariate Markov chains. The relations among these models are addressed in Section 2.3.

2.2.1 Aggregated Markov Chains

An aggregated Markov chain is obtained from a deterministic function of a Markov chain. The family of aggregated Markov chains is closely related to the family of bivariate Markov chains. To demonstrate this relation, suppose that $\{S(t), t \geq 0\}$ is a finite-state continuous-time irreducible univariate Markov chain with state space $\mathbb{S} = \{1, 2, \ldots, r\}$ and a given generator. Consider a function $u : \mathbb{S} \to \mathbb{X}$ where $\mathbb{X} = \{1, 2, \ldots, d\}$ for some $d \leq r$. When the function is injective then $d = r$ and $\mathbb{X} = \mathbb{S}$. Otherwise, u is an aggregating function for which $d < r$. Consider the aggregated Markov chain $X(t) = u(S(t))$. The sets $\{u^{-1}(1), \ldots, u^{-1}(d)\}$ form a partition of $\mathbb{S}$. If we relabel the states $u^{-1}(a)$ for each $a \in \mathbb{X}$ as $\{1, 2, \ldots, r_a\}$, and denote the resulting chain by $\tilde{S}(t)$, then the bivariate process $\tilde{Z} = \{(X(t), \tilde{S}(t)), t \geq 0\}$ is an irreducible Markov chain with transition probability induced by

$$\begin{aligned} &P(X(t) = b,\ S(t) = j \,|\, X(0) = a,\ S(0) = i) \\ &\quad = \begin{cases} P(S(t) = j \,|\, S(0) = i), & \text{if } u(i) = a, u(j) = b \\ 0, & \text{otherwise.} \end{cases} \end{aligned} \tag{2.17}$$

The generator of this bivariate Markov chain has a block matrix representation, where the ath diagonal block is an $r_a \times r_a$ matrix, and the off-diagonal matrices are not necessarily square matrices. Furthermore, the underlying chain of this bivariate Markov chain is not Markov. Conversely, if $\{Z(t), t \geq 0\}$ is a bivariate Markov chain as defined in Section 2.1, we can trivially define a projection function u such that $X(t) = u(Z(t))$, and $X(t)$ is a function of a finite-state continuous-time irreducible Markov chain. The relationship between bivariate and aggregated Markov chains is useful, since it enables application of results developed for one form of the process to its other alternative form.

As an example, consider a Markov chain S with state space $\{\vartheta_1, \vartheta_2, \vartheta_3, \vartheta_4, \vartheta_5\}$, and an aggregating function that maps states $\{\vartheta_1, \vartheta_2\}$ into state a, and states $\{\vartheta_3, \vartheta_4, \vartheta_5\}$ into state b. Now, rename the states associated with the observable state a as $\{1, 2\}$, respectively, and the states associated with the observable state b as $\{1, 2, 3\}$, respectively. For example, the new state $(b, 2)$ of $\tilde{Z}$ is just the old state ϑ_4 of S. The probability of a jump from, say state $(a, 1)$, to say state $(b, 2)$, is the probability that S jumps from state ϑ_1 to state ϑ_4. If the latter probability is positive, then the probability of the simultaneous jump $(a, 1) \to (b, 2)$, of the underlying and observable chains of the equivalent bivariate Markov chain, is positive as well.

Several authors have studied continuous-time aggregated Markov chains, including Rudemo [92] who referred to these processes as "partially observed Markov chains," Colquhoun and Hawkes [27], Rydén [96], and Larget [64]. These processes are also referred to as "hidden Markov chains" and "lumped Markov chains."

2.2.2 Markov Modulated Poisson Process (MMPP)

The MMPP is a doubly stochastic Poisson process [43, 78, 93]. Its rate at any given time is determined by the state of an underlying Markov chain, which is assumed to be finite-state, homogeneous, and irreducible. Given the underlying Markov chain S, the observable process X may be viewed as an non-homogeneous Poisson process, with r possible rates, that are selected according to a Markovian regime. The Poisson rates are denoted by $\{\lambda_1, \ldots, \lambda_r\}$ where $\lambda_i \geq 0$. The observable process X assumes its values in $\mathbb{X} = \{0, 1, \ldots\}$. The only allowed transitions of X are from a to $a + 1$ for any non-negative integer a. It follows that the process $Z = (X, S)$ is a bivariate Markov chain with countable alphabet and some generator G which we specify below. The chains S and X of an MMPP do not jump simultaneously almost surely. Doubly stochastic Poisson processes, not necessarily with an underlying Markov chain, were originally proposed by Cox [28], and are often referred to as Cox processes.

Let $Q = \{q_{ij}\}$ denote the generator of S, and let $\Lambda = \text{diag}\ \{\lambda_1, \ldots, \lambda_r\}$. Since a Poisson process is also a Markov chain, we have

from (2.6), for t sufficiently small, that

$$P(Z(t) = (b, j) \,|\, Z(0) = (a, i)) = \begin{cases} g_{a,a+1}(ij)t + o(t), & b = a+1, j \neq i \\ (\lambda_i t + o(t))(1 + q_{ii}t + o(t)), & b = a+1, j = i \\ (1 - \lambda_i t + o(t))(q_{ij}t + o(t)), & b = a, j \neq i \\ 0, & \text{otherwise} \end{cases} \tag{2.18}$$

Since S and X do not jump simultaneously almost surely, we have from the first line on the rhs of (2.18) that $g_{a,a+1}(ij) = 0$ when $j \neq i$. Furthermore, it follows from (2.18) and (2.4), that the generator of the bivariate Markov chain representing the MMPP is given by the infinite block Toeplitz matrix

$$G = \begin{pmatrix} Q-\Lambda & \Lambda & & & & & \\ & Q-\Lambda & \Lambda & & & & \\ & & Q-\Lambda & \Lambda & & & \\ & & & Q-\Lambda & \Lambda & & \\ & & & & \ddots & \ddots & \end{pmatrix}. \tag{2.19}$$

There is no loss of generality in assuming that the Poisson events are counted modulo-2, since the actual count may always be recovered from the modulo count. When modulo count is used, the observable process can take only $d = 2$ values, which we denote here by $\mathbb{X} = \{1, 2\}$ to be consistent with our earlier notation. Since transitions of X from $1 \to 2$ and from $2 \to 1$ are completely symmetrical, we must have $G_{12} = G_{21}$. In addition, we have as before that $G_{11} = G_{22}$. Thus, the generator of the MMPP may be considered as given by [37]

$$G = \begin{pmatrix} Q-\Lambda & \Lambda \\ \Lambda & Q-\Lambda \end{pmatrix}. \tag{2.20}$$

Since each row of G sums up to zero, this generator has at most r^2 independent entries.

When $r = 2$, and one of the Poisson rates equals zero, the MMPP is referred to as the *interrupted Poisson process* [93]. MMPPs are common models in queuing theory, and have been used in applications such as traffic modeling in computer networks, see [71] and the references therein.

2.2.3 Markov Modulated Markov Process (MMMP)

The MMMP is a slight generalization of the MMPP [36, 41]. Its underlying process S is a finite-state, homogeneous, irreducible Markov chain with generator Q, and its observable process X is a conditionally non-homogeneous Markov chain given S. Similarly to the MMPP, X and S do not jump simultaneously almost surely. When $S = i$, the generator of the conditional Markov chain X is given by $\{g_{ab}(i); a, b \in \mathbb{X}\}$ for some $g_{ab}(i) \geq 0$ when $a \neq b$, and $g_{aa}(i) < 0$ such that $\sum_{b \in \mathbb{X}} g_{ab}(i) = 0$ for any $i \in \mathbb{S}$. The pair (X, S) forms a bivariate Markov chain with generator $G = \{G_{ab}; a, b \in \mathbb{X}\}$. To specify G_{ab}, define the diagonal matrices $\Lambda_{ab} = \text{diag}(g_{ab}(1), \ldots, g_{ab}(r))$. We then have

$$G_{ab} = \begin{cases} Q + \Lambda_{aa}, & b = a \\ \Lambda_{ab}, & b \neq a \\ \mathbf{0}, & \text{otherwise.} \end{cases} \tag{2.21}$$

For example, an MMMP with $d = 3$ observable states has the following generator

$$G = \begin{pmatrix} Q + \Lambda_{11} & \Lambda_{12} & \Lambda_{13} \\ \Lambda_{21} & Q + \Lambda_{22} & \Lambda_{23} \\ \Lambda_{31} & \Lambda_{32} & Q + \Lambda_{33} \end{pmatrix}. \tag{2.22}$$

Important applications of MMMPs are in ion-channel current modeling (see Section 11.1) and phylogenetics [48, 18, 85].

2.2.4 Batch Markovian Arrival Process (BMAP)

The BMAP is a rather general and very useful model for arrival processes in queuing theory [71, 72]. The BMAP generalizes several other models including the MMPP. It is a bivariate Markov chain for which the underlying process S is a finite-state, homogeneous, irreducible Markov chain, and the observable chain X is a counting process. The observable chain X assumes its values in $\mathbb{X} = \{0, 1, \ldots\}$. This model allows for batch arrivals. That is, it allows transitions of X from any non-negative integer a to any integer in $\{a, a + 1, \ldots, a + d - 1\}$. In contrast, the Poisson process, or the observable process of the MMPP, allow at most one arrival at each time instant, i.e., $d = 2$. The generator

of a BMAP is an infinite block Toeplitz matrix given by

$$G = \begin{pmatrix} A_0 & A_1 & A_2 & \dots & A_{d-1} & & \\ & A_0 & A_1 & A_2 & \dots & A_{d-1} & \\ & & A_0 & A_1 & A_2 & \dots & \ddots \\ & & & A_0 & A_1 & A_2 & \ddots \\ & & & & \ddots & \ddots & \ddots \\ & & & & & \ddots & \ddots \end{pmatrix} \tag{2.23}$$

where $\{A_a\}$ are $r \times r$ matrices such that the off-diagonal elements of A_0 are non-negative, the main diagonal elements of A_0 are non-positive, $A_a > 0$ for $a = 1, \dots, d-1$, and each row of G sums up to zero. The generator of the underlying Markov chain S is given by $Q = \sum_{a=0}^{d-1} A_a$. The observable counting process and the underlying Markov chain may jump simultaneously. Thus, an underlying state transition may or may not be associated with a batch arrival. Like the MMPP, this process may also be represented as a finite-state bivariate Markov chain when counts are modulo-d.

Being a bivariate Markov chain, the inter-arrival times for a BMAP are correlated, their distributions are non-exponential, and the batch sizes are correlated. The non-exponential inter-arrival time property is shared by the MMPP and the MMMP, and will be discussed in greater detail in Section 3.6. When $d = 2$, the BMAP becomes the Markovian arrival process (MAP). The Poisson process and the MMPP are particular MAPs and hence particular BMAPs. The versatile Markovian point process of Neuts is also a BMAP [81]. Many other arrival processes are special cases of BMAP. A complete list of such processes may be found in [72].

2.3 Relations Among Models

In this section we outline some relationships among the various models presented so far [71]. We list the processes according to their classes as defined in Section 1.

As we have already pointed out, a hidden Markov model is a discrete-time bivariate Markov process, with possibly uncountably

infinite alphabet. The converse relation does not always hold. A discrete-time bivariate Markov chain does not always have a hidden Markov model representation for two reasons. First, the random variables representing the observable process of the bivariate Markov chain may be conditionally dependent, rather than conditionally independent as in the hidden Markov model, given the underlying process. Second, the underlying process of a bivariate Markov chain need not be Markov. When the underlying chain is Markov, then a discrete-time bivariate Markov process may be represented as a switching autoregressive process, see, e.g., [40, Section IV.B.3]. Switching autoregressive processes generalize hidden Markov models since they allow conditional dependence of the observable random variables given the underlying Markov chain.

For the class of continuous-time bivariate Markov chains, we have seen that every aggregated Markov chain has a bivariate chain representation. Conversely, a function of a bivariate Markov chain is trivially an aggregated Markov chain. By definition, the Poisson process is a particular MMPP, the MMPP is a particular MAP, and the MAP is a particular BMAP. The MMPP is also a particular MMMP.

2.4 Parametrization

The parameter of a bivariate Markov chain comprises the initial distribution of chain, and either the set of independent entries of its generator G in the continuous-time case, or the set of independent entries of its transition matrix in the discrete-time case. When the stationary distribution is used, then this distribution can be excluded from the parameter of the bivariate Markov chain, since it is a function of either the generator or the transition matrix of the process. The maximum number of independent entries of G is $dr(dr-1)$. That number is smaller for particular bivariate Markov chains, for example, in the form of an MMPP or a MAP, due to their doubly symmetrical generators. For MMPPs it is at most r^2, and for MAPs it is at most $2r^2 - r$. In such cases, we may view G as a function of some parameter $\phi \in \Phi$ where Φ is the parameter set. For example, ϕ may comprise the set of independent values of G. Throughout this paper we denote the parameter of the

bivariate Markov chain by $\phi \in \Phi$, the associated probability measure by P_ϕ, an associated density by $p_\phi(\cdot)$, and an expected value w.r.t. P_ϕ by $E_\phi\{\cdot\}$.

2.5 An Auxiliary Result

In this section we present a result from matrix theory, due to Van Loan [110], which has proven extremely useful in recursive estimation of the statistics and parameter of a bivariate Markov chain. These topics are discussed in Sections 4 and 5, and 7, respectively. Van Loan's result provides an efficient way to evaluate an integral involving matrix exponentials, from a related larger matrix exponential, without any numerical integration. Specifically, it was shown in [110, Theorem 1] that if

$$C = \begin{pmatrix} A_1 & B_1 \\ \mathbf{0} & A_2 \end{pmatrix}, \tag{2.24}$$

where A_1, A_2 and B_1 are matrices of appropriate dimensions, and

$$e^{Ct} = \begin{pmatrix} \tilde{A}_1 & \tilde{B}_1 \\ \mathbf{0} & \tilde{A}_2 \end{pmatrix}, \quad t \geq 0, \tag{2.25}$$

then, for $i = 1,2$, $\tilde{A}_i = e^{A_i t}$, and

$$\tilde{B}_1 = \int_0^t e^{A_1(t-s)} B_1 e^{A_2 s} ds. \tag{2.26}$$

Thus, the integral in (2.26) may be obtained from evaluation of the matrix exponential in (2.25). The matrix exponential is usually calculated using Padé approximation which requires on the order of r^3 operations for a matrix of order r [79]. This approach for evaluating the integral in (2.26) is significantly faster than attempting to evaluate that integral using numeric integration.

3

Likelihood Function of Observable Process

In this section we study the likelihood function of the observable process of a continuous-time bivariate Markov chain and some of its properties. The likelihood function plays a central role in maximum likelihood estimation of the parameter of the bivariate Markov chain. The expression for the likelihood function follows from the Markov renewal property of the bivariate Markov chain. We focus on that property as it applies to jumps of the observable process rather than to jumps of the bivariate Markov chain as in Section 2.1.4.

3.1 Markov Renewal Property

Consider a bivariate Markov chain $Z = \{Z(t), t \geq 0\}$, and suppose that the arbitrary time origin at $t = 0$ coincides with a jump of the observable process X. This technical assumption is necessary to guarantee that the first positive sojourn time of the observable process is distributed like any other sojourn time of that process. For $k = 0, 1, 2, \ldots$, let T^k denote the time of the $k+1$st jump of X. Let $X_k = X(T^k)$, $S_k = S(T^k)$, and $Z_k = (X_k, S_k)$. For $k = 1, 2, \ldots$, let $T_k = T^k - T^{k-1}$ denote the sojourn time of X in state X_{k-1}. Let $T_0 = 0$. We denote

by t^k, t_k and z_k realizations of T^k, T_k and Z_k, respectively. Note that $\{T^k, T_k\}$ defined here for the jump points of X, differ from the corresponding random variables $\{\tau_k, \Delta\tau_k\}$ defined in Section 2.1.2 for the jump points of Z.

The jump points of X constitute a subset of the jump points of Z, and hence are stopping times w.r.t. the sigma-field generated by Z. Since the bivariate Markov chain is a Markov jump process, it is strong Markov, see Section 2.1.4. Consequently, the Markov property applies to the jump points of X, and we have for $k = 1, 2, \ldots$,

$$P_\phi(T_k \le t, Z_k = z_k \,|\, T_{k-1} = t_{k-1}, Z_{k-1} = z_{k-1}, \ldots, T_1 = t_1, \\ Z_1 = z_1, Z_0 = z_0) = P_\phi(T_k \le t, Z_k = z_k \,|\, Z_{k-1} = z_{k-1}). \tag{3.1}$$

This is the Markov renewal property, which shows that $\{(T_k, Z_k)\}_{k=0}^{\infty}$ forms a *Markov renewal process*, with transition probability given by the rhs of (3.1). We denote the corresponding density, obtained by differentiating the rhs of (3.1) w.r.t. t, by $p_\phi(t_k, z_k \,|\, z_{k-1})$.

From the chain rule for densities, (3.1) implies that,

$$p_\phi(z_0, t_1, z_1, \ldots, t_n, z_n) = p_\phi(z_0) \prod_{k=1}^{n} p_\phi(t_k, z_k \,|\, z_{k-1}). \tag{3.2}$$

Hence,

$$p_\phi(z_0, z_1, \ldots, z_n) = p_\phi(z_0) \prod_{k=1}^{n} p_\phi(z_k \,|\, z_{k-1}), \tag{3.3}$$

which shows that the sequence of random variables $\{Z_k\}$ forms a discrete-time Markov chain. The transition probability of $\{Z_k\}$ is given by $P_\phi(T_1 \le \infty, Z_1 = z_1 \,|\, Z_0 = z_0)$. As a discrete-time Markov chain, it is also strong Markov [15, Proposition 7.8]. Furthermore, (3.2)–(3.3) imply that

$$p_\phi(t_1, \ldots, t_n \,|\, z_0, z_1, \ldots, z_n) = \prod_{k=1}^{n} p_\phi(t_k \,|\, z_k, z_{k-1}). \tag{3.4}$$

Thus, successive sojourn times $\{T_k\}$ are conditionally independent random variables given the sequence of states $\{Z_k\}$. The distribution of

each T_k depends on Z_{k-1} as well as on Z_k. Note that the Markov chain $\{Z_k\}$, together with the sequence of conditionally independent random variables $\{T_k\}$ given $\{Z_k\}$, do not define a hidden Markov model, since $\{Z_k\}$ is not an underlying process. An exception is given by the MMPP, since for that bivariate Markov chain, $\{X_k\}$ can be inferred from $\{T_k\}$, and $\{S_k\}$ is Markov [13]. We discuss this aspect of the MMPP in further detail in Section 7. The Markov renewal process $\{(T_k, Z_k)\}$ may be envisioned as follows. Starting with an initial state $z_0 \in \mathbb{Z}$, the next state z_1 is chosen according to the transition probability of $\{Z_k\}$, and the process resides in z_0 for a duration T_1 that depends on (z_0, z_1). Then a new state z_2 is chosen, and the process resides in z_1 for a duration T_2 that depends on (z_1, z_2), and so on.

It can be shown that the sequence of successive epoch times $\{T^k\}$ in which a fixed state $a \in \mathbb{X}$ is visited is a *renewal* process [25, Proposition 1.11]. The inter-arrival times of a renewal process are independent identically distributed (iid) random variables.

By homogeneity of the bivariate Markov chain, $P_\phi(T_k \le t, Z_k = z_k \,|\, Z_{k-1} = z_{k-1})$ is independent of k. Hence, assuming $k = 1$, $z_0 = (a, i)$, and $z_1 = (b, j)$, for any states (a, i) and (b, j) in $\mathbb{Z}$ such that $a \neq b$, the transition probability is given by

$$P_\phi(T_1 \le t, Z_1 = (b, j) \,|\, Z_0 = (a, i)). \tag{3.5}$$

The process $\{X(t), t \ge 0\}$, with its staircase sample paths such that $X(t) = X_k$ for $T^k \le t < T^{k+1}$, is a *semi-Markov process*, with state space $\mathbb{X}$, and *semi-Markov kernel* given by the family of transition probabilities of the form in (3.5) for all (a, i) and (b, j) in $\mathbb{Z}$ and $t \ge 0$ [25, Eq. 1.13].

The likelihood function of a sample path of the observable process follows from (3.2) and is given by

$$\begin{aligned} p(x(\tau), \tau \in [0, t^n]) &= p_\phi(x_0, t_1, x_1, \ldots, t_n, x_n) \\ &= \sum_{s_0, \ldots, s_n} p_\phi(z_0) \prod_{k=1}^{n} p_\phi(t_k, z_k \,|\, z_{k-1}). \end{aligned} \tag{3.6}$$

This density can be efficiently evaluated using the notion of a transition density matrix which is introduced in Section 3.2. A recursion

for evaluating Eq. (3.6) is detailed in Section 3.4. It will be shown in Section 3.6, that T_k given X_{k-1} has a continuous phase-type distribution. The family of continuous phase-type distributions is very rich, and it includes the distributions of sums of iid exponential random variables, and mixtures of exponential distributions.

3.2 Transition Density Matrices

Let $f_{ij}^{ab}(t;\phi)$ denote the density obtained from differentiation of (3.5) w.r.t. t. In this section we evaluate this density, and provide a compact form for the $r \times r$ *transition density matrix* defined by

$$f^{ab}(t;\phi) = \{f_{ij}^{ab}(t;\phi); i,j = 1,\dots r\}. \tag{3.7}$$

The density $f_{ij}^{ab}(t;\phi)$ satisfies a *Markov renewal equation*. This is an integral equation, involving the semi-Markov kernel, which has a unique solution [25].

To evaluate the density $f_{ij}^{ab}(t;\phi)$, note that the first transition of X from state a at time zero to state b at time t, while $S(0) = i$ and $S(t) = j$, may occur along two routes. First, the bivariate Markov chain may stay in (a,i) in $[0,t)$ and then jump to (b,j) at time t. Alternatively, the chain may stay in (a,i) during $[0,\tau)$ for some $\tau \le t$, jump at τ to an intermediate state (a,l), and then transit, possibly through several other intermediate states of S, from (a,l) to (b,j) during $[\tau,t]$. This leads to the following Markov renewal equation [76]:

$$\begin{aligned} f_{ij}^{ab}(t;\phi) = {} & \left[g_a(i)e^{-g_a(i)t}\right]\frac{g_{ab}(ij)}{g_a(i)} \\ & + \int_0^t \left[g_a(i)e^{-g_a(i)\tau}\right]\sum_{l\neq i}\frac{g_{aa}(il)}{g_a(i)} f_{lj}^{ab}(t-\tau)d\tau, \end{aligned} \tag{3.8}$$

where $g_a(i) = -g_{aa}(ii) > 0$. Differentiating (3.8) w.r.t. t, and solving the resulting differential equation, yield [27, 87, 76],

$$f^{ab}(t;\phi) = e^{G_{aa}t}G_{ab}, \quad a \neq b, \quad t \ge 0. \tag{3.9}$$

A related useful transition probability is defined as

$$\bar{F}_{ij}^{a}(t;\phi) = P_\phi(T_1 > t, S(t) = j \,|\, Z_0 = (a,i)). \tag{3.10}$$

This is the probability that the underlying chain transits from state i to state j in time t, while the observable chain remains in state a past time t. Using a similar Markov renewal equation, it can be shown that the transition matrix

$$\bar{F}^a(t;\phi) = \{\bar{F}^a_{ij}(t;\phi); i,j = 1,\dots r\} \tag{3.11}$$

satisfies [27, 87, 76],

$$\bar{F}^a(t;\phi) = e^{G_{aa}t}, \quad t \geq 0. \tag{3.12}$$

Properties of G_{aa} and of $e^{G_{aa}t}$ were given in Section 2.1.6.

3.3 Likelihood Function

Let $\nu_{a,i}(\phi) = P_\phi(Z_0 = (a,i))$, and define

$$\begin{aligned} \nu_a(\phi) &= (\nu_{a,1}(\phi), \nu_{a,2}(\phi), \dots, \nu_{a,r}(\phi)) \\ \nu(\phi) &= (\nu_1(\phi), \dots, \nu_d(\phi)). \end{aligned} \tag{3.13}$$

The row vector $\nu(\phi)$ represents the initial distribution of the bivariate Markov chain. The likelihood of the observable process follows from $\nu_{x_0}(\phi)$ in (3.13), from the density (3.6), and by using the definition of the transition density matrix (3.7). This likelihood can be expressed compactly as [27, 44]

$$p_\phi(x(\tau), \tau \in [0, t^n]) = \nu_{x_0}(\phi) \left\{ \prod_{l=1}^{n} f^{x_{l-1}x_l}(t_l;\phi) \right\} \mathbf{1} \tag{3.14}$$

where $\mathbf{1}$ denotes a column vector of all ones. Note that the product of transition density matrices, along with the pre and post vector multiplications, eliminate the dependency on the states $\{S_k\}$ of the underlying process, and thus provides the likelihood of the observable process. The likelihood function of $\{x(\tau), \tau \in [0,T]\}$, when T does not necessarily correspond to a jump of the observable process, i.e., $t^n < T < t^{n+1}$ for some n, is given by

$$\begin{aligned} &p_\phi(x(\tau), \tau \in [0,T]) \\ &\quad = \nu_{x_0}(\phi) \left\{ \prod_{l=1}^{n} f^{x_{l-1}x_l}(t_l;\phi) \right\} \bar{F}^{x_n}(T - t^n;\phi)\mathbf{1} \end{aligned} \tag{3.15}$$

where $\bar{F}^{x_n}(T - t^n;\phi)$ is given in (3.12).

3.4 Forward-Backward Recursions

The form of the likelihood function in (3.14) suggests that it can be evaluated recursively. In this section, we present forward-backward recursions, which follow from the Markov renewal property of the bivariate Markov chain, as presented in Section 3.1. We need only the forward recursion to evaluate the likelihood function. Both the forward and backward recursions, however, will be needed in subsequent sections, and will be used for recursive estimation of various statistics of the bivariate Markov chain. The forward-backward recursions in this section are defined similarly to the forward-backward recursions for the hidden Markov model, see, e.g., [40, Section V-A].

Application of the strong Markov property to $\{(T_k, Z_k)\}$ implies that

$$\begin{aligned} &p_\phi(z_0, t_1, z_1, \ldots, t_k, z_k, \ldots, t_n, z_n) \\ &\quad = p_\phi(z_0, t_1, z_1, \ldots, t_{k-1}, z_{k-1}) p_\phi(t_k, z_k, \ldots, t_n, z_n \,|\, z_{k-1}). \end{aligned} \tag{3.16}$$

Summing both sides over all states of the underlying chain gives

$$\begin{aligned} &p_\phi(x_0, t_1, x_1, \ldots, t_k, x_k, \ldots, t_n, x_n) \\ &\quad = \sum_{s_{k-1}} p_\phi(x_0, t_1, x_1, \ldots, t_{k-1}, z_{k-1}) p_\phi(t_k, x_k, \ldots, t_n, x_n \,|\, z_{k-1}) \end{aligned} \tag{3.17}$$

The first term of the summand is identified as the *forward density*, and is denoted as

$$L_i(k-1;\phi) = p_\phi(x_0, t_1, x_1, \ldots, t_{k-1}, x_{k-1}, S_{k-1} = i). \tag{3.18}$$

The second term of the summand is identified as the *backward density*, and is denoted as

$$R_i(k;\phi) = p_\phi(t_k, x_k, \ldots, t_n, x_n \,|\, x_{k-1}, S_{k-1} = i). \tag{3.19}$$

Define the row vector $L(k-1;\phi) = (L_1(k-1;\phi), \ldots, L_r(k-1;\phi))$. From (3.13), $L(0;\phi) = \nu_{x_0}(\phi)$. From (3.14), for $k = 1, \ldots, n$, we have the following *forward recursion*:

$$\begin{aligned} L(k;\phi) &= \nu_{x_0}(\phi) \prod_{l=1}^{k} f^{x_{l-1}x_l}(t_l;\phi) \\ &= L(k-1;\phi) f^{x_{k-1}x_k}(t_k;\phi). \end{aligned} \tag{3.20}$$

Next, define the column vector $R(k;\phi) = \text{col}\{R_1(k;\phi),\ldots,R_r(k;\phi)\}$, with $R(n+1;\phi) = \mathbf{1}$. From (3.14), we have for $k = n, n-1,\ldots,1$, the following *backward recursion*:

$$\begin{aligned} R(k;\phi) &= \prod_{l=k}^{n} f^{x_{l-1}x_l}(t_l;\phi)\mathbf{1} \\ &= f^{x_{k-1}x_k}(t_k;\phi)R(k+1;\phi). \end{aligned} \tag{3.21}$$

Now, from (3.17), if $S_{k-1} = i$, then for any $k = 1,\ldots,n$,

$$\begin{aligned} &p_\phi(x_0,t_1,x_1,\ldots,t_{k-1},x_{k-1},i,t_k,x_k,\ldots,t_n,x_n) \\ &\quad = L_i(k-1;\phi)R_i(k;\phi). \end{aligned} \tag{3.22}$$

Summing both sides of (3.22) over i gives the likelihood function in (3.14) as follows:

$$p_\phi(x(\tau),\tau\in[0,t^n]) = L(k-1;\phi)R(k;\phi). \tag{3.23}$$

When $k = n+1$, this likelihood is given by $L(n;\phi)\mathbf{1}$.

The forward and backward recursions require recursive scaling to improve their numerical stability [87]. The scaled forward recursion is given by

$$\begin{aligned} \tilde{L}(0;\phi) &= \frac{\nu_{x_0}(\phi)}{c_0}, \\ \tilde{L}(k;\phi) &= \frac{\tilde{L}(k-1;\phi)f^{x_{k-1}x_k}(t_k;\phi)}{c_k} \end{aligned} \tag{3.24}$$

where

$$\begin{aligned} c_0 &= \nu_{x_0}(\phi)\mathbf{1} \\ c_k &= \tilde{L}(k-1;\phi)f^{x_{k-1}x_k}(t_k;\phi)\mathbf{1}, \quad k = 1,2,\ldots,n. \end{aligned} \tag{3.25}$$

The scaled backward recursion is given by

$$\begin{aligned} \tilde{R}(n+1;\phi) &= \mathbf{1} \\ \tilde{R}(k;\phi) &= \frac{f^{x_{k-1}x_k}(t_k;\phi)\tilde{R}(k+1;\phi)}{c_k} \end{aligned} \tag{3.26}$$

where $k = n, n-1,\ldots,1$.

The scaled and unscaled recursions are related by

$$\begin{aligned}\tilde{L}(k;\phi) &= \frac{L(k;\phi)}{\prod_{l=0}^{k} c_l}, \quad k = 0,1,\ldots,n \\ \tilde{R}(k;\phi) &= \frac{R(k;\phi)}{\prod_{l=k}^{n} c_l}, \quad k = 1,2,\ldots,n. \end{aligned} \tag{3.27}$$

The scale factors can be interpreted as conditional densities. Define $Y_0 = X_0$, and for $k = 1,2,\ldots$, define $Y_k = (T_k, X_k)$. The sequence $\{Y_0, Y_1, \ldots, Y_n, \ldots\}$ constitutes the observable process of the bivariate Markov chain. It follows from (3.20)-(3.21) and (3.24)-(3.25), that $c_0 = p_\phi(y_0)$, and for $k = 1,2,\ldots,n$

$$c_k = p_\phi(y_k \,|\, y_{k-1}, y_{k-2}, \ldots, y_0). \tag{3.28}$$

Hence, the likelihood of the observable process is given by

$$p_\phi(x(\tau), \tau \in [0, t^n]) = c_0 \prod_{k=1}^{n} c_k, \tag{3.29}$$

and from (3.23), $\tilde{L}(k-1;\phi)\tilde{R}(k;\phi) = 1$ for $k = 1,\ldots,n$. Finally, we note that the ith component of the scaled forward density equals the conditional probability $P_\phi(S_k = i \,|\, x(\tau), \tau \in [0, t^k])$. The scaled backward density does not enjoy such an intuitive interpretation.

3.5 Sampled Bivariate Markov Chain

The sequence $\{Z_k, k = 0,1,\ldots\}$, obtained from sampling the bivariate Markov chain Z at the jump points of the observable process X, is referred to as the *sampled bivariate Markov chain*. Properties of $\{Z_k\}$ were established in [39]. From (3.5) and (3.9), the transition probability of the sampled bivariate Markov chain is given by

$$\begin{aligned} P_\phi(Z_k = (b,j) \,|\, Z_{k-1} = (a,i)) &= \left[\int_0^\infty e^{G_{aa}t} G_{ab} dt\right]_{ij} \\ &= [-G_{aa}^{-1} G_{ab}]_{ij}. \end{aligned} \tag{3.30}$$

The matrix $-G_{aa}^{-1} > 0$, since $e^{G_{aa}t} > 0$ [39, Corollary 1]. The transition matrix of the sampled bivariate Markov chain is given by the block

matrix $D = \{D_{ab}, a, b = 1, \ldots, d\}$, where

$$D_{ab} = \begin{cases} -G_{aa}^{-1} G_{ab}, & b \neq a \\ \mathbf{0}, & b = a. \end{cases} \tag{3.31}$$

The sampled bivariate Markov chain has one closed set of recurrent, possibly periodic, states, while the remaining states are transient. A state (b, j) is recurrent if and only if it corresponds to a non-zero column of G_{ab} for some $a \neq b$ [39, Lemma 3]. When X has two states, as is the case with the MMPP and the MAP, the recurrent states are always periodic.

The transition matrix D has a unique stationary distribution with zero entries for its transient states. The initial distribution $\nu(\phi)$ is the stationary distribution of the bivariate Markov chain if and only if it satisfies $\nu(\phi) = \nu(\phi)D$. The sampled bivariate Markov chain is stationary if and only if its initial distribution is the stationary distribution.

We have so far encountered two stationary distributions for the bivariate Markov chain. The first was introduced in Section 2.1 as the distribution π which satisfies $\pi(\phi)G = \mathbf{0}$. The second was introduced in the previous paragraph as the distribution ν which satisfies $\nu(\phi) = \nu(\phi)D$. Which distribution should be used to guarantee stationarity of the bivariate Markov chain depends on the setup of the problem. Using $\nu(\phi)$ requires that $t = 0$ coincides with a jump of the observable process, and it guarantees stationarity of the observable process. This mode of stationarity was termed *interval stationarity* in [43]. Using π guarantees stationarity of $\{Z(t), t \geq 0\}$, and $t = 0$ need not correspond to a jump of the observable process. This mode of stationarity was termed *environment stationarity* in [43]. The two stationary distributions are related to each other as follows [43, 76],

$$\nu(\phi) \propto \pi(\phi)\mathrm{diag}(G_{11}, \ldots, G_{dd}). \tag{3.32}$$

3.6 Phase-Type Distributions

This section is concerned with the distribution of the sojourn time of the observable process in any of its states. By homogeneity, this is the

distribution of T_1 given X_0. The density of this distribution is given by,

$$p_\phi(t_1 \,|\, x_0) = \sum_{s_0} \sum_{z_1 : x_1 \neq x_0} p_\phi(t_1, z_1 \,|\, z_0) p_\phi(s_0 \,|\, x_0), \tag{3.33}$$

and it can be obtained from the transition density matrix in (3.9), and the initial distribution in (3.13). Following this approach we have for any $a \in \mathbb{X}$ [27, 87, 76],

$$p_\phi(t \,|\, a) = -\bar{\nu}_a e^{G_{aa} t} G_{aa} \mathbf{1} \tag{3.34}$$

where $\bar{\nu}_a = \nu_a / (\nu_a \mathbf{1})$. This is a continuous phase-type density with r phases and parameter $(\bar{\nu}_a, G_{aa})$.

In this section we focus on continuous phase-type distributions. We shall discuss the analogous discrete phase-type distributions in Section 8.1. Phase-type distributions were introduced by Neuts [82]. The family of continuous phase-type distributions is very rich, and it includes, as particular cases, the Erlang distribution and the hyper-exponential distribution. The Erlang distribution is the distribution of a sum of iid exponential random variables. The hyper-exponential distribution is a mixture of exponential distributions. The set of continuous phase-type distributions is dense in the set of distributions on $[0, \infty)$, see, e.g., [2, Theorem 4.2], [119, Theorem 5.2]. Thus, any continuous distribution on $[0, \infty)$ can be approximated arbitrarily well by continuous phase-type distributions. Continuous phase-type distributions represent a significant departure from the exponential sojourn time distribution characteristics of a Markov chain. Thus, such phase-type distributions may be used where the exponential distribution is inadequate. By symmetry, we may conclude that the distribution of the sojourn time of the underlying process in each of its states is also continuous phase-type.

A phase-type distribution is the distribution of the hitting time of a single absorbing state of a Markov chain, where all of its remaining states are transient. The generator of such a Markov chain, with say m transient states, and one absorbing state, is given by

$$G = \left(\begin{array}{c|c} A & \boldsymbol{\varepsilon} \\ \hline \mathbf{0} & 0 \end{array} \right) \tag{3.35}$$

where $A = \{a_{ij}\}$ is an $m \times m$ matrix with $a_{ii} < 0$ and $a_{ij} \geq 0$ when $i \neq j$, and $\boldsymbol{\varepsilon}$ is an $m \times 1$ non-zero vector with non-negative components such that $A\mathbf{1} + \boldsymbol{\varepsilon} = \mathbf{0}$. This chain may be viewed as a bivariate Markov chain with two observable states, say $\{a, b\}$, such that a is associated with the $r_a = m$ transient states of the underlying chain, and b is associated with the $r_b = 1$ absorbing state of the underlying chain. In this bivariate Markov chain, the states $\{(a, i), i = 1, \ldots, m\}$ are transient, and state $(b, 1)$ is absorbing. This bivariate Markov chain has a single non-zero transition density matrix from the transient states to the absorbing state. From (3.9), this transition density matrix is given by,

$$f^{ab}(t; \phi) = e^{At}\boldsymbol{\varepsilon} \tag{3.36}$$

for $t \geq 0$. Recall that this transition density matrix corresponds to

$$P_\phi(T_1 \leq t, Z(t) = (b, 1) \,|\, Z(0) = (a, i)), \quad \text{for } i = 1, \ldots, m. \tag{3.37}$$

When the initial state of the bivariate Markov chain is the absorbing state $(b, 1)$, then

$$P_\phi(T_1 \leq t, Z(t) = (b, 1) \,|\, Z(0) = (b, 1)) = 1 \tag{3.38}$$

for all $t \geq 0$, and the corresponding density is the Dirac function $\delta(t)$. Let $(\boldsymbol{\rho}, \rho_{m+1})$ denote the initial distribution of the bivariate Markov chain, where $\boldsymbol{\rho}$ is an $1 \times m$ vector. The density of the sojourn time T_1 to absorption is then given by

$$p_\phi(t) = \rho_{m+1}\delta(t) - \boldsymbol{\rho}e^{At}A\mathbf{1}. \tag{3.39}$$

This is the *continuous phase-type density* with parameter $(\boldsymbol{\rho}, A)$ as was originally introduced by Neuts [82]. Note that the stationary distribution of (3.35) is given by $(\mathbf{0}, 1)$, and $p_\phi(t) = \delta(t)$ when the chain is initialized by its stationary distribution.

For a regular bivariate Markov chain (see Section 2.1), the sojourn time at any state is positive almost surely, and hence (3.34) does not contain the Dirac function.

4

Recursive Non-Causal Estimation

In this section, we present recursions for non-causal conditional mean estimation of several statistics of a continuous-time bivariate Markov chain given a sample path $\{x(\tau), \tau \in [0,T]\}$ of the observable process. In particular, we are interested in estimation of the following statistics:

(i) A function $u(\cdot)$ of the state $S(t)$ of the underlying chain for $t \in [0,T]$.
(ii) The number of jumps of the bivariate Markov chain Z, from one state to another, in the given interval $[0,T]$.
(iii) The total sojourn time of the bivariate Markov chain Z, in each of its states, in the given interval $[0,T]$.

We denote by $M_{ij}^{ab}(T)$ the number of jumps of Z from state (a,i) to state (b,j) in $[0,T]$, and by $D_i^a(T)$ the total sojourn time of Z in state (a,i) during $[0,T]$. Conditional mean estimation is performed under the assumption that the true parameter of the bivariate Markov chain is known, and is assumed to be given by ϕ. The conditional mean estimates are given by

$$\hat{u}(S(t)) = E_\phi\{u(S(t)) \,|\, x(\tau), \tau \in [0,T]\} \tag{4.1}$$

$$\hat{M}_{ij}^{ab}(T) = E_\phi\{M_{ij}^{ab}(T)\,|\,x(\tau), \tau \in [0,T]\} \tag{4.2}$$

$$\hat{D}_{i}^{a}(T) = E_\phi\left\{D_{i}^{a}(T)\,|\,x(\tau), \tau \in [0,T]\right\}. \tag{4.3}$$

The general approach to recursive estimation of these statistics was established by Rydén in [95]. In this approach, the conditional density required to evaluate each estimate was obtained using Bayes' rule and the densities associated with the Markov renewal process $\{T_k, Z_k\}$ from Section 3. We demonstrate the approach for estimating a function of the state $S(t)$ in Section 4.1. The approach requires forward and backward recursions, and hence it is a non-causal estimation approach. We will discuss causal estimation of the same statistics in Section 5. We begin with non-causal estimation since it requires less computational effort. It is convenient to update these recursions from one jump point of X to the next jump point in the forward mode, and from a jump point of X to the previous jump point in the backward mode. Hence, we assume that T coincides with a jump point of X, that is, $T = t^n$ for some integer n (see Section 3.1).

The approach was originally applied to MMPPs in [95], and then to BMAPs in [17, 60]. The approach was subsequently supplemented by Van Loan's result (see Section 2.5) in [90], which provided a convenient and efficient way to implement the required integrals of matrix exponentials. These ideas were applied to MMMPs in [41], and to general bivariate Markov chains in [76].

4.1 State Estimation

Suppose that $u(S(t)) = u_i$ when $S(t) = i$. The conditional mean estimate of $u(S(t))$ is given by

$$\hat{u}(S(t)) = \sum_{i=1}^{r} u_i \; P_\phi(S(t) = i\,|\,x(\tau), \tau \in [0,t^n]). \tag{4.4}$$

The conditional probability in (4.4) follows from the conditional probability $P_\phi(Z(t) = (a,i)\,|\,x(\tau), \tau \in [0,t^n])$ which was derived in [76, Proposition 5]. Suppose that $t^k \le t < t^{k+1}$ for some $k \in \{0,1,\ldots,n-1\}$, and that $X_k = a$. Let $\mathbf{1}_i$ denotes a column vector with a one in its ith component and zeros elsewhere. Let $'$ denote a matrix transpose. Using

Bayes' rule, (3.20), (3.11), (3.21), (3.29), (3.24), and (3.26), in that order, we obtain

$$\begin{aligned}
&P_\phi(Z(t) = (a,i) \,|\, x(\tau), \tau \in [0,t^n]) \\
&\quad = \frac{p_\phi(z(t) = (a,i), x_0, t_1, x_1, \ldots, t_n, x_n)}{p_\phi(x_0, t_1, x_1, \ldots, t_n, x_n)} \\
&\quad = \frac{\left\{\nu_{x_0} \prod_{l=1}^{k} f^{x_{l-1}x_l}(t_l;\phi)\right\} \cdot \bar{F}^{x_k}(t - t^k;\phi)\mathbf{1}_i\mathbf{1}_i'}{p_\phi(x_0, t_1, x_1, \ldots, t_n, x_n)} \\
&\qquad \cdot f^{x_k x_{k+1}}(t^{k+1} - t;\phi) \prod_{l=k+2}^{n} f^{x_{l-1}x_l}(t_l;\phi)\mathbf{1} \\
&\quad = \frac{L(k;\phi)\bar{F}^{x_k}(t - t^k;\phi)\mathbf{1}_i\mathbf{1}_i'}{p_\phi(x_0, t_1, x_1, \ldots, t_n, x_n)} f^{x_k x_{k+1}}(t^{k+1} - t;\phi)R(k+2;\phi) \\
&\quad = \frac{1}{c_{k+1}}\Big[f^{x_k x_{k+1}}(t^{k+1} - t;\phi)\tilde{R}(k+2;\phi)\tilde{L}(k;\phi)\bar{F}^{x_k}(t - t^k;\phi)\Big]_{i,i}.
\end{aligned} \tag{4.5}$$

Summing the expression in (4.5) over all $x_k = a \in \mathbb{X}$, and substituting the result into (4.4), yield the desired conditional mean estimate of $u(S(t))$.

4.2 Number of Jumps

The number of jumps of the bivariate Markov chain can be conveniently expressed in terms of the indicator function

$$\varphi_{ai}(t) = \begin{cases} 1, & Z(t) = (a,i) \\ 0, & \text{otherwise.} \end{cases} \tag{4.6}$$

The number of jumps from state (a,i) to state (b,j) in $[0,t^n]$ is given by

$$M_{ij}^{ab}(t^n) = \sum_{0 \le t \le t^n} \varphi_{ai}(t-)\varphi_{bj}(t), \tag{4.7}$$

where the sum is over the jump points of Z in $[0,t^n]$. A jump of the bivariate Markov chain occurs when either the underlying chain S jumps alone, or when the observable chain X jumps, possibly, simultaneously with S. We treat each of these two scenarios separately.

In the first scenario, $i \neq j$ while $a = b$. For this case, application of a limit process to (4.7) [1, 3], shows that the conditional mean estimate of $M_{ij}^{aa}(t^n)$ given $\{x(\tau), \tau \in [0, t^n]\}$ can be written as

$$\hat{M}_{ij}^{aa}(t^n) = \int_0^{t^n} P_\phi(Z(t-) = (a,i), Z(t) = (a,j) \,|\, x(\tau), \tau \in [0,t^n])dt. \tag{4.8}$$

The conditional probability in (4.8) can be developed along the same lines as in (4.5). Once this conditional probability is obtained, the integral is evaluated using Van Loan's result from Section 2.5. This yields the following estimate [76, Proposition 3]:

$$\hat{M}_{ij}^{aa}(t^n) = \left[G_{aa} \circ \sum_{k:x_k=a} \frac{\mathcal{I}_k'}{c_{k+1}} \right]_{ij} \tag{4.9}$$

where $k \in \{0, 1, \ldots, n-1\}$, the symbol $\circ$ indicates the Hadamard product (or Schur product) [55, Section 7.5], i.e., the entrywise product of the two matrices, c_k is given in (3.25), and

$$\mathcal{I}_k = [e^{C_k t_{k+1}}]_{12} \tag{4.10}$$

is the upper right block of the $2r \times 2r$ matrix exponential of $C_k t_{k+1}$ where

$$C_k = \begin{bmatrix} G_{x_k x_k} & G_{x_k x_{k+1}} \tilde{R}(k+2;\phi) \tilde{L}(k;\phi) \\ \mathbf{0} & G_{x_k x_k} \end{bmatrix}. \tag{4.11}$$

In the second scenario, $a \neq b$ while i and j may, or may not, be equal. For this case, the conditional mean of (4.7) is given by

$$\hat{M}_{ij}^{ab}(t^n) = \sum_{\substack{k:x_k=a, \\ x_{k+1}=b}} P_\phi(Z(t^k-) = (a,i), Z(t^k) = (b,j) \,|\, x(\tau), \tau \in [0,t^n]), \tag{4.12}$$

where $k \in \{0, 1, \ldots, n-1\}$. Evaluating the conditional probability as before, we have [76, Proposition 4]

$$\hat{M}_{ij}^{ab}(t^n) = \left[G_{ab} \circ \sum_{\substack{k:x_k=a, \\ x_{k+1}=b}} \frac{\mathcal{J}_k'}{c_{k+1}} \right]_{ij} \tag{4.13}$$

where

$$\mathcal{J}_k = \tilde{R}(k+2;\phi)\tilde{L}(k;\phi)e^{G_{x_k x_k} t_{k+1}}. \tag{4.14}$$

4.3 Total Sojourn Time

The total sojourn time of the bivariate Markov chain in state (a,i) during $[0,t^n]$ is given by

$$D_i^a(t^n) = \int_0^{t^n} \varphi_{ai}(\tau)d\tau. \tag{4.15}$$

The conditional mean estimate of $D_i^a(t^n)$ given $\{x(\tau), \tau \in [0,t^n]\}$, is the integral of the conditional probability of $Z(t) = (a,i)$ given $\{x(\tau), \tau \in [0,t^n]\}$ which is given in (4.5). Using Van Loan's result, we obtain [76, Proposition 5]

$$\hat{D}_i^a(t^n) = \left[\sum_{k:x_k=a} \frac{\mathcal{I}'_k}{c_{k+1}}\right]_{ii} \tag{4.16}$$

where $k \in \{0,1,\ldots,n-1\}$.

4.4 Computational Load

The computational complexity of the recursions presented in this section is dominated by the number of arithmetic operations required to calculate a matrix exponential. From [79], this number is of the order of r^3. It is readily seen that evaluation of the forward recursion (3.24), or the backward recursion (3.26), requires $O(r^3)$ operations per jump of the observable chain. Evaluation of each of the recursions in this section requires a similar $O(r^3)$ operations per jump of the observable chain. Hence, the overall computational complexity of the recursions presented in this section is $O(r^3)$ operations per jump of the observable chain.

5

Recursive Causal Estimation

In this section we present recursions for causal conditional mean estimation of the state, the number of jumps, and the total sojourn time, for a continuous-time bivariate Markov chain. We assume, as in Section 4, that the true parameter of the bivariate Markov chain is known, and is given by ϕ. Causal recursions allow the estimates to be updated as the observations become available, without the need to store the entire data as was the case with the non-causal recursions in Section 4.

A recursion for the state of the bivariate Markov chain was known since the 1970's, see [123, 92] who developed such recursion using different approaches. It turns out that recursions for causal estimation of the number of jumps and the total sojourn time of the bivariate Markov chain, can be developed by adapting the approach for recursive non-causal estimation from Section 4. This was done in [75] by using two key ideas. The first idea is from [128], where the number of jumps and the state are estimated jointly. This idea is also useful in estimating the total sojourn time in a similar way. The second idea is from [105], where the backward density in (3.21) is seen as a function of n and k with a forward mode in n. The approach of [110] for evaluating integrals of matrix exponentials plays here an important role as in Section 4.

In [37], recursions for causal estimation of the same statistics were derived for the MMMP and MMPP using the transformation of measure approach. The principles of that approach are outlined in Section 9.1. That approach systematically provides forward recursions in applicable estimation problems. In that approach, all conditional mean estimates are derived under a reference probability measure that is easier to work with than the original probability measure. Specifically, under the reference measure, the underlying and observable chains, S and X, respectively, are statistically independent, and the probability law of S is the same under both measures. The original measure must be absolutely continuous w.r.t. the reference measure to guarantee the existence of the Radon-Nikodym derivative for the two measures. In [37], choosing such a reference measure was possible, since the underlying and observable chains of the MMMP do not jump simultaneously almost surely under the original measure, and also under the reference measure. For a bivariate Markov chain, the two processes may jump simultaneously under the original measure but not under the reference measure due to independence of S and X. Hence, the original measure cannot be absolutely continuous w.r.t. the reference measure, and the Radon-Nikodym derivative cannot be constructed. Thus, the transformation of measure approach could not be extended to the bivariate Markov chain. The recursions developed in [75] reduce to those developed in [37] for the MMMP and MMPP versions of the bivariate Markov chain.

5.1 State Estimation

The conditional mean estimate of the function $u(S(t))$, given $\{x(\tau), \tau \in [0,t]\}$, is given by

$$\hat{S}(t) = \sum_{i=1}^{r} u_i \; P_\phi(S(t) = i \,|\, x(\tau), \tau \in [0,t]), \tag{5.1}$$

where we have assumed, as in Section 4.1, that $u(S(t)) = u_i$ when $S(t) = i$. When $t^k \leq t < t^{k+1}$, then from (3.18) and (3.11), we have

$$P_\phi(S(t) = i \,|\, x(\tau), \tau \in [0,t]) = \frac{[L(k;\phi)\bar{F}^{x_k}(t - t^k;\phi)]_i}{L(k;\phi)\bar{F}^{x_k}(t - t^k;\phi)\mathbf{1}}. \tag{5.2}$$

5.2 Number of Jumps

In this section we detail the recursion for the causal conditional mean estimate of the number of jumps $M_{ij}^{ab}(t^k)$ given $\{x(\tau), \tau \in [0, t^k]\}$. Following the state augmentation approach of [128], this estimate is obtained from the conditional mean estimate of $M_{ij}^{ab}(t^k)\varphi_l(t^k)$ given $\{x(\tau), \tau \in [0, t^k]\}$, where $\varphi_l(t^k)$ is the state indicator function defined by

$$\varphi_l(t) = \begin{cases} 1, & S(t) = l, \\ 0, & \text{otherwise} \end{cases} \tag{5.3}$$

and $l \in \mathbb{S}$. Define the $1 \times r$ vector $\boldsymbol{M}_{ij}^{ab}(t^k)$ whose lth component is given by $M_{ij}^{ab}(t^k)\varphi_l(t^k)$. Let $\hat{\boldsymbol{M}}_{ij}^{ab}(t^k) = E_\phi\{\boldsymbol{M}_{ij}^{ab}(t^k) \,|\, x(\tau), \tau \in [0, t^k]\}$. The conditional mean estimate of $M_{ij}^{ab}(t^k)$ is obtained from $\hat{\boldsymbol{M}}_{ij}^{ab}(t^k)\mathbf{1}$.

The recursion for $\hat{\boldsymbol{M}}_{ij}^{ab}(t^k)$ is given in terms of the matrix exponential of

$$C_k^j = \begin{bmatrix} G_{x_k x_k} & \mathbf{0} \\ \tilde{L}(k)'\mathbf{1}_j' & G_{x_k x_k}' \end{bmatrix}. \tag{5.4}$$

We use $[\cdot]_{21}$ to denote the lower left block of the referenced matrix.

In estimating the number of jumps, we distinguish between two cases as was done in Section 4.2. When $i \neq j$ while $a = b$, the recursion for the number of jumps is given by [75, Proposition 1]

$$\begin{aligned} \hat{\boldsymbol{M}}_{ij}^{aa}(t^k) = \frac{1}{c_k}\{&\hat{\boldsymbol{M}}_{ij}^{aa}(t^{k-1}) e^{G_{x_{k-1}x_{k-1}} t_k} \\ &+ I(x_{k-1} = a) g_{aa}(ij) \mathbf{1}_i' [e^{C_{k-1}^j t_k}]_{21}\} G_{x_{k-1}x_k}, \end{aligned} \tag{5.5}$$

for $k \geq 1$, with the initialization $\hat{\boldsymbol{M}}_{ij}^{aa}(t_0) = \mathbf{0}$. In (5.5), $I(\cdot)$ denotes the indicator function as defined in connection with (2.12), and c_k is given in (3.25). When $a \neq b$, the recursion for the number of jumps is given by [75, Proposition 2]

$$\begin{aligned} \hat{\boldsymbol{M}}_{ij}^{ab}(t^k) = \frac{1}{c_k}\{&\hat{\boldsymbol{M}}_{ij}^{ab}(t^{k-1}) e^{G_{x_{k-1}x_{k-1}} t_k} G_{x_{k-1}x_k} \\ &+ I(x_{k-1} = a, x_k = b) g_{ab}(ij) \tilde{L}(k-1) e^{G_{x_{k-1}x_{k-1}} t_k} \mathbf{1}_i \mathbf{1}_j'\} \end{aligned} \tag{5.6}$$

for $k \geq 1$, with the initialization $\hat{\boldsymbol{M}}_{ij}^{ab}(t_0) = \mathbf{0}$.

5.3 Total Sojourn Time

The causal conditional mean estimate of $D_i^a(t^k)$ given $\{x(\tau), \tau \in [0, t^k]\}$ is obtained from the conditional mean estimate of $D_i^a(t^k)\varphi_l(t^k)$, $l \in \mathbb{S}$, given $\{x(\tau), \tau \in [0, t^k]\}$. Define the $1 \times r$ vector $\boldsymbol{D}_i^a(t^k)$ whose lth component is $D_i^a(t^k)\varphi_l(t^k)$. Let $\hat{\boldsymbol{D}}_i^a(t^k) = E_\phi\{\boldsymbol{D}_i^a(t^k) \,|\, x(\tau), \tau \in [0, t^k]\}$. The conditional mean estimate of $D_i^a(t^k)$ is obtained from $\hat{\boldsymbol{D}}_i^a(t^k)\mathbf{1}$. The forward recursion for $\hat{\boldsymbol{D}}_i^a(t^k)$ is given by [75, Proposition 2]

$$\begin{aligned}\hat{\boldsymbol{D}}_i^a(t^k) = \frac{1}{c_k}\{&\hat{\boldsymbol{D}}_i^a(t^{k-1})e^{G_{x_{k-1}x_{k-1}}t_k} \\ &+ I(x_{k-1} = a)\mathbf{1}_i'[e^{C_{k-1}^i t_k}]_{21}\}G_{x_{k-1}x_k},\end{aligned} \tag{5.7}$$

for $k \geq 1$, and with the initialization $\hat{\boldsymbol{D}}_i^a(t_0) = \mathbf{0}$.

5.4 Computational Load

The computational complexity of the forward recursion is dominated by the computation of the first term in (5.6). It requires $O(r^2d^2)$ products of a vector by a matrix which implies a computational complexity of $O(r^4d^2)$ per jump of the observable chain.

6

Maximum Likelihood Parameter Estimation

The maximum likelihood parameter estimation approach is currently the method of choice for estimating the parameter of a bivariate Markov chain. The approach is usually implemented using the EM procedure [30, 29]. This is an iterative approach in which all available data is used repeatedly to increase the likelihood of the estimated parameter. In this section, we first review the identifiability problem, and discuss asymptotic optimality of the maximum likelihood parameter estimation approach, for discrete-time and continuous-time bivariate Markov chains. We then detail the EM approach for estimating the parameter of a continuous-time bivariate Markov chain. The EM approach for estimating the parameter of a discrete-time bivariate Markov chain will be detailed in Section 8.2. We conclude this section with a short review of other non-maximum likelihood approaches that have been proposed in the literature before the area was dominated by the EM approach.

6.1 Identifiability

Two different parameters or representations of a bivariate Markov chain may lead to the same finite-dimensional distributions of the

observable process. In that case, the representations are said to be *equivalent*. This may happen, for example, when the states of the bivariate Markov chain are permuted. Equivalent representations may also exist under less obvious conditions. An equivalence class of the true parameter of the bivariate Markov chain contains all representations which produce the same finite-dimensional distributions of the observable process. A bivariate Markov chain is said to be *identifiable* if different representations lead to different finite-dimensional distributions, of some order, of the observable process. When the equivalence class of the true parameter of the bivariate Markov chain contains only representations which result from state permutation, then the process is still considered identifiable. Conditions for identifiability of continuous-time aggregated Markov chains, and hence of bivariate Markov chains (see Section 2.2.1), were given in [96, Theorem 2]. These conditions imply, for example, that an MMPP with an irreducible underlying Markov chain, and distinct Poisson rates, is identifiable. Identifiability of continuous-time (and discrete-time) aggregated Markov chains was also studied by Larget [64]. He developed in [64, Theorem 2], under some mild regularity conditions, a unique canonical representation of the process. This representation contains a minimal parametrization of the equivalence class of the true parameter. Equivalence of aggregated Markov chains may be checked by comparing their canonical representations. The works of Rydén [96] and Larget [64] are based on the work of Ito, Amari and Kobayashi [56] who provided conditions for identifiability of discrete-time aggregated Markov chains. These may be viewed as hidden Markov models with finite alphabet, or as discrete-time bivariate Markov chains.

6.2 Optimality

Optimality of a parameter estimator, such as the maximum likelihood estimator, is usually assessed by its consistency and asymptotic normality, see, e.g., [21, Chap. 12]. Roughly speaking, an estimator $\hat{\phi}_n$ of the true parameter ϕ, obtained from n observations, is said to be *strongly consistent* if $\hat{\phi}_n$ converges almost surely to ϕ as $n \to \infty$. The statement is more involved when equivalence classes of the true parameter

ought to be taken into account, see, e.g., [66, 93]. A consistent estimator is said to be *asymptotically normal* if $n^{1/2}(\hat{\phi}_n - \phi)$ converges weakly to the normal distribution with zero mean and covariance given by the inverse of the Fisher information matrix. Both consistency and asymptotic normality of bivariate Markov chains are notoriously hard to prove.

For discrete-time bivariate Markov chains we have the following result. Strong consistency and asymptotic normality of the maximum likelihood parameter estimator for a hidden Markov model, with finite-state underlying Markov chain and finite alphabet observable process, were first proved in [11, 86].

For discrete-time bivariate Markov processes, in the form of hidden Markov models, with possibly uncountably infinite alphabet for the observable process, we have the following results. Strong consistency of the maximum likelihood parameter estimator for a hidden Markov model with finite-state underlying Markov chain and continuous-alphabet observable process, was proved in [66]. Asymptotic normality of the maximum likelihood parameter estimator for the hidden Markov model in [66] was proved in [13]. Strong consistency and asymptotic normality of the conditional maximum likelihood parameter estimator, of a possibly non-stationary switching autoregressive process, with an underlying Markov chain that has a separable compact state space which is not necessarily finite, was proved in [33]. Conditioning is on the initial observations, and the initial state of the underlying Markov chain. For additional results on hidden Markov models in this class, see [40, Section VI.B], [21, Chap. 12], and [32], and the references therein.

For continuous-time bivariate Markov chains, the picture is not as complete as for the discrete-time bivariate Markov chains. Strong consistency of the maximum likelihood parameter estimator of an MMPP was proved in [93] by adopting the proof of [66]. Strong consistency of the conditional maximum likelihood parameter estimator of a bivariate Markov chain, given the initial observation, was proved in [39] by adopting the proof of [66, 93]. Asymptotic normality of the maximum likelihood parameter estimator for a bivariate Markov chain has not yet been proven. Instead, strong consistency and asymptotic normality of an

alternative parameter estimator for the MMPP, termed the "maximum split-time likelihood estimator," were proved by Rydén [94]. This estimator follows from maximization of a likelihood function, derived under the assumption that the process in consecutive disjoint time intervals is independent. Numerical results show that this estimator performs similarly to the maximum likelihood estimator.

6.3 EM Algorithm

The EM algorithm for estimating the parameter of an MMPP was pioneered by Rydén [95]. In a closely related work, Asmussen et al. [3] developed an EM algorithm for estimating the parameter of a continuous phase-type distribution. The approach was subsequently studied in [90] where some computational aspects were addressed and resulted in a significant speedup of the procedure. The approach was then extended to MMMPs in [41], to BMAPs in [17, 60], and to general continuous-time bivariate Markov chains in [76].

The EM approach is an iterative procedure, for estimating the parameter of a random process, with the eventual goal of obtaining the estimate that has the highest possible likelihood value [30]. The procedure begins with some initial estimate of the parameter, and generates a new estimate with higher likelihood in each iteration. The procedure is terminated when either a stopping criterion is met, or consecutive iterations yield the same likelihood. In the latter case, a fixed point is reached, and the estimated parameter is a stationary point of the likelihood function. Conditions for convergence of the sequence of estimated parameter values were given in [122]. A possible stopping criterion is when the relative difference in likelihood values in two consecutive iterations falls below some threshold. Initialization of the EM procedure is crucially important when the likelihood function has more than one local maximum. We assume that the EM procedure is applied to a given sample path of the observable process, $x_0^T = \{x(\tau), \tau \in [0,T]\}$. We denote the initial parameter estimate by ϕ_0, and the estimate at the end of the mth iteration by ϕ_m for $m = 1, 2, \ldots$.

The iterative nature of the EM procedure follows from the fact that the observable process constitutes only a partial or incomplete

statistic of the random process. The procedure requires specification of a complete statistic which facilitates the estimation of the parameter. For the bivariate Markov chain, the most useful complete statistic comprises the entire process $\{(x_0^T, S_0^T)\}$. In this notation, we have emphasized different roles played by the given sample path, x_0^T, and by the unobserved underlying process S_0^T. Given the parameter estimate ϕ_m, a new parameter estimate ϕ_{m+1} is generated by maximizing the EM auxiliary function

$$E_{\phi_m}\{\log p_\phi(x_0^T, S_0^T)\,|\,x_0^T\}, \tag{6.1}$$

which is the conditional mean of the log-likelihood function of the complete statistic given the observed sample path.

The likelihood function of the complete statistic $\{(X_0^T, S_0^T)\}$ follows from the likelihood function of a continuous-time univariate Markov chain. The latter likelihood function was derived in [1, Theorem 3.2]. Furthermore, it was shown in [1] that the number of jumps of the chain from one state to another in the given interval $[0,T]$, and the total sojourn time in each state in that interval, are sufficient statistics for estimating the generator of the chain. Each entry of the generator is estimated as the ratio of the number of jumps between the two states, and the total sojourn time in the originating state [1, Section 4]. For the bivariate Markov chain, the EM estimate of each entry of the generator, is given by the ratio of the conditional mean estimate of the number of jumps between the two states and the conditional mean estimate of the total sojourn time in the originating state. These two conditional mean estimates are calculated from the given sample path of the observed process using the current estimate of the parameter.

Recall that $M_{ij}^{ab}(T)$ denotes the number of jumps of the bivariate Markov chain from (a,i) to (b,j) in $[0,T]$, and that $D_i^a(T)$ denotes the total sojourn time of the bivariate Markov chain in state (a,i) in $[0,T]$. Given the parameter estimate ϕ_m at the end of the mth iteration, the estimates of these quantities are given by

$$\begin{aligned} \hat{M}_{ij}^{ab}(T) &= E_{\phi_m}\{M_{ij}^{ab}(T)\,|\,x_0^T\} \\ \hat{D}_i^a(T) &= E_{\phi_m}\{D_i^a(T)\,|\,x_0^T\}. \end{aligned} \tag{6.2}$$

The EM estimate of the entry $g_{ab}(ij)$ of the generator of the bivariate Markov chain at the $m+1$st iteration, is given by

$$\hat{g}_{ab}(ij) = \frac{\hat{M}_{ij}^{ab}(T)}{\hat{D}_i^a(T)}, \quad (a,i) \neq (b,j). \tag{6.3}$$

Since T is usually large, we may content ourselves with the assumption that T coincides with a jump of the observable process, i.e., $T = t^n$ for some integer n.

The conditional mean estimators in (6.2) can be implemented using either the recursions from Section 4 for non-causal estimation, or the recursions from Section 5 for causal estimation. The recursions for causal estimation, however, are more computationally intensive, and require per jump of the observable process $O(r^4d^2)$ operations, compared to $O(r^3)$ operations required by the recursions for non-causal estimation. Since each iteration of the EM algorithm requires the entire data set, there is no obvious advantage in using causal estimation for this application. The use of causal estimation of $M_{ij}^{ab}(T)$ and $D_i^a(T)$ does not turn the batch EM approach into a recursive parameter estimation approach. The search for a recursive EM approach has a long history, see, e.g., [108, Eq. 9], [115, Eqs. 19–21]. Optimality of these approaches for estimation from incomplete data has not been established [98].

6.4 Numerical Results

Numerical results, demonstrating the performance of the EM algorithm in estimating the parameters of various bivariate Markov chains, were reported in the literature. We provide a few pointers in this section. In [95, 90], numerical results were provided for estimating MMPPs. Results for estimating the parameter of an MMMP were given in [41]. Additional numerical examples, for estimating the parameters of general bivariate Markov chains, were worked out in [76]. In all of these cases, the EM algorithm was implemented using the recursions for non-causal estimation presented in Section 4. In [60], extensive numerical evaluation of the EM algorithm was performed, in estimating the parameter of the BMAP in applications involving Internet protocol

aggregated traffic modeling. The implementation of the E-step in [60] did not rely on Van Loan's [110] result but rather on an alternative technique termed "randomization."

6.5 Other Parameter Estimation Approaches

The EM algorithm is not the only approach that has been applied to bivariate Markov chains. An excellent review of some of these approaches, as they applied to MMPPs, can be found in [93]. In [78], the parameter and the underlying Markov chain of an MMPP were estimated using alternate maximization of the likelihood function of the underlying and observable chains. In contrast, the EM approach averages over the underlying chain rather than attempting to estimate it. Such joint parameter and state estimation is known to be biased, see, e.g., [19, 107]. Moment based approaches were developed for switched Poisson processes in [52, 91], and for the MAP in [22]. A switched Poisson process is an MMPP with two underlying states, i.e., $r = 2$. Maximum likelihood parameter estimation of an MMPP using general optimization procedures were studied in [88, 93]. In [88], the downhill simplex procedure, which does not require derivatives of the likelihood function, was employed. In [93], a quasi-Newton multidimensional optimization procedure was applied to maximize the likelihood function of the MMPP where derivatives were estimated numerically. All of these approaches, except the more recent one of [22], were compared in [93] in estimating the parameters of various MMPPs. In [87], the parameter of a continuous-time aggregated reversible Markov chain was estimated using the Davisson-Fletcher-Powell approach [73, Section 9.3]. The required derivatives of the likelihood function were evaluated analytically, and then implemented by utilizing a spectral representation of G_{aa}. By reversibility, all eigenvalues of G_{aa}, but the 0 eigenvalue, are negative.

7

Recursive Parameter Estimation

As we have seen in Section 6.3, recursive causal estimation of the statistics of the bivariate Markov chain does not facilitate recursive causal estimation of its parameter using the EM approach.

Recursive parameter estimation for the special bivariate Markov chain, in the form of an MMPP, was pioneered by Lindgren and Holst in [69], [53, Eq. 16]. Applying our notation from Section 3.1 to the MMPP, we use T_k to denote the kth sojourn time of the conditionally Poisson observable process in the state X_{k-1}, for $k = 1, 2, \ldots$, and we let $T_0 = 0$ and $X_0 = 1$ to account for the assumed first jump at $t = 0$. The sampled MMPP is given by the sequence $\{Z_k = (X_k, S_k), k = 0, 1, \ldots\}$. Since X_k counts the number of jumps up to and including the $k + 1$st jump, the value of X_k can be deduced from the sequence $\{T_0, T_1, \ldots, T_k\}$. Thus, when dealing with the MMPP, we can focus on the sequence $\{(T_k, S_k)\}$, rather than on the sequence $\{(T_k, Z_k)\}$. Recall also that for the MMPP, the sequence $\{S_k\}$ is Markov.

The recursion proposed in [69] for estimating the parameter ϕ of an MMPP, was motivated by an earlier recursion for estimating the parameter of a sequence of iid random variables. Suppose that the observations $\{T_k\}$ from the MMPP are iid. Then, for $k = 1, 2, \ldots$, the

recursion is given by

$$\hat{\phi}_k = \hat{\phi}_{k-1} + \frac{1}{k}[\Psi(\hat{\phi}_{k-1})]^{-1}\ \psi(t_k;\hat{\phi}_{k-1}), \tag{7.1}$$

with some initial estimate $\hat{\phi}_0$, where $\hat{\phi}_{k-1}$ denotes the parameter estimate at the kth jump of the observable process, $\psi(t_k;\hat{\phi}_{k-1})$ denotes the score function evaluated at $\hat{\phi}_{k-1}$, and $\Psi(\hat{\phi}_{k-1})$ denotes the Fisher information matrix evaluated at $\hat{\phi}_{k-1}$. The score function is the gradient column vector given by

$$\begin{aligned}\psi(t_k;\phi) &= \text{col}\{\partial \log p_\phi(t_k)/\partial\phi_l,\ l=1,\ldots,\tilde{r}\}\\ &:= D_\phi \log p_\phi(t_k)\end{aligned} \tag{7.2}$$

where $\tilde{r}$ denotes the dimension of ϕ. The Fisher information matrix is defined by

$$\Psi(\phi) = E_\phi\{\psi(T_k;\phi)\psi'(T_k;\phi)\}. \tag{7.3}$$

It was shown in [113] that this recursion follows from maximization over ϕ, of the second order Taylor series expansion of the EM auxiliary function

$$E_{\phi_{k-1}}\{\log p_\phi(t_1,\ldots,t_k,S_0,\ldots,S_k)\,|\,t_1,\ldots,t_k\} \tag{7.4}$$

around $\hat{\phi}_{k-1}$, assuming that the sequence $\{(T_k,S_k)\}$ is iid, and the observed information matrix, given by $\psi(T_k;\phi)\psi'(T_k;\phi)$, is replaced by its expected value which constitutes the Fisher information matrix.

For the MMPP, $\{S_k\}$ is a Markov chain, and the random variables $\{T_k\}$ are conditionally independent given $\{S_k\}$. For each $k \geq 1$, T_k depends on S_k as well as on S_{k-1}, see, Eq. (3.4). This implies that $\{T_k,S_k\}$ has a hidden Markov model representation [93], and the sequence $\{(T_k,S_k)\}$ is not iid. Hence, in [69], the score function of the observable process (7.2) was replaced by

$$\begin{aligned}\tilde{\psi}(t_k;\phi) &= E_\phi\{D_\phi \log p_\phi(t_k,S_k\,|\,S_{k-1})\,|\,t_1,\ldots,t_k\}\\ &= \sum_{s_{k-1},s_k} p_\phi(s_{k-1},s_k\,|\,t_1,\ldots,t_k) D_\phi \log p_\phi(t_k,s_k\,|\,s_{k-1}),\end{aligned} \tag{7.5}$$

and $\Psi(\phi)$ in (7.3) was substituted by the empirical estimate given by

$$\tilde{\Psi}_k = \frac{1}{k}\sum_{l=1}^{k} \psi(t_l;\hat{\phi}_{l-1})\psi'(t_l;\hat{\phi}_{l-1}). \tag{7.6}$$

Clearly, $\tilde{\Psi}_k$ depends on the sequence $\{\hat{\phi}_0,\ldots,\hat{\phi}_{k-1}\}$ of all past estimates of the parameter. The form of the function in (7.5) was possibly motivated by the Markov renewal property (3.1). In (7.5), $p_\phi(s_{k-1},s_k\,|\,t_1,\ldots,t_k)$ can be efficiently calculated using the standard forward recursion of a hidden Markov model, which is given in Eq. (8.13) of Section 8.2. Evaluation of $[\tilde{\Psi}_k]^{-1}$ was done recursively, from $[\tilde{\Psi}_{k-1}]^{-1}$ and $\tilde{\psi}(t_k;\hat{\phi}_{k-1})$, using the matrix inversion lemma. Thus, no explicit matrix inversion was required [69].

The function $\tilde{\psi}(t_k;\phi)$ in (7.5) differs from $D_\phi \log p_\phi(t_k\,|\,t_1,\ldots,t_{k-1})$, and hence is not a score function [97]. Rydén [97] showed that (7.1), together with (7.5) and (7.6), aim at local minimization of the relative entropy rate between the true probability measure of the MMPP and the estimated probability measure. Furthermore, if ϕ denotes the true parameter, and the estimator $\hat{\phi}_k$ is strongly consistent, then $k^{1/2}(\hat{\phi}_{k+1}-\phi)$ is asymptotically normal with zero mean and covariance matrix given by the inverse of $\lim_{k\to\infty} E_\phi\{\tilde{\psi}(T_k;\phi)\tilde{\psi}'(T_k;\phi)\}$.

Recursion (7.1), together with (7.5) and (7.6), was also applied in [54] for estimating the parameter of a switching autoregressive process with Markov regime. Such a process is related to a bivariate Markov chain as we have elaborated on in Section 2.3.

The recursion specified by (7.1) and (7.5) was further studied in [117]. An explicit recursion for $\tilde{\psi}(t_k;\phi)$ in (7.5) was developed, and the Fisher information matrix $\Psi(\phi)$ was evaluated under some simplifying assumptions. The lth component of $\tilde{\psi}(t_k;\phi)$ in (7.5) was shown to satisfy [117, Eq. 6]

$$\tilde{\psi}_l(t_k;\phi) = \frac{L(k-1;\phi)}{c_k}\frac{\partial}{\partial\phi_l}[e^{(Q-\Lambda)t_k}\Lambda]\mathbf{1} \tag{7.7}$$

where $L(k;\phi)$ is the forward recursion defined in (3.20), c_k is the scaling factor defined in (3.25), and $e^{(Q-\Lambda)t}\Lambda$ is a specialization of $e^{G_{aa}t}G_{ab}$ for the MMPP, see Eq. (2.19). An explicit expression for the derivative of the matrix exponential in (7.7), and its efficient implementation using

Van Loan's result [110], were also derived in [117]. In [118], recursions for the score function (7.2) and for the observed information matrix, for vectors of observations from an MMPP, were developed.

A vector version of (7.1) may be applied to a bivariate Markov chain, when vectors of consecutive observations are assumed iid, while the random variables within each vector maintain their dependency. This idea was first proposed in [97] for recursive estimation of the parameter of a hidden Markov model. The recursion in [97] relies on the score function alone, while the Fisher information matrix is taken to be proportional to the identity matrix. Suppose that the recursion in [97] is applied to the vectors $\{\boldsymbol{y}_m, m = 1, 2, \ldots\}$ where $\boldsymbol{y}_m = (y_{(m-1)n}, \ldots, y_{mn})$ is a vector of $n + 1$ successive observations. Following each application, the estimated parameter is projected onto a compact convex subset of the parameter space Φ which contains the true parameter. The projected estimates undergo further averaging which improves their statistical properties.

The recursion from [97] can be summarized as follows. Let $\psi(\boldsymbol{y}; \phi) = D_\phi \log p_\phi(\boldsymbol{y})$ denote the score function. The projected parameter estimate for the $m + 1$st vector is given by

$$\hat{\phi}_{m+1} = \mathcal{P}_\Phi(\hat{\phi}_m + \xi_m \psi(\boldsymbol{y}_{m+1}; \hat{\phi}_m)) \tag{7.8}$$

where $\xi_m = \xi_0 m^{-\alpha}$ for some $\xi_0 > 0$ and $\alpha \in (1/2, 1]$, and $\mathcal{P}_\Phi$ denotes the projection. The estimate of the true parameter at the $m + 1$st vector is given by

$$\bar{\phi}_{m+1} = \frac{1}{m+1} \sum_{k=1}^{m+1} \hat{\phi}_k. \tag{7.9}$$

Asymptotic properties of this recursion, and a numerical study comparing its performance with that of the maximum split-time likelihood estimator [94], for estimating the parameter of a hidden Markov model, were provided in [97].

A recursion for the score function $\psi(\boldsymbol{y}_m; \phi) = D_\phi \log p_\phi(\boldsymbol{y}_m)$, where $\boldsymbol{y}_m$ is a vector of observations from a continuous-time bivariate Markov chain, can be derived using an approach similar to that of [118]. We demonstrate this recursion for $m = 1$ without loss of generality.

For $k = 0, 1, \ldots, n$, let $Y_k = (T_k, X_k)$ denote the kth observation of the bivariate Markov chain. Let $Y_0^n = \{Y_0, Y_1, \ldots, Y_n\}$, and let y_0^n denote, as usual, a realization of Y_0^n. The recursion follows from the gradient of the forward density $p_\phi(y_0^n, s_n)$. For $n \geq 1$, this density satisfies the forward recursion given by,

$$p_\phi(y_0^n, s_n) = \sum_{s_{n-1}} p_\phi(y_0^{n-1}, s_{n-1}) p_\phi(t_n, z_n \mid z_{n-1}), \tag{7.10}$$

with the initialization of $p_\phi(y_0, s_0) = p_\phi(z_0)$. Applying the differentiation product rule to (7.10), and using (3.24), (3.25) and (3.29), provide the desired recursion.

Recall that $\tilde{r}$ denotes the dimension of ϕ. Define the $\tilde{r} \times r$ matrix of gradient vectors,

$$\begin{aligned} \delta_n(\phi) &= \frac{1}{\prod_{k=0}^n c_k} \left\{ \frac{\partial p_\phi(y_0^n, s_n)}{\partial \phi_l}, l = 1, \ldots, \tilde{r}; s_n = 1, \ldots, r \right\} \\ &= \frac{1}{\prod_{k=0}^n c_k} \left[D_\phi p_\phi(y_0^n, 1), D_\phi p_\phi(y_0^n, 2), \ldots, D_\phi p_\phi(y_0^n, r) \right]. \end{aligned} \tag{7.11}$$

Let $\partial_l f^{x_{n-1}x_n}(t_n; \phi)$ denote the $r \times r$ matrix of first-order derivatives of the elements of $f^{x_{n-1}x_n}(t_n; \phi)$ w.r.t. ϕ_l. Define the $\tilde{r} \times r$ matrix $\chi(n-1; \phi)$ whose lth row is given by $\tilde{L}(n-1; \phi)\, \partial_l f^{x_{n-1}x_n}(t_n; \phi)$. Then, $\delta_n(\phi)$ satisfies the following recursion

$$\delta_n(\phi) = \frac{1}{c_n} [\delta_{n-1}(\phi) f^{x_{n-1}x_n}(t_n; \phi) + \chi(n-1; \phi)]. \tag{7.12}$$

The score function is given by

$$D_\phi \log p_\phi(y_0^n) = \delta_n(\phi) \mathbf{1}. \tag{7.13}$$

The recursion in (7.12) requires the derivative of the transition density matrix $f^{ab}(t; \phi) = e^{G_{aa} t} G_{ab}$ w.r.t. each component ϕ_l of the parameter. The derivative of a matrix exponential follows from the expression for the differential of that matrix as given in [23]. Consider an $r \times r$ matrix $A = \{a_{ij}\}$ which is a function of some $\tilde{r}$-dimensional parameter $\theta = \{\theta_l\}$. For $l = 1, \ldots, \tilde{r}$, let $\partial_l A = \{\partial a_{ij} / \partial \theta_l\}$ denote the $r \times r$ matrix of derivatives of the elements of A w.r.t. θ_l. The derivatives of each of the $\{a_{ij}\}$ elements w.r.t. each of the $\{\theta_l\}$ elements are given by the

$r^2 \times \tilde{r}$ Jacobian

$$\nabla A = [\mathrm{vec}(\partial_1 A), \ldots, \mathrm{vec}(\partial_{\tilde{r}} A)] \tag{7.14}$$

where vec is the standard vectorization function. The differential of A is given by the $r \times r$ matrix $dA = \sum_{l=1}^{\tilde{r}} (\partial_l A) d\theta_l$. More compactly, $\mathrm{vec}\,(dA) = \nabla A d\theta$. It was shown in [23, Section 2], using Van Loan's result which we presented in Section 2.5, that

$$\mathrm{vec}\left(de^A\right) = \left[e^C\right]_{12} \ \mathrm{vec}(dA) \tag{7.15}$$

where

$$C = \begin{pmatrix} A' \otimes I_r & I_{r^2} \\ \mathbf{0} & I_r \otimes A \end{pmatrix}, \tag{7.16}$$

$\otimes$ denotes a Kronecker product, and $\left[e^C\right]_{12}$ is the $(1,2)$ $r^2 \times r^2$ block matrix of e^C. Hence,

$$\nabla e^A = \left[e^C\right]_{12} \nabla A. \tag{7.17}$$

The derivative of a product of two matrices is given as follows. From [112, Theorem 1], suppose that the matrices A and B are functions of the parameter θ. Then, the derivative of AB w.r.t. θ_l is given by $(\partial_l A)B + A(\partial_l B)$.

Numerical results obtained by applying the recursion (7.8)-(7.9), using (7.12), for recursive estimation of bivariate Markov chains, may be found in [68].

8

Discrete-Time Bivariate Markov Chains

In this section we introduce the discrete-time bivariate Markov chain. We discuss parameter estimation of this process, and approximation of the parameter of a continuous-time bivariate Markov chain by an estimated parameter of a corresponding discrete-time bivariate Markov chain. The latter process is obtained from sampling of the continuous-time bivariate Markov chain at fixed intervals, rather than at the jump points of the observable process as was done in Section 3.1.

8.1 Structure and Properties

A discrete-time bivariate Markov chain comprises a pair of discrete-time finite-alphabet random processes which are jointly Markov. Each of the two processes alone need not be Markov. The two processes may jump simultaneously. The discrete-time bivariate Markov chain is assumed homogeneous. We keep our notation similar to that used in the continuous-time case, and thus we denote the process as $\{Z(t) = (X(t), S(t)), t = 0, 1, \dots\}$, and assume that it takes values in the same state space $\mathbb{Z}$. The state pairs $\{(a, i) \in \mathbb{Z}\}$ are ordered lexicographically,

and the transition probability is given by

$$h_{ab}(ij) = P_\phi(Z(t+1) = (b,j) \,|\, Z(t) = (a,i)) \tag{8.1}$$

where ϕ is the parameter of the process, that is, ϕ comprises the initial distribution of the chain, and the set of independent entries of its transition matrix. The transition matrix $H = \{h_{ab}(ij)\}$ is written as a block matrix $H = \{H_{ab}; a, b \in \mathbb{X}\}$, where $H_{ab} = \{h_{ab}(ij); i, j \in \mathbb{S}\}$ is an $r \times r$ matrix. The underlying chain S is Markov with transition matrix Q if and only if $\sum_{b\in\mathbb{X}} H_{ab} = Q$ independently of a. A similar condition can be given for the observable chain X to be Markov. When H is irreducible, it has a unique stationary distribution π satisfying $\pi = \pi H$ [51, Theorem 6.9.21]. The process $\{Z(t)\}$ is stationary if and only if $P_\phi(Z(0) = (a,i)) = \pi_{a,i}$ for all $(a,i) \in \mathbb{Z}$.

Sampling $\{Z(t), t = 0,1,2,\ldots\}$ at the jump points of $\{X(t), t = 0,1,2,\ldots\}$, assuming that $t = 0$ coincides with a jump point of X, results in a *discrete-time Markov renewal process* which is denoted here by $\{(T_k, Z_k), k = 0,1,\ldots\}$. Using our notation from Section 3.1, T_k, $k \geq 1$, denotes the sojourn time of the chain in state X_{k-1}, which corresponds to the kth jump of X, and $Z_k = (X_k, S_k)$. Properties of that process were discussed in [83], and are summarized below. The transition probability of the Markov renewal process is given by

$$f_{ij}^{ab}(l;\phi) = P_\phi(T_1 = l, Z_1 = (b,j) \,|\, Z_0 = (a,i)) \tag{8.2}$$

for $l = 1,2,\ldots$, and $a \neq b$. The transition probability matrix, defined as $f^{ab}(l;\phi) = \{f_{ij}^{ab}(l;\phi), i,j = 1,\ldots,r\}$, where $a \neq b$, is given by,

$$f^{ab}(l;\phi) = H_{aa}^{l-1} H_{ab}. \tag{8.3}$$

The probability mass function of the observable process $\{X_0, X_1, \ldots, X_T\}$ is given by an expression identical to (3.14) when T is a jump point of the observable process, there are n jumps in $[0,T]$, and $\nu_{x_0}(\phi)$ is defined analogously to (3.13).

Assume that the matrices H and $\{H_{aa}, a \in \mathbb{X}\}$ are irreducible, and that the diagonal elements of H are positive. From the Perron-Frobenius theorem [63, pp. 536–537], the spectral radius of H_{aa} lies in $(0,1)$, and hence, from [63, p. 531, Theorem 2], $(I - H_{aa})$ is an M-matrix. That is, it is non-singular, and $(I - H_{aa})^{-1} \geq \mathbf{0}$. In fact, under

the above assumptions, we have from [63, p. 533, Exercise 1], that,

$$(I - H_{aa})^{-1} = \sum_{l=1}^{\infty} H_{aa}^{l-1} > 0. \tag{8.4}$$

The transition probability of the sampled bivariate Markov chain $\{Z_k, k = 0, 1, \ldots\}$ is given by

$$\begin{aligned} P_\phi(Z_k = (b,j) \,|\, Z_{k-1} = (a,i)) &= \sum_{l=1}^{\infty} f_{ij}^{ab}(l;\phi)dt \\ &= [(I - H_{aa})^{-1} H_{ab}]_{ij}, \end{aligned} \tag{8.5}$$

and the corresponding transition matrix is given by the block matrix $D = \{D_{ab}; a, b \in \mathbb{X}\}$, where

$$D_{ab} = \begin{cases} (I - H_{aa})^{-1} H_{ab}, & b \neq a \\ \mathbf{0}, & b = a. \end{cases} \tag{8.6}$$

The sampled discrete-time bivariate Markov chain has one closed set of recurrent, possibly periodic, states, while the remaining states are transient. The transition matrix D has a unique stationary distribution with zero entries for its transient states. The sampled discrete-time bivariate Markov chain is stationary if and only if its initial distribution $\nu(\phi)$ satisfies $\nu(\phi) = \nu(\phi)D$.

The distribution of the sojourn time of the observable process in each state in $\mathbb{X}$ follows from (8.2). Its probability mass function is given by [83]

$$p_\phi(l \,|\, a) = \bar{\nu}_a H_{aa}^{l-1}(I - H_{aa})\mathbf{1} \tag{8.7}$$

for $l = 1, 2, \ldots$, where $\bar{\nu}_a = \nu_a/(\nu_a \mathbf{1})$ as in (3.34). This is a *discrete phase-type* probability mass function with parameter $(\bar{\nu}_a, H_{aa})$ [82, p. 46]. The set of discrete phase-type distributions is dense in the set of distributions on $\{0, 1, 2, \ldots\}$ [65, p. 54].

8.2 Parameter Estimation

In this section we denote the observable process of the bivariate Markov chain Z in $[0, t]$ by $X_0^t = \{X(0), X(1), \ldots, X(t)\}$ for any non-negative integer t. We denote a realization of X_0^t by $x_0^t = \{x_0, x_1, \ldots, x_t\}$. We also

use $z_t = (x_t, s_t)$ to denote a realization of $Z(t)$. Previously, we have used z_t to denote a value of the sampled bivariate Markov chain. This minor abuse of notation should not cause any problem since we shall not discuss the sampled bivariate Markov chain in the remaining parts of this section.

The parameter ϕ of the discrete-time bivariate Markov chain Z, may be estimated from a realization x_0^T of the observable process, using a variant of the algorithm developed by Baum and Petrie [11], Baum, Petrie, Soules, and Weiss [12, 10], and Welch [116]. This algorithm is commonly referred to as the "Baum-Welch" algorithm. See also [114] for an application of the algorithm to discrete-time bivariate Markov chains. This is an easier estimation problem than that encountered earlier with the continuous-time bivariate Markov chain.

For this discussion, assume that $\pi_{a,i} = P_\phi(Z(0) = (a,i))$ is any initial distribution of the chain, not necessarily its stationary distribution. Let

$$M_{ij}^{ab}(T) = \sum_{t=1}^{T} \varphi_{ai}(t-1)\varphi_{bj}(t) \tag{8.8}$$

denote the number of transitions of Z from state (a,i) to state (b,j) in $[0,T]$ where (b,j) is not necessarily different from (a,i). This means that we allow here self transitions, and hence $M_{ij}^{ab}(T)$ is not necessarily the number of jumps of the chain from state (a,i) to a different state (b,j). The probability mass function of the bivariate Markov chain is given by

$$\begin{aligned} &P_\phi(Z(0) = z_0, Z(1) = z_1, \ldots, Z(T) = z_T) \\ &\quad = \pi_{z_0} \prod_{(a,i)} \prod_{(b,j)} h_{ab}(ij)^{M_{ij}^{ab}(T)}. \end{aligned} \tag{8.9}$$

Applying a standard EM argument to (8.9), assuming ϕ_m is the parameter estimate at the end of the mth iteration, shows that the estimate of π_{z_0} at the $m+1$st iteration is given by

$$\hat{\pi}_{a,i} = \begin{cases} P_{\phi_m}(S(0) = i \,|\, x_0^T), & x_0 = a \\ 0, & \text{otherwise}, \end{cases} \tag{8.10}$$

and the estimate of $h_{ab}(ij)$ at the conclusion of the $m+1$st iteration is given by

$$\hat{h}_{ab}(ij) = \frac{\hat{M}_{ij}^{ab}(T)}{\sum_{(\beta,k)} \hat{M}_{ik}^{a\beta}(T)} \tag{8.11}$$

where

$$\begin{aligned} \hat{M}_{ij}^{ab}(T) &= E_{\phi_m}\{M_{ij}^{ab}(T) \,|\, x_0^T\} \\ &= \sum_{\substack{t=1: x_{t-1}=a \\ x_t=b}}^{T} P_{\phi_m}(S(t-1)=i, S(t)=j \,|\, x_0^T). \end{aligned} \tag{8.12}$$

The probabilities in (8.10) and in (8.12) may be calculated using the standard forward-backward recursions for hidden Markov models, see, e.g., [10, 40]. Specifically, for a given parameter ϕ, the forward recursion is given by

$$\begin{aligned} F(x_0^t, s_t; \phi) &= P_\phi(X_0^t = x_0^t, S(t) = s_t) \\ &= \sum_{s_{t-1}} F(x_0^{t-1}, s_{t-1}; \phi) h_{x_{t-1},x_t}(s_{t-1}, s_t) \end{aligned} \tag{8.13}$$

where $t = 1, \ldots, T$, and $F(x_0, s_0; \phi) = \pi_{x_0,s_0}$. For the backward recursion we denote $X_t^T = \{X(t), X(t+1), \ldots, X(T)\}$, and the recursion is given by

$$\begin{aligned} B(x_t^T \,|\, z_{t-1}; \phi) &= P_\phi(X_t^T = x_t^T \,|\, Z(t-1) = z_{t-1}) \\ &= \sum_{s_t} B(x_{t+1}^T \,|\, z_t; \phi) h_{x_{t-1},x_t}(s_{t-1}, s_t) \end{aligned} \tag{8.14}$$

where $t = T, \ldots, 1$, and $B(x_{T+1}^T \,|\, s_{T+1}; \phi) = 1$. We also have for $t = 1, \ldots, T$,

$$\begin{aligned} &P_\phi(S(t-1) = s_{t-1}, S(t) = s_t, X_0^T = x_0^T) \\ &\quad = F(x_0^{t-1}, s_{t-1}; \phi) B(x_{t+1}^T \,|\, z_t; \phi) h_{x_{t-1},x_t}(s_{t-1}, s_t). \end{aligned} \tag{8.15}$$

This equation may be used for recursive evaluation of the conditional probability required in (8.12). The forward-backward recursions are recursively scaled to improve their numerical stability by a procedure similar to that described in Section 3.3, see, e.g., [40, Section V-A].

8.3 Approximation by Discrete-Time Bivariate Markov Chains

The relative simplicity of the parameter estimation problem for discrete-time bivariate Markov chains, compared to continuous-time bivariate Markov chains, has motivated some authors to consider estimation of the generator of a continuous-time bivariate Markov chain, from an estimate of the transition matrix of a sampled version of the continuous-time bivariate Markov chain. In this approach, the continuous-time bivariate Markov chain is first sampled at fixed intervals, irrespectively of the jump points of the observable process, and the transition matrix of the resulting discrete-time bivariate Markov chain is estimated using a variant of the Baum-Welch algorithm described in Section 8.2. We denote the estimated transition matrix by $\hat{P}_\phi(\Delta)$ where Δ denotes the sampling period. Given $\hat{P}_\phi(\Delta)$, an estimate of the generator of the continuous-time bivariate Markov chain, say $\hat{G}$, is obtained by attempting to solve (2.8), rewritten here as,

$$\hat{P}_\phi(\Delta) = e^{\hat{G}\Delta}. \tag{8.16}$$

This approach was adopted, for example, in [24] and [114]. In principle, the solution of (8.16) is given by the matrix logarithm of the transition matrix estimate normalized by Δ. But the problem is far more complex due to the infinite number of branches of the logarithm function.

This approach raises two key questions. First, for a given estimated transition matrix $\hat{P}_\phi(\Delta)$, is it always possible to find a *valid* generator $\hat{G}$ that solves (8.16)? Second, if a valid solution exists, is it unique? The first question deals with embeddability of a discrete-time Markov chain in a continuous-time Markov chain. When a valid solution exists, we refer to $\hat{P}_\phi(\Delta)$ as an embeddable matrix. When the solution is unique, we say that $\hat{G}$ is identifiable. As it turns out, the answers to these two questions are far from trivial. An excellent discussion of the embeddability and identifiability problems is given in [102]. We shall follow the discussion from [102] in this section.

An intuitive approach, which relies on the Taylor series expansion of the logarithm function, yields

$$\frac{1}{\Delta}\log \hat{P}_\phi(\Delta) = \frac{1}{\Delta}\sum_{k=1}^{\infty}\frac{(-1)^{k-1}[\hat{P}_\phi(\Delta) - I]^k}{k}. \tag{8.17}$$

When $\hat{P}_\phi(\Delta)$ has distinct eigenvalues $\{\upsilon_i\}$, this series converges if and only if $|\upsilon_i - 1| < 1$ for all i's. Convergence, however, is not necessarily to a valid generator [102, Example 3]. Conversely, $\hat{P}_\phi(\Delta)$ may be compatible with a valid generator, i.e., embeddable, even when the series does not converge [102, Example 4]. These observations follow from the fact that the series (8.17) provides only a partial description of the logarithm of a matrix. When the eigenvalues of $\hat{P}_\phi(\Delta)$ satisfy the above conditions, then (8.17) provides only the principal branch of $\log \hat{P}_\phi(\Delta)$.

Explicit sufficient conditions for a transition matrix to be embeddable are known only for matrices of order two [58]. Such conditions are not useful for bivariate Markov chains whose minimal order rd is always larger than two. A set of necessary conditions, developed by several authors, is given in [102, Section 3.1]. For example, for every embeddable transition matrix, $\det(P_\phi(\Delta)) > 0$ [58]; all eigenvalues $\{\upsilon_i\}$ other than $\upsilon_i = 1$ must satisfy $|\upsilon_i| \neq 1$, and any negative eigenvalue must have even algebraic multiplicity [35]. Another necessary condition implies that only a finite number of branches of $\log \hat{P}_\phi(\Delta)$ ought to be considered when determining the compatibility of a given transition matrix to a generator. These conditions can be used to identify estimated transition matrices that are not embeddable. Furthermore, the last quoted condition enables the use of Sylvester's formula which provides a complete description of $\log \hat{P}_\phi(\Delta)$ by incorporating different branches of the logarithm function. For an $rd \times rd$ matrix A with distinct eigenvalues, and a multi-valued function $u(\cdot)$, Sylvester's formula is given by

$$u(A) = \sum_{i=1}^{rd} u_{a_i}(\upsilon_i)\prod_{j\neq i}\frac{(A - \upsilon_i I)}{(\upsilon_i - \upsilon_j)} \tag{8.18}$$

where $\{u_{a_i}, i = 1, \ldots, rd\}$ represent at most rd different branches of the function u. By applying this formula to $A = \hat{P}_\phi(\Delta)$, and letting $u_{a_i}(A)$ be a branch of the logarithm function, the desired generator can be constructed when $\hat{P}_\phi(\Delta)$ is embeddable [102, Section 3.2a]. A detailed algorithm for constructing the generator from an embeddable transition matrix can be found in [102, Section 3.3a]. An extension of this approach to transition matrices with non-distinct eigenvalues is also provided in [102].

For an embeddable estimated transition matrix to have a unique estimated generator, one of the following sufficient conditions must be met [102, Section 4.1]: i) The eigenvalues of $\hat{P}_\phi(\Delta)$ are distinct and positive; ii) the minimal value of any element on the main diagonal of $\hat{P}_\phi(\Delta)$ is larger than 0.5; iii) $\det(\hat{P}_\phi(\Delta)) > e^{-\pi}$. Under condition i), the series in (8.17) provides the principal branch of $\log(P_\phi(\Delta))$ and will converge to a unique valid generator.

Another aspect of the approach for obtaining $\hat{G}$ discussed in this section, is that it provides little control over the desired structure of the estimated generator. In some applications, such as that of ion-channel current modeling (see Section 11.1), the structure of the true generator G imposes constraints on $e^{G\Delta}$, and the estimated transition matrix by the Baum-Welch algorithm may not fulfil these constraints. Thus, even if the logarithm of the estimated transition matrix produces a unique valid generator, the estimated generator may fail to be of the desired form.

The shortcomings of estimating the generator of a continuous-time bivariate Markov chain from a regularly time-sampled version of that chain, and the increased complexity associated with the use of a necessarily small sampling period, render this approach as inferior to the approach advocated in this paper, where estimation of the generator is performed directly from the continuous-time bivariate Markov chain. As discussed earlier, such estimation becomes possible when the continuous-time bivariate Markov chain is sampled at the jump points of the observable process. This provides a conceptually more meaningful approach which is also more computationally efficient.

9

Hidden Bivariate Markov Chains

A hidden bivariate Markov chain is a discrete-time or a continuous-time bivariate Markov chain observed through a discrete-time or a continuous-time memoryless noisy channel. The output of the channel at time t, denoted here by $Y(t)$, may depend on the joint state $Z(t) = (X(t), S(t))$ of the bivariate Markov chain, or it may be independent of $S(t)$ given $X(t)$. Suppose first that the chain and the channel are discrete-time. The process with the first dependency scenario corresponds to a standard hidden Markov model, albeit with an underlying bivariate Markov chain rather than a univariate Markov chain, see, e.g., [40]. The process with the second dependency scenario corresponds to a hidden semi-Markov process, see, e.g., [9]. The main difference between these two models, is that the sojourn time in each state $(a, i) \in \mathbb{Z}$ of the hidden Markov model is geometrically distributed, while the sojourn time in each state $a \in \mathbb{X}$ of the hidden semi-Markov process has a discrete phase-type distribution. Phase-type distributions are more general and may be more suitable in some applications. The parameter of the hidden bivariate Markov chain in either case may be estimated using a variant of the Baum-Welch algorithm.

A hidden semi-Markov process may also be obtained by supplementing the standard hidden Markov model, which comprises a discrete-time

univariate Markov chain observed through a discrete-time memoryless channel (see, e.g., [40]), with an explicit durational model [42, 124]. While this approach forces the sojourn time distribution to have a desirable form, it requires a far more complex parameter estimation scheme, compared to the Baum-Welch algorithm in the hidden semi-Markov process described in the previous paragraph. Moreover, the desirable form of the durational distribution is rarely known in practice. For example, in speech recognition applications, the desirable sojourn time distribution is not known, and various models have been hypothesized. One example is the Gamma distribution in [67]. It is interesting to note that when the shape parameter of the Gamma distribution is an integer, then it is the distribution of a sum of iid exponential random variables, i.e., it is an Erlang distribution, which is a special continuous phase-type distribution.

In speech recognition applications, the distribution of $Y(t)$ given $X(t)$ is usually normal with parameter that depends solely on $X(t)$. In other applications, such as in reliability theory and DNA analysis, $Y(t)$ has a finite alphabet. The development of finite alphabet hidden bivariate Markov chains, motivated by the desire to obtain more favorable sojourn time distributions, was studied in [9].

Hidden bivariate Markov chains also occur in continuous-time. For example, a continuous-time univariate Markov chain observed through a discrete-time memoryless Gaussian channel, was attributed to the patch-clamp measurements from a single ion-channel [46, 89]. In more elaborate ion-channel models, the univariate Markov chain is replaced by a multivariate Markov chain. That chain is also observed through a discrete-time memoryless Gaussian channel which represents the noise from the patch-clamp. This application is discussed in more detail in Section 11.1.

In this Section we deal with a continuous-time bivariate Markov chain observed through a continuous-time channel. The channel is represented by additive Brownian motion noise. This model is of theoretical importance since it generalizes the model of a univariate Markov chain observed in Brownian motion [121, 127, 128]. It is also of practical interest since measurements from a bivariate Markov chain may be noisy in some applications.

The mathematical tools used so far in this paper are inadequate for our task in this section. Estimation schemes for continuous-time random processes observed in Brownian motion, are conveniently derived through transformation of measure and the generalized Bayes' rule. In the next section, we provide a brief introduction to this approach, which will also be beneficial for our discussion in Section 10. This material is more advanced and requires some background in random processes. Excellent accessible texts are the books by Wong and Hajek [120], and by Klebaner [59].

9.1 Transformation of Measure Approach

The transformation of measure approach is a canonical approach for deriving the conditional mean estimator of a desired signal given an observed signal. It applies to discrete-time as well as continuous-time processes. The approach involves two conceptual steps. First, the probability measure of the desired and observed signals is transformed into a reference probability measure, under which the desired and observed signals are statistically independent. Then, the generalized Bayes' rule is invoked for evaluating the conditional mean estimate of the desired signal, as the ratio of two conditional mean estimates which are calculated under the reference measure. Only one of the two conditional mean estimates under the reference measure needs to be evaluated, since the other provides a simple normalization. The evaluated conditional mean estimate under the reference measure is called the unnormalized conditional mean estimate.

The transformation of the given measure into the reference measure is provided by the Radon-Nikodym derivative [14, Theorem 32.2]. When the two measures possess densities, say with respect to Lebesgue measure, then the Radon-Nikodym derivative is the likelihood ratio given by the ratio of the two probability density functions. Alternatively, when the two measures possess densities with respect to the counting measure, then the Radon-Nikodym derivative is the ratio of the two probability mass functions. The key to this approach is the existence of an explicit expression for the Radon-Nikodym derivative. For problems involving additive white Gaussian noise or Poisson counting noise,

explicit expressions for the Radon-Nikodym derivatives are known, but they depend on stochastic Itô integrals. We next describe these ideas in more concrete terms, and apply them in Section 9.2 for estimating the same statistics of a bivariate Markov chain considered in Sections 4 and 5, except that here the observable chain is seen through a Brownian motion. We shall revisit this approach in Section 10.

In this section, as well as in Section 10, we use P_0 and P_1 to denote probability measures, and E_0 and E_1 to denote expectations w.r.t. these probability measures, respectively. This is standard notation in nonlinear filtering theory. This notation should not be confused with P_ϕ and E_ϕ from earlier sections. Another standard notation is $\pi_t(\cdot)$ which represents the unnormalized conditional expected value of some random process w.r.t. P_0. The exact definition will be given shortly following Eq. (9.5) below. This notation should not be confused with the stationary distribution π of a bivariate Markov chain used in Section 2.1.

Suppose that we are interested in causal conditional mean estimation of a measurable function $u(\cdot)$ of a process $\{Z(t), t \geq 0\}$, not necessarily a bivariate Markov chain, from the observable process

$$Y(t) = \int_0^t v(Z(\tau))d\tau + W(t), \quad t \geq 0, \tag{9.1}$$

where $v(\cdot)$ is some measurable function, and $\{W(t), t \geq 0\}$ denotes a standard Brownian motion. Suppose that P_1 is the probability measure of $\{(Z(t), Y(t)), t \geq 0\}$, and that $\{Z(t), t \geq 0\}$ and $\{W(t), t \geq 0\}$ are statistically independent under P_1. Suppose that a reference probability measure P_0 for $\{(Z(t), Y(t)), t \geq 0\}$ exists, such that: i) the process $\{Z(t), t \geq 0\}$ has the same probability measure under P_0 as under P_1; ii) $\{Y(t), t \geq 0\}$ is a standard Brownian motion under P_0, and iii) $\{Z(t), t \geq 0\}$ and $\{Y(t), t \geq 0\}$ are statistically independent under P_0. Existence of such a probability measure is guaranteed by Girsanov's theorem, see, e.g., [120, Section 2, p. 254], [59, Chap. 10]. Define

$$\begin{aligned} \Upsilon(t) &= \exp\left\{\int_0^t v(Z(\tau))dY(\tau) - \frac{1}{2}\int_0^t v^2(Z(\tau))d\tau\right\} \\ &= 1 + \int_0^t \Upsilon(\tau-)v(Z(\tau))dY(\tau), \end{aligned} \tag{9.2}$$

and assume that $E_0\{\Upsilon(t)\} = 1$. Let $Z_0^t = \{Z(\tau), \tau \in [0,t]\}$, and define Y_0^t similarly. From Girsanov's theorem, P_1 is absolutely continuous w.r.t. P_0, and $\Upsilon(t)$ is the Radon-Nikodym derivative of P_1 w.r.t. P_0, that is,

$$\Upsilon(t) = \frac{dP_1}{dP_0}(Z_0^t, Y_0^t). \tag{9.3}$$

Let $\mathcal{G}_t$ denote the σ-field generated by $\{Z_0^t, Y_0^t\}$. A sufficient condition for $\{\Upsilon(t)\}$ to be a P_0-martingale w.r.t. $\mathcal{G}_t$, with $E_0\{\Upsilon(t)\} = 1$, is given by Novikov's theorem [59, Theorem 8.17]. The martingale property means that for any $\tau > 0$,

$$E_0\{\Upsilon(t+\tau) \,|\, Z_0^t, Y_0^t\} = \Upsilon(t), \quad \text{a.s.} \tag{9.4}$$

When the two measures P_1 and P_0 possess densities, then the Radon-Nikodym derivative is given by the likelihood ratio, or the ratio of the two densities. Girsanov's theorem is far more general since it holds for *any* finite energy signal $v(Z(t))$ on $[0,t]$. Note that the integrals in (9.2) w.r.t. $dY(\tau)$ are Itô integrals [59, Chap. 4].

Let $E_1\{u(Z_t) \,|\, Y_0^t\}$ denote the conditional mean estimate of $u(Z_t)$ given Y_0^t evaluated under the true measure P_1. Similarly, let $E_0\{u(Z_t)\Upsilon(t) \,|\, Y_0^t\}$ denote the conditional mean estimate of $u(Z_t)\Upsilon(t)$ given Y_0^t evaluated under the reference measure P_0. The generalized Bayes' rule (Kallianpur-Striebel formula) [70, Lemma 7.4], states that:

$$E_1\{u(Z_t) \,|\, Y_0^t\} = \frac{E_0\{u(Z_t)\Upsilon(t) \,|\, Y_0^t\}}{E_0\{\Upsilon(t) \,|\, Y_0^t\}}. \tag{9.5}$$

This generalized Bayes' rule can be easily verified when the two measures possess densities simply by substituting $\Upsilon(t)$ with the likelihood ratio.

In the transformation of measure approach, a stochastic differential equation is developed for the unnormalized conditional expected value $\pi_t(u(Z)) := E_0\{u(Z_t)\Upsilon(t) \,|\, Y_0^t\}$, from which the normalized conditional expected value $E_1\{u(Z_t) \,|\, Y_0^t\}$ is obtained as $\pi_t(u(Z))/\pi_t(1)$. The stochastic differential equation follows from application of the product rule [59, p. 220] to $u(Z_t)\Upsilon(t)$, by using the differential form of $\Upsilon(t)$ given in the second line of (9.2), and from the semimartingale

representation of the statistic being estimated [59, Section 9.6]. The semimartingale representation expresses the estimated statistic as the sum of a finite-variation function and a martingale.

The transformation of measure approach has become the method of choice in nonlinear estimation problems. Its striking feature is that it always leads to *linear* forward recursions. Since the noise is a Brownian motion, the resulting recursions are expressed as stochastic differential equations. Recursive estimation of the state of a continuous-time univariate Markov chain observed in Brownian motion was pioneered by Wonham [121] and Zakai [127]. Estimation of the number of jumps of the Markov chain was pioneered by Zeitouni and Dembo [128]. This was done by augmenting the number of jumps process with the state process, and estimating the augmented process using the state recursion from [121, 127]. The transformation of measure approach has been applied to a range of estimation problems in [36]. In particular, the approach was applied to estimation of Markov modulated Markov processes in the absence of noise in [36, 37].

9.2 Noisy Bivariate Markov Chains

In this section we present recursions for estimating the statistics of interest of a continuous-time bivariate Markov chain $\{Z(t), t \geq 0\}$ observed in Brownian motion. We assume that the observable noisy process is given by (9.1), with $v(Z(t)) = \frac{1}{\beta}X(t)$, where β is a constant that determines the signal to noise ratio. The statistics of interest are: i) a function of the state of the bivariate Markov chain; ii) the number of jumps from one state to another in a given time interval; and iii) the total sojourn time of the chain in each state in a given time interval. Estimation of each statistic at time t is performed from Y_0^t. To demonstrate the approach, we detail the derivation of the state recursion, and provide the other two recursions without their proofs. The derivation of the three recursions, along with some numerical results, may be found in [38].

9.2.1 State Estimation

In this section we detail the recursion for the conditional mean estimate of a function $u(Z(t))$ of the state of the bivariate Markov

chain. Suppose that $u(Z(t)) = u_{bj}$ when $Z(t) = (b, j)$. The function can then be expressed as a linear combination of the indicator functions $\{\varphi_{bj}(t), (b,j) \in \mathbb{Z}\}$ defined in (4.6), that is,

$$u(Z(t)) = \sum_{b,j} u_{bj}\varphi_{bj}(t). \tag{9.6}$$

Hence, it suffices to estimate $\{\varphi_{bj}(t)\}$. The conditional mean estimate of the indicator function $\varphi_{bj}(t)$ given Y_0^t, is given by,

$$\hat{\varphi}_{bj}(t) = E_1\{\varphi_{bj}(t)\,|\,Y_0^t\} = \frac{E_0\{\varphi_{bj}(t)\Upsilon(t)\,|\,Y_0^t\}}{E_0\{\Upsilon(t)\,|\,Y_0^t\}} := \frac{\pi_t(\varphi_{bj})}{\pi_t(1)}. \tag{9.7}$$

Clearly, $E_1\{\varphi_{bj}(t)\,|\,Y_0^t\}$ is the P_1-conditional probability of $Z(t) = \varphi_{bj}(t)$ given Y_0^t. We next show how the recursion for $\pi_t(\varphi_{bj})$ is derived.

First, from [59, Thm 9.15], it can be shown that $\varphi_{bj}(t)$ satisfies,

$$\varphi_{bj}(t) = \varphi_{bj}(0) + \sum_{a,i} g_{ab}(ij) \int_0^t \varphi_{ai}(\tau)d\tau + V_{bj}(t) \tag{9.8}$$

where $\{V_{bj}(t)\}$ is a P_0-martingale measurable on the σ-field $\mathcal{F}_t$ generated by Z_0^t. This is the semimartingale representation of $\varphi_{bj}(t)$. Next, from the product rule for semimartingales [59, p. 220],

$$\begin{aligned}\varphi_{bj}(t)\Upsilon(t) \;=\; & \varphi_{bj}(0) + \int_0^t \varphi_{bj}(\tau-)d\Upsilon(\tau) \\ & + \int_0^t \Upsilon(\tau-)d\varphi_{bj}(\tau) + [\varphi_{bj}, \Upsilon](t)\end{aligned} \tag{9.9}$$

where $[\varphi_{bj}, \Upsilon](t)$ denotes the quadratic covariation between $\varphi_{bj}(t)$ and $\Upsilon(t)$. This quadratic covariation equals zero since $\varphi_{bj}(t)$ is of finite variation and $\Upsilon(t)$ is continuous [59, Theorem 1.11]. . Substituting the second line of (9.2) in the first integral of (9.9), and (9.8) in its second integral, we obtain under P_0

$$\begin{aligned}\varphi_{bj}(t)\Upsilon(t) \;=\; & \varphi_{bj}(0) + \frac{1}{\beta}\int_0^t \varphi_{bj}(\tau-)X(\tau)\Upsilon(\tau-)dY_\tau \\ & + \sum_{a,i} g_{ab}(ij) \int_0^t \Upsilon(\tau-)\varphi_{ai}(\tau)d\tau \\ & + \int_0^t \Upsilon(\tau-)\; dV_{bj}(\tau).\end{aligned} \tag{9.10}$$

The recursion for $\pi_t(\varphi_{bj})$ is obtained by applying the conditional expected value under P_0, given Y_0^t, to both sides of (9.10). Using [120, Lemma 3.2, p. 261], it follows that the conditional mean of the last integral in (9.10) equals zero. Furthermore, using predictability of the right-continuous bivariate Markov chain with respect to the σ-field generated by the Brownian motion [59, Corollary 8.36], it follows that the conditional mean of each of the remaining two integrals in (9.10) can be applied directly to their integrands, and conditioning can be reduced from Y_0^t to Y_0^τ. The unnormalized conditional mean estimate $\pi_t(\varphi_{bj})$ obtained in this way satisfies the following recursion

$$\pi_t(\varphi_{bj}) = \pi_0(\varphi_{bj}) + \frac{b}{\beta}\int_0^t \pi_\tau(\varphi_{bj})dY(\tau) + \sum_{a,i} g_{ab}(ij)\int_0^t \pi_\tau(\varphi_{ai})d\tau, \tag{9.11}$$

where $\pi_0(\varphi_{bj})$ is the prior unnormalized probability of $\{X(0) = (b, j)\}$ under P_1. When the underlying chain has only one state, i.e., $r = 1$, (9.11) reduces to the recursion for estimating the state of a univariate Markov chain observed in Brownian motion [121, 127].

9.2.2 Number of Jumps Estimation

In this section we detail the recursion for estimating the number of jumps $M_{ij}^{ab}(t)$ from state (a, i) to state (b, j) in $[0, t]$. We denote the conditional mean estimate of $M_{ij}^{ab}(t)$ given Y_0^t by $\hat{M}_{ij}^{ab}(t)$. Following the state augmentation approach of [128], a recursion is developed for the conditional mean estimate of $\eta_{\gamma k}(t) := M_{ij}^{ab}(t)\varphi_{\gamma k}(t)$, where $\gamma = 1, \ldots, d$ and $k = 1, \ldots, r$, from which $\hat{M}_{ij}^{ab}(t)$ is obtained by summing over all (γ, k).

The recursion for estimating $\eta_{\gamma k}(t)$ was developed in [38] along the lines described in Section 9.2.1. The semimartingale representation of $M_{ij}^{ab}(t)$ was obtained as in [37, Eq. 24], and is given by

$$M_{ij}^{ab}(t) = g_{ab}(ij)\int_0^t \varphi_{ai}(\tau-)d\tau + \int_0^t \varphi_{ai}(\tau-)dV_{bj}(\tau). \tag{9.12}$$

The product rule is applied here twice, once for $M_{ij}^{ab}(t)\Upsilon(t)$ and then for $(M_{ij}^{ab}(t)\Upsilon(t))\varphi_{\gamma k}(t)$ using (9.8). The resulting recursion for the unnormalized conditional mean estimate

$$\pi_t(\eta_{\gamma k}) = E_0\{\eta_{\gamma k}(t)\Upsilon(t)\,|\,Y_0^t\}, \tag{9.13}$$

is given by,

$$\pi_t(\eta_{\gamma k}) = \pi_0(\eta_{\gamma k}) + \frac{\gamma}{\beta}\int_0^t \pi_\tau(\eta_{\gamma k})dY(\tau) + \sum_{\nu,l} g_{\nu\gamma}(lk)\int_0^t \pi_\tau(\eta_{\nu l})d\tau$$

$$+\delta_{jk}\delta_{\gamma b}g_{ab}(ij)\int_0^t \pi_\tau(\varphi_{ai})d\tau \tag{9.14}$$

where δ_{jk} denotes the Kronecker delta.

9.2.3 Total Sojourn Time Estimation

In this section we detail the recursion for estimating the total sojourn time $D_i^a(t)$ in state (a,i) during $[0,t]$. We denote the conditional mean estimate of $D_i^a(t)$ given Y_0^t by $\hat{D}_i^a(t)$. This estimate is also obtained by using the state augmentation approach of [128], see also [36]. A recursion is developed for the conditional mean estimate of $\varsigma_{\gamma k}(t) := D_i^a(t)\varphi_{\gamma k}(t)$, where $\gamma = 1,\ldots,d$ and $k = 1,\ldots,r$, from which $\hat{D}_i^a(t)$ is obtained by summing over all (γ,k).

The recursion for estimating $\varsigma_{\gamma k}(t)$ was developed in [38] along the lines described in Sections 9.2.1-9.2.2. The semimartingale representation of $D_i^a(t)$ is trivial and is given by

$$D_i^a(t) = \int_0^t \varphi_{ai}(\tau)d\tau. \tag{9.15}$$

The recursion for the unnormalized conditional mean estimate

$$\pi_t(\varsigma_{\gamma k}) = E_0\{\varsigma_{\gamma k}(t)\Upsilon(t)\,|\,Y_0^t\} \tag{9.16}$$

is given by,

$$\pi_t(\varsigma_{\gamma k}) = \pi_0(\varsigma_{\gamma k}) + \frac{\gamma}{\beta}\int_0^t \pi_\tau(\varsigma_{\gamma k})dY(\tau)$$

$$+\sum_{\nu,l} g_{\nu\gamma}(lk)\int_0^t \pi_\tau(\varsigma_{\nu l})d\tau + \ \delta_{ik}\delta_{\gamma a}\int_0^t \pi_\tau(\varphi_{ai})d\tau. \tag{9.17}$$

9.2.4 Recursion Implementation

Each of the above three recursions involves a stochastic Itô integral. A common approach for implementing such recursions is based on Clark's transformation [26]. This transformation was applied in [57] for estimating the state, number of jumps, and total sojourn time of a continuous-time univariate Markov chain observed in additive white Gaussian noise. In this approach, the stochastic differential equation is transformed into an ordinary time-varying differential equation which can be solved numerically.

To demonstrate the procedure, consider the state recursion (9.11), and the $1 \times rd$ row vector of state estimates

$$\pi_t(\boldsymbol{\varphi}) := \{\pi_t(\varphi_{a1}), \ldots, \pi_t(\varphi_{ar}), a \in \{1, \ldots, d\}\}. \tag{9.18}$$

Define the block diagonal matrix

$$B = \frac{1}{\beta}\text{diag}[1 \cdot I_r, \ldots, d \cdot I_r], \tag{9.19}$$

where I_r is an $r \times r$ identity matrix. Then, the state vector estimate (9.18) satisfies

$$\pi_t(\boldsymbol{\varphi}) = \pi_0(\boldsymbol{\varphi}) + \int_0^t \pi_\tau(\boldsymbol{\varphi}) B dY(\tau) + \int_0^t \pi_\tau(\boldsymbol{\varphi}) G d\tau. \tag{9.20}$$

Clark's transformation is constructed as follows. Consider a solution of (9.20) in the form of $q_t(\boldsymbol{\varphi}) := \varpi_t(\boldsymbol{\varphi})\mathcal{M}_t$ where $\varpi_t(\boldsymbol{\varphi})$ is a row vector of deterministic differentiable functions and

$$\begin{aligned} \mathcal{M}_t &:= \exp\left\{BY(t) - \frac{1}{2}B^2 t\right\} \\ &= \mathcal{M}_0 + \int_0^t B\mathcal{M}_{\tau-} dY(\tau). \end{aligned} \tag{9.21}$$

The second equality in (9.21) follows from Itô's formula for semimartingales [59, Section 8.10]. Application of the product rule for semimartingales [59, Corollary 8.7] to $q_t(\boldsymbol{\varphi}) := \varpi_t(\boldsymbol{\varphi})\mathcal{M}_t$ provides,

$$q_t(\boldsymbol{\varphi}) = q_0(\boldsymbol{\varphi}) + \int_0^t \varpi_{\tau-}(\boldsymbol{\varphi}) d\mathcal{M}_\tau + \int_0^t d\varpi_\tau(\boldsymbol{\varphi})\mathcal{M}_{\tau-} + [\varpi(\boldsymbol{\varphi}), \mathcal{M}](t). \tag{9.22}$$

The covariation in (9.22) equals zero since $\mathcal{M}_t$ is of finite variation and $\varpi_t(\boldsymbol{\varphi})$ is continuous [59, Section 4.5, Theorem 1.11]. By matching the first (or the second) integral from (9.20) with the corresponding integral from (9.22), using the second line of (9.21) for $d\mathcal{M}_\tau$, it follows that if $\varpi_t(\boldsymbol{\varphi})$ satisfies the ordinary time varying differential equation

$$d\varpi_t(\boldsymbol{\varphi}) = \varpi_t(\boldsymbol{\varphi})\mathcal{M}_t G \mathcal{M}_{t-}^{-1} dt, \tag{9.23}$$

then $\pi_t(\boldsymbol{\varphi}) = q_t(\boldsymbol{\varphi})$ a.s. when $q_0(\boldsymbol{\varphi}) = \pi_0(\boldsymbol{\varphi})$. Thus, $\pi_t(\boldsymbol{\varphi})$ can be obtained from a numerical solution of (9.23) with the initial condition of $\varpi_0(\boldsymbol{\varphi}) = \pi_0(\boldsymbol{\varphi})e^{-BY(0)}$. Note that $\mathcal{M}_{t-} = \mathcal{M}_t$ since under P_0, $\{Y(t)\}$ is a Brownian motion and hence continuous.

A recursion for solving (9.23) numerically, using a first-order Euler approximation, was given in [26]. It follows from discretization of the differential equation at $t = k\delta$ where $k = 0, 1, \ldots$, and δ is a step size. The discretized equation is given by

$$\begin{aligned} \varpi_{(k+1)\delta}(\boldsymbol{\varphi}) &= \varpi_{k\delta}(\boldsymbol{\varphi}) + \delta\varpi_{k\delta}(\boldsymbol{\varphi})\mathcal{M}_{k\delta} G \mathcal{M}_{k\delta}^{-1} \\ q_{(k+1)\delta}(\boldsymbol{\varphi}) &= \varpi_{(k+1)\delta}(\boldsymbol{\varphi})\mathcal{M}_{(k+1)\delta}. \end{aligned} \tag{9.24}$$

Let $\Delta y_{k+1} = y_{(k+1)\delta} - y_{k\delta}$ where $y_{k\delta}$ represents a realization of $Y(k\delta)$. From (9.24) and (9.21)

$$\begin{aligned} q_{(k+1)\delta}(\boldsymbol{\varphi}) &= q_{k\delta}(\boldsymbol{\varphi})(I + \delta G) \exp\left\{ B\Delta y_{k+1} - \frac{1}{2}B^2\delta \right\} \\ q_0(\boldsymbol{\varphi}) &= \pi_0(\boldsymbol{\varphi}), \end{aligned} \tag{9.25}$$

which is the desired forward recursion for the unnormalized conditional mean estimate $\pi_{k\delta}(\boldsymbol{\varphi})$ of the state vector $\boldsymbol{\varphi}$. It is easy to see that each component of $q_{(k+1)\delta}(\boldsymbol{\varphi})$ is positive, whenever the corresponding component of $q_{k\delta}(\boldsymbol{\varphi})$ is positive, provided that $\delta < 1/\min_{a,i}\{-g_{aa}(ii)\}$ [74]. The recursions (9.14) and (9.17) were implemented in a similar manner in [38].

Numerical results using this approach were presented in [57, 38], for estimating the statistics of univariate and bivariate Markov chains, respectively. In [38], the recursions (9.14) and (9.17) were also embedded in the EM approach of Section 6.3, for estimating the parameter of a bivariate Markov chain observed in Brownian motion at various signal to noise ratios.

10

Underlying Diffusion Processes

In this section we focus on two bivariate Markov processes for which the underlying process is a diffusion process. In one case, the diffusion process is observed in Brownian motion. In the other case, the diffusion process modulates the rate of a Poisson process. The pair of processes, comprising the underlying diffusion process and the observable process in each of these two scenarios, is a bivariate Markov process. Moreover, the underlying diffusion process in each case is a Markov process. The second model described above may be considered as an MMPP with an uncountably infinite alphabet underlying Markov process. These processes are of great practical importance in many applications. Their inclusion in this review paper complements the picture of the family of bivariate Markov processes.

For each of these two processes, we present recursions, in the form of stochastic partial differential equations, for estimating the diffusion process. The recursions for both models can be derived using the transformation of measure approach. The principles of that approach were outlined in Section 9.1. The approach was originally developed by Zakai [125] for the conditional mean and conditional density of a diffusion process observed in Brownian motion. See also [80, 34]. A recursion for

estimating the diffusion process in the presence of a Brownian motion and a counting process is given in [120, Section 5, p. 269]. The recursions are given in terms of the unnormalized conditional mean or conditional density estimates of the diffusion process given the observable process.

Recursions for the normalized conditional mean and conditional density estimates of a diffusion process observed in Brownian motion were first developed by Kushner [62]. A recursion for the normalized conditional density of a diffusion process modulating a Poisson process was first derived by Snyder [103]. See also [16, 101, 111].

An EM approach for maximum likelihood estimation of some parameters of a diffusion process observed in Brownian motion was developed in [29].

10.1 Diffusion Process observed in Brownian Motion

In this section we present Zakai's equation for recursive estimation of a time-homogeneous diffusion process observed in Brownian motion [125]. The diffusion process $\{S(t), t \geq 0\}$ satisfies the stochastic differential equation

$$dS(t) = \mu(S(t))dt + \sigma(S(t))dW(t), \tag{10.1}$$

and the observable process $\{X(t), t \geq 0\}$ satisfies the stochastic differential equation

$$dX(t) = \varrho(S(t))dt + d\tilde{W}(t), \tag{10.2}$$

where $\{W(t), t \geq 0\}$ and $\{\tilde{W}(t), t \geq 0\}$ are independent Brownian motions. The functions $\mu(\cdot)$, $\sigma(\cdot)$ and $\mu(\cdot)$ are assumed known. The function $\mu(\cdot)$ is assumed to satisfy the Lipschitz condition, and the function $\sigma(\cdot)$ is assumed to satisfy a Hölder condition of order larger than .5. These conditions guarantee existence and uniqueness of the solution of (10.1) [59, Theorem 5.5]. The process $\{S(t), t \geq 0\}$ is a Markov process [59, Theorem 5.6], and the joint process $\{(X(t), S(t)), t \geq 0\}$ is jointly Markov.

The generator of a time-homogeneous Markov process is the linear operator $\mathcal{L}$ defined by [59, Eq. 6.39]

$$\mathcal{L}u(\alpha) = \lim_{t \downarrow 0} \frac{E\{u(S(t)) \,|\, S(0) = \alpha\} - u(\alpha)}{t} \tag{10.3}$$

for any function u for which the limit exists. In that case, we say that u is in the domain of the generator. Note that (10.3) reduces to (2.4) when $u(\cdot)$ is an indicator function. When u is bounded and twice continuously differentiable, the generator of the diffusion process (10.1) can be shown to satisfy the second order differential equation [59, Eq. 6.30]

$$\mathcal{L}u(\alpha) = \frac{1}{2}\sigma^2(\alpha)\frac{\partial^2}{\partial\alpha^2}u(\alpha) + \mu(\alpha)\frac{\partial}{\partial\alpha}u(\alpha), \tag{10.4}$$

and $\mathcal{L}$ is seen as a differential operator.

Consider the following assumptions on the coefficients $\mu(\alpha)$ and $\sigma(\alpha)$ of the time-homogeneous diffusion process: a1) $\mu(\alpha)$ and $\sigma(\alpha)$ are bounded and continuous; a2) The derivatives of $\mu(\alpha)$ and $\sigma(\alpha)$ w.r.t. α up to order two are bounded and continuous; a3) $\sigma^2(\alpha)$ is bounded away from zero; a4) $\mu(\alpha)$ and $\sigma^2(\alpha)$ satisfy a Hölder condition; a5) The derivative $\dot{\mu}(\alpha)$ of $\mu(\alpha)$ w.r.t. α, and the derivatives $\dot{\sigma}(\alpha)$ and $\ddot{\sigma}(\alpha)$ of $\sigma(\alpha)$ w.r.t. α, are bounded and satisfy a Hölder condition.

When a1) and a2) hold, the stochastic differential equation (10.1) has a unique weak solution (i.e., solution in distribution), which has the strong Markov property [59, Theorem 5.10]. Furthermore, the transition probability function $P(S(\tau) \leq s \,|\, S(\tau - t) = \alpha)$ of the solution depends on τ and $\tau - t$ only through their difference t [59, Theorem 6.10]. Hence, we can focus on $P(S(t) \leq s \,|\, S(0) = \alpha)$. When the density of this transition probability function exists, it is denoted by $p(t, \alpha, s)$. When a1) and a3)–a4) are satisfied, then the density $p(t, \alpha, s)$ is the unique positive fundamental solution of *Kolmogorov's backward equation* given by [59, Theorem 5.15], [59, Eq. 6.31]

$$\frac{\partial}{\partial t}p(t,\alpha,s) = \frac{1}{2}\sigma^2(\alpha)\frac{\partial^2}{\partial\alpha^2}p(t,\alpha,s) + \mu(\alpha)\frac{\partial}{\partial\alpha}p(t,\alpha,s). \tag{10.5}$$

If, in addition, a5) holds, then the density $p(t, \alpha, s)$ satisfies *Kolmogorov's forward equation* in t and s for any fixed α [59, Theorem 5.15], [59, Eq. 6.32]. This equation is given by

$$\frac{\partial}{\partial t}p(t,\alpha,s) = \frac{1}{2}\frac{\partial^2}{\partial s^2}(\sigma^2(s)p(t,\alpha,s)) - \frac{\partial}{\partial s}(\mu(s)p(t,\alpha,s)). \tag{10.6}$$

Equation (10.6) is also known as the *Fokker-Planck equation*. Define the *adjoint operator* of $\mathcal{L}$ as [59, p. 158],

$$(\mathcal{L}^* u)(s) = \frac{1}{2}\frac{\partial^2}{\partial s^2}(\sigma^2(s)u(s)) - \frac{\partial}{\partial s}(\mu(s)u(s)). \tag{10.7}$$

Equations (10.5) and (10.6) may be concisely written as

$$\frac{\partial p}{\partial t} = \mathcal{L}p, \quad \frac{\partial p}{\partial t} = \mathcal{L}^* p \tag{10.8}$$

respectively.

Zakai's equation is a stochastic partial differential equation for the evolution of the unnormalized conditional mean estimate of $u(S(t))$ given X_0^t. The transformation of measure approach described in Section 9.1 was originally developed for this diffusion estimation problem. The approach relies on transformation of the actual probability measure P_1 of (S, X), to a reference probability measure P_0 of (S, X), such that under P_0, X is a Brownian motion, S has the same probability law as under P_1, and S and X are statistically independent. Such transformation is given by Girsanov's theorem from (9.2), when S, X and $\varrho(\cdot)$ take the roles of Z, Y and $v(\cdot)$, respectively. The generalized Bayes' rule defined in (9.5) is used to express the conditional mean estimate of $u(S(t))$ given X_0^t under P_1, as the ratio of $\pi_t(u(S)) := E_0\{u(S(t))\Upsilon(t)\,|\,X_0^t\}$ and $\pi_t(1)$ where E_0 indicates expectation under P_0. Zakai's equation is a stochastic partial differential equation for the evolution of $\pi_t(u(S))$. The derivation of Zakai's equation along these lines may be found in [126], and in [120, Section 5, p. 269]. *Zakai's equation* is given by

$$d\pi_t(u(S)) = \pi_t(u(S)\varrho(S))dX(t) + \pi_t(\mathcal{L}u(S))dt \tag{10.9}$$

where $\mathcal{L}$ is the differential operator defined in (10.4), and $\pi_0(u(S)) = E_0\{u(S(0))\}$. Uniqueness of the solution for Zakai's equation was proved in [125] and more generally in [61].

A second form of Zakai's equation, called the adjoint Zakai equation, follows from (10.9), and provides a stochastic partial differential equation for the evolution of the unnormalized conditional density of $S(t)$ given X_0^t. We denote this density by $q_t(s)$. The conditional density of $S(t)$ given X_0^t under P_1 is given by $q_t(s)\pi_t(1)$. Under some assumptions similar to those in a1)-a5), the *adjoint Zakai equation* is given by [125, Theorem 3]

$$dq_t(s) = q_t(s)\varrho(s)dX(t) + (\mathcal{L}^* q_t)(s)dt \tag{10.10}$$

where $(\mathcal{L}^* q_t)(s)$ is defined in (10.7), and $q_0(s)$ is the prior unnormalized density of $S(0)$ under P_1.

10.2 Diffusion Modulated Poisson Process

Consider the diffusion process $S(t)$ in (10.1), and assume that it modulates the rate λ of a Poisson process $\{N(t), t \geq 0\}$. The functions $\mu(\cdot)$ and $\sigma(\cdot)$ in (10.1), and the rate function $\lambda(\cdot)$, are assumed known. The modulated process may be represented as

$$dN(t) = \lambda(S(t))dt + dM(t) \tag{10.11}$$

where $M(t)$ is a martingale with independent increments on the sigma-field generated by $\{S_0^t, N_0^t\}$. Actually, this representation holds for any right-continuous counting process with finite rate [100, Theorem 1]. The bivariate process $\{(N(t), S(t)), t \geq 0\}$ is jointly Markov. In this section we present the stochastic partial differential equation for the evolution of the unnormalized conditional mean estimate of a function $u(\cdot)$ of the diffusion process given the Poisson events. This is the equation for $\pi_t(u(S)) = E_0\{u(S(t))\Upsilon(t) \,|\, N_0^t\}$ where $\Upsilon(t)$ is the appropriate Radon-Nikodym derivative.

The Radon-Nikodym derivative for this problem is given by [59, Eq. 10.45]

$$\begin{aligned}\Upsilon(t) &= \exp\left\{\int_0^t \ln\lambda(S(\tau))dN(\tau) + \int_0^t (1 - \lambda(S(\tau))d\tau\right\} \\ &= 1 + \int_0^t \Upsilon(\tau-)(\lambda(S(\tau)) - 1)(dN(\tau) - d\tau).\end{aligned} \tag{10.12}$$

Under the reference measure P_0, the diffusion process $\{S(t)\}$ has the same probability law as under the true measure P_1, the observable process $\{N(t)\}$ is homogeneous Poisson with unit rate, and $\{S(t)\}$ and $\{N(t)\}$ are independent.

Application of the transformation of measure approach gives (see, e.g., [126], or [120, Section 5, p. 269]),

$$d\pi_t(u(S)) = \pi_{t-}(u(S)(\lambda(S) - 1))(dN(t) - dt) + \pi_t(\mathcal{L}u(S))dt \tag{10.13}$$

where $\pi_0(u(S)) = E_0\{u(S(0))\}$.

10.3 Numerical Solutions

Zakai's equation, (10.9) for the conditional mean estimate, and (10.10) for the conditional density estimate, describes the evolution of the unnormalized estimates of these quantities by a stochastic partial differential equation in an infinite-dimensional space. Approximate numerical solutions of these equations have been the subject of ongoing research. The literature on this topic is extensive and is beyond the scope of this review paper. The book by Bain and Crisan [4] contains extensive discussion on application of particle filter techniques to Zakai's equation. These are sequential Monte Carlo simulation techniques which avoid setting up a fixed size quantization grid. A relatively recent survey on this and other numerical approaches may be found in [20].

Another interesting approach is based on Galerkin approximation [50]. This approach has recently been studied and expanded to estimation of a diffusion process observed in a mixture of a Brownian motion and a Poisson process [47]. In this approach, Zakai's equation is projected onto a finite-dimensional subspace spanned by smooth basis functions, e.g., Hermite polynomials, and the vector of corresponding Fourier coefficients satisfies an ordinary stochastic differential equation. It was shown in [47, Theorem 3.1], under some regularity conditions, that the Galerkin approximation error converges to zero, uniformly in time, in the mean square error sense, as the subspace dimension increases to infinity. The ordinary stochastic differential equation is solved through the Euler-Maruyama method using time discretization. This method tends to become unstable when the sampling interval is not sufficiently small. To overcome this problem, a splitting-up approach was proposed in which the stochastic and deterministic components of the stochastic differential equation are treated separately.

11

Selected Applications

Bivariate Markov processes have served as powerful models in many applications. Discrete-time bivariate Markov processes, with possibly uncountably infinite alphabet, in the form of hidden Markov models, have been used in numerous applications such as speech recognition, speech enhancement, written character recognition, image recognition, blind channel equalization, target tracking, fault detection, economic forecasting, DNA sequencing, electrocardiograph (ECG) analysis, and meteorology. These applications were briefly reviewed in [40] where references to specific applications were provided. Continuous-time bivariate Markov chains in the form of MMPPs or BMAPs have been extensively used to model arrival processes in queuing theory, see [71, 72], and the references therein. Multivariate Markov chains were used in ion-channel current modeling, see, e.g., [5] and the references therein. An extensive list of applications of point processes in general, and bivariate Markov processes in particular, in medicine and physiology, may be found in [104].

In this section we provide a brief overview of several applications. We begin with ion-channel current estimation where bivariate Markov processes have been extensively studied. We also review two recent

applications in spectrum sensing for cognitive radio, and in modeling of network congestion.

11.1 Ion-channel Current Estimation

An important application of bivariate Markov chains, or their alternative representations as aggregated Markov chains, is in ion-channel current estimation. Ion-channels are protein molecules that span the membrane of living cells. In certain configurations, they allow ions to transfer across the membrane, thus producing weak quantal currents measurable at a few pico-amperes. There are many types of ion-channels, and their cumulative contributions determine the nature of neural currents. Ion-channel currents alternate among several conductance levels, and they stay in each level for random durations. The number of such levels may be as small as two, signifying that the channel is either closed (no current), or open (current flows). Ion-channel currents are measured using the patch clamp technique. Patch clamp recordings are coarse in that they only provide information as to whether the channel is open or closed. They contain no information about the visited conductance levels or their sojourn times. In addition, they are usually characterized by low signal to noise ratio. A good introductory summary of the area of ion-channel currents, with an extensive list of references, was given by Ball and Rice [7].

The theory of Markov processes plays a central role in the study of ion-channel current, see, e.g., [7, 5], and the references therein. A single ion-channel is commonly modeled as a reversible continuous-time finite-state Markov chain [46]. That chain is not observable, and only an aggregating function of the chain is provided by the patch clamp technique. Thus, we have a bivariate Markov chain with one observable chain and an underlying chain. When noise is taken into account, the model becomes that of a hidden bivariate Markov chain. Research in this area has focused on many of the questions that were treated in this paper. Specifically, construction of the likelihood function of the observable process [27, 87, 44]; estimation of the parameter of the bivariate Markov chain [8]; estimation of the state sequence

[45, 87]; and characterization of the distribution of the sojourn time [5, 87].

In practice, it is difficult to isolate the contribution from a single ion-channel, and the measured current may originate from several channels which are not statistically independent. For this situation, a more elaborate model was proposed in [5]. The model is a special multivariate Markov chain with an underlying irreducible continuous-time Markov chain, say $\{S(t)\}$, and m conditionally independent identically distributed irreducible continuous-time Markov chains $\{X_1(t), X_2(t), \ldots, X_m(t)\}$ given $\{S(t)\}$. The model does not allow for simultaneous jumps of $\{S(t)\}$ and any of the processes $\{X_1(t), X_2(t), \ldots, X_m(t)\}$. For $m = 1$, the model becomes the MMMP. Conditions for time reversibility of the multivariate Markov chain were given in [5].

11.2 Spectrum Sensing for Cognitive Radio

The concept of spectrum sensing for cognitive radio was developed to address spectrum scarcity in wireless communication networks. The idea is to continuously monitor usage of a given radio channel, predict in real-time periods during which the channel is idle, and assign the channel to a secondary user during detected idle periods of the primary user. Clearly, a key to the success of this approach is the ability of the cognitive radio system to accurately model the sojourn time of the primary user in the active and idle states, and to predict the onsets of such periods. An alternative to this temporal sensing approach, is spatial spectrum sensing. In the latter approach, the channel may be allocated to a secondary user located sufficiently far from the primary user so that their transmissions do not interfere with each other [77].

In [84, 106], temporal sensing was performed by training a hidden Markov model on real wireless signal measurements from the primary user. A hidden Markov model with two states and two conditionally Gaussian output densities was used. One state represented a busy channel while the other represented an idle channel. The trained model was then attributed to newly received cellular signals, and the states of the signal were decoded using the Viterbi algorithm or the

forward-backward algorithm, see, e.g., [40]. The channel was turned over to a secondary user during periods corresponding to the idle state of the primary user. In [49], it was argued empirically that a geometric sojourn time distribution, typical of a hidden Markov model, is inadequate for reliable representation of the active and idle periods of the primary user, and that a hidden semi-Markov model would be more appropriate. In [83], the hidden Markov model was replaced by a hidden bivariate Markov chain whose sojourn time in each state follows that of a discrete phase-type distribution. The hidden bivariate Markov chain outperformed the standard hidden Markov model by providing lower probability of prediction error for a given false alarm probability.

11.3 Network Congestion

Congestion due to traffic flows exceeding communication resources may cause packet loss and delay across the network. Characterizing network congestion is important for assessing service quality and for designing the network to accommodate current and future demands. In this section we review two approaches for modeling network congestion using bivariate Markov chains.

In [99], a discrete-time bivariate Markov chain, in the form of a hidden Markov model, was used to model the end-to-end packet loss process. In this application, the underlying Markov chain represents different levels of network congestion. The observable process is binary, and it assumes the value 0 when the transmitted packet reaches the destination and the value 1 if this packet is lost. Such model is appropriate for traffic flows in which the packets are transmitted at approximately constant time intervals.

In [114], a continuous-time bivariate Markov chain was proposed to model packet delay and loss. This model is more appropriate than the discrete-time bivariate Markov chain when packets are transmitted at arbitrary time points. In this approach, the observable process represents packet delay, with a maximal delay value attributed to packet loss. The range of delay values was uniformly quantized to conform with the finite-alphabet of the continuous-time bivariate Markov chain. The

possible delay values can be measured by sending a sequence of probing packets from the source host to the destination host at regular intervals. The parameter of this model was estimated from a discrete-time bivariate Markov chain approximation to the continuous-time bivariate Markov chain as discussed in Section 8.3.

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Concluding Remarks

In this paper we have reviewed some properties, and a range of recursive estimation procedures, associated with bivariate Markov processes. This very rich family of random processes contains the hidden Markov model, the Markov modulated Poisson process, the batch Markovian arrival process, the Poisson process whose rate is modulated by a diffusion process, and a diffusion process observed in a Brownian motion. Bivariate Markov processes have produced powerful models in many application areas including signal processing, queuing, communications, and biomedical engineering. Both causal and non-causal estimation of some statistics of the bivariate Markov processes were reviewed. In addition, off-line as well as on-line recursive parameter estimation approaches were covered. The estimation approaches were developed using the Markov renewal property of the bivariate Markov chain, and the transformation of measure approach. Except for the models involving diffusion processes and Brownian motions, all other recursions are explicit and do not require sampling of the continuous-time process at regular sufficiently small intervals or any numerical integration.

An important open problem in this area is that of recursive parameter estimation tailored to the structure of the bivariate Markov chain. A

possible approach to this problem is to estimate recursively and jointly the parameter and associated statistics. In addition, it would be interesting to see whether causal recursive estimation of the statistics of the bivariate Markov chain facilitates forward recursive estimation of its parameter.

We hope that this paper could serve as a springboard for other interested researchers to pursue the study of this rather interesting family of processes. It is also our hope that this paper would be useful in promoting applications of bivariate Markov processes.

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