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A solution to the reversible embedding problem for finite Markov chains

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ABSTRACT

The embedding problem for Markov chains is a famous problem in probability theory and only partial results are available up till now. In this paper, we propose a variant of the embedding problem called the reversible embedding problem which has a deep physical and biochemical background and provide a complete solution to this new problem. We prove that the reversible embedding of a stochastic matrix, if it exists, must be unique. Moreover, we obtain the sufficient and necessary conditions for the existence of the reversible embedding and provide an effective method to compute the reversible embedding. Some examples are also given to illustrate the main results of this paper.

1. Introduction

In 1937, Elfving (1937) proposed the following problem: given an $n \times n$ stochastic matrix P, can we find an $n \times n$ generator matrix Q such that $P = e^Q$? This problem, which is referred to as the embedding problem for stochastic matrices or the embedding problem for finite Markov chains, is still an open problem in probability theory. Let $X = \{X_n : n \geq 0\}$ be a discrete-time homogeneous Markov chain with transition probability matrix P. The embedding problem is equivalent to asking whether we can find a continuous-time homogeneous Markov chain $Y = \{Y_t : t \geq 0\}$ with transition semigroup $\{P(t) : t \geq 0\}$ such that $P = P(1)$. If this occurs, the discrete-time Markov chain X can be embedded as the discrete skeleton of the continuous-time Markov chain Y.

The embedding problem has been studied for a long time (Kingman, 1962; Runnenburg, 1962; Chung, 1967; Speakman, 1967; Cuthbert, 1973; Johansen, 1974; Singer and Spilerman, 1975, 1976; Carette, 1995; Davies, 2010; Chen and Chen, 2011; Guerry, 2013). So far, the embedding problem for 2×2 stochastic matrices has been solved by Kendall and this result is published in Kingman (1962). The embedding problem for 3×3 stochastic matrices has also been solved owing to the work of Johansen (1974), Carette (1995), and Chen and Chen (2011). However, when the order n of the stochastic matrix P is larger than three, only partial results are available and our knowledge on the set of embeddable $n \times n$ stochastic matrices is quite limited. There is also an embedding problem for inhomogeneous Markov chains which has been dealt with by some authors (Goodman, 1970; Johansen, 1973; Frydman and Singer, 1979; Johansen and Ramsey, 1979; Frydman, 1980a,b, 1983; Fuglede, 1988; Lencastre et al., 2016). However, we only focus on the homogeneous case in this paper.

The embedding problem has wide applications in many scientific fields, such as social science (Singer and Spilerman, 1975, 1976), mathematical finance (Israel et al., 2001), statistics (Bladt and Sørensen, 2005; Metzner et al., 2007), biology (Verbyla et al., 2013; Jia et al., 2014), and manpower planning (Guerry, 2014). One of the most important applications of the

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embedding problem is the generator estimation problem in statistics. Let $Y = \{Y_t : t \geq 0\}$ be a continuous-time Markov chain with generator matrix Q. In practice, it often occurs that we can only observe a sufficiently long trajectory of Y at several discrete times $0, T, 2T, \ldots, mT$ with time interval T. Let $P = (p_{ij})$ be the transition probability matrix of Y at time T. Then p_{ij} can be estimated by the maximum likelihood estimator

$$\hat{p}_{ij} = \frac{\sum_{k=0}^{m-1} I_{\{Y_{kT}=i, Y_{(k+1)T}=j\}}}{\sum_{k=0}^{m-1} I_{\{Y_{kT}=i\}}}, \tag{1}$$

where I_A denotes the indicator function of A. A natural question is whether we can obtain an estimator $\hat{Q}$ of the generator matrix Q from the estimator $\hat{P} = (\hat{p}_{ij})$ of the transition probability matrix P. It is reasonable to require the estimators $\hat{P}$ and $\hat{Q}$ to be related by $\hat{P} = e^{\hat{Q}T}$. Therefore, the generator estimation problem in statistics is naturally related to embedding problem for finite Markov chains.

Recently, the generator estimation problem has been widely studied in biology (Verbyla et al., 2013; Jia et al., 2014), since a number of biochemical systems can be modeled by continuous-time Markov chains. In general, there are two types of Markov chains that must be distinguished, reversible chains and irreversible chains. In the reversible case, the detailed balance condition $\mu_i q_{ij} = \mu_j q_{ji}$ holds for any pair of states i and j, where μ_i is the stationary probability of state i and q_{ij} is the transition rate from state i to j (Norris, 1998). From the physical perspective, detailed balance is a thermodynamic constraint for closed systems. In other words, if there is no sustained energy supply, then a biochemical system must satisfy detailed balance (Qian, 2007). In the modeling of many biochemical systems such as enzymes (Cornish-Bowden, 2012) and ion channels (Sakmann and Neher, 2009), detailed balance has become a basic assumption (Alberty, 2004). Therefore, in many realistic biochemical systems, what we are concerned about is not simply to find a generator matrix $\hat{Q}$ such that $\hat{P} = e^{\hat{Q}T}$, but to find a reversible Markov chain with generator matrix $\hat{Q}$ such that $\hat{P} = e^{\hat{Q}T}$.

Here we consider the following problem: given an $n \times n$ stochastic matrix P, can we find a reversible generator matrix Q such that $P = e^Q$? This problem will be referred to as the reversible embedding problem for stochastic matrices or the reversible embedding problem for finite Markov chains in this paper. Compared with the classical embedding problem, the reversible embedding problem has a deeper physical and biochemical background.

In this paper, we provide a complete solution to the reversible embedding problem. We prove that the reversible embedding of stochastic matrices, if it exists, must be unique. Moreover, we give the sufficient and necessary conditions for the existence of the reversible embedding and provide an effective method to compute the reversible embedding. Finally, we use some examples of 3×3 stochastic matrices to illustrate the main results of this paper.

2. Preliminaries

For clarity, we recall several basic definitions.

Definition 1. An $n \times n$ real matrix $P = (p_{ij})$ is called a stochastic matrix if $p_{ij} \geq 0$ for any $i, j = 1, 2, \ldots, n$ and $\sum_{j=1}^n p_{ij} = 1$ for any $i = 1, 2, \ldots, n$.

Definition 2. An $n \times n$ real matrix $Q = (q_{ij})$ is called a generator matrix if $q_{ij} \geq 0$ for any $i \neq j$ and $\sum_{j=1}^n q_{ij} = 0$ for any $i = 1, 2, \ldots, n$.

In this paper, we consider a fixed $n \times n$ stochastic matrix P. For simplicity, we assume that P is irreducible. Otherwise, we may restrict our discussion to an irreducible recurrent class of P. Since P is irreducible, it has a unique invariant distribution $\mu = (\mu_1, \mu_2, \ldots, \mu_n)$ whose components are all positive (Norris, 1998).

Definition 3. P is called reversible if the detailed balance condition $\mu_i p_{ij} = \mu_j p_{ji}$ holds for any $i, j = 1, 2, \ldots, n$. In this case, μ is called a reversible distribution of P.

Definition 4. Let Q be an $n \times n$ generator matrix. Then Q is called reversible if there exists a distribution $\pi = (\pi_1, \pi_2 \cdots, \pi_n)$ such that the detailed balance condition $\pi_i q_{ij} = \pi_j q_{ji}$ holds for any $i, j = 1, 2, \ldots, n$. In this case, π is called a reversible distribution of Q.

In fact, if π is a reversible distribution of Q, then π is also an invariant distribution of Q.

Definition 5. If there exists an $n \times n$ real matrix A such that $P = e^A$, then A is called a real logarithm of P.

Definition 6. P is called embeddable if there exists an $n \times n$ generator matrix Q such that $P = e^Q$. In this case, Q is called an embedding of P.

It is easy to see that if Q is a embedding of P, then Q is also a real logarithm of P.