RELATIVE ENTROPY BETWEEN MARKOV TRANSITION RATE MATRICES

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Relative Entropy Between Markov Transition Rate Matrices*

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Abstract

We derive the relative entropy between two Markov transition rate matrices from sample path considerations. This relative entropy is interpreted as a "level 2.5" large deviations action functional. That is, the level two large deviations action functional for empirical distributions of continuous-time Markov chains can be derived from the relative entropy using the contraction mapping principle [1].

1 Introduction

In this note we derive the relative entropy between two Markov transition rate matrices. We use the relative entropy to obtain an expression for the probability that a Markov chain with a given transition matrix behaves as if it had another transition rate matrix over a long period of time (large deviations).

2 The Main Result

Consider a stationary Markov chain X with rate matrix Q^o and stationary distribution π^o. The jump chain has probability transition matrix

$$P^o_{i,j} = \begin{cases} 0 & i = j \\ -Q^o_{i,j}/Q^o_{i,i} & i \neq j \end{cases} .$$

Let Q be a rate matrix with with jump transition matrix P and stationary distribution π. Consider a trajectory w with n transitions over $[0,T]$ with the k^{th} transition occurring at T_k, $T_0 = 0$ and $T_n = T$. Let $n_i = \sum_{k=1}^{n} 1\{X(T_k) = i\}$, $n_{i,j} = \sum_{k=0}^{n-1} 1\{X(T_k) = i,\ X(T_{k+1}) = j\}$, $\Delta_k = T_{k+1} - T_k$, and $A = -\sum_{i=1}^{m} \pi(i)Q(i,i)$. Note that the invariant of P is μ where $\mu(i) = -A^{-1}\pi(i)Q(i,i)$.

We say that w is Q-typical if

$$\begin{aligned} n_{i,j} &= \mu(i)P(i,j)n + o(n) && (1) \\ &= A^{-1}\pi(i)Q(i,j)n + o(n), && (2) \\ \sum_{k=0}^{n-1} \Delta_k 1\{X(T_k) = i\} &= n\frac{\mu(i)}{-Q(i,i)} + o(n) && (3) \\ &= nA^{-1}\pi(i) + o(n), && (4) \\ \text{and } T_n &= nA^{-1} + o(n). && (5) \end{aligned}$$

Let $X_i = X(T_i)$. Define the likelihood ratio $L(w,n)$ of the Q^o chain with respect to the Q chain evaluated at the trajectory w over $[0, T_n]$. Thus,

$$L(w,n) = \frac{\pi^o(X_0)}{\pi(X_0)} \prod_{k=0}^{n-1} \frac{Q^o(X_k, X_{k+1})e^{Q^o(X_k,X_k)\Delta_k}}{Q(X_k, X_{k+1})e^{Q(X_k,X_k)\Delta_k}}.$$

We now use the assumption that w is Q-typical will to simplify $\log L(w,n)$. Take $\log \frac{0}{0} = 0$ and note that

$$\begin{aligned} \log\left(\prod_{k=0}^{n-1} \frac{Q^o(X_k, X_{k+1})}{Q(X_k, X_{k+1})}\right) &= \sum_{i,j=1}^{m} n_{i,j} \log \frac{Q^o(i,j)}{Q(i,j)} \\ &= nA^{-1} \sum_{i,j=1}^{m} \pi(i)Q(i,j) \log \frac{Q^o(i,j)}{Q(i,j)} + o(n) \ \text{ by (3)} \end{aligned}$$

Also,

$$\log\left(\prod_{k=0}^{n-1}\frac{e^{Q^o(X_k,X_k)\Delta_k}}{e^{Q(X_k,X_k)\Delta_k}}\right) = \sum_{i=1}^{m}(Q^o(i,i)-Q(i,i))\sum_{k=0}^{n-1}\Delta_k 1\{X_k=i\}$$

$$= nA^{-1}\sum_{i=1}^{m}\pi(i)(Q^o(i,i)-Q(i,i))+o(n) \text{ by (5).}$$

Combining the expressions above and substituting equation (5), we get

$$\log L(w,n) = -T_n\sum_{i=1}^{m}\pi(i)\sum_{j=1,j\neq i}^{m}\left(Q(i,j)\log\frac{Q(i,j)}{Q^o(i,j)}+Q^o(i,j)-Q(i,j)\right)+o(n)$$

$$= -T_nH(Q;Q^o)+o(n),$$

where we have defined the relative entropy of the *rate* matrix Q with respect to Q^o as

$$H(Q;Q^o) := \sum_{i=1}^{m}\pi(i)\sum_{j=1,j\neq i}^{m}\left(Q(i,j)\log\frac{Q(i,j)}{Q^o(i,j)}+Q^o(i,j)-Q(i,j)\right).$$

Recall that n, the number of transitions of the jump chain P, is proportional to the amount of simulation time and, by equation (5), so is T_n. Also note that $Q(i,j)\log\frac{Q(i,j)}{Q^o(i,j)}+Q^o(i,j)-Q(i,j)$ is the Legendre transform of the logarithm of the moment generating function of a Poisson random variable with intensity $Q^o(i,j)$ evaluated at $Q(i,j)$.

Assume a trajectory w is Q-typical as described above. Let $\mathbf{P}_T^o$ be the (trajectory) distribution of $\{X(t) : t\in[0,T]\}$, and let $\mathbf{P}_T$ be the distribution of $\{Y(t) : t\in[0,T]\}$

where Y has transition rate matrix Q. By the Radon-Nikodym theorem,

$$\begin{aligned}\mathbf{P}^{o}_{T_n}(w) &= L(w,n)\mathbf{P}_{T_n}(w) \\ &= \exp(-T_n H(Q;Q^o) + o(n))\mathbf{P}_{T_n}(w)\end{aligned}$$

where the last equality is by the argument above for large n. Therefore, the probability that $\{X(t) : t \in [0,T]\}$ has a trajectory that is Q-typical is, for large T, $\exp(-TH(Q;Q^o) + o(T))$ because $\mathbf{P}_T(W_T) \to 1$ as $T \to \infty$ where W_T is the set of all Q-typical trajectories on $[0,T]$.

We refer to H as the level 2.5 large deviations action functional of the Markov chain Q^o because, using the contraction mapping principle, we can obtain the action functional of Donsker/Varadhan for empirical distributions (level 2) of continuous-time Markov chains ([2], p.125-128). For example, take $m = 2$ and *fix* the invariant distribution π. By direct calculation, we find that the level two action functional is

$$\begin{aligned}J_{Q^o}(\pi) &= \left(\sqrt{\pi_1 q^o(1)} - \sqrt{\pi_2 q^o(2)}\right)^2 \\ &= \inf_{Q:\pi Q=0} H(Q;Q^o).\end{aligned}$$

3 Conclusions

We have derived the relative entropy between two Markov transition rate matrices and interpreted it as the level 2.5 large deviations action functional. The sample path argument used above is an adaptation of an argument used by D. Aldous [3] to explain the relative entropy between two (discrete-time) Markov transition probability matrices P and P^o:

$$\sum_{i,j} \mu(i) P(i,j) \log \frac{P(i,j)}{P^o(i,j)}$$

where μ is the invariant of P.

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