On the Optimal Transition Rate Matrix of Markov Process

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Outline

1. Introduction
2. Results on Continuous-time Markov chain
3. Discussion

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- Suppose that $X_0, X_1, \ldots, X_n, \ldots$ is a Markov chain generated by some transition matrix P with stationary distribution π, then the time average $\frac{1}{n}\sum_{k=0}^{n-1} f(X_k)$ is a reasonable approximation to $\pi(f)$.

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- For the continuous-time, it is $\frac{1}{T}\int_0^T f(X_t)dt$.

Referring to [Iosifescu 1980] if P is irreducible, then for any initial distribution μ,

$$\begin{aligned} \nu(f, P, \pi) &= \lim_{n\to\infty} \text{Var}_\mu \left[\frac{\sum_{k=0}^{n-1} f(X_k)}{\sqrt{n}} \right] \\ &= \left\langle \left(\frac{I+P}{I-P} \right) f, f \right\rangle_\pi \\ &= 2 \left\langle (I-P)^{-1} f, f \right\rangle_\pi - \langle f, f \rangle_\pi , \end{aligned}$$

for all f with $\pi(f) = 0$, where $\langle f, g \rangle$ is the weighted inner product defined by π. Note that the inverse $(I-P)^{-1}$ is taken over the space $\mathcal{N} = \{f : \pi(f) = 0\}$. Regarding P as a theoretical algorithm, we would like to find P such that $\nu(f, P, \pi)$ is small.

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(i) Minimize $\nu(P,\pi)$ over all $P \in \mathcal{R}$.
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(i) is solved by Frigessi et al. (1992), and (iv) is solved by Chen et al. (2012).

Theorem (Hwang 2005)

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Lemma

$$\mathit{Trace}(I-P)^{-1} = \sum_j \pi_j E_i(T_j)$$

where T_j is the first hitting time to state j.

Theorem (Chen et al. 2012)

$$tr(I - P_{N\times N})^{-1} \geq \sum_{i=1}^{N}(i-1)\pi_i.$$

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There are 2^{N-2} transition matrices reaching the minimum. Furthermore, for each transition matrix reaching the minimum,

$$p_{i,i} = \begin{cases} 0 & i < N \\ \frac{\pi_N - \pi_{N-1}}{\pi_N} & i = N \end{cases},$$

and one of the following holds:

1. $p_{1,2} = 1$ *and* $p_{i,1} = \frac{\pi_1}{\pi_i}$ *for some* i.
2. $p_{2,1} = \frac{\pi_1}{\pi_2}$ *and* $p_{1,j} = 1$ *for some* j

One of these optimal transition matrices is of the form:

$$P = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ \frac{\pi_1}{\pi_N} & \frac{\pi_2 - \pi_1}{\pi_N} & \frac{\pi_3 - \pi_2}{\pi_N} & \cdots & \frac{\pi_N - \pi_{N-1}}{\pi_N} \end{pmatrix}. \tag{2}$$

The transition rate $q_{i,j}$ is the rate that X_t from i to j.

$$\Pr(X_{t+h} = j | X_t = i) = q_{i,j}h + o(h).$$

Let $q_{i,i} \equiv -\sum_{j \neq i} q_{i,j}$. Then

$$\Pr(X_{t+h} = i | X_t = i) = 1 - q_{i,i}h + o(h).$$

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To minimize the averaged asymptotic variance is equivalent to minimize

$$\text{Mean of the first hitting time} = \sum_j \pi_j E_\pi(T_j) \quad (3)$$

$$= \sum_j \pi_j E_i(T_j) \qquad \forall i. \quad (4)$$

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Solve the equations above:

$$\begin{pmatrix} -\frac{1}{2\pi_1} & \frac{1}{2\pi_1} \\ \frac{1}{2\pi_2} & -\frac{1}{2\pi_2} \end{pmatrix}.$$

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Conjecture

For any transition rate matrix $Q_{N\times N} = (q_{i,j})_{N\times N}$ *which* π *is invariant to, if*

$$-\sum_i \pi_i q_{i,i} = 1, \tag{5}$$

then

$$\sum_{i=1}^{N} E_\pi(T_j) \geq N \sum_{i<j} \pi_i \pi_j. \tag{6}$$

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For the discrete-time

$$\sum_{i=1}^{N} E_\pi(T_j) \geq \sum_i (i-1)\pi_i.$$

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Lemma

$$E_i(T_i^+) = -\frac{1}{q_{ii}\pi_i}.$$

Theorem

For any transition rate matrix $Q_{N\times N} = (q_{i,j})_{N\times N}$ *which* π *is invariant to, if*

$$-\pi_i q_{i,i} = 1/N, \tag{7}$$

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$$\sum_{i=1}^{N} E_\pi(T_j) \geq N \sum_{i<j} \pi_i \pi_j. \tag{8}$$

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Then $E_1T_2 = 2\pi_1$, and

$$\pi_1E_1(T_1) + \pi_2E_2(T_2) = 2\pi_1\pi_2.$$

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To compare the case of $N = n + 1$ with $N = n$, we consider a new

process Y_t which is essentially X_t ignoring all the time staying in state 1.

Let $\tau_0 = 0$. Iteratively, define

$$\rho_{k+1} = \min_{t \geq \tau_k}\{t | X_t = 1\}$$

be the first time after τ_k that $X_t = 1$, and

$$\tau_{k+1} = \min_{t > \rho_{k+1}}\{t | X_t \neq 1\}$$

be the first time after ρ_{k+1} that $X_t \neq 1$. That is, $[\rho_k, \tau_k)$'s are the time intervals that $X_t = 1$. Now define

$$\sigma_t = \max_k\{k | \sum_{i=1}^{k}(\rho_i - \tau_{i-1}) < t\}$$

and

$$\eta_t = t - \sum_{i=1}^{\sigma_t}(\rho_i - \tau_{i-1}).$$

Then the time of $X_s \neq 1$ before $\tau_{\sigma_t} + \eta_t$ is t. Therefore, define $\{Y_t\}$ as

$$Y_t = X_{\tau_{\sigma_t} + \eta_t}.$$

Lemma

$\{Y_t\}$ is a Markov process on the state space $\{2, 3, \cdots, n+1\}$ with the transition matrix $R = (r_{i,j})$

$$r_{i,j} = q_{i,j} - \frac{q_{i,1} \cdot q_{1,j}}{q_{1,1}} \qquad \forall i, j.$$

Furthermore,

$$\mu R = 0,$$

with

$$\mu_i = \frac{\pi_i}{1 - \pi_1} \qquad 2 \le i \le n+1.$$

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Lemma

For $i \neq k$ and arbitrary j,

$$E_i(\textit{time staying in } j \textit{ before } T_k) = \pi_j(E_i(T_k) + E_k(T_j) - E_i(T_j)).$$

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$$-\sum_{i=2}^{n+1} \mu_i r_{i,i} \neq 1.$$

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$$\sum_{i=2}^{n+1} \mu_i E_\mu(S_i) \geq (1-\pi_1)\frac{n+1}{n} \cdot n \sum_{i<j} \mu_i \mu_j = \frac{1}{1-\pi_1}(n+1) \sum_{i<j \text{ and } i,j \neq 1} \pi_i \pi_j.$$

$$(1-\pi_1)[\sum_{i=1}^{n+1}\pi_i E_\pi(T_i)] - \pi_1 E_\pi(T_1) \geq (n+1)\sum_{i<j \text{ and } i,j\neq 1}\pi_i\pi_j.$$

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True of ignoring any k.

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Now take sum over k:

$$\sum_k \left[(1-\pi_k)[\sum_{i=1}^{n+1}\pi_i E_\pi(T_k)] - \pi_k E_\pi(T_k)\right] \geq (n+1)\sum_k \sum_{i<j \text{ and } i,j\neq k} \pi_i\pi_j.$$

$$Q = \begin{pmatrix} -\frac{1}{N\pi_1} & \frac{1}{N\pi_1} & 0 & \cdots & 0 \\ 0 & -\frac{1}{N\pi_2} & \frac{1}{N\pi_2} & \cdots & 0 \\ \vdots & 0 & \ddots & \ddots & \vdots \\ 0 & \vdots & \ddots & \ddots & \frac{1}{N\pi_{N-1}} \\ \frac{1}{N\pi_N} & 0 & \cdots & 0 & -\frac{1}{N\pi_N} \end{pmatrix}.$$

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$$E_1(T_i) = \sum_{j=1}^{i-1} E_j(T_{j+1}) = N \sum_{j=1}^{i-1} \pi_j.$$

Therefore,

$$\sum_i \pi_i E_1(T_i) = \sum_i \pi_i N \sum_{j=1}^{i-1} \pi_j = N \sum_{i<j} \pi_i \pi_j.$$

$$Q = \begin{pmatrix} -\frac{1}{N\pi_1} & \frac{1}{N\pi_1} & 0 & \cdots & 0 \\ 0 & -\frac{1}{N\pi_2} & \frac{1}{N\pi_2} & \cdots & 0 \\ \vdots & 0 & \ddots & \ddots & \vdots \\ 0 & \vdots & \ddots & \ddots & \frac{1}{N\pi_{N-1}} \\ \frac{1}{N\pi_N} & 0 & \cdots & 0 & -\frac{1}{N\pi_N} \end{pmatrix}.$$

Then $E_i(T_{i+1}) = N\pi_i$ for $i < N$.

$$E_1(T_i) = \sum_{j=1}^{i-1} E_j(T_{j+1}) = N \sum_{j=1}^{i-1} \pi_j.$$

Therefore,

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There are (N-1)! optimal transition rate matrices.

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Compare the results between Discrete and Continuous:

$$\begin{aligned} N\sum_{i<j}\pi_i\pi_j &= N\sum_{j=1}^{N}\sum_{i=1}^{j-1}\pi_i\pi_j \\ &= \sum_{j=1}^{N}\pi_j N\sum_{i=1}^{j-1}\pi_i \\ &\leq \sum_{j=1}^{N}\pi_j(j-1). \end{aligned}$$

The corresponding transition rate is $\pi_{N-1} + \sum_{k=1}^{N-1} \pi_k$.

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$$
\begin{aligned}
\pi_{N-1} + \sum_{k=1}^{N-1} \pi_k &= \sum_{k=1}^{j-1} \pi_k + \pi_{N-1} + \sum_{k=j}^{N-1} \pi_k \\
&\geq \sum_{k=1}^{j-1} \pi_k + (N-j+1) \cdot \frac{1}{j-1} \sum_{k=1}^{j-1} \pi_k = \frac{N}{j-1} \sum_{k=1}^{j-1} \pi_k,
\end{aligned}
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\pi_{N-1} + \sum_{k=1}^{N-1} \pi_k &= \sum_{k=1}^{j-1} \pi_k + \pi_{N-1} + \sum_{k=j}^{N-1} \pi_k \\
&\geq \sum_{k=1}^{j-1} \pi_k + (N-j+1) \cdot \frac{1}{j-1} \sum_{k=1}^{j-1} \pi_k = \frac{N}{j-1} \sum_{k=1}^{j-1} \pi_k,
\end{aligned}$$

$$\begin{aligned}
\frac{N}{\pi_{N-1} + \sum_{k=1}^{N-1} \pi_k} \sum_{i<j} \pi_i \pi_j &= \sum_{j=1}^{N} \pi_j N \sum_{i=1}^{j-1} \pi_i \frac{1}{\pi_{N-1} + \sum_{k=1}^{N-1} \pi_k} \\
&\leq \sum_{j=1}^{N} \pi_j N \sum_{i=1}^{j-1} \pi_i \frac{1}{\frac{N}{j-1} \sum_{k=1}^{j-1} \pi_k} \\
&= \sum_{j=1}^{N} \pi_j (j-1).
\end{aligned}$$

Thank You