8. 固有値とmixing time

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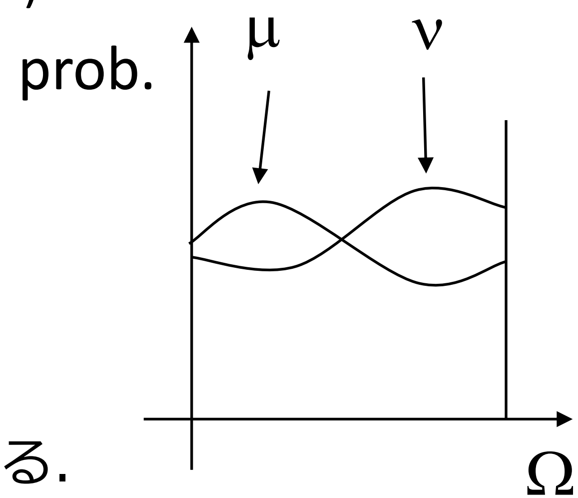
マルコフ連鎖のmixing time

誤差

- Ω上の分布μ, νの**総変動距離 (total variation distance)**

$$d_{\mathrm{TV}}(\mu,\nu) := \max_{Q\subseteq\Omega}\left\{\sum_{x\in Q}\big(\mu(x)-\nu(x)\big)\right\}$$
$$= \frac{1}{2}\sum_{x\in\Omega}|\mu(x)-\nu(x)|$$



- エルゴード的マルコフ連鎖Mの定常分布を$\boldsymbol{\pi}$とする.

$\epsilon\ (0<\epsilon<1)$に対して,

$$\tau(\epsilon) := \max_{x\in\Omega}\{\min\{t \mid \forall s \geq t, d_{\mathrm{TV}}(P_x^s, \pi) \leq \epsilon\}\}$$

をMの**mixing time**という.

- $\tau(\epsilon) \leq \mathrm{poly}(\log|\Omega|, \epsilon^{-1})$のとき, **rapidly mixing**という.

例題

例 3.

$$P=\begin{pmatrix}1/3 & 1/2 & 1/6\\ 1/2 & 1/6 & 1/3\\ 1/6 & 1/3 & 1/2\end{pmatrix}$$ のP^nを求めよ.

Pを対角化する．特性方程式を立てると.

$$\left(\frac{1}{3}-\lambda\right)\left(\frac{1}{6}-\lambda\right)\left(\frac{1}{2}-\lambda\right)+\frac{1}{2}\cdot\frac{1}{3}\cdot\frac{1}{6}+\frac{1}{6}\cdot\frac{1}{2}\cdot\frac{1}{3}-\left(\frac{1}{3}-\lambda\right)\frac{1}{3}\cdot\frac{1}{3}-\frac{1}{2}\cdot\frac{1}{2}\left(\frac{1}{2}-\lambda\right)-\frac{1}{6}\left(\frac{1}{6}-\lambda\right)\frac{1}{6}$$

$$=-\lambda^3+\lambda^2-\frac{11}{36}\lambda+\frac{1}{36}+\frac{1}{36}+\frac{1}{36}-\frac{1}{9}\left(\frac{1}{3}-\lambda\right)-\frac{1}{4}\left(\frac{1}{2}-\lambda\right)-\frac{1}{36}\left(\frac{1}{6}-\lambda\right)$$

$$=-\lambda^3+\lambda^2+\frac{1}{12}\lambda-\frac{1}{12}=(1-\lambda)\left(\lambda^2-\frac{1}{12}\right)=(1-\lambda)\left(\frac{\sqrt{3}}{6}-\lambda\right)\left(-\frac{\sqrt{3}}{6}-\lambda\right)$$

固有値と右固有ベクトルは $\left(1,\begin{pmatrix}1\\1\\1\end{pmatrix}\right),\left(\frac{\sqrt{3}}{6},\begin{pmatrix}2\\ \sqrt{3}-1\\ -\sqrt{3}-1\end{pmatrix}\right),\left(-\frac{\sqrt{3}}{6},\begin{pmatrix}2\\ -\sqrt{3}-1\\ \sqrt{3}-1\end{pmatrix}\right)$

$$\begin{pmatrix}\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}}\\ \frac{2}{\sqrt{12}} & \frac{\sqrt{3}-1}{\sqrt{12}} & \frac{-\sqrt{3}-1}{\sqrt{12}}\\ \frac{2}{\sqrt{12}} & \frac{-\sqrt{3}-1}{\sqrt{12}} & \frac{\sqrt{3}-1}{\sqrt{12}}\end{pmatrix}\begin{pmatrix}\frac{1}{3} & \frac{1}{2} & \frac{1}{6}\\ \frac{1}{2} & \frac{1}{6} & \frac{1}{3}\\ \frac{1}{6} & \frac{1}{3} & \frac{1}{2}\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{3}} & \frac{2}{\sqrt{12}} & \frac{2}{\sqrt{12}}\\ \frac{1}{\sqrt{3}} & \frac{\sqrt{3}-1}{\sqrt{12}} & \frac{-\sqrt{3}-1}{\sqrt{12}}\\ \frac{1}{\sqrt{3}} & \frac{-\sqrt{3}-1}{\sqrt{12}} & \frac{\sqrt{3}-1}{\sqrt{12}}\end{pmatrix}=\begin{pmatrix}1 & 0 & 0\\ 0 & \frac{\sqrt{3}}{6} & 0\\ 0 & 0 & \frac{-\sqrt{3}}{6}\end{pmatrix}$$

例題

例 3.

$P=\begin{pmatrix}1/3 & 1/2 & 1/6\\ 1/2 & 1/6 & 1/3\\ 1/6 & 1/3 & 1/2\end{pmatrix}$ の P^n を求めよ.

$$\begin{pmatrix}\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}}\\ \frac{2}{\sqrt{12}} & \frac{\sqrt{3}-1}{\sqrt{12}} & \frac{-\sqrt{3}-1}{\sqrt{12}}\\ \frac{2}{\sqrt{12}} & \frac{-\sqrt{3}-1}{\sqrt{12}} & \frac{\sqrt{3}-1}{\sqrt{12}}\end{pmatrix}\begin{pmatrix}\frac{1}{3} & \frac{1}{2} & \frac{1}{6}\\ \frac{1}{2} & \frac{1}{6} & \frac{1}{3}\\ \frac{1}{6} & \frac{1}{3} & \frac{1}{2}\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{3}} & \frac{2}{\sqrt{12}} & \frac{2}{\sqrt{12}}\\ \frac{1}{\sqrt{3}} & \frac{\sqrt{3}-1}{\sqrt{12}} & \frac{-\sqrt{3}-1}{\sqrt{12}}\\ \frac{1}{\sqrt{3}} & \frac{-\sqrt{3}-1}{\sqrt{12}} & \frac{\sqrt{3}-1}{\sqrt{12}}\end{pmatrix}=\begin{pmatrix}1 & 0 & 0\\ 0 & \frac{\sqrt{3}}{6} & 0\\ 0 & 0 & \frac{-\sqrt{3}}{6}\end{pmatrix}$$

したがって,

$$P^n=\begin{pmatrix}\frac{1}{\sqrt{3}} & \frac{2}{\sqrt{12}} & \frac{2}{\sqrt{12}}\\ \frac{1}{\sqrt{3}} & \frac{\sqrt{3}-1}{\sqrt{12}} & \frac{-\sqrt{3}-1}{\sqrt{12}}\\ \frac{1}{\sqrt{3}} & \frac{-\sqrt{3}-1}{\sqrt{12}} & \frac{\sqrt{3}-1}{\sqrt{12}}\end{pmatrix}\begin{pmatrix}1^n & 0 & 0\\ 0 & \left(\frac{\sqrt{3}}{6}\right)^n & 0\\ 0 & 0 & \left(\frac{-\sqrt{3}}{6}\right)^n\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}}\\ \frac{2}{\sqrt{12}} & \frac{\sqrt{3}-1}{\sqrt{12}} & \frac{-\sqrt{3}-1}{\sqrt{12}}\\ \frac{2}{\sqrt{12}} & \frac{-\sqrt{3}-1}{\sqrt{12}} & \frac{\sqrt{3}-1}{\sqrt{12}}\end{pmatrix}$$

$n\to\infty$ を考えると.

$$P^\infty=\begin{pmatrix}1/3 & 1/3 & 1/3\\ 1/3 & 1/3 & 1/3\\ 1/3 & 1/3 & 1/3\end{pmatrix}$$

mixing timeは第2固有値で決まる

定理 8.1. (上界).

Lazyな**reversible**マルコフ連鎖に対して,

$$\boldsymbol{\tau(\varepsilon)} \leq \frac{\ln \pi_{\min}^{-1} + \ln \varepsilon^{-1}}{1 - \lambda_2}$$

ただし$\pi_{\min} = \min_{i \in \Omega} \pi_i$, λ_2はPの**第二固有値**.

定理 8.2. (下界).

Lazyなreversibleマルコフ連鎖に対して,

$$\tau(\varepsilon) \geq \frac{\lambda_2 \ln\left((2\varepsilon)^{-1}\right)}{2(1 - \lambda_2)}$$

準備 1

- 有限マルコフ連鎖Mが**lazy**
  - 任意の$i \in \Omega$に対して，$p_{ii} \geq \frac{1}{2}$.

補題 8.3.
Reversibleマルコフ連鎖$M = (\Omega, P)$はlazyとする．
このとき，Pは半正定値(すべての固有値は実数で非負).

証明の概略

$P' = 2P - I$は確率行列．さらにマルコフ連鎖$M' = (\Omega, P')$はreversible．Reversibleマルコフ連鎖は実対角化可能(後述)．また，Gershgorinの定理からP'の固有値λ'_iはすべて$-1 \leq \lambda'_i \leq 1$．$P = \frac{P'+I}{2}$より，$P$の固有値は$\frac{\lambda'_i+1}{2}$となり，非負.

まとめ:

Pはreversibleかつlazyとする.

- ✓ Pの固有値はすべて実数．$\lambda_1 \geq \cdots \geq \lambda_n$とする.
- ✓ $\lambda_1 = 1$
- ✓ $\lambda_2 < 1$ (Perron-Frobeniusの定理; λ_2を**第二固有値**という)
- ✓ $\lambda_n \geq 0$

準備 2

補題 8.4.

reversibleマルコフ連鎖の推移確率行列Pは実対角化可能.

$$\Pi^{\frac{1}{2}} := \mathrm{diag}(\sqrt{\pi_1}, \sqrt{\pi_2}, \dots, \sqrt{\pi_n})$$

$$\Pi^{-\frac{1}{2}} := \mathrm{diag}\left(\frac{1}{\sqrt{\pi_1}}, \frac{1}{\sqrt{\pi_2}}, \dots, \frac{1}{\sqrt{\pi_n}}\right)$$

$$\Pi^{\frac{1}{2}} P \Pi^{-\frac{1}{2}} = \begin{pmatrix} \sqrt{\pi_1} & & 0 \\ & \sqrt{\pi_2} & \\ 0 & & \sqrt{\pi_n} \end{pmatrix} (p_{ij}) \begin{pmatrix} \frac{1}{\sqrt{\pi_1}} & & 0 \\ & \frac{1}{\sqrt{\pi_2}} & \\ 0 & & \frac{1}{\sqrt{\pi_n}} \end{pmatrix} = \left(\sqrt{\frac{\pi_i}{\pi_j}} p_{ij}\right)$$

!

$$= \left(\sqrt{\frac{p_{ji}}{p_{ij}}} p_{ij}\right) = \left(\sqrt{p_{ij} p_{ji}}\right)$$

$$[\pi_i p_{ij} = \pi_j p_{ji}] \Leftrightarrow \left[\frac{\pi_i}{\pi_j} = \frac{p_{ji}}{p_{ij}}\right]$$

$\Pi^{\frac{1}{2}} P \Pi^{-\frac{1}{2}}$は実対称行列なので，対角化できる.

!

$$\Pi^{\frac{1}{2}} P \Pi^{-\frac{1}{2}} = \begin{pmatrix} \sqrt{\pi_1} & & & 0 \\ & \sqrt{\pi_2} & & \\ & & \ddots & \\ 0 & & & \sqrt{\pi_n} \end{pmatrix} (p_{ij}) \begin{pmatrix} \frac{1}{\sqrt{\pi_1}} & & & 0 \\ & \frac{1}{\sqrt{\pi_2}} & & \\ & & \ddots & \\ 0 & & & \frac{1}{\sqrt{\pi_n}} \end{pmatrix}$$

$$= \begin{pmatrix} \sqrt{\pi_1} & & & 0 \\ & \sqrt{\pi_2} & & \\ & & \ddots & \\ 0 & & & \sqrt{\pi_n} \end{pmatrix} \left(\begin{array}{c|c|c|c} \frac{p_{11}}{\sqrt{\pi_1}} & \frac{p_{12}}{\sqrt{\pi_2}} & \cdots & \frac{p_{1n}}{\sqrt{\pi_n}} \\ \frac{p_{21}}{\sqrt{\pi_1}} & \frac{p_{22}}{\sqrt{\pi_2}} & \cdots & \frac{p_{2n}}{\sqrt{\pi_n}} \\ \vdots & \vdots & & \vdots \\ \frac{p_{n1}}{\sqrt{\pi_1}} & \frac{p_{n2}}{\sqrt{\pi_2}} & \cdots & \frac{p_{nn}}{\sqrt{\pi_n}} \end{array} \right)$$

$$= \begin{pmatrix} \sqrt{\frac{\pi_1}{\pi_1}} p_{11} & \sqrt{\frac{\pi_1}{\pi_2}} p_{12} & \cdots & \sqrt{\frac{\pi_1}{\pi_n}} p_{1n} \\ \sqrt{\frac{\pi_2}{\pi_1}} p_{21} & \sqrt{\frac{\pi_2}{\pi_2}} p_{22} & \cdots & \sqrt{\frac{\pi_2}{\pi_n}} p_{2n} \\ \vdots & \vdots & & \vdots \\ \sqrt{\frac{\pi_n}{\pi_1}} p_{n1} & \sqrt{\frac{\pi_n}{\pi_2}} p_{n2} & \cdots & \sqrt{\frac{\pi_n}{\pi_n}} p_{nn} \end{pmatrix}$$

準備3

補題 8.5.

$$\max_x(\mu_x - \nu_x) \le d_{\mathrm{TV}}(\mu,\nu) \le \max_x\left(1 - \frac{\nu_x}{\mu_x}\right)$$

$$\begin{aligned} d_{\mathrm{TV}}(\mu,\nu) &= \sum_{x\in\Omega:\mu_x>\nu_x} (\mu_x - \nu_x) \\ &\ge \max_{x\in\Omega}(\mu_x - \nu_x) \end{aligned}$$

$$\begin{aligned} d_{\mathrm{TV}}(\mu,\nu) &= \sum_{x\in\Omega:\mu_x>\nu_x} (\mu_x - \nu_x) \\ &= \sum_{x\in\Omega:\mu_x>\nu_x} \mu_x\left(1 - \frac{\nu_x}{\mu_x}\right) \\ &\le \max_{x\in\Omega}\left(1 - \frac{\nu_x}{\mu_x}\right) \sum_{x\in\Omega:\mu_x>\nu_x} \mu_x \\ &\le \max_{x\in\Omega}\left(1 - \frac{\nu_x}{\mu_x}\right) \end{aligned}$$

上界の証明（アウトライン）

定理 8.1 (上界).

Lazyな**reversible**マルコフ連鎖に対して,

$$\boldsymbol{\tau(\varepsilon)} \leq \frac{\ln \pi_{\min}^{-1} + \ln \varepsilon^{-1}}{1 - \lambda_2}$$

ただし$\pi_{\min} = \min_{i \in \Omega} \pi_i$, λ_2はPの**第二固有値**.

証明の方針 (proof strategy)

- ■ Perron FrobeniusよりPの最大固有値は1.
  それ以外は1未満 (済みとする).
- □ $(P^t)_{ij} = \pi_j + \sqrt{\frac{\pi_j}{\pi_i}} \sum_{k=2}^{n} \lambda_k^t b_{ki} b_{kj}$.
  ただしb_{ij}は$\Pi^{\frac{1}{2}} P \Pi^{-\frac{1}{2}}$の固有ベクトルの成分.
- □ $d_{\mathrm{TV}}\left(P_{i\cdot}^t, \boldsymbol{\pi}\right) = \sum_{j=1}^{n} |(P^t)_{ij} - \pi_j| \leq \frac{\lambda_2^t}{\pi_{\min}}$.
- □ $\frac{\lambda_2^{\tau^*}}{\pi_{\min}} \leq \epsilon$.

上界の証明 1/5

$\Pi^{\frac{1}{2}} P \Pi^{-\frac{1}{2}}$は実対称行列なので，対角化できる．

$$\Pi^{\frac{1}{2}} P \Pi^{-\frac{1}{2}} = B^\top \Lambda B$$
$$= \sum_{k=1}^{n} \lambda_k \begin{pmatrix} b_{k1} \\ \vdots \\ b_{kn} \end{pmatrix} (b_{k1}, \ldots, b_{kn})$$
$$= \sum_{k=1}^{n} \lambda_k \, \boldsymbol{b}_{\boldsymbol{k}}^\top \boldsymbol{b}_{\boldsymbol{k}} \, .$$

ただし，

- $1 = \lambda_1 > \lambda_2 \geq \cdots \geq \lambda_n \geq 0$,
- $B = \begin{pmatrix} \boldsymbol{b}_1 \\ \vdots \\ \boldsymbol{b}_n \end{pmatrix}$.

このとき，Bは**直交行列**に注意 (線形代数).

$$
\begin{aligned}
\Pi^{\frac{1}{2}} P \Pi^{-\frac{1}{2}} &= B^\top \Lambda B \\
&= \left(\begin{array}{c|c|c|c} b_{11} & b_{21} & \cdots & b_{n1} \\ b_{12} & b_{22} & \cdots & b_{n2} \\ \vdots & \vdots & & \vdots \\ b_{1n} & b_{2n} & \cdots & b_{nn} \end{array}\right) \begin{pmatrix} \lambda_1 & & & 0 \\ & \lambda_2 & & \\ & & \ddots & \\ 0 & & & \lambda_n \end{pmatrix} \left(\begin{array}{cccc} b_{11} & b_{12} & \cdots & b_{1n} \\ \hline b_{21} & b_{22} & \cdots & b_{2n} \\ \hline \vdots & \vdots & & \vdots \\ \hline b_{n1} & b_{n2} & \cdots & b_{nn} \end{array}\right) \\
&= \left(\begin{array}{c|c|c|c} b_{11} & b_{21} & \cdots & b_{n1} \\ b_{12} & b_{22} & \cdots & b_{n2} \\ \vdots & \vdots & & \vdots \\ b_{1n} & b_{2n} & \cdots & b_{nn} \end{array}\right) \left(\begin{array}{cccc} \lambda_1 b_{11} & \lambda_1 b_{12} & \cdots & \lambda_1 b_{1n} \\ \hline \lambda_2 b_{21} & \lambda_2 b_{22} & \cdots & \lambda_2 b_{2n} \\ \hline \vdots & \vdots & & \vdots \\ \hline \lambda_n b_{n1} & \lambda_n b_{n2} & \cdots & \lambda_n b_{nn} \end{array}\right) \\
&= \begin{pmatrix} \sum_{k=1}^{n} \lambda_k b_{k1}^2 & \sum_{k=1}^{n} \lambda_k b_{k1} b_{k2} & \cdots & \sum_{k=1}^{n} \lambda_k b_{k1} b_{kn} \\ \sum_{k=1}^{n} \lambda_k b_{k2} b_{k1} & \sum_{k=1}^{n} \lambda_k b_{k2}^2 & \cdots & \sum_{k=1}^{n} \lambda_k b_{kn} b_{k1} \\ \vdots & \vdots & & \vdots \\ \sum_{k=1}^{n} \lambda_k b_{kn} b_{k1} & \sum_{k=1}^{n} \lambda_k b_{kn} b_{k2} & \cdots & \sum_{k=1}^{n} \lambda_k b_{kn}^2 \end{pmatrix} \\
&= \sum_{k=1}^{n} \lambda_k \begin{pmatrix} b_{k1}^2 & b_{k1} b_{k2} & \cdots & b_{k1} b_{kn} \\ b_{k2} b_{k1} & b_{k2}^2 & \cdots & b_{k2} b_{kn} \\ \vdots & \vdots & & \vdots \\ b_{kn} b_{k1} & b_{kn} b_{k2} & \cdots & b_{kn}^2 \end{pmatrix} \\
&= \sum_{k=1}^{n} \lambda_k \boldsymbol{b}_k^\top \boldsymbol{b}_k
\end{aligned}
$$

上界の証明 2/5

このとき，Bは**直交行列**に注意 (線形代数).

補題 8.6.(直交行列の基本性質)

- $|b_{ij}| \leq 1$
- $\sum_{k=1}^{n} b_{ki} b_{kj} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$

補題 8.7.

$\Pi^{\frac{1}{2}} P \Pi^{-\frac{1}{2}}$の固有値1の固有ベクトルは

$$\boldsymbol{b}_{\boldsymbol{1}} = (\sqrt{\pi_1}, \ldots, \sqrt{\pi_n})$$

証明

$\Pi^{\frac{1}{2}} P \Pi^{-\frac{1}{2}} = \left(\sqrt{p_{ij} p_{ji}}\right)$より，

$$\boldsymbol{b}_{\boldsymbol{1}} \Pi^{\frac{1}{2}} P \Pi^{-\frac{1}{2}} \boldsymbol{b}_{\boldsymbol{1}}^{\top} = \sum_{i=1}^{n} \sum_{j=1}^{n} \sqrt{\pi_i} \sqrt{p_{ij} p_{ji}} \sqrt{\pi_j} = \sum_{i=1}^{n} \sum_{j=1}^{n} \pi_i p_{ij} = \sum_{i=1}^{n} \pi_i = 1.$$

上界の証明 3/5

補題 8.8.

$$(P^t)_{ij} = \pi_j + \sqrt{\frac{\pi_j}{\pi_i}} \sum_{k=2}^{n} \lambda_k^t b_{ki} b_{kj}$$

$$P^t = \Pi^{-\frac{1}{2}} B^\top \Lambda^t B \Pi^{\frac{1}{2}}$$

$$= \sum_{k=1}^{n} \lambda_k^t \, \Pi^{-\frac{1}{2}} \begin{pmatrix} b_{k1} \\ \vdots \\ b_{kn} \end{pmatrix} (b_{k1}, \dots, b_{kn}) \Pi^{\frac{1}{2}}$$

!!

P^tの各要素は

$$(P^t)_{ij} = \sqrt{\frac{\pi_j}{\pi_i}} \sum_{k=1}^{n} \lambda_k^t b_{ki} b_{kj}$$

$$= \sqrt{\frac{\pi_j}{\pi_i}} b_{1i} b_{1j} + \sqrt{\frac{\pi_j}{\pi_i}} \sum_{k=2}^{n} \lambda_k^t b_{ki} b_{kj}$$

$$= \pi_j + \sqrt{\frac{\pi_j}{\pi_i}} \sum_{k=2}^{n} \lambda_k^t b_{ki} b_{kj}$$

補題 7.

$\Pi^{\frac{1}{2}} P \Pi^{-\frac{1}{2}}$の固有値1の固有ベクトルは

$$\boldsymbol{b_1} = (\sqrt{\pi_1}, \dots, \sqrt{\pi_n})$$

!!

$$
\begin{aligned}
P^t &= \Pi^{-\frac{1}{2}} B^\top \Lambda^t B \Pi^{\frac{1}{2}} \\
&= \sum_{k=1}^{n} \lambda_k^t \begin{pmatrix} \frac{1}{\sqrt{\pi_1}} & & & 0 \\ & \frac{1}{\sqrt{\pi_2}} & & \\ & & \ddots & \\ 0 & & & \frac{1}{\sqrt{\pi_n}} \end{pmatrix} \begin{pmatrix} b_{k1}^2 & b_{k1}b_{k2} & \cdots & b_{k1}b_{kn} \\ b_{k2}b_{k1} & b_{k2}^2 & \cdots & b_{k2}b_{kn} \\ \vdots & \vdots & & \vdots \\ b_{kn}b_{k1} & b_{kn}b_{k2} & \cdots & b_{kn}^2 \end{pmatrix} \begin{pmatrix} \sqrt{\pi_1} & & & 0 \\ & \sqrt{\pi_2} & & \\ & & \ddots & \\ 0 & & & \sqrt{\pi_n} \end{pmatrix} \\
&= \sum_{k=1}^{n} \lambda_k^t \begin{pmatrix} \frac{1}{\sqrt{\pi_1}} & & & 0 \\ & \frac{1}{\sqrt{\pi_2}} & & \\ & & \ddots & \\ 0 & & & \frac{1}{\sqrt{\pi_n}} \end{pmatrix} \begin{pmatrix} \sqrt{\pi_1} b_{k1}^2 & \sqrt{\pi_2} b_{k1}b_{k2} & \cdots & \sqrt{\pi_n} b_{k1}b_{kn} \\ \sqrt{\pi_1} b_{k2}b_{k1} & \sqrt{\pi_2} b_{k2}^2 & \cdots & \sqrt{\pi_n} b_{k2}b_{kn} \\ \vdots & \vdots & & \vdots \\ \sqrt{\pi_1} b_{kn}b_{k1} & \sqrt{\pi_2} b_{kn}b_{i2} & \cdots & \sqrt{\pi_n} b_{kn}^2 \end{pmatrix} \\
&= \sum_{k=1}^{n} \lambda_k^t \begin{pmatrix} \sqrt{\frac{\pi_1}{\pi_1}} b_{k1}^2 & \sqrt{\frac{\pi_2}{\pi_1}} b_{k1}b_{k2} & \cdots & \sqrt{\frac{\pi_n}{\pi_1}} b_{k1}b_{kn} \\ \sqrt{\frac{\pi_1}{\pi_2}} b_{k2}b_{k1} & \sqrt{\frac{\pi_2}{\pi_2}} b_{k2}^2 & \cdots & \sqrt{\frac{\pi_n}{\pi_2}} b_{k2}b_{kn} \\ \vdots & \vdots & & \vdots \\ \sqrt{\frac{\pi_1}{\pi_n}} b_{kn}b_{k1} & \sqrt{\frac{\pi_2}{\pi_n}} b_{kn}b_{k2} & \cdots & \sqrt{\frac{\pi_n}{\pi_n}} b_{kn}^2 \end{pmatrix}
\end{aligned}
$$

上界の証明 4/5

$$
\begin{aligned}
d_{\mathrm{TV}}\left(P_{i\cdot}^t, \boldsymbol{\pi}\right) &= \frac{1}{2}\sum_{j=1}^{n}\left|P_{ij}^t - \pi_j\right| \\
&\leq \max_j \frac{\left|P_{ij}^t - \pi_j\right|}{\pi_j} \\
&= \max_j \left(\frac{1}{\pi_j}\left|\sqrt{\frac{\pi_j}{\pi_i}}\sum_{k=2}^{n}\lambda_k^t b_{ki} b_{kj}\right|\right) \\
&= \max_j \left(\left|\frac{1}{\sqrt{\pi_i \pi_j}}\sum_{k=2}^{n}\lambda_k^t b_{ki} b_{kj}\right|\right) \\
&\leq \lambda_2^t \max_j \left(\left|\frac{1}{\sqrt{\pi_i \pi_j}}\sum_{k=2}^{n} b_{ki} b_{kj}\right|\right) \\
&\leq \lambda_2^t \max_j \left(\frac{1}{\sqrt{\pi_i \pi_j}}\right) \\
&\leq \lambda_2^t \max_j \left(\frac{1}{\pi_j}\right) \\
&= \frac{\lambda_2^t}{\pi_{\min}}
\end{aligned}
$$

補題 8.5.

$$\max_x (\mu_x - \nu_x) \leq d_{\mathrm{TV}}(\mu, \nu) \leq \max_x \left(1 - \frac{\nu_x}{\mu_x}\right)$$

補題 8.8.

$$(P^t)_{ij} = \pi_j + \sqrt{\frac{\pi_j}{\pi_i}}\sum_{k=2}^{n}\lambda_k^t b_{ki} b_{kj}$$

補題 8.6.(直交行列の基本性質)

- $\left|b_{ij}\right| \leq 1$
- $\sum_{k=1}^{n} b_{ki} b_{kj} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$

上界の証明 5/5

定理 8.1 (上界).
Lazyな**reversible**マルコフ連鎖に対して,

$$\boldsymbol{\tau(\varepsilon)} \le \frac{\ln \pi_{\min}^{-1} + \ln \varepsilon^{-1}}{1-\lambda_2}$$

ただし$\pi_{\min} = \min_{i\in\Omega} \pi_i$, λ_2はPの**第二固有値**.

$\tau^* = \frac{\ln \pi_{\min}^{-1} + \ln \varepsilon^{-1}}{1-\lambda_2}$とおいて,

$$\frac{\lambda_2^{\tau^*}}{\pi_{\min}} \le \frac{1}{\pi_{\min}} \lambda_2^{\frac{\ln \pi_{\min}^{-1} + \ln \epsilon^{-1}}{1-\lambda_2}}$$

$$\le \frac{1}{\pi_{\min}} \exp\left(\frac{\ln \lambda_2}{1-\lambda_2}\left(\ln \pi_{\min}^{-1} + \ln \epsilon^{-1}\right)\right)$$

$$\le \frac{1}{\pi_{\min}} \exp\left(-\left(\ln \pi_{\min}^{-1} + \ln \epsilon^{-1}\right)\right)$$

$$= \epsilon$$

$x^{\frac{1}{1-x}} \le e^{-1} \quad (\because x \le e^{x-1})$

□

定理 8.2 (下界).

Lazyなreversibleマルコフ連鎖に対して，

$$\tau(\varepsilon) \geq \frac{\lambda_2 \ln\left((2\varepsilon)^{-1}\right)}{2(1-\lambda_2)}$$

補題 8.5.

$$\max_x(\mu_x - \nu_x) \leq d_{\mathrm{TV}}(\mu, \nu) \leq \max_x \left(1 - \frac{\nu_x}{\mu_x}\right)$$

証明

$$\begin{aligned} d_{\mathrm{TV}}\left(P_{i\cdot}^t, \boldsymbol{\pi}\right) &\geq \max_j \left|P_{ij}^t - \pi_j\right| \\ &\geq \left|\pi_i - P_{ii}^t\right| \\ &= \left|-\sqrt{\frac{\pi_i}{\pi_i}} \sum_{k=2}^n \lambda_k^t b_{ki} b_{ki}\right| \\ &= \left|\sum_{k=2}^n \lambda_k^t b_{ki}^2\right| \\ &\geq \lambda_2^t \end{aligned}$$

上界同様，代入して題意を得る． □

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おわり