



# Analysis of non-reversible Markov chains

Michael Choi

Cornell University  
School of ORIE  
cc2373@cornell.edu

May 22, 2017



# Introduction

---

- Consider a Markov chain  $P$  with time-reversal  $\hat{P}$  on state space  $\mathcal{X}$

# Introduction

---

- Consider a Markov chain  $P$  with time-reversal  $\hat{P}$  on state space  $\mathcal{X}$
- Non-reversible Markov chains are of great theoretical and applied interest

# Introduction

---

- Consider a Markov chain  $P$  with time-reversal  $\hat{P}$  on state space  $\mathcal{X}$
- Non-reversible Markov chains are of great theoretical and applied interest
- The major theoretical challenge is to analyze non-self-adjoint operators

# Introduction

---

- Consider a Markov chain  $P$  with time-reversal  $\hat{P}$  on state space  $\mathcal{X}$
- Non-reversible Markov chains are of great theoretical and applied interest
- The major theoretical challenge is to analyze non-self-adjoint operators
- From a Markov chain Monte Carlo perspective, it has been demonstrated that non-reversibility can improve the rate of convergence:
  - Hwang et al. '93 and '05: acceleration by adding anti-symmetric drift
  - Diaconis et al. '00: proposes a non-reversible sampler
  - Sun et al. '10, Bierkens '16: non-reversible Metropolis-Hastings by vortices/perturbations
  - Duncan et al. '13: non-reversible Langevin samplers

## Literature review

---

A historical account for analyzing non-reversible Markov chains:

- Kendall '59: dilation by Sz.-Nagy's dilation theorem
- Fill '91, Paulin '15: reversiblizations
- Kontoyiannis and Meyn '12: recasting to a weighted- $L^\infty$  space
- Patie and Savov '15, Miclo '16, Choi and Patie '16: intertwining/similarity orbit

We will focus on the similarity orbit and the reversiblization approach today.

- 1 Introduction
- 2 Analysis of non-reversible Markov chains via similarity orbit
- 3 Metropolis-Hastings reversiblizations
- 4 Summary

# The $\mathcal{S}$ class

---

Definition (The  $\mathcal{S}$  class: A class of Markov chain Similar to normal Markov chain)

We say that  $P \in \mathcal{S}$  if

$$P\Lambda = \Lambda Q$$

where

- $P$ : transition kernel of **general** chain on  $\mathcal{X}$
- $\Lambda$ : a bounded link kernel with bounded inverse
- $Q$ : transition kernel of **normal** chain, i.e.  $Q\hat{Q} = \hat{Q}Q$ .



## The $\mathcal{S}$ class

---

Definition (The  $\mathcal{S}$  class: A class of Markov chain Similar to normal Markov chain)

We say that  $P \in \mathcal{S}$  if

$$P\Lambda = \Lambda Q$$

where

- $P$ : transition kernel of **general** chain on  $\mathcal{X}$
- $\Lambda$ : a bounded link kernel with bounded inverse
- $Q$ : transition kernel of **normal** chain, i.e.  $Q\hat{Q} = \hat{Q}Q$ .

Remark: Recall that we analyzed the spectral theory where  $P$  is upward skip-free and  $Q$  is a birth-death chain

## The $\mathcal{S}$ class

---

Definition (The  $\mathcal{S}$  class: A class of Markov chain Similar to normal Markov chain)

We say that  $P \in \mathcal{S}$  if

$$P\Lambda = \Lambda Q$$

where

- $P$ : transition kernel of **general** chain on  $\mathcal{X}$
- $\Lambda$ : a bounded link kernel with bounded inverse
- $Q$ : transition kernel of **normal** chain, i.e.  $Q\hat{Q} = \hat{Q}Q$ .

Remark: If  $\Lambda$  is a Markov kernel, then  $P$  and  $Q$  are said to be intertwined by the link  $\Lambda$ .

- ① Introduction
  
- ② Analysis of non-reversible Markov chains via similarity orbit
  - (i). Spectral theory
  - (ii). Convergence to equilibrium
  - (iii). Example: Ehrenfest model
  - (iv). Cutoff phenomena
  
- ③ Metropolis-Hastings reversiblizations
  
- ④ Summary

# The $\mathcal{S}$ class: Spectral theory

## Theorem

Assume that  $P \in \mathcal{S}$  with  $P \stackrel{\Lambda}{\sim} Q$ . Then the following holds.

- Denote the self-adjoint spectral measure of  $Q$  by  $\mathcal{E} = \{E_B; B \in \mathcal{B}(\mathbb{C})\}$ , then  $\{F_B := \Lambda E_B \Lambda^{-1}; B \in \mathcal{B}(\mathbb{C})\}$  defines a spectral measure and  $P$  is a spectral scalar-type operator with spectral resolution given by

$$P = \int_{\sigma(P)} \lambda dF_\lambda,$$

$$\widehat{P} = \int_{\sigma(\widehat{P})} \lambda dF_\lambda^*.$$

Note that

$$\sigma(P) = \sigma(Q), \sigma(P) = \overline{\sigma(\widehat{P})}, \sigma_c(P) = \sigma_c(Q), \sigma_p(P) = \sigma_p(Q), \sigma_r(P) = \sigma_r(Q),$$

and the multiplicity of each eigenvalue in  $\sigma_p(P)$  is the same as that of  $\sigma_p(Q)$ .

# The $\mathcal{S}$ class: Spectral theory

---

## Theorem

Assume that  $P \in \mathcal{S}$  with  $P \stackrel{\Delta}{\sim} Q$ . Then the following holds.

- For analytic and single valued function  $f$  on  $\sigma(P)$ , we have

$$f(P) = \int_{\sigma(P)} f(\lambda) dF_{\lambda}.$$

# The $\mathcal{S}$ class: Spectral theory

## Theorem

Assume that  $P \in \mathcal{S}$  with  $P \stackrel{\Delta}{\sim} Q$ . Then the following holds.

- In particular, if  $P$  is compact on  $\mathcal{X} = \llbracket 0, \mathfrak{r} \rrbracket$  with distinct eigenvalues then for any  $f \in \ell^2(\pi)$  and  $n \in \mathbb{N}$ ,

$$P^n f = \sum_{k=0}^{\mathfrak{r}} \lambda_k^n \langle f, f_k^* \rangle_{\pi} f_k,$$

where the set  $(f_k)_{k=0}^{\mathfrak{r}}$  are eigenfunctions of  $P$  associated to the eigenvalues  $(\lambda_k)_{k=0}^{\mathfrak{r}}$  and form a Riesz basis of  $\ell^2(\pi)$ , and the set  $(f_k^*)_{k=0}^{\mathfrak{r}}$  is the unique Riesz basis biorthogonal to  $(f_k)_{k=0}^{\mathfrak{r}}$ . For any  $x, y \in \mathcal{X}$  and  $n \in \mathbb{N}$ , the spectral expansion of  $P$  is given by

$$P^n(x, y) = \sum_{k=0}^{\mathfrak{r}} \lambda_k^n f_k(x) f_k^*(y) \pi(y).$$

# The $\mathcal{S}$ class: Spectral theory

---

**Eigentime identity** (Aldous and Fill '02, Cui and Mao '10, Miclo '15):

1. Sample two points  $x, y$  independently from  $\pi$

# The $\mathcal{S}$ class: Spectral theory

---

**Eigentime identity** (Aldous and Fill '02, Cui and Mao '10, Miclo '15):

1. Sample two points  $x, y$  independently from  $\pi$
2. Calculate the expected hitting time from  $x$  to  $y$ :  $\mathbb{E}_x(\tau_y)$



# The $\mathcal{S}$ class: Spectral theory

---

**Eigentime identity** (Aldous and Fill '02, Cui and Mao '10, Miclo '15):

1. Sample two points  $x, y$  independently from  $\pi$
2. Calculate the expected hitting time from  $x$  to  $y$ :  $\mathbb{E}_x(\tau_y)$
3. Expected value of this procedure is the sum of the inverse of the non-zero (and negative of the) eigenvalues of the generator:

$$\sum_{x, y \in \mathcal{X}} \mathbb{E}_x(\tau_y) \pi(x) \pi(y) = \sum_{i=1, \lambda_i \neq 0}^{|\mathcal{X}|} \frac{1}{\lambda_i}$$

# The $\mathcal{S}$ class: Spectral theory

---

## Corollary (Eigentime identity)

*Suppose that  $\mathcal{X}$  is a finite state space. If  $L \in \mathcal{S}(G)$  with eigenvalues  $(-\lambda_i)_{i \in \llbracket \mathcal{X} \rrbracket}$ , then  $(P_t)_{t \geq 0}$  and  $(Q_t)_{t \geq 0}$  share the same eigentime identity.*

$$\sum_{x, y \in \mathcal{X}} \mathbb{E}_x(\tau_y^Q) \pi_Q(x) \pi_Q(y) = \sum_{x, y \in \mathcal{X}} \mathbb{E}_x(\tau_y^P) \pi(x) \pi(y) = \sum_{i=1, \lambda_i \neq 0}^{|\mathcal{X}|} \frac{1}{\lambda_i}.$$

- ① Introduction
  
- ② Analysis of non-reversible Markov chains via similarity orbit
  - (i). Spectral theory
  - (ii). Convergence to equilibrium
  - (iii). Example: Ehrenfest model
  - (iv). Cutoff phenomena
  
- ③ Metropolis-Hastings reversiblizations
  
- ④ Summary

## The $\mathcal{S}$ class: Convergence to equilibrium

---

Two notations:

- Second largest eigenvalue in modulus of  $P$ :

$$\lambda_* = \lambda_*(P) := \sup\{|\lambda| \in \sigma(P); \lambda \neq 1\}$$

- Second largest singular value of  $P$ :

$$\sigma_* = \sigma_*(P) := \sqrt{\lambda_*(P\hat{P})}$$

- $\lambda_* \leq \sigma_*$  (with equality holds if  $P$  is normal)
- For a general  $P$ ,

$$\lambda_*^n \leq \|P^n - \pi\|_{\ell^2(\pi) \rightarrow \ell^2(\pi)} \leq \sigma_*^n$$

- For a reversible  $P$ ,

$$\|P^n - \pi\|_{\ell^2(\pi) \rightarrow \ell^2(\pi)} = \lambda_*^n$$

## The $\mathcal{S}$ class: Convergence to equilibrium

---

### Theorem ( $\ell^2(\pi)$ distance)

Let  $P \in \mathcal{S}$  with stationary distribution  $\pi$ . For  $n \in \mathbb{N}$ ,

$$\lambda_*^n \leq \|P^n - \pi\|_{\ell^2(\pi) \rightarrow \ell^2(\pi)} \leq \sigma_*^n \mathbf{1}_{\{n < n^*\}} + \kappa_\Lambda \lambda_*^n \mathbf{1}_{\{n \geq n^*\}},$$

where  $n^* = \lceil \frac{\ln \kappa_\Lambda}{\ln \sigma_* - \ln \lambda_*} \rceil$  and  $\kappa_\Lambda = \|\Lambda\| \|\Lambda^{-1}\| \geq 1$  is the condition number of  $\Lambda$ .

## The $\mathcal{S}$ class: Convergence to equilibrium

### Theorem ( $\ell^2(\pi)$ distance)

Let  $P \in \mathcal{S}$  with stationary distribution  $\pi$ . For  $n \in \mathbb{N}$ ,

$$\lambda_*^n \leq \|P^n - \pi\|_{\ell^2(\pi) \rightarrow \ell^2(\pi)} \leq \sigma_*^n \mathbf{1}_{\{n < n^*\}} + \kappa_\Lambda \lambda_*^n \mathbf{1}_{\{n \geq n^*\}},$$

where  $n^* = \lceil \frac{\ln \kappa_\Lambda}{\ln \sigma_* - \ln \lambda_*} \rceil$  and  $\kappa_\Lambda = \|\Lambda\| \|\Lambda^{-1}\| \geq 1$  is the condition number of  $\Lambda$ .

- A sufficient condition for which  $\lambda_* < \sigma_*$  is given by  $\max_i P(i, i) > \lambda_*$  using Sing-Thompson theorem.

## The $\mathcal{S}$ class: Convergence to equilibrium

### Theorem ( $\ell^2(\pi)$ distance)

Let  $P \in \mathcal{S}$  with stationary distribution  $\pi$ . For  $n \in \mathbb{N}$ ,

$$\lambda_*^n \leq \|P^n - \pi\|_{\ell^2(\pi) \rightarrow \ell^2(\pi)} \leq \sigma_*^n \mathbf{1}_{\{n < n^*\}} + \kappa_\Lambda \lambda_*^n \mathbf{1}_{\{n \geq n^*\}},$$

where  $n^* = \lceil \frac{\ln \kappa_\Lambda}{\ln \sigma_* - \ln \lambda_*} \rceil$  and  $\kappa_\Lambda = \|\Lambda\| \|\Lambda^{-1}\| \geq 1$  is the condition number of  $\Lambda$ .

- A sufficient condition for which  $\lambda_* < \sigma_*$  is given by  $\max_i P(i, i) > \lambda_*$  using Sing-Thompson theorem.
- Recall the notion of hypocoercivity (Villani '06), i.e. there exists a constant  $C < \infty$  and  $\rho \in (0, 1)$  such that

$$\|P^n - \pi\|_{\ell^2(\pi) \rightarrow \ell^2(\pi)} \leq C \rho^n.$$

We provide an *explicit* spectral interpretation of the constant  $C$  by  $\kappa_\Lambda$ , and the convergence rate seems to be more involved.

## The $\mathcal{S}$ class: Convergence to equilibrium

---

Theorem (total variation distance)

Let  $P \in \mathcal{S}$  with stationary distribution  $\pi$ . For  $n \in \mathbb{N}$ ,

$$\|P^n(x, \cdot) - \pi\|_{TV} \leq \frac{1}{2} \sqrt{\frac{1 - \pi(x)}{\pi(x)}} \left( \sigma_*^n \mathbf{1}_{\{n < n^*\}} + \kappa_\Lambda \lambda_*^n \mathbf{1}_{\{n \geq n^*\}} \right)$$



## The $\mathcal{S}$ class: Convergence to equilibrium

### Theorem (total variation distance)

Let  $P \in \mathcal{S}$  with stationary distribution  $\pi$ . For  $n \in \mathbb{N}$ ,

$$\|P^n(x, \cdot) - \pi\|_{TV} \leq \frac{1}{2} \sqrt{\frac{1 - \pi(x)}{\pi(x)}} \left( \sigma_*^n \mathbf{1}_{\{n < n^*\}} + \kappa_\Lambda \lambda_*^n \mathbf{1}_{\{n \geq n^*\}} \right)$$

Remark: Recall the notion of geometrically ergodicity (Kendall '59, Meyn and Tweedie '94, Baxendale '05), i.e. there exists a constant  $C_x < \infty$  and  $\rho \in (0, 1)$  such that for  $x \in E$  and  $n \in \mathbb{N}$ ,

$$\|P^n(x, \cdot) - \pi\|_{TV} \leq C_x \rho^n$$

The constant  $\kappa_\Lambda$  provides an *explicit* and *computable* interpretation, and the rate of convergence seems to be more involved.

- ① Introduction
  
- ② Analysis of non-reversible Markov chains via similarity orbit
  - (i). Spectral theory
  - (ii). Convergence to equilibrium
  - ③ (iii). Example: Ehrenfest model
  - (iv). Cutoff phenomena
  
- ③ Metropolis-Hastings reversiblizations
  
  
- ④ Summary

## Example: Ehrenfest model

---

- Ehrenfest model: a birth-death process  $(Q_t)_{t \geq 0}$  on  $\llbracket 0, N \rrbracket$  with parameter  $0 < p < 1$  and
  - birth rate  $\lambda_x = p(N - x)$
  - death rate  $\mu_x = (1 - p)x$
  - stationary distribution: binomial distribution  $\pi_Q$  with parameters  $N, p$
  - eigenfunctions: Krawtchouk polynomials

$$\phi_j(x) = {}_2F_1 \left( \begin{matrix} -j, -x \\ -N \end{matrix} \middle| p^{-1} \right)$$

- spectral representation:

$$Q_t(x, y) = \pi_Q(y) \sum_{j=0}^N e^{-jt} \phi_j(x) \phi_j(y) \frac{(-1)^{-j} p^j}{j!(1-p)^j} (-N)_j$$

# Example: Ehrenfest model

---

- Three orbits:
  - Permutation orbit  $\Lambda_\sigma$
  - (Zhou '08, Diaconis and Miclo '15) Random walk orbit  $\Lambda_{rw}$
  - (In thesis) Pure birth orbit  $\Lambda_{pb}$

## Example: Ehrenfest model

- Three orbits:
  - Permutation orbit  $\Lambda_\sigma : \Lambda_\sigma = (\mathbf{1}_{y=\sigma(x)})_{x,y \in \mathcal{X}}$ ,  $\Lambda_\sigma^{-1} = \Lambda_\sigma^T$
  - (Zhou '08, Diaconis and Miclo '15) Random walk orbit  $\Lambda_{rw}$  : For  $j = 1, 3, \dots, 2N - 1$ , the eigenvalue  $\beta_j$ , right eigenfunction  $\psi_j$  and left eigenfunction  $\Psi_j$  are given by

$$\beta_j := \cos\left(\frac{j\pi}{2N+1}\right),$$

$$\psi_j(x) := \cos\left(\frac{(2x+1)j\pi}{2(2N+1)}\right), \quad x \in \llbracket 0, N \rrbracket,$$

$$\Psi_j(x) := \begin{cases} \psi_j(x), & \text{for } x \in \llbracket 0, N-1 \rrbracket, \\ \frac{(-1)^{(j+1)/2}}{2} \cot\left(\frac{j\pi}{2(2N+1)}\right), & \text{for } x = N, \end{cases}$$

$$\Lambda_{rw} = \sum_{j \in \{0, 1, 3, \dots, 2N-1\}} \beta_j \psi_j \Psi_j^T,$$

- (In thesis) Pure birth orbit  $\Lambda_{pb}$

# Example: Ehrenfest model

	Permutation orbit $\Lambda_\sigma$
Is $\Lambda$ unitary?	✓
Is $P_t$ reversible?	✓
Spectral representation of $P_t$	$P_t(x, y) = \sum_{j=0}^N e^{-jt} f_j(x) f_j^*(y) \frac{(-1)^{-j} p^j}{j!(1-p)^j} (-N)_j$
$f_j(x)$	$\phi_j(\sigma^{-1}(x))$
$f_j^*(y)$	$\phi_j(\sigma^{-1}(y)) \pi_Q(\sigma^{-1}(y))$
$\ P_t - \pi\ _{\ell^2(\pi) \rightarrow \ell^2(\pi)}$	$e^{-t} = \kappa_{\Lambda_\sigma} e^{-t}$
Eigentime identity	$\sum_{j=1}^N \frac{1}{j}$

# Example: Ehrenfest model

	Random walk orbit $\Lambda_{rw}$
Is $\Lambda$ unitary?	<b>X</b>
Is $P_t$ reversible?	<b>X</b>
Spectral representation of $P_t$	$P_t(x, y) = \sum_{j=0}^N e^{-jt} f_j(x) f_j^*(y) \frac{(-1)^{-j} p^j}{j!(1-p)^j} (-N)_j$
$f_j(x)$	discrete cosine transform of $(\beta_k^{-1} \langle \Psi_k, \phi_j \rangle)_{\text{oddk}}$
$f_j^*(y)$	$\sum_{k \in \{0, 1, 3, \dots, 2N-1\}} \beta_k \langle \psi_k, \phi_j \rangle_{\pi_Q} \Psi_k(y)$
$\ P_t - \pi\ _{\ell^2(\pi) \rightarrow \ell^2(\pi)}$	$\leq \kappa_{\Lambda_{rw}} e^{-t}$
Eigentime identity	$\sum_{j=1}^N \frac{1}{j}$

## Example: Ehrenfest model

---

Remarks:

- More examples and their orbits in the thesis:  $M/M/\infty$  queue, linear and quadratic birth-death processes.
- We can consider  $d$ -dimensional *non-reversible* chains via *tensorized* orbits, e.g.

$$P_t \Lambda_{rw}^{\otimes d} = \Lambda_{rw}^{\otimes d} Q_t,$$

where  $(Q_t)_{t \geq 0}$  is a multivariate reversible Markov chain, e.g. generalized Bernoulli-Laplace (Khare and Zhou '09), Dirichlet-multinomial Gibbs sampler (Khare and Zhou '09), Griffiths and Spano '13, Griffiths '16...



- ① Introduction
- ② Analysis of non-reversible Markov chains via similarity orbit
  - (i). Spectral theory
  - (ii). Convergence to equilibrium
  - (iii). Example: Ehrenfest model
  - (iv). Cutoff phenomena
- ③ Metropolis-Hastings reversiblizations
- ④ Summary

## Cutoff phenomena

---

- Separation cutoff: generalizes the “spectral gap times mixing time going to infinity” criterion to a subclass  $\mathcal{GMC} \subset \mathcal{S}$ .
- $L^2$ -cutoff: generalizes the  $L^2$ -cutoff criteria for reversible chains to the class  $\mathcal{S}$  using the Laplace transform cutoff criteria in Chen and Saloff-Coste '09.

- 1 Introduction
- 2 Analysis of non-reversible Markov chains via similarity orbit
- 3 Metropolis-Hastings reversiblizations**
- 4 Summary

# The Metropolis reversiblization (Aldous and Fill '02)

326 CHAPTER 9. A SECOND LOOK AT GENERAL MARKOV CHAINS (APRIL 21, 1995)

## 9.4 Making reversible chains from irreversible chains

Let  $\mathbf{P}$  be an irreducible transition matrix on  $I$  with stationary distribution  $\pi$ . The following straightforward lemma records several general ways in which to construct from  $\mathbf{P}$  a transition matrix  $\mathbf{Q}$  for which the associated chain still has stationary distribution  $\pi$  but is *reversible*. These methods all involve the time-reversed matrix  $\mathbf{P}^*$


$$\pi_i p_{ij} = \pi_j p_{ji}^*$$

and so in practice can only be used when we know  $\pi$  explicitly (as we have observed several times previously, in general we cannot write down a useful explicit expression for  $\pi$  in the irreversible setting).

**Lemma 9.20** *The following definitions each give a transition matrix  $\mathbf{Q}$  which is reversible with respect to  $\pi$ .*

The additive reversiblization:  $\mathbf{Q}^{(1)} = \frac{1}{2}(\mathbf{P} + \mathbf{P}^*)$

The multiplicative reversiblization:  $\mathbf{Q}^{(2)} = \mathbf{P}\mathbf{P}^*$

The Metropolis reversiblization;  $\mathbf{Q}_{i,j}^{(3)} = \min(p_{i,j}, p_{j,i}^*), j \neq i.$  

# The Metropolis reversiblization

## Definition (Classical MH kernel)

The first MH chain, with transition kernel denoted by  $M_1 := M_1(P)$ , is the MH kernel with proposal kernel  $P$  and target distribution  $\pi$ . That is, let

$$\alpha_1(x, y) = \begin{cases} \min\left(\frac{\pi(y)p(y, x)}{\pi(x)p(x, y)}, 1\right) & \text{if } \pi(x)p(x, y) > 0, \\ 0 & \text{otherwise,} \end{cases}$$

$$m_1(x, y) = \alpha_1(x, y)p(x, y) = \min\{\hat{p}(x, y), p(x, y)\},$$

$$r_1(x) = \int_{y \neq x} (1 - \alpha_1(x, y))p(x, y) \mu(dy),$$

then  $M_1$  is given by

$$M_1(x, dy) = m_1(x, y)\mu(dy) + r_1(x)\delta_x(dy).$$

# Metropolis-Hastings reversiblizations

---

Nothing new so far...

# Metropolis-Hastings reversiblizations

---

## Definition (The second MH kernel)

The second MH kernel  $M_2$  and density  $m_2$  are given by

$$m_2(x, y) = \max\{\hat{p}(x, y), p(x, y)\},$$
$$M_2(x, dy) = m_2(x, y)\mu(dy) - r_1(x)\delta_x(dy).$$

# Metropolis-Hastings reversiblizations

## Definition (The second MH kernel)

The second MH kernel  $M_2$  and density  $m_2$  are given by

$$m_2(x, y) = \max\{\widehat{p}(x, y), p(x, y)\},$$
$$M_2(x, dy) = m_2(x, y)\mu(dy) - r_1(x)\delta_x(dy).$$

## Lemma

1.  $P + \widehat{P} = M_1 + M_2$ .
2.  $M_1$  and  $M_2$  are self-adjoint bounded operators on  $L^2(\pi)$ .
3.  $M_1 = M_2 = P$  if and only if  $P$  is reversible with respect to  $\pi$ .
4.  $M_i(P) = M_i(\widehat{P})$  for  $i = 1, 2$ .

Remark: Note that  $M_2$  may not even be a contraction kernel.



- ① Introduction
- ② Analysis of non-reversible Markov chains via similarity orbit
- ③ Metropolis-Hastings reversiblizations
  - (i). Weyl's inequality
  - (ii). Comparison theorem
  - (iii). MH-spectral gap
  - (iv). Variance bounds
- ④ Summary

## Weyl's inequality

---

Suppose that  $\mathcal{X}$  is a finite state space with  $n = |\mathcal{X}|$ , and arrange eigenvalues of a symmetric matrix  $M$  in non-increasing order by  $\lambda_1(M) \geq \dots \geq \lambda_n(M)$ .

Theorem (Weyl's inequality for additive reversibilization)

1. For  $i, j, k \in \llbracket n \rrbracket$  and  $i + 1 = j + k$ ,

$$\lambda_i(P + \widehat{P}) \leq \lambda_j(M_1) + \lambda_k(M_2).$$

2. For  $i, l, m \in \llbracket n \rrbracket$  and  $i + n = l + m$ ,

$$\lambda_i(P + \widehat{P}) \geq \lambda_l(M_1) + \lambda_m(M_2).$$

## Weyl's inequality

### Corollary (Spectral gap bound via Weyl's inequality)

Denote

$$L := \max_{l+m=2+n} \{\lambda_l(M_1) + \lambda_m(M_2)\},$$

$$U := \min_{j+k=3} \{\lambda_j(M_1) + \lambda_k(M_2)\}.$$

Then

$$1 - \frac{1}{2}U \leq \gamma(P) \leq 1 - \frac{1}{2}L.$$

Remark: This bound is tight for asymmetric  $(p, q)$  simple random walk on  $n$ -cycle, which gives

$$1 - \frac{1}{2}U = \max\{p, q\}(1 - \cos(2\pi/n)) \leq 1 - \cos(2\pi/n) = \gamma(P) = 1 - \frac{1}{2}L.$$

More examples can be found in the thesis.

# Weyl's inequality

---

## Corollary

*If  $P$  is a lazy and ergodic Markov kernel on a finite state space, then  $M_2$  is a contraction kernel.*

- ① Introduction
- ② Analysis of non-reversible Markov chains via similarity orbit
- ③ Metropolis-Hastings reversiblizations
  - (i). Weyl's inequality
  - (ii). Comparison theorem
  - (iii). MH-spectral gap
  - (iv). Variance bounds
- ④ Summary

# Comparison theorem

---

## Theorem

For real-valued function  $f \in L^2(\pi)$ ,

$$\langle M_2 f, f \rangle_\pi \leq \langle P f, f \rangle_\pi \leq \langle M_1 f, f \rangle_\pi.$$

In particular,

$$\lambda(M_2) \leq \lambda(M_1), \quad \Lambda(M_2) \leq \Lambda(M_1),$$

where for  $i = 1, 2$ ,

$$\lambda(M_i) := \inf\{\alpha : \alpha \in \sigma(M_i), \alpha < 1\},$$

$$\Lambda(M_i) := \sup\{\alpha : \alpha \in \sigma(M_i), \alpha < 1\}.$$

# Comparison theorem

---

Remarks:

- $\langle Pf, f \rangle_\pi \leq \langle M_1 f, f \rangle_\pi$  is known as Peskun ordering in MCMC.
- This kind of inequality is more generally known as comparison theorems of Markov chains - Diaconis and Saloff-Coste '93, Dyer et al. '06
- This allows us to state a variant of Cheeger's inequality for non-reversible chains.

## (Higher-order) Cheeger's inequality

Theorem (Lee et al. '12, Wang '14, Miclo '15)

Suppose that  $P$  is the transition kernel of a reversible finite Markov chain with eigenvalues  $1 = \lambda_1 \geq \dots \geq \lambda_n$ . For  $k \in \llbracket n \rrbracket$ ,

$$\frac{1 - \lambda_k}{2} \leq \Phi_*(k) \leq O(k^4) \sqrt{1 - \lambda_k},$$

where  $\Phi_*(k)$  is the  $k$ -way expansion defined to be

$$\Phi_*(k) := \min_{(A_1, \dots, A_k) \in \mathcal{D}_k} \max_{i \in \llbracket k \rrbracket} \frac{\langle P \mathbf{1}_{A_i}, \mathbf{1}_{A_i^c} \rangle_\pi}{\langle \mathbf{1}_{A_i}, \mathbf{1}_{A_i} \rangle_\pi},$$

and  $\mathcal{D}_k$  is the set of  $k$ -uples of disjoint and  $\pi$ -non-negligible subsets of  $\mathcal{X}$ .



# (Higher-order) Cheeger's inequality

---

## Corollary

For non-reversible  $P$  and  $k \in \llbracket n \rrbracket$ ,

$$\frac{1 - \lambda_k(M_1)}{2} \leq \Phi_*(k) \leq O(k^4) \sqrt{1 - \lambda_k(M_2)}.$$

- ① Introduction
- ② Analysis of non-reversible Markov chains via similarity orbit
- ③ Metropolis-Hastings reversiblizations
  - (i). Weyl's inequality
  - (ii). Comparison theorem
  - (iii). MH-spectral gap
  - (iv). Variance bounds
- ④ Summary

## MH-spectral gap

---

Suppose that  $P$  is the transition kernel of a non-reversible chain with time-reversal  $\hat{P}$  on a finite state space with stationary distribution  $\pi$  and spectral gap  $\gamma(P)$ .

$$\|P^n(x, \cdot) - \pi\|_{TV} \leq C_x \beta^n,$$

where  $\beta$  can be (possibly with a different  $C_x$ ):

- $\sigma_*(P)$  (Fill '91)
- $1 - \gamma((P + \hat{P})/2)$  for lazy chain (Fill '91)
- $\sqrt{1 - \gamma_{ps}}$  with  $\gamma_{ps} = \max_{k \geq 1} \gamma(\hat{P}^k P^k)/k$  (“*Pseudo*” spectral gap, Paulin '15)
- We now propose a gap based on  $M_1$  and  $M_2$ .

# MH-spectral gap

---

## Definition (MH-spectral gap)

Denote

$$\mathcal{C} := \{n \in \mathbb{N} : |\lambda(M_2(P^n))| < 1, \Lambda(M_1(P^n)) < 1\},$$
$$\beta^{MH} := \sup_{n \in \mathcal{C}} \{|\lambda(M_2(P^n))|^{1/n}, \Lambda(M_1(P^n))^{1/n}\}.$$

The MH-spectral gap  $\gamma^{MH} = \gamma^{MH}(P)$  is given by

$$\gamma^{MH} := 1 - \beta^{MH}.$$

Remark: For reversible  $P$ ,  $\gamma^{MH} = \gamma$ , the classical  $L^2$ -spectral gap.

# MH-spectral gap

---

## Theorem

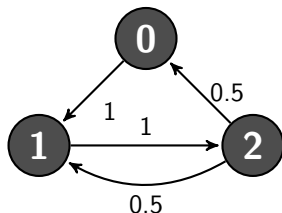
If  $|\mathcal{C}^c| < \infty$ , then for all  $n \in \mathbb{N}$  and  $x \in \mathcal{X}$ ,

$$\|P^n(x, \cdot) - \pi\|_{TV} \leq C_x (\beta^{MH})^n.$$

Remark: In some (but not all) numerical examples, the convergence rate  $\beta^{MH}$  outperform the rate of Fill '91 and Paulin '15. See the thesis.

## MH-spectral gap

Non-reversible Markov chain on triangle (Montenegro and Tetali '06)



$$\|P^n(x, \cdot) - \pi\|_{TV} \leq C_x \beta^n$$

where  $\beta$  can be

- $\sigma_*(P) = 1$  (Fill '91)
- $1 - \gamma((P + \hat{P})/2)$  for lazy chain (Fill '91)
- $\sqrt{1 - \gamma_{ps}} = 0.866$  (Paulin '15)
- $\beta^{MH} = 0.849$  ☺

- ① Introduction
- ② Analysis of non-reversible Markov chains via similarity orbit
- ③ Metropolis-Hastings reversiblizations
  - (i). Weyl's inequality
  - (ii). Comparison theorem
  - (iii). MH-spectral gap
  - (iv). Variance bounds
- ④ Summary

## Variance bounds

### Theorem (Variance bounds for reversible chains)

For reversible  $P$  and  $f \in L^2(\pi)$ ,

$$V_f := \text{Var}_\pi(f),$$

$$\sigma_{as}^2 := \lim_{n \rightarrow \infty} \frac{1}{n} \text{Var}_\pi \left( \sum_{i=1}^n f(X_i) \right).$$

Then,

$$\text{Var}_\pi \left( \sum_{i=1}^n f(X_i) \right) \leq n V_f \left( \frac{2}{\gamma} \right),$$

$$\left| \text{Var}_\pi \left( \sum_{i=1}^n f(X_i) \right) - n \sigma_{as}^2 \right| \leq V_f \left( \frac{4}{\gamma^2} \right).$$



## Variance bounds

Theorem (Variance bounds for non-reversible chains, Paulin '15)

For non-reversible  $P$  and  $f \in L^2(\pi)$ ,

$$V_f := \text{Var}_\pi(f),$$

$$\sigma_{as}^2 := \lim_{n \rightarrow \infty} \frac{1}{n} \text{Var}_\pi \left( \sum_{i=1}^n f(X_i) \right).$$

Then,

$$\text{Var}_\pi \left( \sum_{i=1}^n f(X_i) \right) \leq n V_f \left( \frac{4}{\gamma_{ps}} \right),$$

$$\left| \text{Var}_\pi \left( \sum_{i=1}^n f(X_i) \right) - n \sigma_{as}^2 \right| \leq V_f \left( \frac{16}{\gamma_{ps}^2} \right).$$

## Variance bounds

Theorem (Variance bounds for non-reversible chains)

For non-reversible  $P$  and  $f \in L^2(\pi)$ ,

$$V_f := \text{Var}_\pi(f),$$

$$\sigma_{as}^2 := \lim_{n \rightarrow \infty} \frac{1}{n} \text{Var}_\pi \left( \sum_{i=1}^n f(X_i) \right).$$

Then,

$$\text{Var}_\pi \left( \sum_{i=1}^n f(X_i) \right) \leq n V_f \left( |\mathcal{C}^c| + \frac{4}{\gamma^{MH}} \right),$$

$$\left| \text{Var}_\pi \left( \sum_{i=1}^n f(X_i) \right) - n \sigma_{as}^2 \right| \leq V_f 4 \left( 1 + |\mathcal{C}^c| + \frac{4(\beta^{MH})^{|\mathcal{C}^c|+1}}{\gamma^{MH}} \right)^2.$$

- 1 Introduction
- 2 Analysis of non-reversible Markov chains via similarity orbit
- 3 Metropolis-Hastings reversiblizations
- 4 Summary

# Summary

---

## 1. Similarity orbit of normal Markov chains

- Spectral theory and functional calculus for Markov chains in this  $\mathcal{S}$  class
- Eigentime identity
- Convergence to equilibrium
- Separation and  $L^2$ -cutoff
- New non-reversible examples with known spectral expansion, eigenfunction and stationary distribution

## 2. Metropolis-Hastings reversiblizations

- Weyl's inequality
- Comparison theorem
- MH-spectral gap
- Variance bounds

# Summary

---

## 1. Similarity orbit of normal Markov chains

- Spectral theory and functional calculus for Markov chains in this  $\mathcal{S}$  class
- Eigentime identity
- Convergence to equilibrium
- Separation and  $L^2$ -cutoff
- New non-reversible examples with known spectral expansion, eigenfunction and stationary distribution

## 2. Metropolis-Hastings reversiblizations

- Weyl's inequality
- Comparison theorem
- MH-spectral gap
- Variance bounds

# Summary

---

## 1. Similarity orbit of normal Markov chains

- Spectral theory and functional calculus for Markov chains in this  $\mathcal{S}$  class
- Eigentime identity
- Convergence to equilibrium
- Separation and  $L^2$ -cutoff
- New non-reversible examples with known spectral expansion, eigenfunction and stationary distribution

## 2. Metropolis-Hastings reversiblizations

- Weyl's inequality
- Comparison theorem
- MH-spectral gap
- Variance bounds

# Summary

---

## 1. Similarity orbit of normal Markov chains

- Spectral theory and functional calculus for Markov chains in this  $\mathcal{S}$  class
- Eigentime identity
- Convergence to equilibrium
- Separation and  $L^2$ -cutoff
- New non-reversible examples with known spectral expansion, eigenfunction and stationary distribution

## 2. Metropolis-Hastings reversiblizations

- Weyl's inequality
- Comparison theorem
- MH-spectral gap
- Variance bounds

# Summary

---

## 1. Similarity orbit of normal Markov chains

- Spectral theory and functional calculus for Markov chains in this  $\mathcal{S}$  class
- Eigentime identity
- Convergence to equilibrium
- Separation and  $L^2$ -cutoff
- New non-reversible examples with known spectral expansion, eigenfunction and stationary distribution

## 2. Metropolis-Hastings reversiblizations

- Weyl's inequality
- Comparison theorem
- MH-spectral gap
- Variance bounds



# Summary

---

## 1. Similarity orbit of normal Markov chains

- Spectral theory and functional calculus for Markov chains in this  $\mathcal{S}$  class
- Eigentime identity
- Convergence to equilibrium
- Separation and  $L^2$ -cutoff
- New non-reversible examples with known spectral expansion, eigenfunction and stationary distribution

## 2. Metropolis-Hastings reversiblizations

- Weyl's inequality
- Comparison theorem
- MH-spectral gap
- Variance bounds

# Summary

---

## 1. Similarity orbit of normal Markov chains

- Spectral theory and functional calculus for Markov chains in this  $\mathcal{S}$  class
- Eigentime identity
- Convergence to equilibrium
- Separation and  $L^2$ -cutoff
- New non-reversible examples with known spectral expansion, eigenfunction and stationary distribution

## 2. Metropolis-Hastings reversiblizations

- Weyl's inequality
- Comparison theorem
- MH-spectral gap
- Variance bounds

# Summary

---

## 1. Similarity orbit of normal Markov chains

- Spectral theory and functional calculus for Markov chains in this  $\mathcal{S}$  class
- Eigentime identity
- Convergence to equilibrium
- Separation and  $L^2$ -cutoff
- New non-reversible examples with known spectral expansion, eigenfunction and stationary distribution

## 2. Metropolis-Hastings reversiblizations

- Weyl's inequality
- Comparison theorem
- MH-spectral gap
- Variance bounds

# Summary

---

## 1. Similarity orbit of normal Markov chains

- Spectral theory and functional calculus for Markov chains in this  $\mathcal{S}$  class
- Eigentime identity
- Convergence to equilibrium
- Separation and  $L^2$ -cutoff
- New non-reversible examples with known spectral expansion, eigenfunction and stationary distribution

## 2. Metropolis-Hastings reversiblizations

- Weyl's inequality
- Comparison theorem
- MH-spectral gap
- Variance bounds

# Summary

---

## 1. Similarity orbit of normal Markov chains

- Spectral theory and functional calculus for Markov chains in this  $\mathcal{S}$  class
- Eigentime identity
- Convergence to equilibrium
- Separation and  $L^2$ -cutoff
- New non-reversible examples with known spectral expansion, eigenfunction and stationary distribution

## 2. Metropolis-Hastings reversiblizations

- Weyl's inequality
- Comparison theorem
- MH-spectral gap
- Variance bounds

# Summary

---

## 1. Similarity orbit of normal Markov chains

- Spectral theory and functional calculus for Markov chains in this  $\mathcal{S}$  class
- Eigentime identity
- Convergence to equilibrium
- Separation and  $L^2$ -cutoff
- New non-reversible examples with known spectral expansion, eigenfunction and stationary distribution

## 2. Metropolis-Hastings reversiblizations

- Weyl's inequality
- Comparison theorem
- MH-spectral gap
- Variance bounds

# References

---

This talk is based on

- M.C.H. Choi and P. Patie. Skip-free Markov chains. Submitted.
- M.C.H. Choi and P. Patie. Analysis of non-reversible Markov chains via similarity orbit. Submitted.
- M.C.H. Choi. Metropolis-Hastings reversibilizations of non-reversible chains. Submitted.

Thank you! Question(s)?