# Current developments in MCMC III: Comparisons theorems for slice sampling


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**Dynstoch Satellie Spring School**

May 2024

# Overview

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In this final talk we'll consider Slice Sampling and also study Hybrid variants, [Besag and Green (1993), Higdon (1998), Neal (2003)], which was pioneered as an alternative to Random Walk, which will involve further comparisons.

Power, S., Rudolf, D., Sprungk, B., Wang, A.Q., 2024. Weak Poincaré inequality comparisons for ideal and hybrid slice sampling. https://arxiv.org/abs/2402.13678 .

# Metropolis–Hastings

**Algorithm 1** Metropolis–Hastings (MH)

*initialise:* $X_0 = x_0, i = 0$
**while** $i < N$ **do**
  $i \leftarrow i + 1$
  simulate $Y_i \sim Q(X_{i-1}, \cdot)$
  $\alpha(X_{i-1}, Y_i) = 1 \wedge \frac{q(Y_i, X_{i-1})\pi(Y_i)}{q(X_{i-1}, Y_i)\pi(X_{i-1})}$
  **with probability** $\alpha(X_{i-1}, Y_i)$
    $X_i \leftarrow Y_i$
  **else**
    $X_i \leftarrow X_{i-1}$
**return** $(X_i)_{i=1,\dots,N}$

# Random walk Metropolis recap

Have seen: Random Walk Metropolis (RWM) [Metropolis et. al. (1953)]:
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Slice Sampling was introduced to try and circumvent these deficiencies.

# Slice Sampling [Neal (2003)]

Target: $\pi(\mathrm{d}x) = \varpi(x)\nu(\mathrm{d}x)$ on $\mathcal{X}$, reference measure $\nu$.

$$G(t) := \{x \in \mathcal{X} : \varpi(x) > t\}, \quad \nu_t := \frac{\nu(\cdot \cap G(t))}{\nu(G(t))}.$$

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**Algorithm 3** Ideal Slice Sampling

*initialise:* $X_0 = x_0, i = 0$
**while** $i < N$ **do**
    $i \leftarrow i + 1$
    **Sample** $t \sim \mathrm{Unif}([0, \varpi(x)])$;
    **Sample** $Y \sim \nu_t$;
    **Set** $X_i = Y$.
**return** $(X_i)_{i=1,\dots,N}$

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(Similar to going from Gibbs sampling $\rightsquigarrow$ Metropolis-within-Gibbs.)

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**Algorithm 5** Hybrid Slice Sampling (HSS)

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**while** $i < N$ **do**
  $i \leftarrow i + 1$
  **Sample** $t \sim \mathrm{Unif}([0, \varpi(x)])$;
  **Sample** $Y \sim H_t(X_{i-1}, \cdot)$;
  **Set** $X_i = Y$.
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This is still a $\pi$-reversible Markov chain.

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HSS also defines a $\pi$-reversible Markov chain.

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Question: how much worse?

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$\nu = \mathcal{N}(0, \mathbf{C})$, $Q(x, \cdot) = \mathcal{N}\left(\rho x, (1 - \rho^2) \cdot \mathbf{C}\right)$, preconditioned Crank–Nicolson.

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Thus our subsequent results allow us to study such chains.

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Intuitively, it relates the convergence of HSS to the convergence rate of ISS in terms of the convergence rates of the $(H_t)$ kernels.

We will do this comparison using the framework of weak Poincaré inequalities introduced earlier.

This will enable us to give quantitative bounds, convering cases when there is no spectral gap, i.e. the convergence is subgeometric, substantially extending previous results [Qin et. al. (2023), Łatuszyński & Rudolf (2014)].

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However some chains have 0 spectral gap and have only subgeometric convergence;

$$\|P^n f - \pi(f)\|_2^2 \leq \gamma(n)\Phi(f),$$

where

$$\Phi(f) = \|f\|_{\mathrm{osc}}^2 = (\operatorname{ess\,sup} f - \operatorname{ess\,inf} f)^2.$$

# Standard Poincaré inequalities

We work on $\mathrm{L}^2(\mu) = \{f : \mathcal{X} \to \mathbb{R} : \|f\|_2^2 < \infty\}$, $\quad \langle f, g \rangle := \int fg \, \mathrm{d}\mu$,
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For a $\mu$-invariant Markov transition kernel $P$ with $\mathrm{L}^2(\mu)$-adjoint $P^*$, consider the Dirichlet form $\mathcal{E}(P^*P, f)$, for $f \in \mathrm{L}^2_0(\mu)$:

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## Standard Poincaré inequality (SPI)

A SPI holds if there exists a constant $C_{\mathrm{P}} > 0$ such that for all $f \in \mathrm{L}_0^2(\mu)$,

$$C_{\mathrm{P}} \|f\|_2^2 \leq \mathcal{E}(P^*P, f).$$

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$$\begin{aligned} C_{\mathrm{P}} \|f\|_2^2 \leq \mathcal{E}(P^* P, f) &= \|f\|_2^2 - \langle P^* P f, f \rangle \\ &= \|f\|_2^2 - \|Pf\|_2^2 \\ \Rightarrow \|Pf\|_2^2 \leq (1 - C_{\mathrm{P}}) \|f\|_2^2. \end{aligned}$$

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The rest is by induction. □

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E.g. $\beta(s) = c_0 s^{-c_1}$.

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Define

$$\begin{aligned} K(u) &:= u\beta(1/u), \qquad u \geq 0, \\ K^*(v) &:= \sup_{u\geq 0}\{uv - K(u)\}, \quad v \geq 0, \\ F(x) &:= \int_x^1 \frac{\mathrm{d}v}{K^*(v)}, \qquad 0 < x \leq 1. \end{aligned}$$

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## Theorem ([Andrieu, Lee, Power, W. (2022)])

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Intuition: the faster $\beta$ decays, the faster the rate of convergence.

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Earlier on [Andrieu, Lee, Power, W. (2022)], we used this machinery to study pseudo-marginal MCMC.

# Comparisons of Markov chains II

Suppose we are able to establish the comparison: $\forall s > 0$, $f \in \mathrm{L}^2_0(\mu)$,

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Suppose the 'ideal' chain $P$ possesses a spectral gap, i.e. it satisfies a SPI:

$$C_{\mathrm{P}}\|f\|_2^2 \leq \mathcal{E}(P, f).$$

# Comparisons of Markov chains II

Suppose we are able to establish the comparison: $\forall s > 0$, $f \in \mathrm{L}^2_0(\mu)$,

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Suppose the 'ideal' chain $P$ possesses a spectral gap, i.e. it satisfies a SPI:

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from which a convergence bound for $\tilde{P}$ can be obtained.

# Comparison of Markov chains

## WPIs

We have discussed WPIs of the form:

$$\|f\|_2^2 \le s\mathcal{E}(P,f) + \beta(s)\Phi(f), \quad \forall s > 0, \quad \forall f \in \mathrm{L}_0^2(\mu). \tag{1}$$

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In order to compare Markov chains, we will consider a more general form of inequalities.

## General comparison inequality

For two (reversible) Markov kernels $P$, $P_2$:

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Indeed, (1) is a special case of (2) where $P_1(x, \mathrm{d}y) = \mu(\mathrm{d}y)$ corresponds to perfect sampling.

Intuition: (2) gives a bound on the convergence of $P_2$ relative to the convergence rate of $P_1$.

# General comparison result

**Theorem ([Andrieu, Lee, Power, W. (2022)])**

*Let* $P_1, P_2$ *be two* $\mu$*-invariant Markov kernels on* $\mathsf{E} \times \mathcal{F}$. *Assume that for any* $(x, B) \subset \mathsf{E} \times \mathcal{F}$,

$$P_2(x, B \backslash \{x\}) \geq \int_{B \backslash \{x\}} \epsilon(x, y) P_1(x, \mathrm{d}y),$$

*for some* $\epsilon : \mathsf{E}^2 \to (0, \infty)$.

*Then for any* $s > 0$, $f \in \mathrm{L}_0^\infty(\mu) \subset \mathrm{L}_0^2(\mu)$,

$$\mathcal{E}(P_1, f) \leq s\,\mathcal{E}(P_2, f) + \frac{1}{2} \mu \otimes P_1(A(s)^\complement \cap \{X \neq Y\}) \Phi(f),$$

*where* $A(s) := \{(x, y) \in \mathsf{E}^2 : s\,\epsilon(x, y) > 1\}$, *and* $\Phi(f) := \|f\|_{\mathrm{osc}}^2$.

# General comparison result - remarks

What we need to show is

$$P_2(x, B\backslash\{x\}) \geq \int_{B\backslash\{x\}} \epsilon(x, y) P_1(x, \mathrm{d}y),$$

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If $\inf_{x,y} \epsilon(x,y) > 0$, then we will get a SPI / geometric convergence.

If we aren't interested in comparisons, but want want an (absolute) WPI, note that if $P(x, \mathrm{d}y) = \pi(\mathrm{d}y)$ represents perfect sampling, then $\mathcal{E}(P, f) = \|f\|_2^2$, and there is the useful representation (exercise!)

$$\|f\|_2^2 = \frac{1}{2} \int \pi(x)\pi(y)[f(y) - f(x)]^2 \, \mathrm{d}x \, \mathrm{d}y.$$

# Independence Sampler: geometric case

The Independence Sampler (IS) is one the simplest MCMC methods: given target $\pi$, at each step sample proposal $Y_i \sim q$, and accept with probability

$$\alpha(X_{i-1}, Y_i) = 1 \wedge \frac{q(X_{i-1})\pi(Y_i)}{\pi(X_{i-1})q(Y_i)} = 1 \wedge \frac{w(Y_i)}{w(X_{i-1})}.$$

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Well-known that there is a spectral gap if and only if the weights are bounded:

$$w(x) := \frac{\pi(x)}{q(x)} \leq M, \quad \forall x \in \mathcal{X}.$$

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(E.g. if so, then you can just do rejection sampling.) The kernel is

$$P(x, \mathrm{d}y) = q(y) \cdot 1 \wedge \frac{w(y)}{w(x)} \,\mathrm{d}y + (1 - \alpha(x))\delta_x(\mathrm{d}y).$$

# Independence Sampler exercises

$$P(x, \mathrm{d}y) = q(y) \cdot 1 \wedge \frac{w(y)}{w(x)}\, \mathrm{d}y + (1 - \alpha(x))\delta_x(\mathrm{d}y), \quad w(x) := \frac{\pi(x)}{q(x)}.$$

# Independence Sampler exercises

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1. Use the general comparison theorem to establish a WPI for the Independence Sampler (i.e. show that $P(x, y) \geq \epsilon(x, y)\pi(y)$ for an appropriate function $\epsilon(x, y)$).
2. Directly deduce a WPI for the Independence Sampler using the useful representations below.

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Useful representations (exercise!):

$$\|f\|_2^2 = \frac{1}{2} \int \pi(x)\pi(y)[f(y) - f(x)]^2 \, \mathrm{d}x \, \mathrm{d}y,$$

$$\mathcal{E}(P, f) = \frac{1}{2} \int \pi(x)\pi(y) \left( w^{-1}(x) \wedge w^{-1}(y) \right) [f(x) - f(y)]^2 \, \mathrm{d}x \, \mathrm{d}y.$$

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Suppose the weights are unbounded, namely

$$\sup_{x \in \mathcal{X}} w(x) = \sup_{x \in \mathcal{X}} \frac{\pi(x)}{q(x)} = \infty.$$

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The previous representation of $\mathcal{E}(P, f)$ immediately gives us a WPI for the subgeometric IS: take

$$\epsilon(x, y) = \left( w^{-1}(x) \wedge w^{-1}(y) \right),$$

then

$$A(s) = \left\{ (x, y) \in \mathsf{E} \times \mathsf{E} : \left( w^{-1}(x) \wedge w^{-1}(y) \right) \geq 1/2 \right\}.$$

# Overview

# Main result

We have $\pi(\mathrm{d}x) = \varpi(x)\nu(\mathrm{d}x)$

$$m_t := \nu(G(t)),$$

recall $\nu_t = \nu(\cdot \cap G(t))/m_t$ . Let's write $U$ for Ideal Slice Sampling, $H$ for Hybrid Slice Sampling.

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**Theorem (Rudolf, Power, Sprungk, W. (2023+))**

*Suppose each $H_t$ is $\nu_t$-reversible, positive and satisfies a WPI with function $\beta_t$. We have the comparison: $\forall s > 0$, $f \in \mathrm{L}^2_0(\mu)$,*

$$\mathcal{E}(U, f) \leq s \cdot \mathcal{E}(H, f) + \beta(s)\Phi(f),$$

*where $\beta : (0, \infty) \to [0, \infty)$ is given by*

$$\beta(s) := \int_0^{\|\varpi\|_\infty} \beta_t(s)\, m_t \,\mathrm{d}t,$$

# Comments

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We see that the convergence rate of $U$ is a kind of weighted average of the convergence rates of each $H_t$.

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If we further have a convergence estimate for $U$ e.g. [Natarovskii et. al. (2021)], then these can be combined to give a convergence bound for $H$.

This significantly extends the previous work of [Łatuszyński & Rudolf (2014)].

# Example: Independent Metropolis–Hastings (IMH)

Recall the IMH$(\pi, q)$ chain: at each iteration with $X_n = x$, propose $Y \sim q$, and accept this proposal with probability

$$\alpha(x, Y) = 1 \wedge \frac{\pi(Y)q(x)}{\pi(x)q(Y)}.$$

It is known that the IMH $(\pi, q)$ satisfies an SPI with constant $\left\|\mathrm{d}\pi/\mathrm{d}q\right\|_\infty^{-1}$ [Mengersen and Tweedie (1996)].

# Explicit example: Exponential distributions

Consider the case when $\mathcal{X} = [0, \infty)$, $\pi(x) = \exp(-x)$, and $\nu(\mathrm{d}x) = \lambda \exp(-\lambda x)\,\mathrm{d}x$ for some $\lambda > 0$.

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$$\pi(x) = \lambda^{-1} \exp(-(1-\lambda)x)\, \nu(\mathrm{d}x).$$

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**Lemma**

*This Ideal Slice Sampler has a spectral gap which can be lower-bounded explicitly:*

- *When $\lambda \in (0, 1)$, the slice sampler has a spectral gap of at least $\frac{1+\lambda}{2}$;*
- *When $\lambda > 1$, the slice sampler has a spectral gap of at least $(2\lambda - 1)^{-2}$.*

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Derived using a contractivity argument.

# Hybrid case

Consider doing now performing an IMH with proposal $\nu$ on each slice:

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When $\lambda \in (0,1)$, we obtain the following comparison for the IMH:

$$\beta(s) = \frac{1}{4} + \frac{1}{4}(1 - s^{-1})^{1/\lambda}\left(\frac{1}{\lambda(s-1)} - 1\right) \sim s^{-1},$$

and a WPI for the IMH-within-Slice Sampler with $\tilde{\beta}(s) = \frac{2\beta\big((1+\lambda)s/2\big)}{1+\lambda} \sim s^{-1}$.

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When $\lambda > 1$, we obtain the following comparison for the IMH:

$$\beta(s) = \frac{\lambda - 1}{4\lambda} s^{-1/\lambda},$$

and a WPI for the IMH-within-Slice Sampler with $\tilde{\beta}(s) = (2\lambda - 1)^2 \beta\left((2\lambda - 1)^{-2} s\right)$.

# Example: Hit-and-Run

An example of a HSS: on each slice, pick a random direction, then sample a uniform point on this line intersected with the slice.

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From [Lovàsz and Vempala (2004)], we deduce that for $L$-smooth and $m$-strongly concave potentials the spectral gap of hit-and-run on a bounded set in dimension $d$ is at least

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where $\kappa = L/m$ is the condition number.

Thus we arrive at the comparison

$$\mathcal{E}(U, f) \leq (2^{33} \kappa d^2)\, \mathcal{E}(H, f).$$

I.e. spectral gap of $H$ is at least $2^{-33} \kappa d^{-2}$ times the spectral gap of $U$.

# Overview

# Concluding remarks

We have derived quantitative comparison theorems relating Simple Slice Sampling with Hybrid Slice Sampling, which covers the subgeometric setting.

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We have further applied this to look at IMH on the slice and Hit-and-run.

This is a nice complement to the pseudo-marginal example from talk II: for pseudo-marginal, we perturbed the acceptance rate; for hybrid slice sampling, we perturbed the proposal mechanism.

# Overall conclusion

We have discussed $L^2$ bounds for MCMC chains, in three different settings.

This is one current line of research, and fits within the wider trend of nonasymptotic convergence guarantees for MCMC methods based on functional inequalities.

There are lots of exciting questions, please come and talk to me if you're interested!

# Thanks for listening! I


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# Thanks for listening! II


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# Convergence of MCMC

What is the criteria for an MCMC chain to be 'good'?

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**Theorem ([?, ?])**

*RWM converges to equilibrium exponentially fast if* and only if* $\pi$ *has an exponential moment (e.g.* $\pi(x) \propto \exp(-\|x-\mu\|^\alpha)$, $\alpha \geq 1$.*). Otherwise, the chain converges at a subgeometric (e.g. polynomial) rate.*

# $L^2$ convergence and Dirichlet forms

We work on $\mathrm{L}^2(\pi) = \{f : \mathcal{X} \to \mathbb{R} : \|f\|_2^2 < \infty\}$, $\langle f, g \rangle := \int fg \, \mathrm{d}\pi$,
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For a $\pi$-invariant Markov transition kernel $P$ with $\mathrm{L}^2(\pi)$-adjoint $P^*$, define the Dirichlet form $\mathcal{E}(P^*P, f)$, for $f \in \mathrm{L}_0^2(\pi)$:

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Furthermore if $P$ is reversible and positive (so its spectrum $\sigma(P) \subset [0, 1]$), we have that

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So it will be sufficient to lower bound $\mathcal{E}(P, f)$.

# Conductance and spectral profiles

## Lemma ([?])

*For nonconstant nonnegative* $g \in \mathrm{L}^2_0(\pi)$*, we have the lower bound*

$$\mathcal{E}(P, g) \geq \mathrm{Var}_\pi(g) \cdot \frac{1}{2} \cdot \Lambda_P \left( \frac{4[\pi(g)]^2}{\mathrm{Var}_\pi(g)} \right),$$

*where* $\Lambda_P$ *is the spectral profile of* $P$*.*

## Lemma

*For* $\pi$*-reversible* $P$*, we have the further lower bound*

$$\Lambda_P(v) \geq \begin{cases} \frac{1}{2}\Phi_P(v)^2 & 0 < v \leq 1/2, \\ \frac{1}{2}[\Phi_P^*]^2 & v > 1/2. \end{cases}$$

# Proof of convergence bound (I)

Fix $f \in \mathrm{L}^2_0(\mu)$. Have that

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Call this final inequality optimized WPI (oWPI).

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Now define

$$F(x) := \int_x^1 \frac{\mathrm{d}v}{K^*(v)}, \quad x \in (0, a], \qquad h_n := \frac{\|P^n f\|_2^2}{\Phi(f)}.$$

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So we invert this to obtain

$$\|P^n f\|_2^2 \leq \Phi(f) F^{-1}(n). \quad \square$$