# Explicit convergence bounds for preconditioned Crank–Nicolson

Andi Q. Wang

University of Warwick

Joint with: Christophe Andrieu, Anthony Lee, Sam Power.

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# Overview

# Sampling

We wish to evaluate integrals

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We simulate a $\pi$-reversible ergodic Markov chain,

$$X_1, X_2, \ldots$$

where $X_n \to \pi$ in distribution and considering

$$I_n := \frac{1}{n}\sum_{i=1}^{n} f(X_i) \approx I = \int_{\mathcal{X}} f(x)\pi(x)\,\mathrm{d}x.$$

# 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** $(X_i)_{i=1,\ldots,n}$

# Setting: Bayesian Inverse Problems

## Target density

We assume that we are targeting a density on $\mathbb{R}^d$ of the form

$$\pi(\mathrm{d}x) \propto \mathcal{N}(\mathrm{d}x; 0, C) \cdot \exp(-\Psi(x)),$$

where $\Psi$ is assumed convex, $L$-smooth and minimized at $x = 0$, and $\mathcal{N}$ denotes a Gaussian density, where $C$ is a positive definite covariance matrix.

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Such densities arise naturally in Bayesian Inverse Problems, where $C$ is a finite section of some infinite-dimensional trace-class covariance operator.

In this case $\nu(\mathrm{d}x) := \mathcal{N}(\mathrm{d}x; 0, C)$ is the prior and $\Psi$ is the (log-)likelihood term corresponding to the observed data.

# Preconditioned Crank–Nicolson

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The preconditioned Crank–Nicolson algorithm (pCN) [Beskos et. al. (2008), Stuart (2010), Example 5.3] is a Metropolis–Hastings chain with $\nu$-reversible Gaussian proposal $Q$: for fixed $\rho \in (0, 1)$,

$$Q(x, A) = \int \mathbf{1}_A(\rho x + \eta z)\, \nu(\mathrm{d}z),$$

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where $\rho^2 + \eta^2 = 1$.

pCN remains stable even in infinite dimensions, since the proposal preserves the (prior) measure $\nu$, unlike pure Random Walk Metropolis.

# Tuning of pCN

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$\eta^2$ too small $\Rightarrow$ proposing tiny moves; wasted computational effort.

We will be interested to derive non-asymptotic bounds on the resulting spectral gap, which can be applied for a given target and given step-size. (C.f. optimal scaling framework of [Roberts, Gelman, Gilks (1997)].)

# Spectral gap

Recall that a reversible $\pi$-invariant Markov kernel $P$ defines an operator on $L^2(\pi)$, and its convergence to equilibrium can be bounded by the spectral gap $\gamma$ (and this is the best rate):

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Want an explicit bound; see related work of [Hairer, Stuart, Vollmer (2014)].

# Main result

Recall we assumed potential $\Psi$ is convex, $L$-smooth.

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

*Under our previous assumptions on $\pi$, setting $\eta = \varsigma \cdot (L \cdot \mathrm{Tr}(C))^{-1/2}$, we have the following bound on the spectral gap:*

$$\gamma \geq 2^{-9} \cdot C_{\mathrm{g}}^2 \cdot \exp(-2\varsigma^2) \cdot \varsigma^2 \cdot (L \cdot \mathrm{Tr}(C))^{-1}.$$

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$$\gamma \geq 3.62784 \times 10^{-5} \cdot (L \cdot \mathrm{Tr}(C))^{-1}.$$

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This is an explicit lower bound, which only depends on the dimension through $\mathrm{Tr}(C)$.

# Overview

1. Introduction: MCMC
2. Convergence framework: conductance and isoperimetry
   - Isoperimetry
   - Close coupling
3. Application to pCN

# Conductance

## Definition: Conductance

The conductance profile of a $\pi$-invariant Markov kernel $P$ is

$$\Phi_P(v) := \inf \left\{ \frac{(\pi \otimes P)(A \times A^{\complement})}{\pi(A)} : \pi(A) \leq v \right\}, \quad v \in (0, 1/2].$$

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**Theorem (Cheeger inequalities)**

*For a positive chain, such as pCN, we have the bounds on the spectral gap,*

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## Theorem (Cheeger inequalities)

*For a positive chain, such as pCN, we have the bounds on the spectral gap,*

$$\frac{1}{2} \cdot [\Phi_P^*]^2 \leq \gamma \leq \Phi_P^*.$$

Thus our goal is to lower bound the conductance.

# Isoperimetry

Fix target density $\pi$ on metric space $(\mathrm{E}, \mathrm{d})$.

**Definition: isoperimetric profile / minorant, c.f. [Milman (2009)]**

Given a measurable set $A$, define the $r$-enlargment of $A$ via $A_r := \{x \in \mathrm{E} : \mathrm{d}(x, A) \leq r\}$, and set

$$\pi^+(A) := \liminf_{r \downarrow 0} \frac{\pi(A_r) - \pi(A)}{r}.$$

Then the isoperimetric profile of $\pi$ is

$$I_\pi(p) := \inf\{\pi^+(A) : A \in \mathcal{E}, \pi(A) = p\}, \quad p \in (0, 1).$$

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A function $\tilde{I}_\pi : (0,1) \to (0,\infty)$ is a regular isoperimetric minorant of $\pi$ if $\tilde{I}_\pi$ is continuous, monotone increasing, symmetric about $1/2$ and $\tilde{I}_\pi \leq I_\pi$.

# Close coupling

**Definition: close coupling**

Given $\epsilon, \delta > 0$, we say that a Markov kernel $P$ is $(\mathsf{d}, \delta, \epsilon)$-close coupling if

$$\mathsf{d}(x, y) \leq \delta \Rightarrow \|P(x, \cdot) - P(y, \cdot)\|_{\mathrm{TV}} \leq 1 - \epsilon, \quad \forall x, y \in \mathsf{E}.$$

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## Lemma: close coupling for Metropolis chains

For Metropolis chains, we have the bound:

$$\|P(x, \cdot) - P(y, \cdot)\|_{\mathrm{TV}} \leq \|Q(x, \cdot) - Q(y, \cdot)\|_{\mathrm{TV}} + 1 - \alpha_0,$$

$$\alpha_0 := \inf_{x \in \mathrm{E}} \alpha(x), \quad \alpha(x) := \int \alpha(x, y) Q(x, \mathrm{d}y).$$

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$$\alpha_0 := \inf_{x \in \mathrm{E}} \alpha(x), \quad \alpha(x) := \int \alpha(x,y) Q(x, \mathrm{d}y).$$

Thus we can establish $P$ is close coupling provided we can bound $\alpha_0$!

# Close coupling, conductance and isoperimetry

**Theorem: Conductance lower bound; c.f. [Dwivedi et. al. (2019)]**

Suppose $\tilde{I}_\pi$ is a regular, concave isoperimetric minorant of $\pi$. Let $P$ be $(\mathrm{d}, \delta, \epsilon)$-close coupling. Then for any $v \in (0, 1/2]$,

$$\Phi_P(v) \geq \frac{1}{4} \cdot \epsilon \cdot 1 \wedge \left( \frac{\delta}{2} \cdot \frac{\tilde{I}_\pi(v/2)}{v/2} \right).$$

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This result thus breaks the problem into two pieces:

- For a given target $\pi$, establish a regular concave isoperimetric minorant $\tilde{I}_\pi$.
- For the chain $P$, establish close coupling.

# Overview

# Isoperimetric minorants for $\pi$

There are various ways to establish isoperimetric minorants: for example, they can be derived from functional inequalities, e.g. Poincaré inequalities, log-Sobolev inequalities, c.f. [Bobkov (1999)].

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The specific case of interest for this talk:

**Lemma**

*Under our assumptions on $\pi$, we have minorant*

$$I_\pi(p) \geq \varphi(\Phi^{-1}(p)) =: \tilde{I}_\pi(p),$$

*with respect to metric $d = |\cdot|_C^{-1}$, where $\varphi, \Phi$ are the standard Gaussian p.d.f. and c.d.f., and furthermore*

$$\tilde{I}_\pi(1/4) = C_{\mathrm{g}},$$

*where $C_{\mathrm{g}} \geq 0.317776$.*

# Controlling acceptance probabilities

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Through a direct calculation, we obtain:

**Lemma**

*Let* $\eta = \varsigma \cdot (L \cdot \mathrm{Tr}(\mathsf{C}))^{-1/2}$*, some* $\varsigma > 0$*. Then*

$$\alpha_0 \geq \frac{1}{2} \cdot \exp\left(-\frac{\varsigma^2}{2}\right).$$

# Main result

Putting together all of these pieces, we obtain the main result.

**Theorem**

*We obtain the lower bound on the spectral gap of pCN, for* $\eta = \varsigma \cdot (L \cdot \mathrm{Tr}(C))^{-1/2}$

$$\gamma \geq 2^{-9} \cdot C_{\mathrm{g}}^2 \cdot \varsigma^2 \cdot \exp(-2\varsigma^2) \cdot (L \cdot \mathrm{Tr}(C))^{-1}.$$

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In this convex, $L$-smooth case, we have a nice isoperimetric minorant; but can be applied in other cases too.

# Concluding remarks

I have presented explicit lower bound on the spectral gap of the pCN algorithm, focussing on the convex, $L$-smooth case.

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However the general framework developed is applicable much more broadly!

Furthermore the full conductance profile can give much more detailed mixing time bounds (not presented today; see paper).

Our paper actually discusses Random Walk Metropolis as the main example; see my Algorithms Seminar.

Natural next steps would be to consider more advanced algorithms such as MALA, HMC, etc...

# Thanks for listening! I


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# Thanks for listening! II


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# Convergence framework

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**Lemma ([Doucet et. al. (2015)])**

*pCN with Gaussian proposals is a positive chain.*

# Close coupling for pCN

Prevously: provided we can choose $\delta$ such that $|x - y| \leq \delta \Rightarrow \|Q(x, \cdot) - Q(y, \cdot)\|_{\mathrm{TV}} \leq \alpha_0/2$, we obtain that $P$ is close coupling with $\epsilon \geq \alpha_0/2$.

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Since we have Gaussian $\mathcal{N}(0, \sigma^2 \mathbf{I}_d)$ proposals, we can use Pinsker's inequality to obtain

**Lemma**

*For $v > 0$,*

$$|x - y|_{C^{-1}} \leq v \cdot \frac{\eta}{\rho} \Rightarrow \|Q(x, \cdot) - Q(y, \cdot)\|_{\mathrm{TV}} \leq v/2.$$

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*Thus by taking $v = \alpha_0$, i.e. $\delta = \alpha_0 \cdot \eta/\rho$, we have that $P$ is close coupling with $\epsilon = \alpha_0/2$.*

So all that remains is to get a handle on $\alpha_0$.

# Convergence of MCMC

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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 $\mathrm{L}^2(\pi) = \{f : \mathcal{X} \to \mathbb{R} : \|f\|_2^2 < \infty\}$, $\quad \langle f, g \rangle := \int fg \, \mathrm{d}\pi$,
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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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This acts like a discrete derivative, and we will seek to lower bound it.

# $L^2$ convergence and Dirichlet forms

We work on $\mathrm{L}^2(\pi) = \{f : \mathcal{X} \to \mathbb{R} : \|f\|_2^2 < \infty\}$, $\quad \langle f, g\rangle := \int fg \, \mathrm{d}\pi$,
$\mathrm{L}^2_0(\pi) := \{f \in \mathrm{L}^2(\pi) : \pi(f) = 0\}$.

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 $f \in \mathrm{L}^2_0(\pi)$:

$$\mathcal{E}(P^*P, f) := \langle (I - P^*P)f, f\rangle = \|f\|^2 - \|Pf\|^2.$$

This acts like a discrete derivative, and we will seek to lower bound it.

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

$$\mathcal{E}(P^*P, f) = \mathcal{E}(P^2, f) \geq \mathcal{E}(P, f).$$

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

# Conductance and spectral profiles

## Lemma ([Goel et. al. (2006)])

*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*

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