Explicit convergence bounds for Metropolis Markov chains

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Overview

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See arXiv preprint! `https://arxiv.org/abs/2211.08959`.

Statistical modelling

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Seek learn or infer values of the parameter x which are commensurate with the observed dataset y.

The Bayesian approach

Encode prior beliefs into a prior distribution $\nu(x)$, and define likelihood $\ell_y(x) := f_x(y)$.

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We are then interested in quantities of the form

$$I = \pi(f) = \int_{\mathcal{X}} f(x)\pi(x)\,\mathrm{d}x,$$

e.g. $f(x) = \|x\|^p$ (posterior moments), $f(x) = 1_A(x)$ (credible sets / posterior tail probabilities), etc.

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So instead, approximate I by sampling $X_1, X_2, \ldots, X_n \sim \pi$ and consider

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

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There are also optimization-based approaches such as Variational Inference, INLA, ...

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We simulate a π-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 $(X_i)_{i=1,\ldots,n}$

Random walk Metropolis

We will focus on Random Walk Metropolis (RWM) [Metropolis et. al. (1953)]:
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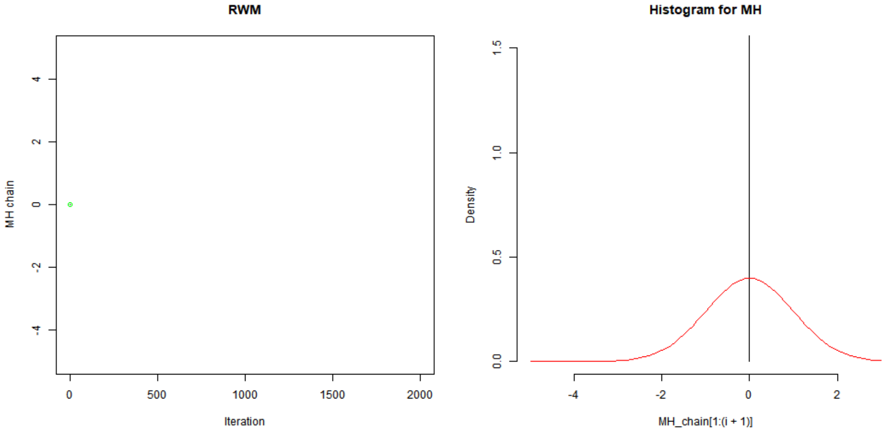
But tuning of $\sigma^2 \cdot \mathbf{I}$ is critical for good performance.

And suprisingly some things were still unknown! (Spectral gap.)

MH example


RWM
MH chain
4
2
0
-2
-4
0
500
1000
1500
2000
Iteration
Histogram for MH
Density
1.5
1.0
0.5
0.0
-4
-2
0
2
MH_chain[1:(i + 1)]

Tuning of RWM

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One beautiful way to approach this problem is optimal scaling [Roberts, Gelman, Gilks (1997)]:

It was shown that for a restricted class of targets π, in the high-dimensional limit, when scaling the variance like $\sigma^2 \sim d^{-1}$, the RWM chain has a stable acceptance ratio, and converges to a Langevin diffusion, and that the cost is like $O(d)$.

Optimal scaling

So optimal scaling tells us that for certain targets π, we should choose $\sigma^2 \sim d^{-1}$ to get a stable acceptance ratio in high dimensions, and even that we should aim for average acceptances rates of 0.234.

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But optimal scaling is purely asymptotic and does not say anything about any particular algorithm.

For example, suppose I am doing Bayesian logistic regression in $d = 1000$ and I have chosen $\sigma^2 = 5 \times 10^{-4}$. How long should I run my chain for?

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However we are restricted to considering RWM, as opposed to MALA/HMC [Dwivedi et. al. (2019), Chen et. al. (2019)].

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

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Under the common assumptions of L-smoothness and m-strong convexity of the potential U [Dwivedi et. al. (2019), Chen et. al. (2019)], we can give straightforward results (but framework more general!).

Such densities can be sandwiched between $\mathcal{N}(x_*, L^{-1}\mathbf{I}_d)$ and $\mathcal{N}(x_*, m^{-1}\mathbf{I}_d)$ densities.

Main result

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

For an L-smooth and m-strongly convex and twice differential potential U on $\mathbb{R}^d$, RWM targeting $\pi \propto \exp(-U)$ with proposal increments $\mathcal{N}(0, \sigma^2 \mathbf{I}_d)$ has spectral gap γ satisfying

$$C \cdot L \cdot d \cdot \sigma^2 \cdot \exp(-2Ld\sigma^2) \cdot \frac{m}{L} \cdot \frac{1}{d} \leq \gamma \leq \frac{L \cdot \sigma^2}{2} \wedge (1 + m \cdot \sigma^2)^{-d/2},$$

where $C = 1 \times 10^{-4}$.

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where $C = 1 \times 10^{-4}$.

To maximise the lower bound, take $\sigma = \varsigma \cdot L^{-1/2} \cdot d^{-1/2}$, and then

$$C \cdot \varsigma^2 \cdot \exp(-2\varsigma^2) \cdot \frac{m}{L} \cdot \frac{1}{d} \leq \gamma \leq \frac{\varsigma^2}{2} \cdot \frac{1}{d}.$$

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So indeed we see the spectral gap of RWM is $O(d^{-1})$.

Note that this applies for any d and for any ς, i.e. it actually says something about the algorithm you are running!

Overview

Conductance

Definition: Conductance

The conductance of a π-invariant Markov kernel P is

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

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Theorem (Cheeger inequalities)

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

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Thus our goal is to lower bound the conductance.

Isoperimetry

Fix target density π on metric space (E, d).

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

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

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

Then the isoperimetric profile of π 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 π 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:

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

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

Thus we can choose δ such that $|x - y| \le \delta \Rightarrow \|Q(x, \cdot) - Q(y, \cdot)\|_{\mathrm{TV}} \le \alpha_0/2$ to obtain P is close coupling with $\epsilon \ge \alpha_0/2$, provided we can bound α_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 π. Let P be $(\mathrm{d}, \delta, \epsilon)$-close coupling. Then

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

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So we have a lower bound on the conductance Φ_P^*, and hence on the spectral gap.

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So we have a lower bound on the conductance Φ_P^*, and hence on the spectral gap.

This result thus breaks the problem into two pieces:

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

Overview

Isoperimetric minorants for π

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The specific case of interest for this talk:

Lemma (Strongly convex case)

Suppose $\pi \propto \exp(-U)$ possesses an m-strongly convex potential U. Then

$$I_\pi(p) \geq m^{1/2} \cdot \varphi(\Phi^{-1}(p)) =: \tilde{I}_\pi(p),$$

where φ, Φ are the standard Gaussian p.d.f. and c.d.f., and furthermore

$$\tilde{I}_\pi(1/4) = m^{1/2} \cdot C_{\mathrm{g}},$$

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

Close coupling for RWM

Prevously: provided we can choose δ 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 $v > 0$,

$$|x - y| \leq v \cdot \sigma \Rightarrow \|Q(x,\cdot) - Q(y,\cdot)\|_{\mathrm{TV}} \leq v/2.$$

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

Close coupling for RWM

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

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

Lemma

For $v > 0$,

$$|x-y| \le v \cdot \sigma \Rightarrow \|Q(x,\cdot)-Q(y,\cdot)\|_{\mathrm{TV}} \le v/2.$$

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

So all that remains is to get a handle on α_0.

Controlling acceptance probabilities

We now assume that the potential U is *m-strongly convex* and *L-smooth*:

$$\frac{m}{2}|h|^2 \leq U(x+h) - U(x) - \langle \nabla U(x), h \rangle \leq \frac{L}{2}|h|^2, \quad x, h \in \mathsf{E}.$$

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Then through a direct calculation, we obtain:

Lemma

Let $\sigma = \varsigma \cdot d^{-1/2} \cdot L^{-1/2}$, 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 RWM, for $\sigma = \varsigma \cdot d^{-1/2} \cdot L^{-1/2}$

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

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The upper bound on the spectral gap is derived through direct calculations.

In the strongly convex, smooth case had a nice isoperimetric minorant; but can be applied in other cases too.

Using the full conductance profile can get much more intricate analysis of the mixing times.

Overview

Concluding remarks

I have presented explicit lower and upper bounds on the spectral gap of the RWM algorithm, focussing on the case of strongly convex and smooth potentials.

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Our paper also discusses the preconditioned Crank–Nicolson (pCN) algorithm a popular MCMC method for Bayesian Inverse Problems, which can be analysed in an analogous manner.

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

Overview

Thanks for listening! I

- Andrieu, C., Lee, A., Power, S., Wang, A. Q. (2022). Poincaré inequalities for Markov chains: a meeting with Cheeger, Lyapunov and Metropolis. *Technical report*. `https://doi.org/10.48550/arxiv.2208.05239`.
- **Andrieu, C., Lee, A., Power, S., Wang, A. Q. (2022)**. Explicit convergence bounds for Metropolis Markov chains: isoperimetry, spectral gaps and profiles. `https://doi.org/10.48550/arxiv.2211.08959`.
- Baxendale, P. H. (2005). Renewal theory and computable convergence rates for geometrically ergodic Markov chains. *Ann. Appl. Probab.*, 15(1B), 700738.
- Belloni, A., Chernozhukov, V. (2009). On the computational complexity of MCMC-based estimators in large samples. *Ann. Statist.*, 37(4), 20112055.
- Bobkov, S. G. (1999). Isoperimetric and analytic inequalities for log-concave probability measures. *Ann. Probab.*, 27(4), 19031921.
- Chen, Y., Dwivedi, R., Wainwright, M. J., Yu, B. (2019). Fast mixing of Metropolized Hamiltonian Monte Carlo: Benefits of multi-step gradients. *J. Mach. Learn. Res.*, 21.
- Dwivedi, R., Chen, Y., Wainwright, M. J., Yu, B. (2019). Log-concave sampling: Metropolis-Hastings algorithms are fast. *J. Mach. Learn. Res.*, 20, 142.
- Goel, S., Montenegro, R., Tetali, P. (2006). Mixing time bounds via the spectral profile. *Elec. J. Probab.*, 11(2000), 126.
- Jarner, S. F., Hansen, E. (2000). Geometric ergodicity of Metropolis algorithms. *Stoc. Proc. Appl.*, 85(2), 341361.

Thanks for listening! II

Livingstone, S., Zanella, G. (2022). The Barker proposal: Combining robustness and efficiency in gradient-based MCMC. *J. Roy. Statist. Soc. Ser. B: Statist. Meth.*, 84(2), 496523.

Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N., Teller, A. H., Teller, E. (1953). Equation of State Calculations by Fast Computing Machines. *J. Chem. Phys.*, 21(6), 10871092.

Milman, E. (2009). On the role of convexity in isoperimetry, spectral gap and concentration. *Invent. Math.*, 177(1), 143.

Roberts, G. O., Gelman, A., Gilks, W. R. (1997). Weak Convergence and Optimal Scaling of random walk Metropolis algorithms. *Ann. Appl. Probab.*, 7(1), 110120.

Roberts, G., Tweedie, R. L. (1996). Geometric convergence and central limit theorems for multidimensional Hastings and Metropolis algorithms. *Biometrika*, 83(1), 95110.

Convergence framework

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Lemma ([Baxendale (2005)])

RWM with Gaussian proposals is a positive chain.

Convergence of MCMC

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One measure of the former is to look at rates of convergence:

Theorem ([Roberts and Tweedie (1996), Jarner and Hansen (2000)])

RWM converges to equilibrium exponentially fast if and only if π 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 π-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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$$\mathcal{E}(P^*P, f) = \mathcal{E}(P^2, f) \geq \mathcal{E}(P, f).$$

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

Conductance

Definition: Conductance

The conductance profile of a π-invariant Markov kernel P is

$$\Phi_P(v) := \inf \left\{ \frac{(\pi \otimes P)(A \times A^\complement)}{\pi(A)} : \pi(A) \leq v \right\}.$$

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Theorem (Cheeger inequalities)

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Thus our goal is to lower bound the conductance.

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 Λ_P *is the spectral profile of* P.

Lemma

For π*-reversible* P*, we have the further lower bound*

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

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