Current developments in MCMC I: Explicit convergence bounds for Metropolis Markov chains

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Overview

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

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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

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- 1940s: Von Neumann and Stanislav Ulam
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- [Girolami and Calderhead (2011)]: Riemannian manifold HMC
- ...recent trends: next slide!

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  - Privacy / federated learning: [Dai, Pollock, Roberts (2023)], [Vono et. al. (2022)];
- Nonasymptotic convergence bounds via functional inequalities
  - [Chen et. al. (2019)], [Chewi et. al. (2021)], these lectures!

Overview of lectures

- Lecture 1 (now!): Andrieu, C., Lee, A., Power, S., Wang, A. Q. (2022+). Explicit convergence bounds for Metropolis Markov chains: isoperimetry, spectral gaps and profiles. To appear in *Ann. Appl. Probab.*
- Lecture 2: Andrieu, C., Lee, A., Power, S., Wang, A. Q. (2022). Comparison of Markov chains via weak Poincaré inequalities with application to pseudo-marginal MCMC. The *Ann. Statist.*, 50(6), 3592-3618.
- Lecture 3: 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`.

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I will present fundamental bounds on the spectral gap of Random Walk Metropolis, which has been an open problem for many years!

Along the way I will introduce a new technique for deriving convergence bounds based on isoperimetry and conductance.

We also have follow up work for the subgeometric case (not discussed today).

Andrieu, C., Lee, A., Power, S., Wang, A. Q. (2023). Weak Poincaré Inequalities for Markov chains: theory and applications. `https://arxiv.org/abs/2312.11689`

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

We will focus on Random Walk Metropolis (RWM) [Metropolis et. al. (1953)]: $Q(X_{i-1}, \cdot) = \mathcal{N}(X_{i-1}, \sigma^2 \cdot \mathbf{I})$.

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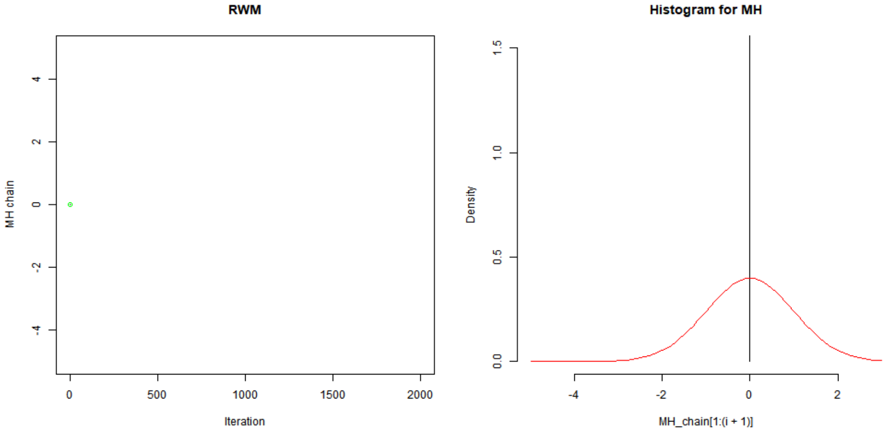
And suprisingly some things were still unknown! (Spectral gap.)

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 $O(d)$.

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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?

Our approach

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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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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

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

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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

Convergence framework: Conductance

Definition: Conductance

The conductance of a π-invariant Markov kernel P is

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

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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 $A_r := \{x \in \mathrm{E} : \mathrm{d}(x, A) \leq r\}$, 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 $(\mathrm{d}, \delta, \epsilon)$-close coupling if

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

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Lemma: close coupling for Metropolis chains

For Metropolis chains, we have the bound:

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

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

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Thus we can choose δ such that $|x - y| \leq \delta \Rightarrow \|Q(x,\cdot) - Q(y,\cdot)\|_{\mathrm{TV}} \leq \alpha_0/2$ to obtain P is close coupling with $\epsilon \geq \alpha_0/2$, 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 for any $v \in (0, 1/2]$,

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

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Hence we have a lower bound 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

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 (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

Previously: 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

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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 $\epsilon = \alpha_0/2$.

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., Doucet, A., Holenstein, R. (2010). Particle Markov chain Monte Carlo methods. *J. Roy. Statist. Soc. Ser. B: Stat. Methodol.*, 72(3), 269-342.
- 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`.
- Andrieu, C., Roberts, G. O. (2009). The pseudo-marginal approach for efficient Monte Carlo computations. *Ann. Statist.*, 37(2), 697-725.
- Bardenet, R., Doucet, A., Holmes, C. (2017). On Markov chain Monte Carlo methods for tall data. Journal of Machine Learning Research, 18, 1-43.
- Baxendale, P. H. (2005). Renewal theory and computable convergence rates for geometrically ergodic Markov chains. *Ann. Appl. Probab.*, 15(1B), 700-738.
- Belloni, A., Chernozhukov, V. (2009). On the computational complexity of MCMC-based estimators in large samples. *Ann. Statist.*, 37(4), 2011-2055.
- Bierkens, J., Fearnhead, P., Roberts, G. (2019). The Zig-Zag process and super-efficient sampling for Bayesian analysis of big data. *Ann. Statist.*, 47(3), 1288-1320.
- Bobkov, S. G. (1999). Isoperimetric and analytic inequalities for log-concave probability measures. *Ann. Probab.*, 27(4), 1903-1921.

Thanks for listening! II

- Bouchard-Côté, A., Vollmer, S. J., Doucet, A. (2018). The Bouncy Particle Sampler: A Nonreversible Rejection-Free Markov Chain Monte Carlo Method. *J. Amer. Statist. Assoc.*, 113(522), 855-867.
- Girolami, M., Calderhead, B. (2011). Riemann manifold Langevin and Hamiltonian Monte Carlo methods. *J. Roy. Statist. Soc. Ser. B*, 73(2), 123-214.
- Cao, Y., Lu, J., Wang, L. (2023). On Explicit L2 -Convergence Rate Estimate for Underdamped Langevin Dynamics. *Arch. Rational Mech. Anal.*, 247(5), 1-34.
- 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.
- Chewi, S., Erdogdu, M. A., Li, M. B., Shen, R., Zhang, M. (2021). Analysis of Langevin Monte Carlo from Poincaré to Log-Sobolev. `https://arxiv.org/abs/2112.12662`
- Dai, H., Pollock, M., Roberts, G. O. (2023). Bayesian fusion: Scalable unification of distributed statistical analyses. *J. Roy. Statist. Soc. Ser. B*, 85(1), 84-107.
- Dalalyan, A. S. (2016). Theoretical guarantees for approximate sampling from smooth and log-concave densities. *J. Roy. Statist. Soc. Ser. B*, 79(3), 651-676.
- Duane, S., Kennedy, A. D., Pendleton, B. J., Roweth, D. (1987). Hybrid Monte Carlo. *Phys. Lett. B*, 195(2), 216-222.
- Durmus, A., Moulines, E. (2017). Nonasymptotic convergence analysis for the unadjusted Langevin algorithm. *Ann. Appl. Probab.*, 27(3), 1551-1587.

Thanks for listening! III

- Dwivedi, R., Chen, Y., Wainwright, M. J., Yu, B. (2019). Log-concave sampling: Metropolis-Hastings algorithms are fast. *J. Mach. Learn. Res.*, 20, 1-42.
- Geman, Stuart, and Donald Geman. (1984) Stochastic relaxation, Gibbs distributions, and the Bayesian restoration of images. *IEEE Trans. patt. anal. mach. intell.* 6: 721-741.
- Goel, S., Montenegro, R., Tetali, P. (2006). Mixing time bounds via the spectral profile. *Elec. J. Probab.*, 11(2000), 1-26.
- Green, P. J. (1995). Reversible Jump Markov Chain Monte Carlo Computation and Bayesian Model Determination. *Biometrika*, 82(4), 711-732.
- Hastings, W. K. (1970). Monte Carlo sampling methods using Markov chains and their applications. *Biometrika*, 57(1), 97-109.
- Haario, H., Saksman, E., Tamminen, J. (1999). Adaptive proposal distribution for random walk Metropolis algorithm. *Comput. Statist.*, 14, 375-395.
- Jacob, P. E., OLeary, J., Atchadé, Y. F. (2020). Unbiased Markov chain Monte Carlo methods with couplings. *J. Roy. Statist. Soc. Ser. B*, 82(3), 543-600.
- Jarner, S. F., Hansen, E. (2000). Geometric ergodicity of Metropolis algorithms. *Stoc. Proc. Appl.*, 85(2), 341-361.
- 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), 496-523.

Thanks for listening! IV

- 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), 1087-1092.
- Meyn, S. P., Tweedie, R. L. (1993). *Markov Chains and Stochastic Stability*. Springer-Verlag.
- Milman, E. (2009). On the role of convexity in isoperimetry, spectral gap and concentration. *Invent. Math.*, 177(1), 1-43.
- Neal, R. M. (1995). *Bayesian Learning for Neural Networks*. PhD Thesis, University of Toronto.
- Neal, R. M. (2003). Slice sampling. *Ann. Statist.*, 31(3), 705-767.
- Propp, J. G., Wilson, D. B. (1996). Exact Sampling with Coupled Markov Chains and Applications to Statistical Mechanics. *Rand. Struct. Alg.*, 9(2), 223-252.
- Roberts, G. O., Gelman, A., Gilks, W. R. (1997). Weak Convergence and Optimal Scaling of random walk Metropolis algorithms. *Ann. Appl. Probab.*, 7(1), 110-120.
- Roberts, G., Tweedie, R. L. (1996). Geometric convergence and central limit theorems for multidimensional Hastings and Metropolis algorithms. *Biometrika*, 83(1), 95-110.
- Rossky, P. J., Doll, J. D., Friedman, H. L. (1978). Brownian dynamics as smart Monte Carlo simulation. *J. Chem. Phys.*, 69(10), 4628-4633.
- Syed, S., Bouchard-Côté, A., Deligiannidis, G., Doucet, A. (2022). Non-reversible parallel tempering: A scalable highly parallel MCMC scheme. *J. Roy. Statist. Soc. Ser. B*, 84(2), 321-350.

Thanks for listening! V

Tavaré, S., Balding, D. J., Griffiths, R. C., Donnelly, P. (1997). Inferring coalescence times from DNA sequence data. *Genetics*, 145(2), 505-518.

Vono, M., Plassier, V., Durmus, A., Dieuleveut, A., Moulines, E. (2022). QLSD: Quantised Langevin Stochastic Dynamics for Bayesian Federated Learning. *Proceedings of AISTATS*, 151, 6459-6500.

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

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

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

Convergence framework

We focus now on lower bounding the spectral gap γ of the RWM.

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Lemma ([Baxendale (2005)])

RWM with Gaussian proposals is a positive chain.

Convergence framework: Conductance

Definition: Conductance

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

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

The conductance of P is $\Phi_P^* := \Phi_P(1/2)$.

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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.

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 $(\mathsf{d}, \delta, \epsilon)$-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.

Conductance and spectral profiles

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

For nonconstant nonnegative $g \in \mathrm{L}_0^2(\pi)$, 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

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