A calculus for Markov chain Monte Carlo studying approximations in algorithms

Rocco Caprio joint work with Adam M Johansen

January 2024



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Markov chain Monte Carlo algorithms are based on the construction of a Markov chain  $\{X_n\}_{n\in\mathbb{N}}$  with transition probabilities

$$\mathbb{P}(X_n \in A | X_{n-1} = x) = P_{\mu}(x, A)$$

 $\mu$  here is the *invariant distribution* of the Markov Chain  $P_{\mu}$ :

$$P_{\mu}(\mu, A) = \int \mu(\mathsf{d} x) P_{\mu}(x, A) = \mu(A)$$

If  $P_{\mu}$  is good enough, we can conclude  $I_n := n^{-1} \sum_{i=1}^n f(X_i) \to I$ .

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#### Algorithm 1 Hastings algorithm

Starting with  $X_0 = x$ . For  $i = 1, \ldots, n$ ,

• Draw 
$$Y \sim Q(X_{i-1}, \cdot)$$

• Compute 
$$r_{\mu}(X_{i-1}, Y) := \frac{\mu(Y)Q(Y, X_{i-1})}{\mu(X_{i-1})Q(X_{i-1}, Y)}$$
.

Set  $X_i = Y$  with probability  $g(r_{\mu}(X_{i-1}, Y))$ , otherwise set  $X_i = X_{i-1}$ .

Where g(x) = xg(1/x),  $g(x) \le 1$  is an acceptance/balancing function. With  $g(x) = \min(1, x)$  this is the Metropolis-Hastings algorithm.

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- In particular, we will check that if the derivative in the invariant distribution of P is bounded, then  $P_{\mu}$  and  $P_{\nu}$  move alike if  $\mu$  and  $\nu$  are close;

 This provides a natural theoretical framework to analyze approximation-based algorithms. There are usually many possible Markov chains for each given invariant distribution. We first need to restrict the space of Markov kernels.

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### Definition

A family of Markov kernels  $\{P_{\star}\}$  is a collection of Markov kernels indexed by an open, convex subset of invariant distributions.

If for some  $\mu, \nu \in \mathcal{P}(X)$ ,  $P_{\mu}, P_{\nu} \in \{P_{\star}\}$ , then the curve  $\mu_t := (1 - t)\mu + t\nu$ interpolating  $\mu$  and  $\nu$  satisfies  $P_{\mu_t} \in \{P_{\star}\}$ .

Your best friends are Markov families!

# Example

The Hastings family

$$\begin{split} P_{\mu}(x,f) &:= \int f(y)Q(x,\mathrm{d}y)g(r_{\mu}(x,y)) + f(x)(1 - \int Q(x,\mathrm{d}y)g(r_{\mu}(x,y))) \\ \text{with } r_{\mu}(x,y) &:= \frac{\mu(y)Q(y,x)}{\mu(x)Q(x,y)}, \ g(x) = xg(1/x), \ g(x) \leq 1. \end{split}$$

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Many other choices are possible. Gibbs, MALA, Metropolis-in-Gibbs families... Let  $\{P_{\star}\}$  be a Markov family. We define the derivative of P by first fixing a starting distribution and a test function. Consider the functional  $P.(\rho, f) : \mu \in \mathcal{P}(\mathsf{X}) \mapsto P_{\mu}(\rho, f) \in \mathbb{R}$  for some fixed  $(\rho, f)$ .

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#### Definition

The derivative of  $P_{\cdot}(\rho, f)$  in the invariant distribution at  $\mu \in \mathcal{P}_{\lambda}(X)$  is the functional  $\partial_{\pi} P_{\mu}(\rho, f)[\cdot] : \mathcal{M}_{\lambda,0}(X) \mapsto \mathbb{R}$  such that for all  $\nu \in \mathcal{P}_{\lambda}(X)$ ,

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}P_{\mu+t(\nu-\mu)}(\rho,f)\right|_{t=0}=\partial_{\pi}P_{\mu}(\rho,f)[\nu-\mu].$$

Where  $\mathcal{M}_{\lambda,0}(X) := \{ set of 0-mass measures with Lebesgue-density \}$ 

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Where  $\mathcal{M}_{\lambda,0}(X) := \{ \text{set of } 0 \text{-mass measures with Lebesgue-density} \}$ 

The derivative of  $P(\rho, \cdot)$  is defined in the oblivious way: it is the operator

 $\partial_{\pi} P_{\mu}(\rho, \cdot)[\cdot] : f \in \{\text{some set}\} \mapsto \partial_{\pi} P_{\mu}(\rho, f)[\cdot]$ 

For  $\rho \in \mathcal{P}_{\lambda}(X)$ , the action of the functional  $\partial_{\pi} P_{\mu}(\rho, f)$  will be expressible in *integral form*: for some function  $\partial_{\pi} P_{\mu}(\rho, f)(\cdot) : X \mapsto \mathbb{R}$ 

$$\partial_{\pi} P_{\mu}(\rho, f)[\nu - \mu] = \int (\nu(y) - \mu(y))\partial_{\pi} P_{\mu}(\rho, f)(y)\lambda(dy)$$
 and  
 $\mu(\partial_{\pi} P_{\mu}(\rho, f)(\cdot)) = 0.$ 

 $\partial_{\pi} P_{\mu}(\rho, f)(\cdot)$ , if it exists, is the *first variation* of  $P_{\cdot}(\rho, f)$ . We call it the *density* of the derivative in the invariant distribution.

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However, for  $\rho \notin \mathcal{P}_{\lambda}(X)$  (e.g.  $\rho = \delta_{x}$ ),  $\partial_{\pi} P_{\mu}(\rho, f)$  will have no density:

$$\partial_{\pi} P_{\mu}(x,f)[
u-\mu] = (a \textit{ density part}) + (a \textit{ singular part})$$

Getting to know  $\partial_{\pi} P_{\mu}(\rho, f)$ 

∂<sub>π</sub>P<sub>µ</sub>(ρ, ·) describes how P<sub>µ</sub>(ρ, ·) changes when we perturb the distribution µ infinitesimally by a 0-mass measure.

 $\Rightarrow$  If  $\partial_{\pi} P_{\mu}(\rho, \cdot)$  is large,  $P(\rho, \cdot)$  is not robust to changes in the invariant.

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Interestingly, it always hold

$$\partial_{\pi}P_{\mu}(\mu,f)(y)=f(y)-P_{\mu}(y,f).$$

(minus) the generator of P! So...

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# Theorem (Ergodic Theorem with derivatives)

Suppose that  $\{X_n\}_{n\in\mathbb{N}}$  is an aperiodic,  $\mu$ -irreducible Markov Chain with transition probabilities  $P_{\mu}$  and invariant distribution  $\mu$ . If there exists some petite set C, some  $b < \infty$  and a non-negative finite function f bounded on C such that

$$-\partial_{\pi}P_{\mu}(\mu,f)(x)\leq -1+b\mathbf{1}_{\mathcal{C}}(x), \quad x\in\mathsf{X}$$

whenever such kernel derivative exists, then for all  $x \in X$ , as  $k \to \infty$ ,

$$\left\|P_{\mu}^{k}(x,\cdot)-\mu\right\|_{\mathrm{tv}}\to 0.$$

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Consider the Hastings family. Let  $W_H := \{\rho \in \mathcal{P}_\lambda(\mathsf{X}) : \rho/\mu^2 \text{ is bounded}\} - \text{ and}$  assume that g is differentiable.

### Proposition

The Hastings kernel  $P_{\cdot}(\rho, \cdot)$  is differentiable in the invariant distribution at  $\mu$  for all  $\rho \in W_{H}$ . The derivative  $\partial_{\pi} P_{\mu}(\rho, \cdot)$  admits an integral representation, with its density given by

$$\partial_{\pi} P_{\mu}(\rho, f)(y) = \int (f(y) - f(z)) rac{
ho(z)}{\mu(z)} g'(r_{\mu}(z, y)) Q(y, dz) \ - rac{
ho(y)}{\mu(y)^2} \int (f(z) - f(y)) q(z, y) g'(r_{\mu}(y, z)) \mu(dz).$$

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ho(y)}{\mu(y)^2} \int (f(z) - f(y)) q(z, y) g'(r_{\mu}(y, z)) \mu(\mathrm{d}z).$$

This rules out Metropolis-Hastings but don't worry.

# Proposition (cont.)

Under some regularity conditions,  $P_{\cdot}(x, \cdot)$  is also differentiable for all  $x \in X$ .  $\partial_{\pi}P_{\mu}(x, \cdot)$  is given by

$$\partial_{\pi} P_{\mu}(x, f)[\nu - \mu] = \underbrace{\int (f(y) - f(x)) \frac{g'(r_{\mu}(x, y))q(y, x)}{\mu(x)} (\nu - \mu)(dy)}_{\substack{density \ part}} \underbrace{-\frac{(\nu - \mu)(x)}{\mu(x)^2} \int (f(y) - f(x))q(y, x)g'(r_{\mu}(x, y))\mu(dy)}_{\substack{density \ part}}.$$

singular part

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#### Theorem

For all  $\rho$  such that  $P_{\cdot}(\rho, \cdot)$  is differentiable at  $\mu_t := (1 - t)\mu + t\nu$  for all  $t \in [0, 1]$ 

$$P_{\mu}(
ho,\cdot)-P_{\nu}(
ho,\cdot)=\int_{0}^{1}\partial_{\pi}P_{\mu_{t}}(
ho,\cdot)[
u-\mu]\,\mathrm{d}t.$$

# Definition

We say that a differentiable Markov kernel  $P_{\cdot}(\rho, \cdot)$  has a bounded derivative at  $\mu$  towards  $\nu$  if there exist constants  $M_{1,\rho}, M_{2,\rho} < \infty$  such that

$$\left\| P_{\mu}(\rho, \cdot) - P_{\nu}(\rho, \cdot) \right\|_{\text{tv}} \le M_{1,\rho} \|\mu - \nu\|_{\text{tv}} + M_{2,\rho}\rho(|\mu - \nu|).$$
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(1)

•  $d(\mu, \nu) = ||\mu - \nu||_{tv} + \rho(|\mu - \nu|)$  is a metric, so this could be written as Lipschitz continuity w.r.t. d, with constant given by  $\max(M_{1,\rho}, M_{2,\rho})$ . However, (1) separates contributions.

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- $d(\mu, \nu) = \|\mu \nu\|_{tv} + \rho(|\mu \nu|)$  is a metric, so this could be written as Lipschitz continuity w.r.t. *d*, with constant given by  $\max(M_{1,\rho}, M_{2,\rho})$ . However, (1) separates contributions.
- When ρ ∈ P<sub>λ</sub>(X), this definition is equivalent to the existence of a constant M<sub>ρ</sub> < ∞ such that</p>

$$\left\| \mathsf{P}_{\mu}(\rho, \cdot) - \mathsf{P}_{\nu}(\rho, \cdot) \right\|_{\mathrm{tv}} \leq M_{\rho} \|\mu - \nu\|_{\mathrm{tv}}.$$

whereas if  $\rho = \delta_x$ , it becomes

$$\left\| \mathcal{P}_{\mu}(x,\cdot) - \mathcal{P}_{\nu}(x,\cdot) \right\|_{\mathrm{tv}} \leq M_{1,x} \left\| \mu - \nu \right\|_{\mathrm{tv}} + M_{2,x} \left| \mu(x) - \nu(x) \right|.$$

# Proposition

For Hastings kernels, if  $P(\rho, \cdot)$  is differentiable in  $\mu_t = (1 - t)\mu + t\nu$  for all  $t \in [0, 1]$  and a boundedness condition on the derivative holds, then  $P(\rho, \cdot)$  will have a bounded derivative in the invariant distribution at  $\mu$  towards  $\nu$ . The "mean-value" inequalities

$$\left\| \mathsf{P}_{\mu}(\rho, \cdot) - \mathsf{P}_{\nu}(\rho, \cdot) \right\|_{\mathrm{tv}} \leq M_{\rho} \left\| \mu - \nu \right\|_{\mathrm{tv}}$$

$$\|P_{\mu}(x,\cdot) - P_{\nu}(x,\cdot)\|_{tv} \le M_{1,x}\|\mu - \nu\|_{tv} + M_{2,x}|\mu(x) - \nu(x)|$$

hold, with some explicit values for the 'Lipschitz constants'  $M_{\rho}$ ,  $M_{1,x}$ ,  $M_{2,x}$ .

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hold, with some explicit values for the 'Lipschitz constants'  $M_{\rho}$ ,  $M_{1,x}$ ,  $M_{2,x}$ .

By considering  $g_j(x) := (x + \dots + x^j)/(1 + x + \dots + x^j) \rightarrow \min(1, x)$  we can also obtain similar mean-value inequalities for the Metropolis-Hastings family.

The Metropolis-Hastings kernel is an example of non-differentiable but Lipschitz mapping of its invariant distribution!

#### These inequalities seem to be fairly tight!



Figure: The mean value inequality  $\|P_{\mu}(x,\cdot) - P_{\nu}(x,\cdot)\|_{tv} \le \|\mu - \nu\|_{tv} M_{1,x} + |\mu(x) - \nu(x)|M_{2,x}$  for RW MH as a function of  $x \in X$ 

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With a bounded derivative  $P_{\mu_n}$  chain moves similarly to  $P_{\mu}$  if  $\mu_n$  and  $\mu$  are close. An alternative is to minimize fluctuations  $P_{\mu_n}$  around  $P_{\mu}$ . Suppose that  $\{\mu_n\}_{n\in\mathbb{N}}\in\mathcal{P}(X)$  are random, and that  $n^{-1/2}[\mu_n-\mu](f) \Rightarrow N(0,v(f))$ .

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### Proposition

If  $P_{\cdot}(\rho, f)$  is differentiable, then

$$n^{-1/2}(P_{\mu_n}(\rho,f)-P_{\mu}(\rho,f)) \Rightarrow N(0,\nu(\partial_{\pi}P_{\mu}(\rho,f))).$$

The random fluctuations of  $P_{\mu_n}(\rho, f)$  around  $P_{\mu}(\rho, f)$  depend explicitly on the derivative  $\partial_{\pi} P_{\mu}(\rho, f)$ .

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- It is natural to think of ν as an approximation of μ. In this sense we are investigating when an "approximated" Markov chain P<sub>ν</sub> moves like the limiting P<sub>μ</sub>, which is desirable.

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- It is natural to think of ν as an approximation of μ. In this sense we are investigating when an "approximated" Markov chain P<sub>ν</sub> moves like the limiting P<sub>μ</sub>, which is desirable.
- ▶ Roughly speaking (and under some other regularity conditions), if  $P_{\cdot}(x, \cdot)$  has a bounded derivative in the invariant distribution at  $\mu$  towards  $\nu$ , and  $\nu$  is somewhat close to  $\mu$ , the "approximated" Markov chain  $P_{\nu}$  will achieve the same asymptotic variance of  $P_{\mu}$  plus an additional variability due the fluctuations of  $\nu$  around  $\mu$ .

Suppose that we can write  $\mu = \Phi(\eta)$ , for some transformation  $\Phi : \mathcal{P}(X) \mapsto \mathcal{P}(X)$ .

#### Algorithm 2 Sequential MCMC

- 1. Simulate  $Y'_{i+1} \sim P_{\eta}(Y'_i, \cdot)$  for  $i = 0, \ldots, n$ ; set  $\eta_n := n^{-1} \sum_{i=0}^n \delta_{Y'_i}$ .
- 2. Simulate  $Y_{i+1} \sim P_{\Phi(\eta_n)}(Y_i, \cdot)$  for  $i = 0, \ldots, n$ .

Typically  $\Phi$  is the Boltzmann-Gibbs transformation associated to some Feynman-Kac model, and this algorithm is popular in the context of particle filtering where



See Berzuini et al., 1997; Golightly and Wilkinson, 2006; Septier et al., 2009; Li et al., 2023; Finke, Doucet, and Johansen, 2020...

Denote with  $\sigma^2$  the asymptotic variance achieved by the Markov chain  $P_{\mu}$  and let  $\mu_n := \Phi(\eta_n)$ .

### Theorem

Assume that

- P. has a bounded derivative in the invariant distribution at μ towards every μ<sub>n</sub>;
- $\mu_n(x) \rightarrow \mu(x)$  for all  $x \in X$  and  $n^{-1/2}[\mu_n \mu](f) \Rightarrow N(0, v(f))$ .

P satisfies an uniform drift and minorization condition.

Then,

$$n^{-1/2} \sum_{i=0}^{n} f(Y_i) - \mu(f) \Rightarrow N(0, \sigma^2(f) + v^2(f)).$$

Extends the theoretical guarantees for sMCMC of Finke, Doucet, and Johansen, 2020!

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- The methods and the strategy developed can be adapted to other contexts. A calculus with proposals and/or other distributions the kernel depends on?
- Many directions to explore, in terms of development of the theory (second order derivatives, Taylor-type theorems...) and/or employing these or similar results in interesting contexts.



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