Convergence of Adaptive and Interacting MCMC algorithms

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Examples of adaptive MCMC

Convergence of the marginals for adaptive MCMC samplers

Law of large numbers for adaptive MCMC samplers

Convergence of the stationary distributions π_{θ_n}

Applications

I. Two examples of adaptive MCMC samplers

1. an Adaptive MCMC algorithm
2. an Interacting MCMC algorithm

Example 1: The Adaptive Metropolis

[Haario et al. (1999)]

Consider the Metropolis-Hastings algorithm

- with target density π on X — $\mathsf{X} \subseteq \mathbb{R}^d$, density w.r.t. the Lebesgue measure
- with Gaussian proposal $q_{\theta}(x, y) = \mathcal{N}_d(x, \theta)[y]$

$\hookrightarrow$ How to choose the design parameter θ ?

Example 1: The Adaptive Metropolis

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$\hookrightarrow$ How to choose the design parameter θ ?

Ans: covariance matrix of π up to a scalar, [ROBERTS ET AL. (1997)] iteratively estimated by the empirical covariance matrix or a robust estimator

$$\theta_{n+1} = \frac{n}{n+1}\theta_n + \frac{1}{n+1}\left\{(X_{n+1} - \mu_{n+1})(X_{n+1} - \mu_{n+1})^T + \kappa \ \mathrm{Id}_d\right\}$$

$$\mu_{n+1} = \mu_n + \frac{1}{n+1}(X_{n+1} - \mu_n)$$

This yields the adaptive Metropolis algorithm: iteratively

- draw $X_{n+1} \sim P_{\theta_n}(X_n, \cdot)$ transition kernel of a HM algo with Gaussian proposal with covariance matrix $\propto \theta_n$
- update the parameter θ_{n+1}, based on θ_n and $X_{1:n+1}$

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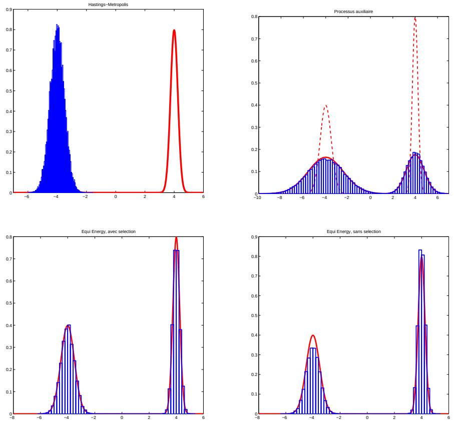
In this example

- $\pi P_\theta = \pi$ i.e. same invariant distribution
- $\theta_n \in \Theta$ where Θ is a finite dimensional parameter space.

Example 2: The Equi-Energy sampler (simplified) [Kou et al. (2006)]

$\hookrightarrow$ For the simulation of multi-modal density π.



Let

- a transition kernel P such that $\pi P = \pi$.
- a probability of swap: $\epsilon \in (0,1)$
- an auxiliary process $\{Y_n, n \geq 0\}$ that “targets” the tempered density $\pi^{1-\beta}$ $\quad (\beta \in (0,1))$

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Define iteratively the process of interest $\{X_n, n \geq 0\}$

- with probability $(1-\epsilon)$: draw $X_{n+1} \sim P(X_n, \cdot)$
- with probability ϵ: draw at random Y through the past values $Y_{0:n}$ and accept or not Y as the new value, with an acceptation-rejection algorithm.

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- with probability ϵ: draw at random Y through the past values $Y_{0:n}$ and accept or not Y as the new value, with an acceptation-rejection algorithm. (simplified EE)

This yields the (simplified) Equi-Energy sampler: $X_{n+1} \sim P_{\theta_n}(X_n, \cdot)$

where $$\theta_{n+1} = \frac{1}{n+1} \sum_{k=0}^{n} \delta_{Y_k}$$

$$P_\theta(x, A) = (1-\epsilon) P(x, A) + \epsilon \left\{ \int_A \alpha(x,y) \theta(\mathrm{d}y) + \mathbb{1}_A(x) \int (1-\alpha(x,y)) \theta(\mathrm{d}y) \right\}$$

and $\alpha(x, y)$ defined such that $\pi P_{\theta_\star} = \pi$ where $\theta_\star = \lim_n \theta_n \propto \pi^{1-\beta}$

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In this example

- $\pi_\theta P_\theta = \pi_\theta$ i.e. invariant distributions depending upon θ
- $\theta_n \in \Theta$ where Θ is an infinite dimensional parameter space.

Conclusion

Let a family of transition kernels on X, $\{P_\theta, \theta \in \Theta\}$.

Consider a X $\times$ Θ-valued process $\{(X_n, \theta_n), n \geq 0\}$ such that

- it is adapted to a filtration $\mathcal{F}_n$.
- $\mathbb{P}(X_{n+1} \in A | \mathcal{F}_n) = P_{\theta_n}(X_n, A)$

$\hookrightarrow$ What kind of conditions on the adaption mecanism $\{\theta_n, n \geq 0\}$ and on the transition kernels $\{P_\theta, \theta \in \Theta\}$ imply that there exists a distribution π such that

- convergence of the marginals: $\mathbb{E}\left[f(X_n)\right] \to \pi(f)$ $\quad$ f bounded
- law of large numbers: $n^{-1} \sum_{k=1}^{n} f(X_k) \xrightarrow{\text{a.s.}} \pi(f)$ $\quad$ f unbounded

II. Convergence of the marginals for adaptive MCMC samplers

For a bounded function f,

$$\mathbb{E}\left[f(X_n)\right] - \pi(f) \to 0$$

Even in the case the kernels P_θ have <u>*the same*</u> *invariant distribution, it is NOT true that ergodicity holds since the kernels are chosen at random. Conditions on the adaptation mecanism are required*

Sketch of the proof

We write

$$\mathbb{E}\left[f(X_n)\right] - \pi(f) = \mathbb{E}\left[f(X_n) - P^N_{\theta_{n-N}} f(X_{n-N})\right] + \mathbb{E}\left[P^N_{\theta_{n-N}} f(X_{n-N}) - \pi_{\theta_{n-N}}(f)\right] + \mathbb{E}\left[\pi_{\theta_{n-N}}(f)\right] - \pi(f)$$

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$\hookrightarrow$ [A] condition on the ergodicity of the transition kernels

"Usually", the transition kernels $\{P_\theta, \theta \in \Theta\}$ are geometrically ergodic :

$$\sup_{f, |f| \leq 1} |P^n_\theta f(x) - \pi_\theta(f)| \leq C_\theta \ \rho^n_\theta \ V(x) \qquad \rho_\theta \in (0,1)$$

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$\hookrightarrow$ [B] condition on the adaptation mecanism since

$$\left|\mathbb{E}\left[f(X_n) - P^N_{\theta_{n-N}} f(X_{n-N})\right]\right| \leq \sum_{j=1}^{N-1} (N-j)\mathbb{E}\left[\sup_x \left\| P_{\theta_{n-N+j}}(x,\cdot) - P_{\theta_{n-N+j-1}}(x,\cdot)\right\|_{\mathrm{TV}}\right]$$

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$\hookrightarrow$ [C] when $\pi_\theta \neq \pi$, condition on the convergence of $\{\pi_{\theta_n}, n \geq 0\}$ to π

Sketch of the proof

We write

$$\mathbb{E}\left[f(X_n)\right] - \pi(f) = \mathbb{E}\left[f(X_n) - P^{r(n)}_{\theta_{n-r(n)}} f(X_{n-r(n)})\right] + \mathbb{E}\left[P^{r(n)}_{\theta_{n-r(n)}} f(X_{n-r(n)}) - \pi_{\theta_{n-r(n)}}(f)\right] + \mathbb{E}\left[\pi_{\theta_{n-r(n)}}(f)\right] - \pi(f)$$

The conditions can be weakened by replacing N by $r(n)$. This allows to consider situations when the *transition kernels are not simultaneously ergodic*

$$\sup_{f,|f|\leq 1} |P^n_{\theta} f(x) - \pi_{\theta}(f)| \leq C_{\theta} \; \rho^n_{\theta} \; V(x) \qquad \rho_{\theta} \in (0,1)$$

and even cases where $C_{\theta_n} \vee (1-\rho_{\theta_n})^{-1}$ is not bounded (a.s.).

Result [Fort et al. 2010]

A. (Ergodicity of the transition kernels)

- $\exists \pi_\theta$ s.t. $\pi_\theta P_\theta = \pi_\theta$
- for any $\epsilon > 0$, there exists a non-decreasing positive sequence $\{r_\epsilon(n), n \geq 0\}$ such that $\limsup_{n\to\infty} r_\epsilon(n)/n = 0$ and

$$\limsup_{n\to\infty} \mathbb{E}\left[\left\| P^{r_\epsilon(n)}_{\theta_{n-r_\epsilon(n)}}(X_{n-r_\epsilon(n)}, \cdot) - \pi_{\theta_{n-r_\epsilon(n)}} \right\|_{\mathrm{TV}} \right] \leq \epsilon \; .$$

B. (Diminishing adaptation) For any $\epsilon > 0$,

$$\lim_{n\to\infty} \sum_{j=0}^{r_\epsilon(n)-1} \mathbb{E}\left[\sup_x \left\| P_{\theta_{n-r_\epsilon(n)+j}}(x, \cdot) - P_{\theta_{n-r_\epsilon(n)}}(x, \cdot) \right\|_{\mathrm{TV}} \right] = 0$$

C. (Convergence of the invariant distributions) $\exists\ \pi$ and a bounded non-negative function f s.t. $\lim_n \pi_{\theta_n}(f) = \pi(f)$ a.s.

Then $\lim_n \mathbb{E}\left[f(X_n) \right] = \pi(f)$.

Comparison with the literature pioneering work by [Roberts & Rosenthal, 2007]

1. Our conditions both weaken the *containment condition* and the *diminishing adaptation condition* of [Roberts & Rosenthal, 2007]. We are able to consider cases when the transition kernels are ergodic but not necessarily uniformly-in-θ.

$$\sup_{f, |f| \leq 1} |P_\theta^n f(x) - \pi_\theta(f)| \leq C_\theta \; \rho_\theta^n \; V(x)$$

Nevertheless, it is required to have an explicit control of ergodicity s.t. $C_{\theta_n} \vee (1-\rho_{\theta_n})^{-1}$ does not "explode too rapidly".

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   Nevertheless, it is required to have an explicit control of ergodicity s.t. $C_{\theta_n} \vee (1-\rho_{\theta_n})^{-1}$ does not "explode too rapidly".

2. π_θ can depend upon θ provided we are able to prove that $\pi_{\theta_n}(f)$ converges to $\pi(f)$.

III. Law of large numbers for adaptive MCMC samplers

For an (unbounded) function f s.t. $\cdots$

$$\frac{1}{n}\sum_{k=1}^{n} f(X_k) \xrightarrow{\text{a.s.}} \pi(f).$$

Sketch of the proof

We write

$$n^{-1}\sum_{k=1}^{n} f(X_k) - \pi(f) = n^{-1}\sum_{k=1}^{n}\left\{f(X_k) - \pi_{\theta_{k-1}}(f)\right\} + \frac{1}{n}\sum_{k=1}^{n}\pi_{\theta_{k-1}}(f) - \pi(f)$$

For the second term, $\hookrightarrow$ [A] condition on $\pi_{\theta_n}(f) \xrightarrow{\text{a.s.}} \pi(f)$

Sketch of the proof

$$n^{-1}\sum_{k=1}^{n} f(X_k) - \pi(f) = n^{-1}\sum_{k=1}^{n}\left\{f(X_k) - \pi_{\theta_{k-1}}(f)\right\} + \frac{1}{n}\sum_{k=1}^{n}\pi_{\theta_{k-1}}(f) - \pi(f)$$

For the first term, Tool : Poisson equation so that

$$n^{-1}\sum_{k=1}^{n}\left\{f(X_k) - \pi_{\theta_{k-1}}(f)\right\} = n^{-1}\underbrace{\sum_{k=1}^{n}\Delta M_k}_{\text{sum of martingale increments}} + \underbrace{R_n^{(1)}}_{\text{Rest due to the adaptation}} + \underbrace{R_n^{(2)}}_{\text{Rest}}$$

Sketch of the proof

$$n^{-1}\sum_{k=1}^{n} f(X_k) - \pi(f) = n^{-1}\sum_{k=1}^{n}\left\{f(X_k) - \pi_{\theta_{k-1}}(f)\right\} + \frac{1}{n}\sum_{k=1}^{n}\pi_{\theta_{k-1}}(f) - \pi(f)$$

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- Martingale increments : $\hookrightarrow$ [B] moment conditions of the form

$$\exists \alpha > 1, \qquad \sum_k \frac{1}{k^\alpha}\, \mathbb{E}\left[|\Delta M_k|^\alpha | \mathcal{F}_{k-1}\right] < +\infty \quad \text{a.s.}$$

Sketch of the proof

$$n^{-1}\sum_{k=1}^{n} f(X_k)-\pi(f) = n^{-1}\sum_{k=1}^{n}\left\{f(X_k)-\pi_{\theta_{k-1}}(f)\right\}+\frac{1}{n}\sum_{k=1}^{n}\pi_{\theta_{k-1}}(f)-\pi(f)$$

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- $R_n^{(1)}$: $\hookrightarrow$ [C] condition on the adaptation: “diminishing adaptation”
- $R_n^{(2)}$: $\hookrightarrow$ very weak conditions ! (more or less, a consequence of the other conditions).

Result

[Fort et al. 2010]

A. (Ergodicity of the transition kernels) There exist $C_\theta, \rho_\theta \in (0,1)$ s.t.

$$\|P_\theta^n(x,\cdot) - \pi_\theta\|_V \leq C_\theta \; \rho_\theta^n \; V(x)$$

B. (Martingale term) $\exists \alpha > 1$

$$\sum_k \frac{1}{k^\alpha} \; \left(C_{\theta_k} \vee (1-\rho_{\theta_k})^{-1}\right)^{2\alpha} \; P_{\theta_k} V^\alpha(X_k) < +\infty \;\; \text{a.s.}$$

C. (Strenghtened diminishing adaptation)

$$\sum_k \frac{1}{k} \left(C_{\theta_k} \vee (1-\rho_{\theta_k})^{-1}\right)^6 \; V(X_k) \; \sup_x \; \sup_{f, |f| \leq V} \frac{|P_{\theta_k} f(x) - P_{\theta_{k-1}} f(x)|}{V(x)} < \infty \;\; \text{a.s.}$$

D. (Convergence of the inv. distributions) for f s.t. $|f| \leq V^a, a \in (0,1)$

$$\pi_{\theta_n}(f) \xrightarrow{\text{a.s.}} \pi(f)$$

Then, $\quad n^{-1} \sum_{k=1}^n f(X_k) \xrightarrow{\text{a.s.}} \pi(f)$

Comparison with the literature

[Atchadé & Rosenthal (2005), Andrieu & Moulines (2006), Roberts & Rosenthal (2007), Saksman & Vihola (2008), Vihola (2009), Atchadé & Fort (2010), Atchad et al. (2010) $\cdots$]

- We are able to prove a strong law of large numbers, for unbounded functions
- without assuming a uniform-in-θ ergodic behavior on the transition kernels (neither the state space X nor the parameter space Θ have to be compact/countable/finite)
- under the condition that the adaptation is diminishing which does not require that the sequence $\{\theta_n, n \geq 0\}$ converges (for example, adaptation based on a stochastic approximation dynamic: "$\theta_n = \theta_{n-1} + \gamma_n H_n(\theta_n, W_{n+1})$" is OK)
- without assuming the stability of the sequence $\{\theta_n, n \geq 0\}$ for example in the finite dimensional case, control of the form "$\limsup_n n^{-\tau} |\theta_n| < +\infty$ a.s. for $\tau > 0$" is OK (at least when $\pi_\theta = \pi \cdots$ - see next section)

IV. Convergence of the stationary distributions

Under the (main) assumption There exists $\theta_\star$ s.t. for any $x \in \mathsf{X}, A \in \mathcal{X}$

$$\exists \Omega_{x,A}, \qquad \mathbb{P}(\Omega_{x,A}) = 1 \qquad \forall \omega \in \Omega_{x,A} \qquad \lim_n P_{\theta_n(\omega)}(x,A) = P_{\theta_\star}(x,A)$$

we prove that for any bounded and continuous function f,

$$\exists \Omega_\star, \qquad \mathbb{P}(\Omega_\star) = 1 \qquad \forall \omega \in \Omega_\star \qquad \lim_n \pi_{\theta_n(\omega)}(f) = \pi_{\theta_\star}(f) \; .$$

well, we have even a stronger result, $\Omega_\star$ does not depend upon f

We write

$$\pi_{\theta_n}(f) - \pi_{\theta_\star}(f) = \left(\pi_{\theta_n}(f) - P^k_{\theta_n} f(x)\right) + \left(P^k_{\theta_n} f(x) - P^k_{\theta_\star} f(x)\right) + \left(P^k_{\theta_\star} f(x) - \pi_{\theta_\star}(f)\right)$$

and control the blue terms by a condition on the ergodicity of the transition kernels.

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and control the blue terms by a condition on the ergodicity of the transition kernels.

For the control of the red term, we write

$$P^k_{\theta_n} f(x) - P^k_{\theta_\star} f(x) = \int \left(P_{\theta_n}(x, \mathrm{d}y) - P_{\theta_\star}(x, \mathrm{d}y)\right) P^{k-1}_{\theta_\star} f(y) + \int P_{\theta_n}(x, \mathrm{d}y) \left(P^{k-1}_{\theta_n} f(y) - P^{k-1}_{\theta_\star} f(y)\right)$$

Starting from :

$$\forall x \in \mathsf{X}, A \in \mathcal{X}, \quad \exists \Omega_{x,A}, \quad \mathbb{P}(\Omega_{x,A}) = 1 \quad \forall \omega \in \Omega_{x,A} \quad \lim_n P_{\theta_n(\omega)}(x, A) = P_{\theta_\star}(x, A)$$

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the steps are:

$$\forall x \in \mathsf{X}, \quad \exists \Omega_x, \qquad \mathbb{P}(\Omega_x) = 1 \qquad \forall \omega \in \Omega_x \qquad \lim_n P_{\theta_n(\omega)}(x, \cdot) \xrightarrow{w} P_{\theta_\star}(x, \cdot)$$

$\hookrightarrow$ Tool: separable metric space X (ex. Polish)

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$\hookrightarrow$ Tool: Polish space X + equicontinuity of $\{P_\theta f - P_{\theta_\star} f, \theta \in \Theta\}$

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$$\exists \Omega_\star, \qquad \mathbb{P}(\Omega_\star) = 1 \qquad \forall \omega \in \Omega_\star \qquad \lim_n P^k_{\theta_n(\omega)}(x, \cdot) \xrightarrow{w} P^k_{\theta_\star}(x, \cdot) \ ,$$

$\hookrightarrow$ Tool: Feller properties of the kernels $\{P_\theta, \theta \in \Theta\}$

Result

[FORT ET AL. 2010]

A. (Ergodicity of the transition kernels)

B. X is Polish

C. $P_{\theta_\star}$ is Feller and for any bounded continuous function f,
$\{P_\theta f, \theta \in \Theta\}$ is equicontinuous.

D. (Convergence of the transition kernels) for any $x \in \mathsf{X}$,
$P_{\theta_n}(x, \cdot) \xrightarrow{w} P_{\theta_\star}(x, \cdot)$ a.s..

Then for any bounded continuous function f, $\pi_{\theta_n}(f) \xrightarrow{\text{a.s.}} \pi_{\theta_\star}(f)$.

Result [Fort et al. 2010]

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C. $P_{\theta_\star}$ is Feller and for any bounded continuous function f, $\{P_\theta f, \theta \in \Theta\}$ is equicontinuous.

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Then for any bounded continuous function f, $\pi_{\theta_n}(f) \xrightarrow{\text{a.s.}} \pi_{\theta_\star}(f)$.

Rmk: Extensions to unbounded continuous functions by (standard) moment conditions.

V. Application to the convergence of adaptive and interacting MCMC algorithms

Ergodicity criteria: checked in practice by

- drift inequality $P_\theta V \leq \lambda_\theta V + b_\theta$
- minorization condition $P_\theta(x, \cdot) \geq \delta_\theta \; \nu_\theta(\cdot) \mathbb{1}_{\mathcal{C}_\theta}(x)$
- conditions on the decay of the rate ξ s.t.

  $\limsup_n \xi(n) \; \left(b_{\theta_n} \vee \delta_{\theta_n}^{-1} \vee (1-\lambda_{\theta_n})^{-1}\right) < +\infty$

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Diminishing adaptation: checked in practice by

$$\mathrm{distance}(P_\theta, P_{\theta'}) \leq C \; \mathrm{distance}(\theta, \theta') \qquad \text{for some "distance"}$$

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  $\limsup_n \xi(n) \ \left(b_{\theta_n} \vee \delta_{\theta_n}^{-1} \vee (1-\lambda_{\theta_n})^{-1} \right) < +\infty$

Diminishing adaptation: checked in practice by

$$\mathrm{distance}(P_\theta, P_{\theta'}) \leq C \ \mathrm{distance}(\theta, \theta') \qquad \text{for some "distance"}$$

Convergence of $\{\pi_{\theta_n}(f), n \geq 0\}$ when $\pi_\theta \neq \pi$: based on the convergence of $\{\theta_n, n \geq 0\}$

Adaptive MCMC

We prove

- when the target density π is *lighter than exponential*
- with $\mathcal{N}_d$ (adapted) proposal distribution s.t. the eigenvalues of the cov matrix are larger than κ.

1. Ergodicity: $\lim_n \sup_{f,|f|_\infty \leq 1} \mathbb{E}\left[f(X_n)\right] = \pi(f)$. contemporaneous work by (Bai et al., 2010)
2. Strong law of large numbers for any function f such that $|f(x)| \leq \pi^{-s}(x)$, $s \in (0,1)$. pioneering work by (Saksman & Vihola, 2009); we use many ideas of their paper!

Convergence of the (simplified) Equi-Energy sampler

We prove

- when the target density π is *lighter than exponential*, on a Polish space X
- whatever the nbr of stages, the probability of swap $\epsilon \in (0,1)$, the successive tempered distributions and the "hottest" one $\pi^{1/T_\star}$, $T_\star > 1$
- when the "first" auxiliary process is an ergodic Markov chain
- when P is a RWHM algorithm with Gaussian proposal distribution

1. Ergodicity: $\lim_n \mathbb{E}\left[f(X_n)\right] = \pi(f)$ for any bounded functions f.
2. Strong law of large numbers for any continuous function f such that $|f(x)| \leq \pi^{-s}(x)$, $s \in (0, 1/T_\star)$.

extensions of the works by (Atchadé, 2007), (Andrieu et al. 2009)

All the details in

G. Fort, E. Moulines, P. Priouret (2010). *Convergence of adaptive MCMC algorithms: ergodicity and law of large numbers*