Eric MOULINES

Telecom Paris Tech CNRS - LTCI

Joint work with **G. FORT** & S. LE CORFF (TELECOM ParisTech, France), P. PRIOURET (Univ. Paris VI, France), P. VANDEKHERKOVE (Univ. Marne La Vallée),

Outline

- 1. MCMC algorithms are a flexible family of algorithms to sample distributions, known up to a normalisation factor.
- 2. This flexibility comes at a price... badly tuned MCMC can be very slow to converge and lack of convergence may be difficult to diagnose.
- 3. In the last 10 years, several algorithms have been proposed to **increase** the sampling efficiency of the MCMC, without requiring much additional user supervision.
- 4. The common idea is to improve the sampling strategy by **learning** from the past simulations.

Outline of the talk

1. Algorithm design

- Adaptive Markov chain : a single chain whose kernel is gradually modified
- Interacting Markov chains : multiple chains which interact
- 2. Some numerical examples
- 3. Convergence of the algorithms

An elementary example : the Adaptive Metropolis Algorithm

- ► $Y_{k+1} = X_k + Z_{k+1}$ where $Z_{k+1} \sim_{i.i.d.} \bar{q}$, and \bar{q} is symmetric (i.e. $\bar{q}(z) = \bar{q}(-z)$)
- ▶ In this case, $q(x, y) = q(y, x) = \overline{q}(y x) = \overline{q}(x y)$ and the acceptance rate does not depend on the proposal distribution

$$\alpha(x,y) = 1 \land \frac{\pi(y)}{\pi(x)}$$

▶ ... biased random walk where some moves get rejected.

Influence of the scaling

- ► If the variance is either **too small** or **too large**, then the convergence rate of the Markov chain is slow :
 - 1. **too small**... almost all the proposal are accepted. Nevertheless, the stepsizes are small, and the algorithm visits the state space very slowly.
 - 2. too large... many propositions fall in regions where π is very small. These proposals are often rejected and the algorithm get stuck at a point.

Finding a proper scale is thus mandatory ! but it is not always obvious to say what small or large mean for a given distribution π and a given function.

Scaling



Optimal Scaling of the RWM

- A useful idea to get a better understanding of the influence of scaling is to consider a high-dimensional limit, *i.e.* the state space X = ℝ^d where we let the dimension d → ∞.
- Under appropriate assumptions, each coordinate of the Markov chain $\{X_{k,i}^{(d)}\}_{i=1}^d$ converges to a diffusion limit.
- The choice of an optimal scaling then translates into the optimization of the limiting diffusion speed, which is rather easy to handle.

Diffusive Limits

- ► Stationary distribution : $\pi^{(d)}(x_1, \dots, x_d) = \prod_{i=1}^d f(x_i)$ on \mathbb{R}^d $(d \to \infty)$
- Metropolis proposal : $q_{\theta}^{(d)}(x_1, \ldots, x_d) \sim \mathcal{N}(0, (\theta^2/d)\mathbf{I}_d)...$ with variance decreasing as 1/d.
- ► Interpolated process : Z_t^(d) = X_{[td],1}^(d)... we consider a single component and we speed up the time scale by d.
- ▶ When *d* becomes large, a single component becomes independent from the other components which globally act as a random environment.



FIGURE: Diffusive limits for different values of d

Diffusive Limits

 $Z^{(d)} \Rightarrow_d Z$ in the Skorokhod space, where Z is a solution the Langevin SDE

$$dZ_t = v^{1/2}(\theta) dB_t + (1/2)v(\theta)\nabla \log f(Z_t) dt$$
$$v(\theta) = \theta^2 \tau^{(\infty)} [\theta, I(f)]$$

where,

$$\tau^{(\infty)}\left[\theta, I(f)\right] = \lim_{d \to \infty} \tau^{(d)}(\theta)$$

is the limit of the acceptance rate in stationarity,

$$\tau^{(d)}(\theta) = \iint \pi^{(d)}(\mathbf{x}) q_{\theta}^{(d)}(\mathbf{y} - \mathbf{x}) \left\{ 1 \wedge \frac{\pi^{(d)}(\mathbf{y})}{\pi^{(d)}(\mathbf{x})} \right\} \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{y}$$

with $\mathbf{x} = (x_1, x_2, \dots, x_d)$ and

$$I(f) = \int \left[\left(\frac{\mathrm{d}\log f(x)}{\mathrm{d}x} \right)' \right]^2 \mathrm{d}x \; .$$

Diffusion speed

► $v(\theta) = 2\theta^2 \tau^{(\infty)} [\theta, I(f)]$ is the **speed** of the limiting diffusion : $Z_t = \tilde{Z}_{v(\theta)t}$ where $\{\tilde{Z}_t\}$ is a solution of the Langevin SDE

 $\mathrm{d}\tilde{Z}_t = \mathrm{d}B_t + (1/2)\nabla \log f(\tilde{Z}_t)\mathrm{d}t \; .$

• Optimizing the scale amounts to find θ which maximizes the diffusion speed.

Diffusion speed optimization

► The limiting acceptance rate is given

$$\tau^{(\infty)}\left[\theta\right] = 2\Phi\left(\theta\frac{\sqrt{I(f)}}{2}\right) \iff \theta = \frac{2}{\sqrt{I(f)}}\Phi^{-1}\left(\tau^{(\infty)}\left[\theta\right]/2\right) .$$

Since v(θ) = θ²τ^(∞) [θ] the speed may be rewritten as a function of the mean acceptance rate in stationarity

$$v(\theta) \propto w \left[\tau^{(\infty)}(\theta) \right] \quad w: \tau \mapsto \tau \Phi^{-1}(\tau/2) .$$

- The speed is maximized if the scale is chosen so that τ^(∞) [θ_⋆], where τ̄ is the maximum of w.
- \blacktriangleright The optimum value of the acceptance rate may be shown to be $\bar{\tau}\approx 0.234...$

Pros and Cons of diffusion limits

- Empirically this 0.234 rule has been observed to be approximately right much more generally.
- Extensions and generalisations of this result can be found in (Roberts and Rosenthal, 2001) and (Bedard, 2007), (Pillai, Stuart, 2009), (Bedard, Douc, Fort, Moulines, 2010).
- The focus of much of this work is in trying to characterise when the 0.234 rule holds and to explain how and why it breaks down in other situations.
- One major disadvantage of the diffusion limit work is its reliance on asymptotics in the dimensionality of the problem. Although it is often empirically observed that the limiting behaviour can be seen in rather small dimensional problems, (see for example Gelman et al., 1996), it is difficult to quantify this in any general way.

How to control the Acceptance Rate

• **Objective** : Finding the scale θ therefore amounts to solve

$$h(\theta) \stackrel{\text{def}}{=} \iint \left\{ 1 \wedge \frac{\pi(y)}{\pi(x)} \right\} \frac{1}{\theta} q\left(\frac{y-x}{\theta}\right) \pi(x) \mathrm{d}x \mathrm{d}y - \bar{\tau} = 0,$$

- Under appropriate assumptions, $\theta \to h(\theta)$ is monotone with $\lim_{\theta \to 0^+} h(\theta) = 1 \overline{\tau} > 0$ and $\lim_{\theta \to \infty} h(\theta) = -\overline{\tau} < 0...$ But $h(\theta)$ cannot be computed explicitly !
- Suggest to use a stochastic approximation procedure to adapt the scale θ.

Adaptive Scaling Metropolis Algorithm

Proposition & Accept/Reject

$$\begin{split} Y_{k+1} &= X_k + \theta_k \mathcal{N}(0, \text{Id}) \\ X_{k+1} &= \begin{cases} Y_{k+1} & \text{with prob. } \alpha(X_k, Y_{k+1}) \\ X_k & \text{otherwise} \end{cases} \end{split}$$

Update the scaling factor

$$\log(\theta_{k+1}) = \log(\theta_k) + \gamma_{k+1} \left\{ \alpha(X_k, Y_{k+1}) - \bar{\tau} \right\}$$

where $\lim_{k\to\infty} \gamma_k = 0$ and $\sum_{k=1}^{\infty} \gamma_k = \infty$.



Multidimensional scaling

• Same asymptotic analysis $(d \to \infty)$ with

$$\pi_{\Sigma_d}^{(d)}(\mathbf{x}) = |\Sigma_d|^{-1} \pi^{(d)} \left(\Sigma_d^{-1} \mathbf{x} \right), \quad \pi^{(d)}(x_1, \dots, x_d) = \prod_{i=1}^d f(x_i)$$
$$q \sim N(0, (\sigma^2/d) \mathrm{Id})$$

then $Z_t^{(d)} = X_{[td],1}$ converges to the solution a Langevin SDE.

- the target acceptance rate (0.234...) which maximizes the speed of the limiting diffusion is independent from the covariance but the maximal achievable speed is strongly affected.
- Idea : adapt the scale and the covariance of the proposal.

Adaptive and Interacting MCMC algorithms
Adaptive MCMC
Multidimensional Scaling

Adaptive MCMC with multidimensional scaling

1. Simulate

$$\begin{split} Y_{k+1} &= X_k + \mathcal{N}(0, \sigma_k \Gamma_k) \\ X_{k+1} &= \begin{cases} Y_{k+1} & \text{with proba. } \alpha(X_k, Y_{k+1}) \\ X_k & \text{otherwise} \end{cases} \end{split}$$

2. Update the target mean and covariance

$$\mu_{k+1} = \mu_k + \gamma_{k+1} (X_{k+1} - \mu_k)$$

$$\Gamma_{k+1} = \Gamma_k + \gamma_{k+1} \left\{ (X_{k+1} - \mu_k) (X_{k+1} - \mu_k)^T - \Gamma_k \right\}$$

3. Control the global scale of the proposal

$$\log(\sigma_{k+1}) = \log(\sigma_k) + \gamma_{k+1} \left(\alpha(X_k, Y_{k+1}) - \bar{\tau} \right)$$

- Adaptive MCMC

Multidimensional Scaling



FIGURE: d = 12, $\pi \sim \mathcal{N}(0, \Gamma)$, $\operatorname{cond}(\Gamma) \approx 100$, $q \sim \mathcal{N}(0, (2.32^2/d) \mathrm{I})$

- Adaptive MCMC

Multidimensional Scaling



FIGURE: d = 12, $\pi \sim \mathcal{N}(0, \Gamma)$, cond $(\Gamma) \approx 100$, $q \sim \mathcal{N}(0, (2.32^2/d)\Gamma)$

- Adaptive MCMC

Multidimensional Scaling



FIGURE: d = 12, $\pi \sim \mathcal{N}(0, \Gamma)$, $\operatorname{cond}(\Gamma) \approx 100$, $q \sim \mathcal{N}(0, \sigma_k \Gamma_k)$, with adaptive multidimensional scaling

Tempering

- The adaptive Metropolis-Hastings algorithm outlined above can run into difficulties if the target probability distribution is multi-modal.
- ► The MCMC can become trapped in a local mode and fail to fully explore other modes which are significant.
- This problem is very similar to the one encountered in finding a global minimum in nonlinear optimisation. One solution to that problem was to use simulated annealing by introducing a temperature parameter.
- The analogous process applied to drawing samples from a target probability distribution is often referred to as tempering : instead of cooling down to make the distribution sharper and sharper, we rather heating up the distribution to make it flatter and flatter...

Parallel tempering

In parallel tempering algorithm by Geyer (1991) is to run parallel Metropolis sampling at different temperatures

 $T_1 \geq T_2 \geq \cdots \geq T_K = 1$, with target distributions $\left\{\pi^{1/T_k}\right\}_{k=1}^K$.

- At intervals, a pair of adjacent level is chosen and a proposal made to swap their states. If the swap is accepted then these states are interchanged.
- ▶ The acceptance probability for the swap between the state at temperature T_{k-1} and T_k ($k \in \{2, ..., K\}$) is computed to ensure that the joint states of all the parallel chains is reversible with respect to the tensor product $\pi^{1/T_1} \otimes \cdots \otimes \pi^{1/T_K}$ of the heated up probability :

$$\alpha_k\left(x^{(k-1)}, x^{(k)}\right) = 1 \wedge \frac{\pi^{1/T_{k-1}}(x^{(k)})\pi^{1/T_k}(x^{(k-1)})}{\pi^{1/T_{k-1}}\left(x^{(k-1)}\right)\pi^{1/T_k}\left(x^{(k)}\right)} \,.$$

Parallel tempering

- This swap allows for an exchange of information across the population of parallel simulations.
- In the higher temperature simulations, radically different configurations can arise.
- By making exchanges, we can capture and improve configurations by putting them into lower temperature simulations.
- Drawback : The temperature levels should be close enough to achieve a significant acceptance probability for a swap.

Interacting Tempering

- The Interacting Tempering Algorithm exploits the parallel tempering idea : the algorithm runs several chains at different temperatures.
- The idea is to replace an instantaneous swap by an interaction with the whole past of a neighboring process.
- ▶ Idea : At time n, find in the past samples of the chain $X_{\star}^{(k-1)} \in \{X_0^{(k-1)}, \ldots, X_n^{(k-1)}\}$ run at temperature T_{k-1} a state such that the probability of accepting the move

$$\frac{\pi^{1/T_{k-1}}(X_n^{(k)})\pi^{1/T_k}(X_\star^{(k-1)})}{\pi^{1/T_{k-1}}\left(X_\star^{(k-1)}\right)\pi^{1/T_k}\left(X_n^{(k)}\right)} \ .$$

is large enough.

Interacting Tempering (at temperature T_i)

- ▶ a transition kernel $P^{(k)}$ with stationary distribution π^{1/T_k} : $\pi^{1/T_k}P^{(k)} = \pi^{1/T_k}$ (typically, a MH algorithm run with the target distribution π^{1/T_k}).
- a probability of interaction $\epsilon \in (0, 1)$

Iteration n : with probability $(1-\epsilon)$ draw $X_{n+1}^{(k)} \sim P^{(k)}(X_n^{(k)}, \cdot)$

$$P_{\theta_n^{(k-1)}}^{(k)}(X_n^{(k)}, A) = (1 - \epsilon)P^{(k)}(X_n^{(k)}, A) + \cdots$$

Interacting Tempering

with probability ϵ ,

- ▶ select a state in $X_{\star}^{(k-1)} \in \left\{X_{\ell}^{(k-1)}\right\}_{\ell=0}^{n}$ with probability $\left\{g(X_{n}^{(k)}, X_{\ell}^{(k-1)})\right\}_{\ell=0}^{n}$;
- \blacktriangleright accept the proposal with probability $\alpha_k(X_n^{(k)},X_\star^{(k-1)})$

$$P_{\theta_n^{(k-1)}}(X_n^{(k)}, A) = (1-\epsilon)P^{(k)}(X_n^{(k)}, A) + \epsilon \left\{ \int_A \theta_n^{(k-1)}(\mathrm{d}y)\alpha_k(X_n^{(k)}, y) + \mathbb{1}_A(X_n^{(k)}) \int \theta_n^{(k-1)}(\mathrm{d}y) \left\{ 1 - \alpha_k(X_n^{(k)}, y) \right\} \right\}$$

where $\theta_n^{(k-1)}(\mathrm{d} y) = \frac{1}{n+1}\sum_{\ell=1}^n \delta_{X_\ell^{(k-1)}}(\mathrm{d} y)$ and

$$\alpha_k(x,y) = \frac{g(x,y)}{\int \theta_n^{(k-1)}(\mathrm{d}y)g(x,y)} \left(1 \wedge \frac{\pi^{1/T_k}(y)\pi^{1/T_{k-1}}(x)}{\pi^{1/T_{k-1}}(y)\pi^{1/T_k}(x)}\right) \ .$$

An example

- 1. Mixture of Gaussians : 4 components in dimension 10.
- 2. Dimension : d = 10 (only the first two components are shown) Interactions : 5 %
- 3. Temperatures : 50,40,30,25,20,15,10,5,2.5,1
- 4. 50 Energy rings (adapted from the empirical quantiles)
- 5. Basic Kernel : random walk Metropolis with covariance (4/d) * I (optimally adapted to individual components).

Interactions : 5 %



A General Framework

- Let (Θ, \mathcal{T}) be a measurable space and (X, \mathcal{X}) a general state space.
- Let (P_θ, θ ∈ Θ) be a collection of Markov transition kernels indexed by θ ∈ Θ, which can be either finite or infinite dimensional (e.g. an empirical distribution).
- For each $\theta \in \Theta$, P_{θ} admits a single probability distribution π_{θ} : $\pi_{\theta} = \pi_{\theta} P_{\theta}$.
- ► Consider a X × Θ -valued process $\{(X_n, \theta_n), n \ge 0\}$ on a filtered probability space $(\Omega, \mathcal{A}, \{\mathcal{F}_n, n \ge 0\}, \mathbb{P})$ such that $\{(X_n, \theta_n), n \ge 0\}$ is \mathcal{F}_n -adapted and for any bounded measurable function f

$$\mathbb{E}\left[f(X_{n+1}) \,|\, \mathcal{F}_n\right] = P_{\theta_n} f(X_n) \;.$$

Problems

- Problem : Find conditions such that :
 - 1. Ergodicity : $\lim_{n\to\infty} \mathbb{E}[f(X_n)] = \pi(f)$ where π is the target distribution.
 - 2. Strong Law of Large Numbers : $\lim_{n\to\infty} n^{-1} \sum_{k=1}^n f(X_k) \to \pi(f)$ \mathbb{P} -a.s.
- **Problem :** $\{X_k\}$ is **not** a Markov Chain.
- Existing results :
 - Adaptive Markov Chains : Andrieu, Moulines (2006), Roberts and Rosenthal (2007), Atchadé and Fort (2009)
 - Interacting Markov Chains : Del Moral and Miclo (2004), Andrieu, Del Moral, Doucet, Jasra (2006,2007,2010), Del Moral and Doucet (2009), Bercu, Del Moral and Doucet (2009)

Ergodicity

Outline of the proof

Error decomposition

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

- Ergodicity

Outline of the proof

Error decomposition

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

 \hookrightarrow [A] condition on the ergodicity of the transition kernels Most often, the transition kernels $\{P_{\theta}, \theta \in \Theta\}$ are geometrically ergodic :

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

Ergodicity

Outline of the proof

Error decomposition

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

 \hookrightarrow [B] condition on the adaptation mechanism

Ergodicity

Outline of the proof

Error decomposition

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

 \hookrightarrow [C] when $\pi_{ heta}
eq \pi$, condition on the convergence of $\{\pi_{ heta_n}, n \geq 0\}$ to π

- Ergodicity

└─ Outline of the proof

Error decomposition

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

The conditions can be weakened by replacing N by r(n). This allows to consider situations where the ergodicity constant of the Markov kernels get worse when θ approaches the parameter set boundary

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

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

Ergodicity

└─ Main result

Result

[Fort et al. 2010]

A. (Ergodicity of the transition kernels)

- There exists π_{θ} 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

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

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) There exist π and a bounded non-negative function f s.t. $\lim_n \pi_{\theta_n}(f) = \pi(f)$ a.s. Then $\lim_n \mathbb{E}[f(X_n)] = \pi(f)$

Law of large numbers for adaptive MCMC samplers

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

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

Law of large numbers for adaptive MCMC samplers

Sketch of the proof

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

Law of large numbers for adaptive MCMC samplers

Sketch of the proof

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

$$n^{-1}\sum_{k=1}^{n}\left\{f(X_k) - \pi_{\theta_{k-1}}(f)\right\} = n^{-1} \qquad \underbrace{\sum_{k=1}^{n} \Delta M_k}_{\text{Remainder due to the adaptation}} + \underbrace{R_n^{(2)}}_{\text{Remainder due to the adaptation}} + \underbrace{R_$$

sum of martingale increments

Law of large numbers for adaptive MCMC samplers

Sketch of the proof

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

$$n^{-1}\sum_{k=1}^{n}\left\{f(X_k) - \pi_{\theta_{k-1}}(f)\right\} = n^{-1} \qquad \underbrace{\sum_{k=1}^{n} \Delta M_k}_{\text{Remainder due to the adaptation}} + \underbrace{R_n^{(2)}}_{\text{Remainder due to the adaptation}} + \underbrace{R_$$

sum of martingale increments

• Martingale increments : \hookrightarrow [B] moment conditions : for some $\alpha > 1$,

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

Law of large numbers for adaptive MCMC samplers

Sketch of the proof

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

$$n^{-1}\sum_{k=1}^{n}\left\{f(X_k) - \pi_{\theta_{k-1}}(f)\right\} = n^{-1}\sum_{\substack{k=1\\ \text{curred particular interpreter}}}^{n}\Delta M_k + \underbrace{R_n^{(1)}}_{\text{Remainder due to the adaptation}} + \underbrace{R_n^{(2)}}_{\text{Remainder due to the adaptation}} + \underbrace{R_n^{(2)}$$

sum of martingale increments

*R*_n⁽¹⁾ :→ [C] condition on the adaptation : "diminishing adaptation"
 *R*_n⁽²⁾ : → very weak conditions ! (more or less, a consequence of the other conditions).

Law of large numbers for adaptive MCMC samplers

Main result

Result

[Fort et al. 2010]

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

$$||P_{\theta}^{n}(x,\cdot) - \pi_{\theta}||_{V} \le C_{\theta} \rho_{\theta}^{n} V(x)$$

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

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

C. (Strengthened 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 invariant distributions) for f s.t. $|f| \le V^a, a \in (0, 1)$

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

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

Law of large numbers for adaptive MCMC samplers

Main result

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 $x \in X$, $P_{\theta_n}(x, \cdot) \rightarrow_{\mathrm{d}} P_{\theta_*}(x, \cdot)$ a.s..
- Then for any **bounded continuous** function $f, \pi_{\theta_n}(f) \xrightarrow{a.s.} \pi_{\theta_\star}(f)$.

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

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

Diminishing adaptation : checked in practice by

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

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

Diminishing adaptation : checked in practice by

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

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

Adaptive MCMC

Adaptive MCMC

We prove

- when the target density π is *lighter than exponential*
- ► with N_d (adapted) proposal distribution s.t. the eigenvalues of the cov matrix are larger than κ.
- 2. Strong law of large numbers for any function f such that $|f(x)| \le \pi^{-s}(x)$, $s \in (0, 1)$. pioneering work by (Saksman & Vihola, 2009); we use many ideas of their paper!

- Applications

Convergence of the Equi-Energy sampler

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
- \blacktriangleright 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 $|f(x)| \le \pi^{-s}(x), s \in (0, 1/T_*)$. extensions of the works by (Atchadé, 2007). (Andrieu et al. 2009)