Adaptive MCMC : theory and methods

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We will provide sufficient conditions so that

the process $\{X_n, n \geq 0\}$ produced by an adaptive MCMC sampler approximates a target density $\pi_\star$ i.e.

- (convergence of the marginals) for any bounded function f

$$\lim_n \mathbb{E}\left[f(X_n)\right] = \pi_\star(f)$$

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- (convergence of the marginals) for any bounded function f

$$\lim_n \mathbb{E}\left[f(X_n)\right] = \pi_\star(f)$$

- (strong LLN) for any function f in a large class of functions

$$\frac{1}{n} \sum_{k=1}^{n} f(X_k) \longrightarrow \pi_\star(f) \qquad \mathbb{P} - a.s.$$

1. Examples
2. Sufficient conditions for convergence of the marginals
3. Sufficient conditions for strong LLN

Example 1 : Adaptive SRWM

- MCMC depends on some design parameters.

Ex. for the **S**ymmetric **R**andom **W**alk **M**etropolis (SRWM) with normal proposal distribution, the design parameter is the variance Σ_q of the Gaussian proposal.

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Ex. for the **S**ymmetric **R**andom **W**alk **M**etropolis (SRWM) with normal proposal distribution, the design parameter is the variance Σ_q of the Gaussian proposal.

- Tune these design parameters "on the fly", during the run of the algorithm.

Ex. (to follow)

based on results obtained by the scaling technique, choose $\Sigma_q \propto \Sigma_\pi$.

usually, Σ_π is unknown : at iteration n, replace it by an estimation computed with the samples $\{X_k, \, k \leq n\}$.

This yields the adaptive SRWM

- P_{θ} : kernel of a SRWM algorithm with proposal $\mathcal{N}_d(0,\theta)$
- Iteration n
  - draw $X_{n+1} \sim P_{\theta_n}(X_n,\cdot)$
  - update the estimate of Σ_π : $\qquad \theta_{n+1} = \phi_n(\theta_n,X_{n+1})$.

This is an example of the following general framework :

- let a family of transition kernels $\{P_\theta, \theta \in \Theta\}$
- with the same invariant probability distribution $\pi_\star$.

- define a process $\{(X_n, \theta_n), n \geq 0\}$ as follows
  - given the past (a filtration $\mathcal{F}_n$), draw

$$X_{n+1} \sim P_{\theta_n}(X_n, \cdot)$$

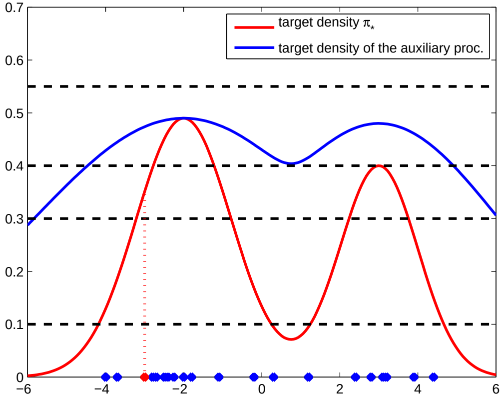
  - update the 'parameter' with an "internal adaptation" scheme

$$\theta_{n+1} \longleftrightarrow \text{built from the process } \{X_k, k \leq n\} \text{ itself}$$

Example 2: Equi-Energy sampler

- Given

  a transition kernel P s.t. $\pi_\star P = \pi_\star$
  a probability of swap $\epsilon \in (0,1)$
  an auxiliary process $\{Y_n, n \geq 0\}$ target : $\pi_\star^\beta$



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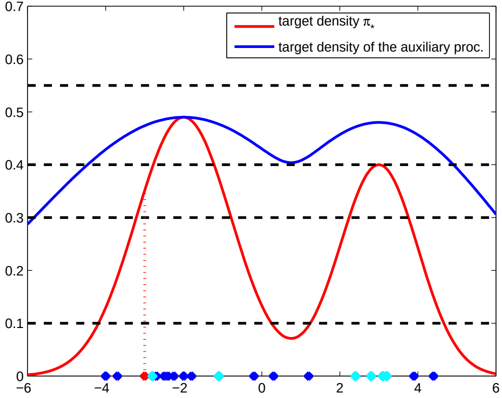

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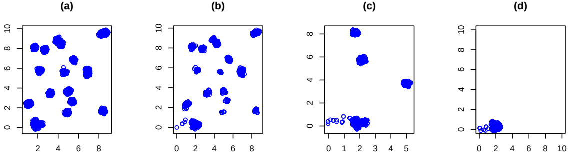

FIG.: Example : Mixture of a 2D-Normal distribution [target / EE / Parallel Tempering / SRWM]

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  an auxiliary process $\{Y_n, n \geq 0\}$ target : $\pi_\star^\beta$

- Iteration n :

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

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

Example 2: Equi-Energy sampler

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  a transition kernel P s.t. $\pi_\star P = \pi_\star$
  a probability of swap $\epsilon \in (0,1)$
  an auxiliary process $\{Y_n, n \geq 0\}$ target : $\pi_\star^\beta$

- Iteration n :

(b) with probability ϵ, draw a point $Y_\star$ among $\{Y_1, \cdots, Y_n\}$ and accept/reject with probability $\alpha(X_n, Y_\star)$

$$P_{\theta_n}(X_n, A) = (1-\epsilon) P(X_n, A) + \epsilon \left\{ \int_A \theta_n(dy)\ \alpha(X_n, y) + \mathbb{1}_A(X_n) \int \theta_n(dy)\ \{1 - \alpha(X_n, y)\} \right\}$$

where

$$\theta_n(dy) = \frac{1}{n} \sum_{k=1}^{n} \delta_{Y_k}(dy).$$

In practice

- Choose the auxiliary process $\{Y_n, n \geq 0\}$ such that $\lim_n \theta_n = \tilde{\pi}$ in some sense, so that asymptotically, "$P_{\theta_n} \approx P_{\tilde{\pi}}$".
- Choose the acceptation-rejection mecanism $\alpha(x,y)$ so that $\pi_\star P_{\tilde{\pi}} = \pi_\star$, so that asymptotically, "$\pi_\star$ is invariant for P_{θ_n}".
- When sampling in the past of the auxiliary process, select the points : introduce a selection $g(x,y)$ (such that $g(x,y) = g(y,x)$)

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This yields :

$$P_{\theta_n}(X_n,A) = (1-\epsilon)P(X_n,A) + \epsilon \, \left\{ \int_A \frac{g(x,y)\theta_n(dy)}{\int g(x,y)\theta_n(dy)} \alpha(X_n,y) + \mathbb{1}_A(X_n) \int \frac{g(x,y)\theta_n(dy)}{\int g(x,y)\theta_n(dy)} \{1-\alpha(X_n,y)\} \right\}$$

where

$$\theta_n(dy) = \frac{1}{n}\sum_{k=1}^{n} \delta_{Y_k}(dy) \qquad \alpha(x,y) = 1 \wedge \frac{\pi(y)\ \tilde{\pi}(x)}{\tilde{\pi}(y)\ \pi(x)}$$

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$$P_{\theta_n}(X_n,A) = (1-\epsilon_{\theta_n}(x))P(X_n,A)+\epsilon_{\theta_n}(x) \left\{ \int_A \frac{g(x,y)\theta_n(dy)}{\int g(x,y)\theta_n(dy)}\alpha(X_n,y) + \mathbb{1}_A(X_n) \int \frac{g(x,y)\theta_n(dy)}{\int g(x,y)\theta_n(dy)}\{1-\alpha(X_n,y)\} \right\}$$

where

$$\theta_n(dy) = \frac{1}{n}\sum_{k=1}^{n} \delta_{Y_k}(dy) \qquad \alpha(x,y) = 1 \wedge \frac{\pi(y)\;\tilde{\pi}(x)}{\tilde{\pi}(y)\;\pi(x)} \qquad \epsilon_\theta(x) := \epsilon \mathbb{1}_{\int \theta(dy) g(x,y) >$$

This is an example of the following general framework :

- let a family of transition kernels $\{P_\theta, \theta \in \Theta\}$
- with their own invariant probability distribution π_θ : $\pi_\theta P_\theta = \pi_\theta$

- define a process $\{(X_n, \theta_n), n \geq 0\}$ as follows
  - given the past (a filtration $\mathcal{F}_n$), draw

$$X_{n+1} \sim P_{\theta_n}(X_n, \cdot)$$

  - update the 'parameter' with an "external adaptation" scheme

$$\theta_{n+1} \longleftrightarrow \text{built from } \underline{\text{an auxiliary}} \text{ process } \{Y_k, k \leq n\}$$

Conclusion of Section I

We have

- a family of transition kernels $\{P_\theta, \theta \in \Theta\}$,
- with invariant distribution : π_θ or $\pi_\star$.

We define a filtration $\mathcal{F}_n$, and a process $\{(X_n, \theta_n), n \geq 0\}$ s.t.

- component θ_n : $\mathcal{F}_n$ adapted — with internal / external adaptation
- component X_n (**process of interest**):

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

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Suff Cond for : the existence of $\pi_\star$ s.t.

$$\lim_n \mathbb{E}\left[f(X_n)\right] = \pi_\star(f)$$

for any **bounded** function f.

Idea, when $\forall \theta, \quad \pi_\theta = \pi_\star$

$$
\begin{aligned}
\mathbb{E}\left[f(X_n)\right] &= \mathbb{E}\left[\mathbb{E}\left[f(X_n)|\mathcal{F}_{n-N}\right]\right] \\
&= \mathbb{E}\Bigg[\underbrace{\mathbb{E}\left[f(X_n)|\mathcal{F}_{n-N}\right] - P^N_{\theta_{n-N}} f(X_{n-N})}_{\text{comparison with a frozen chain with transition } P_{\theta_{n-N}}} \\
&\quad + \underbrace{P^N_{\theta_{n-N}} f(X_{n-N}) - \pi_\star(f)}_{\text{ergodicity of the frozen chain}}\Bigg] + \pi_\star(f).
\end{aligned}
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\end{aligned}$$

Conditions on

- (Diminishing adaptation) two successive transition kernels are similar : "$\|P_{\theta_n}(x,\cdot) - P_{\theta_{n-1}}(x,\cdot)\|_{\mathrm{TV}} \to 0$"
- (Containment condition) ergodicity of the transition kernel " $\|P^n_\theta(x,\cdot) - \pi_\star\|_{\mathrm{TV}} \to 0$ *uniformly*"

Result, when $\forall \theta, \quad \pi_\theta = \pi_\star$

Define

$$M_\epsilon(x,\theta) := \inf\{n \geq 1, \|P_\theta^n(x,\cdot) - \pi_\star\|_{\mathrm{TV}} \leq \epsilon\}$$

Theorem

Assume

1. *(Diminishing adaptation)*

$$\sup_x \|P_{\theta_n}(x,\cdot) - P_{\theta_{n-1}}(x,\cdot)\|_{\mathrm{TV}} \longrightarrow_{\mathbb{P}} 0$$

2. *(Containment condition)*

$$\lim_M \limsup_n \mathbb{P}\left(M_\epsilon(X_n,\theta_n) \geq M\right) = 0.$$

Then

$$\lim_n \sup_{f,|f|_\infty \leq 1} \left|\mathbb{E}\left[f(X_n)\right] - \pi_\star(f)\right| = 0$$

How to check these conditions?

- (Diminishing adaptation)

$$\sup_x \|P_{\theta_n}(x,\cdot) - P_{\theta_{n-1}}(x,\cdot)\|_{\mathrm{TV}} \longrightarrow_{\mathbb{P}} 0$$

$\hookrightarrow$ Problem specific.
For ex. we can have

$$\sup_x \|P_{\theta_n}(x,\cdot) - P_{\theta_{n-1}}(x,\cdot)\|_{\mathrm{TV}} \leq C \; \|\theta_n - \theta_{n-1}\|_{\mathbf{xxx}}$$

so that convergence in probability is implied by the **adaptation scheme**.

How to check these conditions?

- (Containment condition)

$$\lim_M \limsup_n \mathbb{P}\left(M_\epsilon(X_n,\theta_n) \geq M\right) = 0, \qquad M_\epsilon(x,\theta) := \inf\{n \geq 1, \|P_\theta^n(x,\cdot) - \pi_\star\|_{\mathrm{TV}} \leq \epsilon\}$$

$\hookrightarrow$ usually, deduced from **uniform-in-θ ergodicity** : if

$$\sup_\theta \|P_\theta^n(x,\cdot) - \pi_\star\|_{\mathrm{TV}} \leq \rho(n)\ U(x) \qquad \lim_n \rho(n) = 0$$

then

$$M_\epsilon(x,\theta) \leq \rho^{-1}\left(\epsilon C^{-1} U^{-1}(x)\right).$$

Hence : Containment Cond is proved if $\tilde{U}(X_n)$ **is bounded in probability**.

It can thus be proved from uniform-in-θ conditions of the form :

- $\exists \varepsilon > 0, \nu, \mathcal{C} \qquad P_\theta(x,\cdot) \geq \varepsilon \nu(\cdot) \mathbb{1}_\mathcal{C}(x)$
- $P_\theta V(x) \leq V(x) - \phi \circ V(x) + b \mathbb{1}_\mathcal{C}(x)$.

Idea, when $\pi_\theta P_\theta = \pi_\theta$

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Conditions on

- (same) : Diminishing adaptation, Containment condition
- Convergence of the invariant measures $\{\pi_{\theta_n}, n \geq 0\}$ to some $\pi_\star$

Result when $\pi_\theta P_\theta = \pi_\theta$

Theorem

Assume

1. *(Diminishing adaptation)*

$$\sup_x \|P_{\theta_n}(x,\cdot) - P_{\theta_{n-1}}(x,\cdot)\|_{\mathrm{TV}} \longrightarrow_{\mathbb{P}} 0$$

2. *(Containment condition)*

$$\lim_M \limsup_n \mathbb{P}\left(M_\epsilon(X_n,\theta_n) \geq M\right) = 0.$$

3. *(Convergence of the invariant distributions)*

$$\pi_{\theta_n}(f) - \pi_\star(f) \to_{\mathbb{P}} 0.$$

Then

$$\lim_n \ \left|\mathbb{E}\left[f(X_n)\right] - \pi_\star(f)\right| = 0$$

How to check these conditions?

- (Convergence of the invariant distributions)

$$\pi_{\theta_n}(f) - \pi_\star(f) \to_{\mathbb{P}} 0.$$

We proved that if

(i) there exist x s.t.

$$\lim_n \sup_\theta \|P_\theta^n(x,\cdot) - \pi_\theta\|_{\mathrm{TV}} = 0,$$

(ii) there exist $\theta_\star \in \Theta$ and a set A such that $\mathbb{P}(A) = 1$ and

$$\forall \omega \in A, x \in \mathsf{X}, B \in \mathcal{B}(\mathsf{X}) \qquad \lim_n P_{\theta_n(\omega)}(x,B) = P_{\theta_\star}(x,B)$$

(iii) the state space X is Polish

then for any bounded function f,

$$\pi_{\theta_n}(f) \longrightarrow_{a.s.} \pi_{\theta_\star}(f)$$

Conclusion : when applied to the Equi-Energy sampler

Let $\pi_\star$ be positive and continuous on X s.t. $\sup_{\mathsf{X}} \pi_\star < +\infty$.
Let $\beta \in (0,1)$.

- On the auxiliary process :
- On the transition kernel P:
- On the probability of swap ϵ:

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Let $\pi_\star$ be positive and continuous on X s.t. $\sup_{\mathsf{X}} \pi_\star < +\infty$.
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- On the auxiliary process : for any bounded function f,

$$\frac{1}{n} \sum_{k=1}^{n} f(Y_k) \longrightarrow_{a.s.} \pi_\star^{\beta}(f).$$

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- On the transition kernel P: P is phi-irreducible, $\pi_\star P = \pi_\star$, the level sets $\{\pi \geq p\}$ are 1-small and

$$PV(x) \leq \lambda V(x) + b\mathbb{1}_{\mathcal{C}}(x) \qquad V(x) = \left(\frac{\pi(x)}{\sup_{\mathsf{X}} \pi}\right)^{-\tau(1-\beta)}$$

  for some $\lambda \in (0,1)$, $b < +\infty$, a set $\mathcal{C}$, $\tau \in (0,1]$.

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- On the probability of swap ϵ:

$$0 \leq \epsilon < \frac{1-\lambda}{1-\lambda+\tau(1-\tau)^{(1-\tau)/\tau}}$$

Under these conditions,

- the diminishing adaptation condition holds
- a <u>uniform-in-θ drift</u> condition holds

$$\tilde{\lambda} \in (0,1), \qquad P_\theta V(x) \leq \tilde{\lambda} V(x) + b \mathbb{1}_{\mathcal{C}}(x),$$

  and we prove the containment condition.
- the invariant measures a.s. converge : $\lim_n \pi_{\theta_n}(f) = \pi_\star(f)$ a.s. for any bounded function.

Hence, for any bounded function f

$$\mathbb{E}\left[f(X_n)\right] \longrightarrow_n \pi_\star(f).$$

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for any function f in a large class of functions.

Idea : use the Poisson equation

$$\frac{1}{n}\sum_{k=1}^{n} f(X_k) - \pi_\star(f) = \underbrace{\frac{1}{n}\sum_{k=1}^{n}\{f(X_k) - \pi_{\theta_{k-1}}(f)\}}_{\text{“Poisson term”}} + \underbrace{\frac{1}{n}\sum_{k=1}^{n}\pi_{\theta_{k-1}}(f) - \pi_\star(f)}_{\text{Cesaro mean (is null when } \pi_\theta = \pi_\star)}$$

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About the convergence of the invariant measures: we prove that

if

(i) uniform-in-θ V-ergodicity for some x,

$$\lim_n \sup_\theta \|P_\theta^n(x,\cdot) - \pi_\theta\|_V = 0,$$

(ii) There exist $\theta_\star \in \Theta$ and A s.t. $\mathbb{P}(A) = 1$ and

$$\forall \omega \in A, x, B \qquad P_{\theta_n(\omega)}(x,B) \longrightarrow P_{\theta_\star}(x,B)$$

(iii) Polish state space X

then

$$\pi_{\theta_n}(f) \longrightarrow_{a.s.} \pi_{\theta_\star}(f) \qquad \text{for any } f \in \mathcal{L}_{V^\alpha},\ \alpha \in [0,1)$$

About the "Poisson" term we write

$$\frac{1}{n}\sum_{k=1}^{n}\{f(X_k)-\pi_{\theta_{k-1}}(f)\} = n^{-1}\underbrace{\sum_{k=1}^{n}\{\hat{f}_{\theta_{k-1}}(X_k)-P_{\theta_{k-1}}\hat{f}_{\theta_{k-1}}(X_{k-1})\}}_{\text{martingale term}}$$

$$+\underbrace{\frac{1}{n}\sum_{k=1}^{n-1}\{P_{\theta_k}\hat{f}_{\theta_k}(X_k)-P_{\theta_{k-1}}\hat{f}_{\theta_{k-1}}(X_k)\}}_{\text{Remainder term (I)}}+\underbrace{n^{-1}\{P_{\theta_0}f_{\theta_0}(X_0)-P_{\theta_{n-1}}f_{\theta_{n-1}}(X_{n-1})\}}_{\text{Remainder term (II)}}$$

where $\hat{f}_\theta$ solves $f-\pi_\theta(f)=\hat{f}_\theta-P_\theta\hat{f}_\theta$.

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$$+\underbrace{\frac{1}{n}\sum_{k=1}^{n-1}\{P_{\theta_k}\hat{f}_{\theta_k}(X_k)-P_{\theta_{k-1}}\hat{f}_{\theta_{k-1}}(X_k)\}}_{\text{Remainder term (I)}}+\underbrace{n^{-1}\{P_{\theta_0}f_{\theta_0}(X_0)-P_{\theta_{n-1}}f_{\theta_{n-1}}(X_{n-1})\}}_{\text{Remainder term (II)}}$$

where $\hat{f}_\theta$ solves $f-\pi_\theta(f)=\hat{f}_\theta-P_\theta\hat{f}_\theta$.

- a.s. convergence of the martingale : conditions on the L^p-moments of the increment $\hookrightarrow$ in practice, **uniform-in-θ drift conditions** on the kernels P_θ.

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$$+\underbrace{\frac{1}{n}\sum_{k=1}^{n-1}\{P_{\theta_k}\hat f_{\theta_k}(X_k)-P_{\theta_{k-1}}\hat f_{\theta_{k-1}}(X_k)\}}_{\text{Remainder term (I)}}+\underbrace{n^{-1}\{P_{\theta_0}f_{\theta_0}(X_0)-P_{\theta_{n-1}}f_{\theta_{n-1}}(X_{n-1})\}}_{\text{Remainder term (II)}}$$

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- a.s. convergence of the martingale : conditions on the L^p-moments of the increment $\hookrightarrow$ in practice, **uniform-in-θ drift conditions** on the kernels P_θ.
- a.s. convergence of the remainder terms : regularity in θ of the solution to the Poisson equation $\hookrightarrow$ in practice, **strenghtened diminishing adaptation condition**.

Define

$$D_V(\theta,\theta') := \sup_x \frac{\|P_\theta(x,\cdot) - P_{\theta'}(x,\cdot)\|_V}{V(x)}$$

Theorem

Assume

(i) *(uniform ergodic behavior)* P_θ *is phi-irreducible,*

$$P_\theta V \leq \lambda V + b\mathbb{1}_{\mathcal{C}} \qquad \lambda \in (0,1), b < +\infty,$$

and level sets of V *are* 1*-small.*

(ii) *(strenghtened D.A.)* $\sum_k \frac{1}{k} V^\alpha(X_k) \;\; D_{V^\alpha}(\theta_k,\theta_{k-1}) < +\infty$ *a.s.*

(iii) *(convergence of the invariant measures)*

Then : if $\mathbb{E}[V(X_0)] < \infty$, *for any* $\alpha \in [0,1)$ *and any* $f \in \mathcal{L}_{V^\alpha}$

$$\frac{1}{n}\sum_{k=1}^{n} f(X_k) \longrightarrow_{a.s.} \pi_\star(f),$$

Conclusion : when applied to the Equi-Energy sampler

Let $\pi_\star$ be positive and continuous on X s.t. $\sup_{\mathsf{X}} \pi_\star < +\infty$.
Let $\beta \in (0,1)$.

- On the transition kernel P:
- On the probability of swap ϵ:
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Note that : it is assumed that a strong LLN holds for the auxiliary process and any function $f \in \mathcal{L}_{V^\alpha}$, $\alpha \in (0,1)$; in order to prove a strong LLN for the process of interest and any function $f \in \mathcal{L}_{V^\alpha}$, $\alpha \in (0,1)$.

$\hookrightarrow$ repeat the mecanism and prove the convergence of the marginals + a strong LLN for the K-levels Equi-Energy sampler

Conclusion of the talk

- We prove convergence of the marginals + strong LLN for general adaptive MCMC samplers with the main ingredients
  - (strenghtened) diminishing adaptation
  - "uniform" ergodic behavior of the kernels
  - `when` $\pi_\theta \neq \pi_\star$: a.s. convergence of the invariant measures π_{θ_n}

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- And illustrate the conditions by considering the Equi-Energy sampler.

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- And illustrate the conditions by considering the Equi-Energy sampler.
- Extensions (not discussed here) : uniform-in-θ ergodicity conditions have been proved by showing that the transition kernels are **geometrically ergodic**. We also provide examples in which they are only **sub-geometrically ergodic**. For ex. in the case

$$P_\theta V \leq V - c\, V^{1-\alpha} + b\mathbb{1}_{\mathcal{C}}$$

  we prove a strong LLN for functions increasing like V^β for any $\beta \in [0,1-\alpha)$.