Gersende FORT

CNRS (LTCI) Paris, France

Free Energy Calculations: A mathematical perspective Oaxaca, July 2015

Introduction

Goal:

Explore the support of a distribution π and/or compute integrals w.r.t. π

$$\int_{\{x\in\mathbb{R}^n:\xi(x)\in\mathcal{O}\}}\,\mathsf{d}\pi(x).$$

when

- π highly metastable
- and π is a distribution on \mathbb{R}^n , n large.

Monte Carlo: a stochastic approximation

- propose sample from a (proposal) distribution π_{\star}
- \bullet correct the samples in order to approximate π
- Markov chain Monte Carlo: $\{X_1, X_2, \dots\}$ Markov chain with stationary distribution π

$$\int \phi(x) \mathsf{d}\pi(x) \approx \frac{1}{N} \sum_{k=1}^{N} \phi(X_k)$$

its construction depends on a proposal distribution π_{\star}

2 Importance Sampling: $\{X_1, X_2, \cdots\}$ from a proposal distribution π_*

$$\int \phi(x) \mathsf{d}\pi(x) = \int \phi(x) \frac{\mathsf{d}\pi(x)}{\mathsf{d}\pi_{\star}(x)} \mathsf{d}\pi_{\star}(x) \approx \frac{1}{N} \sum_{k=1}^{N} \phi(X_k) \frac{\mathsf{d}\pi(X_k)}{\mathsf{d}\pi_{\star}(X_k)}$$

Monte Carlo: a stochastic approximation

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2 Importance Sampling: $\{X_1, X_2, \dots\}$ from a proposal distribution π_*

$$\int \phi(x) \mathrm{d}\pi(x) = \int \phi(x) \frac{\mathrm{d}\pi(x)}{\mathrm{d}\pi_{\star}(x)} \mathrm{d}\pi_{\star}(x) \approx \frac{1}{N} \sum_{k=1}^{N} \phi(X_k) \frac{\mathrm{d}\pi(X_k)}{\mathrm{d}\pi_{\star}(X_k)}$$

 \hookrightarrow the efficiency of these samplers depends on the choice of π_{\star}

Naïve Monte Carlo samplers



COMPANY.

x 10⁶

1.2 1.4 1.6 1.8 2

Adaptive Monte Carlo

- choose a family of proposal distributions $\{\pi_{\theta}, \theta \in \Theta\}$
- at iteration t+1,

based on the past behavior of the sampler: X_1, \cdots, X_t ,

(a) Sample X_{t+1} by using the proposal distribution π_{θ_t}

(b) Update the parameter θ : $\theta_t \rightarrow \theta_{t+1}$

Example: Wang-Landau based-algorithms (Self Healing Umbrella Sampling, Well Tempered Metadynamics, · · ·) are Adaptive Importance Samplers

- Reaction Coordinate: $\xi : \mathbb{R}^n \to \{1, \cdots, d\}$
- The distributions π_{θ} :

$$\pi_{\theta}(x) \propto \sum_{i=1}^{d} \mathrm{1}_{\{x \in \mathbb{R}^{n}: \xi(x)=i\}} \pi(x) \, \exp(-\ln(\theta(i)))$$

•
$$\theta = (\theta(1), \cdots, \theta(d)) \in (\mathbb{R}_+)^d$$
 such that $\sum_{i=1}^d \theta(i) = 1$

Example: Wang-Landau based-algorithms (Self Healing Umbrella Sampling, Well Tempered Metadynamics, · · ·) are Adaptive Importance Samplers

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•
$$\theta = (\theta(1), \cdots, \theta(d)) \in (\mathbb{R}_+)^d$$
 such that $\sum_{i=1}^d \theta(i) = 1$

Algorithm: repeat

Sample Draw X_{t+1} "from" π_{θ_t} Update Update the parameter:

$$\tilde{\theta}_{t+1} = \tilde{\theta}_t + \mathsf{C}(\theta_t, X_{t+1}, t)$$

and set

$$\theta_{t+1} = \frac{\theta_{t+1}}{\sum_{\ell=1}^{d} \tilde{\theta}_{t+1}(\ell)}$$

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•
$$\theta = (\theta(1), \cdots, \theta(d)) \in (\mathbb{R}_+)^d$$
 such that $\sum_{i=1}^d \theta(i) = 1$

Algorithm: repeat

Sample Draw X_{t+1} "from" π_{θ_t} Update Update the parameter:

$$\tilde{\theta}_{t+1}(i) = \tilde{\theta}_t(i) \left(1 + \gamma_{t+1} \mathbb{1}_{\{x:\xi(x)=i\}}(X_{t+1}) \right)$$

and set

$$\theta_{t+1} = \frac{\theta_{t+1}}{\sum_{\ell=1}^{d} \tilde{\theta}_{t+1}(\ell)}$$

Adaptation for · · ·

• Optimal proposal mecanism $\pi_{\theta_{\star}}$ where

$$\theta_{\star}$$
 solves $h(\theta_{\star}) = 0$

• No explicit solution: define an iterative mecanism $\theta_1, \theta_2, \cdots$, such that (hopefully) $\lim_t \theta_t = \theta_*$.

Example: Wang Landau based algorithms

$$\pi_{\theta}(x) \propto \sum_{i=1}^{d} \mathbb{I}_{\{x \in \mathbb{R}^{n}: \xi(x)=i\}} \pi(x) \, \exp(-\ln(\theta(i))$$

Optimality criterion: θ_{\star} is such that

$$\forall \ell, \qquad \int_{\{x \in \mathbb{R}^n : \xi(x) = \ell\}} \pi_{\theta_\star}(x) \mathsf{d}x = \frac{1}{d}$$

• we look for the $(-\ln)$ free energy: $heta_\star = (heta_\star(1), \cdots, heta_\star(d))$

$$\theta_{\star}(\ell) = \int_{\{x \in \mathbb{R}^n : \xi(x) = \ell\}} \pi(x) \mathsf{d}x$$

Example: Wang Landau based algorithms

$$\pi_{\theta}(x) \propto \sum_{i=1}^{d} \mathbb{I}_{\{x \in \mathbb{R}^{n}: \xi(x)=i\}} \pi(x) \, \exp(-\ln(\theta(i))$$

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• we look for the $(-\ln)$ free energy: $heta_\star = (heta_\star(1), \cdots, heta_\star(d))$

$$\theta_{\star}(\ell) = \int_{\{x \in \mathbb{R}^n : \xi(x) = \ell\}} \pi(x) \mathsf{d}x$$

• which is also defined as the root of

$$h(\theta) = \left(\sum_{i=1}^{d} \frac{\theta_{\star}(i)}{\theta(i)}\right)^{-1} (\theta_{\star} - \theta) = \int H_{\theta}(x) \pi_{\theta}(x) dx$$

In this talk



Simultaneously

() How to obtain draws $\{X_n, n \ge 0\}$ approximating π_{θ_*} ?

$$\frac{1}{N}\sum_{k=1}^{N}\phi(X_k)\to\int\phi(x)\pi_{\theta_\star}(x)\mathsf{d}x$$

2 How to obtain a converging sequence $\{\theta_n, n \ge 0\}$ with a limit θ_{\star} solving

$$h(\theta) = 0$$

when only a Monte Carlo approximation of h is available?

Not in this talk

• We produced
$$\{X_1, X_2, \cdots\}$$
 such that

$$\frac{1}{N}\sum_{t=1}^{N}\phi(X_{t})\to\int\phi(x)\pi_{\theta_{\star}}(x)\mathrm{d}x$$

 $\bullet\,$ The samples can be corrected to approximate $\pi\,$

$$\frac{d}{N}\sum_{t=1}^{N}\phi(X_{t}) \ \theta_{t}\left(\xi(X_{t})\right) \rightarrow \int \phi(x)\pi(x)\mathrm{d}x$$

Outline

1 Introduction

- 2 Adaptive Monte Carlo samplers
 - Controlled Markov chains
 - Sufficient conditions for the cvg in distribution
 - In the literature

3 Stochastic Approximation Algorithms

4 Conclusion

Controlled Markov chains (1/2)

 $P_{\theta}, \theta \in \Theta$: family of Markov kernels. π_{θ} invariant distribution of P_{θ} .

• The draws $(X_t)_t$ are from a controlled Markov chain

 $X_{t+1}|\text{past}_t \sim P_{\theta_t}(X_t, \cdot)$

• Question: Even in the case $\pi_{\theta} = \pi$ for all θ : does $(X_t)_t$ converge (say in distribution) to π ?

Mathematical aspects of adaptive samplers: application to free energy calculation $\[label{eq:application}]$ Adaptive Monte Carlo samplers

Controlled Markov chains

Controlled Markov chains (2/2)

- Answer: No.
- For example:

$$X_{t+1} \sim \begin{cases} P_0(X_t, \cdot) & \text{if } X_t = 0\\ P_1(X_t, \cdot) & \text{if } X_t = 1 \end{cases}$$

where

$$P_{\ell} = \begin{pmatrix} 1 - t_{\ell} & t_{\ell} \\ t_{\ell} & 1 - t_{\ell} \end{pmatrix}.$$

We have $\pi P_{\ell} = \pi$ with $\pi \propto (1,1)$.

The transition matrix of $(X_t)_t$ is

$$ilde{P} = egin{pmatrix} 1 - t_0 & t_0 \\ t_1 & 1 - t_1 \end{pmatrix}$$
 with invariant distribution $ilde{\pi} \propto (t_1, t_0)$

Adaptive Monte Carlo samplers

Sufficient conditions for the cvg in distribution

Sufficient conditions for the cvg in distribution



Adaptive Monte Carlo samplers

L-Sufficient conditions for the cvg in distribution

Sufficient conditions for the cvg in distribution

Compare the two mecanisms

$$P_{\theta_{t-N}} \to P_{\theta_{t-N+1}} \to \dots \to P_{\theta_{t-1}}$$
$$P_{\theta_{t-N}} \to P_{\theta_{t-N}} \to \dots \to P_{\theta_{t-N}}$$

which is small as soon as $P_{\theta_{j+1}}$ and $P_{\theta_{j}}$ are close

• Diminishing adaption condition Roughly speaking:

$$\operatorname{dist}(P_{\theta}, P_{\theta'}) \leq \operatorname{dist}(\theta, \theta')$$
 and $\lim_{t} (\theta_{t+1} - \theta_t) = 0$

Adaptive Monte Carlo samplers

Sufficient conditions for the cvg in distribution

Sufficient conditions for the cvg in distribution



Adaptive Monte Carlo samplers

L_Sufficient conditions for the cvg in distribution

• Containment condition Roughly speaking:

 $\lim_{N \to \infty} \operatorname{dist}(P^N_\theta, \pi_\theta) = 0$

at some rate depending smoothly on θ .

Adaptive Monte Carlo samplers

Sufficient conditions for the cvg in distribution

Sufficient conditions for the cvg in distribution



Adaptive Monte Carlo samplers

└─ Sufficient conditions for the cvg in distribution

• Regularity in θ of π_{θ} so that

$$\lim_{t} \theta_t = \theta_\star \implies \operatorname{dist} \left(\pi_{\theta_t} - \pi_{\theta_\star} \right) \to 0$$

- Adaptive Monte Carlo samplers

Sufficient conditions for the cvg in distribution

Sufficient conditions for the cvg in distribution

Theorem (F., Moulines, Priouret (2012))

Assume

A. (Containment condition)

- $\exists \pi_{\theta} \ s.t. \ \pi_{\theta} P_{\theta} = \pi_{\theta}$
- 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

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

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

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

C. (Convergence of the invariant distributions) $(\pi_{\theta_t})_t$ converges weakly to π_{θ_\star} almost-surely.

Then for any bounded and continuous function f

$$\lim_{n} \mathbb{E}\left[g(X_{n})\right] = \int g(x) \, \pi_{\theta_{\star}}(x) \mathsf{d}x$$

Mathematical aspects of adaptive samplers: application to free energy calculation
Adaptive Monte Carlo samplers
In the literature

In the literature

Sufficient conditions for

- Convergence in distribution of $(X_t)_t$
- Strong law of large numbers for $(X_t)_t$
- Central Limit Theorem for $(X_t)_t$

▶ Roberts, Rosenthal. Coupling and Ergodicity of Adaptive Markov chain Monte Carlo algorithms. J. Appl. Prob. (2007)

► F., Moulines, Priouret. Convergence of adaptive MCMC algorithms: ergodicity and law of large numbers. *Ann. Statist.* (2012)

▶ F., Moulines, Priouret and Vandekerkhove. A Central Limit Theorem for Adaptive and Interacting Markov Chain. *Bernoulli* (2013).

Conditions successfully applied to establish the convergence of Adaptive Hastings-Metropolis, Wang-Landau, SHUS, Well-tempered, ···

► F., Jourdain, Kuhn, Lelièvre and Stoltz. Convergence of the Wang-Landau algorithm. *Mathematics of Computation (2014)*

► F., Jourdain, Lelièvre and Stoltz. Self-Healing Umbrella Sampling: convergence and efficiency. *arXiv math.PR* 1410.2109 (2014)

Outline

1 Introduction

2 Adaptive Monte Carlo samplers

3 Stochastic Approximation Algorithms

- Introduction
- Stability
- \blacksquare Recurrence of any neighborhood of $\mathcal L$
- Convergence of $\{\theta_t, t \ge 0\}$
- Conclusion

4 Conclusion

Mathematical aspects of adaptive samplers: application to free energy calculation
Stochastic Approximation Algorithms
Introduction

Stochastic Approximation (SA) Algorithm

Find the roots of:
$$h(\theta) = \int H_{\theta}(x) \ \pi_{\theta}(\mathsf{d}x)$$

• Natural idea: NOT possible here since h is not explicit

$$\theta_{t+1} = \theta_t + \gamma_{t+1} \ h(\theta_t)$$

SA algorithm

 $\theta_{t+1} = \theta_t + \gamma_{t+1} \ H_{\theta_t}(X_{t+1})$

where

- $\{\gamma_t, t \ge 0\}$ sequence of positive stepsizes
- $X_{t+1} \sim \pi_{\theta_t}$ OR $X_{t+1} \sim P_{\theta_t}(X_t, \cdot)$ where P_{θ} is a Markov transition kernel with inv. dist. π_{θ} .

Example: Wang Landau is a Stochastic Approximation Algorithm

$$\tilde{\theta}_{t+1}(i) = \tilde{\theta}_t(i) \left\{ 1 + \gamma_{t+1} \mathbb{I}_{\{\xi(x)=i\}}(X_{t+1}) \right\}$$
$$= \tilde{\theta}_t(i) + \gamma_{t+1} \tilde{\theta}_t(i) \mathbb{I}_{\{\xi(x)=i\}}(X_{t+1})$$

Example: Wang Landau is a Stochastic Approximation Algorithm

$$\tilde{\theta}_{t+1}(i) = \tilde{\theta}_t(i) \left\{ 1 + \gamma_{t+1} \mathrm{I}_{\{\xi(x)=i\}}(X_{t+1}) \right\}$$
$$= \tilde{\theta}_t(i) + \gamma_{t+1}\tilde{\theta}_t(i) \mathrm{I}_{\{\xi(x)=i\}}(X_{t+1})$$
$$\sum_{i=1}^d \tilde{\theta}_{t+1}(i) = \sum_{i=1}^d \tilde{\theta}_t(i) + \gamma_{t+1} \sum_{i=1}^d \tilde{\theta}_t(i) \mathrm{I}_{\{\xi(x)=i\}}(X_{t+1})$$
$$= \sum_{i=1}^d \tilde{\theta}_t(i) + \gamma_{t+1} \tilde{\theta}_t(\xi(X_{t+1}))$$
$$= \left(\sum_{i=1}^d \tilde{\theta}_t(i)\right) \left\{ 1 + \gamma_{t+1} \theta_t(\xi(X_{t+1})) \right\}$$

Example: Wang Landau is a Stochastic Approximation Algorithm

$$\begin{split} \tilde{\theta}_{t+1}(i) &= \tilde{\theta}_t(i) \left\{ 1 + \gamma_{t+1} \mathrm{I}_{\{\xi(x)=i\}}(X_{t+1}) \right\} \\ &= \tilde{\theta}_t(i) + \gamma_{t+1} \tilde{\theta}_t(i) \mathrm{I}_{\{\xi(x)=i\}}(X_{t+1}) \\ \sum_{i=1}^d \tilde{\theta}_{t+1}(i) &= \sum_{i=1}^d \tilde{\theta}_t(i) + \gamma_{t+1} \sum_{i=1}^d \tilde{\theta}_t(i) \mathrm{I}_{\{\xi(x)=i\}}(X_{t+1}) \\ &= \sum_{i=1}^d \tilde{\theta}_t(i) + \gamma_{t+1} \tilde{\theta}_t\left(\xi(X_{t+1})\right) \\ &= \left(\sum_{i=1}^d \tilde{\theta}_t(i)\right) \left\{ 1 + \gamma_{t+1} \theta_t\left(\xi(X_{t+1})\right) \right\} \end{split}$$

$$\theta_{t+1}(i) = \frac{\tilde{\theta}_{t+1}(i)}{\sum_{\ell=1}^{d} \tilde{\theta}_{t+1}(\ell)} = \theta_t(i) \frac{1 + \gamma_{t+1} \mathbb{1}_{\{\xi(x)=i\}}(X_{t+1})}{1 + \gamma_{t+1} \theta_t(\xi(X_{t+1}))} \\ = \theta_t(i) + \gamma_{t+1} H_{\theta_t}(X_{t+1}) + O(\gamma_{t+1}^2)$$

Convergence of SA algorithms to the limit set ${\cal L}$

$$\theta_{t+1} = \theta_t + \gamma_{t+1} \ H_{\theta_t}(X_{t+1})$$

Prove successively

- Stability: the sequence $\{\theta_t, t \ge 0\}$ is in a compact set of Θ
- Attractive limiting set \mathcal{L} :

 $\liminf_{t} \operatorname{dist} \left(\theta_t, \mathcal{L} \right) = 0.$

• Convergence :

 $\lim_t \operatorname{dist} \left(\theta_t, \mathcal{L}\right) = 0.$

Stability of the SA algorithm: $\theta_{t+1} = \theta_t + \gamma_{t+1}H_{\theta_t}(X_{t+1})$

Theorem

Assume $h: \Theta \to \mathbb{R}^d$ is continuous and

(i) Lyapunov function: $V: \Theta \to \mathbb{R}^+$ is C^1 and

- the level sets $\{\theta \in \Theta : V(\theta) \le M\}$ are compact subsets of Θ
- $\nabla V(\theta) \cdot h(\theta) \le 0$
- $\mathcal{L} = \{\theta \in \Theta : \nabla V(\theta) \cdot h(\theta) = 0\}$ is in a compact level set $\{V \le M_0\}$

(ii) Noise: $H_{\theta_t}(X_{t+1}) = h(\theta_t) + \xi_{t+1}$ and

$$\lim_{L} \sum_{t=1}^{L} \gamma_t \xi_t \text{ exists.}$$

(iii) Step-size sequence: $\lim_t \gamma_t = 0$.

(iv) **Recurrence:** $\{\theta_t, t \ge 0\}$ is i.o. in a compact subset of $\Theta \subseteq \mathbb{R}^d$

Then: $\{\theta_t, t \ge 0\}$ remains in a compact subset of Θ .

Mathematical aspects of adaptive samplers: application to free energy calculation Stochastic Approximation Algorithms Stability



Recurrence : θ_t infinitely often in $\{V \leq M\}$.

The Lyapunov property:

for any \mathcal{K} compact s.t. $\mathcal{K} \cap \mathcal{L} = \emptyset$,

there exist $\delta, \gamma_{\star}, \beta_{\star} > 0$ s.t.

 $[\gamma \leq \gamma_{\star}, |\xi| \leq \beta_{\star}, u \in \mathcal{K}] \Longrightarrow V(u + \gamma h(u) + \gamma \xi) \leq V(u) - \gamma \delta$

Stochastic Approximation Algorithms

Recurrence of any neighborhood of L

Any neighboorhood of \mathcal{L} is recurrent

Theorem

Assume $h: \Theta \to \mathbb{R}^d$ is continuous and

- (i) Lyapunov function: (idem)
- (ii) Noise: (idem)
- (iii) Step-size sequence: $\sum_t \gamma_t = +\infty$
- (iv) Stability: $\{\theta_t, t \ge 0\}$ is in a compact subset of Θ

Then: $\liminf_t d(\theta_t, \mathcal{L}) = 0.$

Stochastic Approximation Algorithms

Recurrence of any neighborhood of L



Stability: $\theta_t \in \{V \leq M\}$ for any t

The Lyapunov property:

for any \mathcal{K} compact s.t. $\mathcal{K} \cap \mathcal{L} = \emptyset$, there exist $\delta, \gamma_{\star}, \beta_{\star} > 0$ s.t. $[\gamma \leq \gamma_{\star}, |\xi| \leq \beta_{\star}, u \in \mathcal{K}] \Longrightarrow V(u + \gamma h(u) + \gamma \xi) \leq V(u) - \gamma \delta$

Stepsize: $\sum_t \gamma_t = +\infty$ and $\lim_t \gamma_t = 0$

Stochastic Approximation Algorithms

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Convergence of $\{\theta_t, t \ge 0\}$: $\theta_{t+1} = \theta_t + \gamma_{t+1}H_{\theta_t}(X_{t+1})$

Theorem

Assume $h: \Theta \to \mathbb{R}^d$ is continuous and

- (i) Lyapunov function: (idem)
- (ii) Noise: (idem)
- (iii) Step-size sequence: (idem)
- (iv) Stability: (idem)
- (v) Excursions outside \mathcal{L} : $\lim_t V(\theta_t)$ exists

Then: $\lim_t \mathrm{dist}\,(heta_t,\mathcal{L})=0$ and also: convergence to a connected component of $\mathcal L$

Stochastic Approximation Algorithms



Stability:

The Lyapunov property:

Stepsize:

Shorter length of the excursions outside \mathcal{L}_{α} : " $\lim_t V(\theta_t)$ exists" implies that the time

$$\sum_{j=k}^{\tau_{\alpha}(k)} \gamma_{j}$$

arbitrary small when k large enough.

Conclusion

Conclusion: stability and convergence

Theorem

Assume $h: \Theta \to \mathbb{R}^d$ is continuous and

- (i) Lyapunov function: $V: \Theta \to \mathbb{R}^+$ is C^1 and
 - the level sets $\{\theta \in \Theta : V(\theta) \leq M\}$ are compact subsets of Θ
 - $\nabla V(\theta) \cdot h(\theta) \le 0$
 - $\mathcal{L} = \{ \theta \in \Theta : \overline{\nabla}V(\theta) \cdot h(\theta) = 0 \}$ is in a compact level set $\{ V \leq M_0 \}$

(ii) Noise:

$$\lim_{L \to \infty} \sum_{t=1}^{L} \gamma_t \xi_t \qquad \text{exists}$$

- (iii) Step-size sequence: $\sum_t \gamma_t = \infty$ $\lim_t \gamma_t = 0$
- (iv) Recurrence: $\{\theta_t, t \geq 0\}$ is i.o. in a compact subset of $\Theta \subseteq \mathbb{R}^d$
- (v) Excursions outside \mathcal{L} : $\lim_t V(\theta_t)$ exists

Then: $\{\theta_t, t \ge 0\}$ remains in a compact subset of Θ and $\lim_t \operatorname{dist}(\theta_t, \mathcal{L}) = 0$.

Conclusion: on the noise

We write

$$H_{\theta_t}(X_{t+1}) = h(\theta_t) + \xi_{t+1}$$

In practice,

$$X_{t+1} \sim P_{\theta_t}(X_t, \cdot)$$
 Markov transition with inv. dist. π_{θ_t}

- Biased approximation: $\mathbb{E}\left[\xi_{t+1}\right] \neq 0$
- Cumulated noise

$$\sum_{t=1}^{L} \gamma_{t+1} \{ H_{\theta_t}(X_{t+1}) - h(\theta_t) \}$$

converges under assumptions

- $\sum_t \gamma_t^2 < \infty$
- ergodicity of the transition kernels P_{θ}
- "smoothness-in- θ " of the transition kernels P_{θ}

Mathematical aspects of adaptive samplers: application to free energy calculation
Stochastic Approximation Algorithms
Conclusion

In the literature

• On Stochastic Approximation

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▶ Benaïm. Dynamics of stochastic approximation algorithms. Séminaire de Probabilités de Strasbourg (1999)

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• Applied to the convergence of ABP samplers

► Dama, Parrinello, Voth. Well tempered Metadynamics converges asymptotically. *Physical Review Letters (2014)*

► F., Jourdain, Kuhn, Lelièvre and Stoltz. Convergence of the Wang-Landau algorithm. *Mathematics of Computation (2014)*

► F., Jourdain, Lelièvre and Stoltz. Self-Healing Umbrella Sampling: convergence and efficiency. *arXiv math.PR* 1410.2109 (2014)

Outline

1 Introduction

- 2 Adaptive Monte Carlo samplers
- **3** Stochastic Approximation Algorithms
- 4 Conclusion

As a global conclusion - a theorem solving the two questions

Theorem (F., Jourdain, Lelièvre, Stoltz (2014))

In the case $\theta_{t+1} = \theta_t + \gamma_{t+1} H_{\theta_t}(X_{t+1})$ and $\sup_{\theta,x} |H_{\theta}(x)| < \infty$

- (i) Lyapunov function with limit set $\mathcal{L} = \{\theta_{\star}\}; \{\theta_t, t \geq 0\}$ visits i.o. a compact set of $\Theta; \sum_t \gamma_t = +\infty, \sum_t \gamma_t^2 < \infty.$
- (ii) There exists $\rho \in (0,1)$ such that for any $\theta \in \Theta$

$$\sup_{x} \|P_{\theta}^{n}(x,\cdot) - \pi_{\theta}\|_{TV} \le 2\rho^{n}$$

(iii) There exists C s.t. for all $\theta, \theta' \in \Theta$

$$\sup_{x} \|P_{\theta}(x,\cdot) - P_{\theta'}(x,\cdot)\|_{TV} \le C|\theta - \theta'|$$

(iv) There exists C s.t. for all $\theta, \theta' \in \Theta$

$$\sup_{x} |H_{\theta}(x) - H_{\theta'}(x)| \le C|\theta - \theta'|$$

Then: $\lim_t \theta_t = \theta_*$ a.s. and for any bounded function g

$$\lim_{N} \frac{1}{N} \sum_{t=1}^{N} g(X_t) = \int g(x) \ \pi_{\theta_{\star}}(\mathsf{d}x) \qquad \text{a.s.}$$

Collaborations

Talk based on joint works with

- Eric Moulines (Telecom ParisTech, France)
- Benjamin Jourdain (ENPC, France)
- Tony Lelièvre (ENPC, France)
- Gabriel Stöltz (ENPC, France)
- Pierre Priouret (Univ. Paris VI, France)
- Matti Vihola (Univ. Jyvaskyla, Finland)
- Pierre Vandekerkhove (Univ. Marne-la-Vallée, France)