Convergence and Efficiency of Adaptive Importance Sampling techniques with partial biasing

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Joint work with
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Talk based on the paper
G. Fort, B. J., T. Lelièvre, G. Stoltz Convergence and Efficiency of Adaptive Importance Sampling techniques with partial biasing, arXiv:1610.0919
Goal:

Explore the support of a distribution \( \pi \, d\lambda \) with density \( \pi \) w.r.t. the Lebesgue measure \( \lambda \) on \( D \subseteq \mathbb{R}^d \) and/or compute integrals w.r.t. \( \pi \)

\[
\int_D f(x) \, \pi(x) d\lambda(x)
\]

when \( \pi \) is highly metastable, \( d \) is large.

Solution: based on Importance Sampling (IS)

Sample \( X_1, \ldots, X_n, \ldots \) i.i.d. \( \tilde{\pi} \, d\lambda \)

Define the IS approximation

\[
\int_D f \, \pi d\lambda \approx \frac{1}{n} \sum_{k=1}^{n} \frac{\pi(X_k)}{\tilde{\pi}(X_k)} f(X_k).
\]

importance ratio
Motivation (2/4) - How to choose $\tilde{\pi}$?

- Define a partition of the support $\mathcal{D}$ in $I$ strata

$$\mathcal{D} = \bigcup_{i=1}^{I} \mathcal{D}_i \quad \mathcal{D}_i \cap \mathcal{D}_j = \emptyset \text{ for } i \neq j$$

- A family of auxiliary distribution based on a local biasing

For all probability $\theta = (\theta(1), \cdots, \theta(I))$ on $\{1, 2, \ldots, I\}$ with $\theta(i) > 0, \forall i$, let

$$\pi_\theta(x) \overset{\text{def}}{=} \left( \sum_{i=1}^{I} \frac{\theta_*(i)}{\theta(i)} \right)^{-1} \sum_{i=1}^{I} \frac{\pi(x)}{\theta(i)} \mathbb{I}_{\mathcal{D}_i}(x),$$

where

$$\theta_*(i) \overset{\text{def}}{=} \int_{\mathcal{D}_i} \pi d\lambda$$

If $\mathcal{D}_i = \xi^{-1}([a_i, a_{i+1}))$ with $\xi : \mathbb{R}^d \to \mathbb{R}$ a collective variable (reaction coordinate) and $a_1 < a_2 < \ldots < a_{I+1}$ then $\log \theta_*(i)$ is the free-energy (up to an additive constant)
Motivation (2/4) - How to choose $\widetilde{\pi}$?

- Define a partition of the support $\mathcal{D}$ in $I$ strata

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If $\mathcal{D}_i = \xi^{-1}([a_i, a_{i+1}))$ with $\xi : \mathbb{R}^d \to \mathbb{R}$ a collective variable (reaction coordinate) and $a_1 < a_2 < \ldots < a_{I+1}$ then $\log \theta_*(i)$ is the free-energy (up to an additive constant)

Key property: $\pi_{\theta_*}(\mathcal{D}_i) = 1/I$ – all the strata have the same weight: efficient to tackle multimodality! but $\theta_*$ is unknown.
An *iterative* algorithm which

- Will learn on the fly the weight vector $\theta_\star$ though a Stochastic Approximation algorithm
  
  $\theta_{n+1} = \theta_n + \gamma_{n+1}H(\theta_n, X_{n+1})$

  where $H$ is chosen so that $\theta_\star$ is the unique solution of
  
  $$\int H(\theta, x) \, \pi_\theta(x) \, d\lambda(x) = 0.$$  

- from draws $X_{n+1} \sim P_{\theta_n}(X_n, \cdot)$ where $P_\theta(x, \cdot)$ is a kernel with invariant distribution $\pi_\theta$ (e.g. a Metropolis-Hastings kernel)
Motivation - Adaptive Importance Sampling (3/4)

An *iterative* algorithm which

- Will learn on the fly the weight vector $\theta_*$ though a Stochastic Approximation algorithm

  \[ \theta_{n+1} = \theta_n + \gamma_{n+1} H(\theta_n, X_{n+1}) \]

  where $H$ is chosen so that $\theta_*$ is the unique solution of

  \[ \int H(\theta, x) \pi_\theta(x) \, d\lambda(x) = 0. \]

- from draws $X_{n+1} \sim P_{\theta_n}(X_n, \cdot)$ where $P_\theta(x, \cdot)$ is a kernel with invariant distribution $\pi_\theta$ (e.g. a Metropolis-Hastings kernel)

If convergence is established, this yields

- an estimator of the free energy: $\lim_n \theta_n = \theta_*$. 
- an approximation of the target distribution $\pi$ - computed on the fly/online

  \[ \int f \, \pi \, d\lambda = \lim_n \frac{I}{n} \sum_{k=1}^n f(X_k) \left( \sum_{i=1}^I \theta_k(i) \mathbb{I}_{\mathcal{D}_i}(X_k) \right) \]
A family of algorithms: Wang Landau, Self Healing Umbrella Sampling (SHUS), Well-Tempered Metadynamics, $\text{SHUS}_{\rho}^{g}$
on the form

1. Given a new draw $X_{n+1} \sim P_{\theta_n}(X_n, \cdot)$ with inv. dist. $\pi_{\theta_n}$
2. Update a counter of the visits to a stratum

$$C_{n+1}(i) = C_n(i) + (\cdots)^2 \mathbb{I}_{D_i}(X_{n+1}) \quad i = 1, \cdots, I$$

3. Normalize the counter to obtain a probability measure on $\{1, 2, \ldots, I\}$

$$\theta_{n+1}(i) = \frac{C_{n+1}(i)}{\sum_{j=1}^{I} C_{n+1}(j)} = \theta_n(i) + \gamma_{n+1} \cdots + O(\gamma_{n+1}^2) \quad i = 1, \cdots, I$$

**Fundamental:** if $X_{n+1} \in D_i$

$$C_{n+1}(i) > C_n(i), \quad C_{n+1}(j) = C_n(j), j \neq i$$

$$\implies \pi_{\theta_{n+1}}(D_i) < \pi_{\theta_n}(D_i), \quad \pi_{\theta_{n+1}}(D_j) > \pi_{\theta_n}(D_j), j \neq i.$$
Wang-Landau (WL) update
(adapted from) the Wang-Landau algorithm  
(Wang and Landau, 2001)

**Input:**
- initial values: a point $X_0 \in \mathcal{D}$ and a counter $C_0 \in (\mathbb{R}^*_+)^I$
- a positive (deterministic) stepsize sequence $\{\gamma_n, n \geq 0\}$

For $n = 0, 1, \cdots$
- Normalize the counter
  \[
  \theta_n(i) = \frac{C_n(i)}{\sum_{j=1}^{I} C_n(j)}, \quad \forall i = 1, \cdots, I
  \]
- Draw a new point: $X_{n+1} \sim P_{\theta_n}(X_n, \cdot)$ kernel with inv. dist. $\pi_{\theta_n}$
- Update the counter of the visited stratum
  \[
  C_{n+1}(i) = C_n(i) + \gamma_{n+1} C_n(i) \mathbb{I}_{\mathcal{D}_i}(X_{n+1}), \quad \forall i = 1, \cdots, I
  \]
\[ \theta_{n+1}(i) = \theta_n(i) + \gamma_{n+1} \theta_n(i) \left( \mathbb{1}_{D_i}(X_{n+1}) - \sum_{j=1}^I \theta_n(j) \mathbb{1}_{D_j}(X_{n+1}) \right) + \gamma_{n+1}^2 O_{w.p.1}. (1). \]
a WL based algorithm - convergence results (2/3)

\[
\theta_{n+1}(i) = \theta_n(i) + \gamma_{n+1} \theta_n(i) \left( \mathbb{I}_{D_i}(X_{n+1}) - \sum_{j=1}^{I} \theta_n(j) \mathbb{I}_{D_j}(X_{n+1}) \right) + \gamma_{n+1}^2 O_{w.p.1}. (1)
\]

\[
\int_{\mathbb{R}^d} H(\theta, x) \pi_\theta(x)dx = \left( \sum_{i=1}^{I} \theta_*(i)/\theta(i) \right)^{-1}(\theta_* - \theta)
\]

Under conditions on
- the strata and the target: \( 0 < \inf_D \pi \leq \sup_D \pi < \infty \).
- the kernels \( P_\theta \) : satisfied by Metropolis-Hastings kernels, with proposal \( q(x, y) d\lambda(y) \) such that \( q(x, y) = q(y, x) \) and \( \inf_{(x,y) \in D^2} q(x, y) > 0 \).
- the stepsize sequence \( \gamma_n \): \( \sum_n \gamma_n = +\infty, \sum_n \gamma_n^2 < \infty \)

it is proved asymptotic results (Fort, J., Kuhn, Lelièvre, Stoltz, 2015a)

1. The a.s. convergence of the sequence \( \theta_n \) to \( \theta_* \).
2. The ”convergence” of the samples \( \{X_1, \cdots, X_n, \cdots\} \)

\[
\int f \pi d\lambda = \lim_n \frac{I}{n} \sum_{k=1}^{n} f(X_k) \left( \sum_{i=1}^{I} \theta_k(i) \mathbb{I}_{D_i}(X_k) \right) \quad a.s.
\]

\( \leftrightarrow \) bad Efficiency Factor
and role of the stepsize sequence (Fort, J., Kuhn, Lelièvre, Stoltz, 2015b) in the transient phase

Figure: Left: level curves of the target density. Right: typical trajectory for $\beta = 15$ when $\gamma_n = \gamma_*/n^{0.6}$ with $\alpha = 0.6$ and $\gamma_* = 1$.

- The density depends on a parameter $\beta$: large values of $\beta$ increases the metastability phenomenon.
- We choose $\gamma_n = \gamma_*/n^\alpha$, $\alpha \in (1/2, 1]$

$$\ln T_{(\alpha<1)} = C(\alpha, \gamma_*) + \frac{1}{1-\alpha} \ln \beta \quad \ln T_{(\alpha=1)} = C(\gamma_*) + \frac{\mu_0}{1 + \gamma_*} \beta$$

$\hookrightarrow$ "self tuned" step size $\gamma_n$
An Adaptive Importance Sampling Algorithm with
- self-tuned stepsize sequence
- partial biasing to improve the IS step

$\text{SHUS}_{\rho}^{g}$
A new algorithm

Self-tuned and Partially biasing algorithm  (F., Jourdain, Leliévre, Stoltz (2016))

**Input:**
- initial values: a point $X_0 \in \mathcal{D}$ and a counter $C_0 \in (\mathbb{R}^*_+)^I$
- a biasing function $\rho : (0,1) \to \mathbb{R}_+$ and a stepsize function $g : \mathbb{R}_+ \to \mathbb{R}_+$,

Set $\pi_{\rho(\theta)}(x) \overset{\text{def}}{=} \left(\sum_{i=1}^I \frac{\theta_\star(i)}{\rho(\theta(i))}\right)^{-1} \sum_{i=1}^I \frac{\pi(x)}{\rho(\theta(i))} \mathbb{I}_{\mathcal{D}_i}(x)$.

For $n = 0, 1, \cdots$
- Normalize the counter $\theta_n(i) = C_n(i)/\sum_{j=1}^I C_n(j), \quad \forall i = 1, \cdots, I$
- Draw a new point: $X_{n+1} \sim P_{\rho(\theta_n)}(X_n, \cdot)$ kernel with inv. dist. $\pi_{\rho(\theta_n)}$
- Update the counter of the visited stratum $\forall i = 1, \cdots, I$

$$C_{n+1}(i) = C_n(i) + \left\lfloor \frac{\gamma}{g \left(\sum_{j=1}^I C_n(j)\right)} \right\rfloor \begin{pmatrix} I \\ \sum_{j=1}^I C_n(j) \end{pmatrix} \rho(\theta_n(i)) \mathbb{I}_{\mathcal{D}_i}(X_{n+1}),$$

$= C_n(i)$ if $\rho(t) \equiv t$
The intuition for this new update rule of $C_n$

The samples $X_n \sim_{i.i.d.} \pi$;

- A counter of the visits to each stratum

\[
C_{n+1}(i) = C_n(i) + \gamma \mathbb{I}_{D_i}(X_{n+1}) = C_0(i) + \gamma \sum_{k=1}^{n+1} \mathbb{I}_{D_i}(X_k) \Rightarrow C_{n+1}(i) \sim \gamma n \theta_\star(i)
\]

\[
= C_n(i) + \frac{\gamma}{\sum_{j=1}^{I} C_n(j)} \left( \sum_{j=1}^{I} C_n(j) \right) \mathbb{I}_{D_i}(X_{n+1})
\]

- The estimate of $\theta_\star$

\[
\theta_{n+1}(i) = \theta_n(i) + \gamma_{n+1} \left( \mathbb{I}_{D_i}(X_{n+1}) - \theta_n(i) \sum_{j=1}^{I} \mathbb{I}_{D_j}(X_{n+1}) \right) + O(\gamma_{n+1}^2)
\]

- For approximation of integrals

\[
\int f \pi d\lambda \approx \frac{1}{n} \sum_{k=1}^{n} f(X_k)
\]
The intuition for this new update rule of $C_n$

The samples $X_n \overset{i.i.d.}{\sim} \pi \rho(\theta_*) \propto \sum_{i=1}^{I} \frac{\pi}{\rho(\theta_*(i))} \mathbb{I}_{D_i}$;

- A counter of the visits to each stratum

$$C_{n+1}(i) = C_n(i) + \gamma \frac{\sum_{j=1}^{I} C_n(j)}{\sum_{j=1}^{I} C_n(j)} \left( \sum_{j=1}^{I} C_n(j) \right)^{-1} \rho(\theta_*(i)) \mathbb{I}_{D_i}(X_{n+1})$$

$\gamma_{n+1} = O(1/n)$

$$C_n(i) \sim \left( \sum_{j=1}^{I} \frac{\theta_*(j)}{\rho(\theta_*(j))} \right)^{-1} \gamma_n \theta_*(i)$$

- The estimate of $\theta_*$

$$\theta_{n+1}(i) = \theta_n(i) + \gamma_{n+1} \left( \rho(\theta_*(i)) \mathbb{I}_{D_i}(X_{n+1}) - \theta_n(i) \sum_{j=1}^{I} \rho(\theta_*(j)) \mathbb{I}_{D_j}(X_{n+1}) \right) + O(\gamma_{n+1}^2)$$

- For approximation of integrals

$$\int f \pi d\lambda \approx \left( \sum_{j=1}^{I} \frac{\theta_*(j)}{\rho(\theta_*(j))} \right) \frac{1}{n} \sum_{k=1}^{n} f(X_k) \left( \sum_{j=1}^{I} \rho(\theta_*(j)) \mathbb{I}_{D_j}(X_k) \right)$$

The discrepancy between the weights is modified through $\rho$. ex. $t^a$, $0 < a < 1$
The intuition for this new update rule of $C_n$

The samples $X_n \overset{i.i.d.}{\sim} \pi \rho(\theta_*) \propto \sum_{i=1}^{I} \frac{\pi}{\rho(\theta_*(i))} \mathbb{I}_{D_i}$;

- A counter of the visits to each stratum

$$C_{n+1}(i) = C_n(i) + \frac{\gamma}{g\left(\sum_{j=1}^{I} C_n(j)\right)} \left(\sum_{j=1}^{I} C_n(j)\right) \rho(\theta_*(i)) \mathbb{I}_{D_i}(X_{n+1})$$

- The estimate of $\theta_*$

$$\theta_{n+1}(i) = \theta_n(i) + \gamma_{n+1} \left(\rho(\theta_*(i)) \mathbb{I}_{D_i}(X_{n+1}) - \theta_n(i) \sum_{j=1}^{I} \rho(\theta_*(j)) \mathbb{I}_{D_j}(X_{n+1})\right) + \mathcal{O}(\gamma_{n+1}^2)$$

- For approximation of integrals

$$\int f \pi d\lambda \approx \left(\sum_{j=1}^{I} \frac{\theta_*(j)}{\rho(\theta_*(j))}\right) \frac{1}{n} \sum_{k=1}^{n} f(X_k) \left(\sum_{j=1}^{I} \rho(\theta_*(j)) \mathbb{I}_{D_j}(X_k)\right)$$

The discrepancy between the weights is modified through $\rho$. ex. $t^a$, $0 < a < 1$

Control the step size through a function $g$
The intuition for this new update rule of $C_n$

The samples $X_{n+1} \sim P_{\rho(\theta_n)}(X_n,.)$ and the weight $\theta_\star$ is learnt along iterations

- A counter of the visits to each stratum

$$C_{n+1}(i) = C_n(i) + \frac{\gamma}{g\left(\sum_{j=1}^{I} C_n(j)\right)} \left(\sum_{j=1}^{I} C_n(j)\right) \rho(\theta_n(i)) \mathbb{I}_{D_i}(X_{n+1})$$

- The estimate of $\theta_\star$

$$\theta_{n+1}(i) = \theta_n(i) + \gamma_{n+1} \left(\rho(\theta_n(i)) \mathbb{I}_{D_i}(X_{n+1}) - \theta_n(i) \sum_{j=1}^{I} \rho(\theta_n(j)) \mathbb{I}_{D_j}(X_{n+1})\right) + O(\gamma_{n+1}^2)$$

- For approximation of integrals

$$\int f \pi d\lambda \approx \frac{1}{n} \sum_{k=1}^{n} \left(\sum_{j=1}^{I} \frac{\theta_{k-1}(j)}{\rho(\theta_{k-1}(j))}\right) f(X_k) \left(\sum_{j=1}^{I} \rho(\theta_{k-1}(j)) \mathbb{I}_{D_j}(X_k)\right)$$

The discrepancy between the weights is modified through $\rho$. ex. $t^a$, $0 < a < 1$

Control the step size through a function $g$
1. On the target density: \( \sup_{\mathcal{D}} \pi < \infty \) and \( \min_{1 \leq i \leq I} \theta_\star(i) > 0 \)

2. On the kernels \( P_\theta \): satisfied by Metropolis-Hastings kernels, with proposal \( q(x, y) d\lambda(y) \) such that \( q(x, y) = q(y, x) \) and \( \inf_{(x,y) \in \mathcal{D}^2} q(x, y) > 0 \)

3. On the function \( \rho \longrightarrow \): satisfied with \( \rho(t) = \max(t_0, t)^a \) with \( t_0, a \in [0, 1) \).
   See (Dama, Hocky, Sun, Voth, 2015) and (McCarty, Valsson, Tiwary, Parrinello, 2015) for motivations to choose \( t_0 > 0 \).

4. On the function \( g \), chosen of the form

\[
g(s) = \begin{cases} 
(\ln(1 + s))^{\alpha/(1-\alpha)} \text{ with } \alpha \in (1/2, 1) \\
 s^\mu \text{ with } \mu > 0 \rightarrow \text{ corresponds to } \alpha = 1
\end{cases}
\]
Convergence results (1/2)

By using sufficient conditions for convergence of Adaptive MCMC samplers Fort, Moulines, Priouret (2012) and convergence of Stochastic Approximation algo with controlled Markovian dynamics Andrieu, Moulines, Priouret (2005)

► On the random sequence $\gamma_n$ almost-surely,

$$\lim_{n} \gamma_n n^\alpha = (1 - \alpha)^\alpha \gamma^{1-\alpha} \left( \sum_{j=1}^{I} \frac{\theta_*(j)}{\rho(\theta_*(j))} \right) \quad \text{a.s.}$$

► On the weight sequence $\theta_n$ almost-surely,

$$\lim_{n} \theta_n = \theta_*$$

► On the Importance Sampling step almost-surely,

$$\lim_{n} \frac{1}{n} \sum_{k=1}^{n} \left( \sum_{j=1}^{I} \frac{\theta_{k-1}(j)}{\rho(\theta_{k-1}(j))} \right) f(X_k) \left( \sum_{j=1}^{I} \rho(\theta_{k-1}(j)) \mathbb{I}_{D_j}(X_k) \right) = \int f \pi d\lambda$$
We wrote the results in the case

$$\rho(t) = \max(t_0, t)^a$$ with $$t_0, a \in [0, 1)$$

$$g(s) = \begin{cases} 
(\ln(1 + s))^{\alpha/(1-\alpha)} & \text{with } \alpha \in (1/2, 1) \\
 s^\mu & \text{with } \mu > 0 \rightarrow \text{corresponds to } \alpha = 1
\end{cases}$$

Applies to a discrete version of the Well-Tempered metadynamics algorithm (Barducci, Bussi and Parrinello (2008)) where $$\rho(t) = t^a$$ and $$g(s) = s^{1-a}$$ with $$a \in (0, 1)$$, $$\gamma_n = O(1/n)$$

The ”partial biasing” and ”self-tuned stepsize” parameters are one to one.

Convergence also holds in the case $$\rho(t) = t$$ and $$g$$ as above (Fort, J., Lelièvre, Stoltz, 2016).

Additional assumption $$\inf_D \pi > 0$$ needed to prove recurrence $$\limsup_{n \to \infty} \min_{1 \leq i \leq I} \theta_n(i) > 0$$.

Indeed when $$\theta_n(i)$$ small and $$X_{n+1} \in D_i$$, the increase of the counter

$$C_{n+1}(i + 1) - C_n(i) \propto \rho(\theta_n(i))$$ is smaller than when $$\rho(t) = t^a$$ with $$a < 1$$.

Applies to the Self Healing Umbrella Sampling algorithm (Marsili et al. 2006) where $$g(s) = s$$ and $$\rho(t) = t$$ ”no partial biasing”.
Elements of proof

We prove cv of the Generalized Wang-Landau algorithm where for $n \in \mathbb{N}$,

$$C_{n+1}(i) = C_n(i) \left(1 + \gamma_{n+1} \frac{\rho(\theta_n(i))}{\theta_n(i)} \mathbb{I}_{D_i}(X_{n+1})\right)$$

$$= C_n(i) + \gamma_{n+1} \left(\sum_{j=1}^{I} C_n(j)\right) \rho(\theta_n(i)) \mathbb{I}_{D_i}(X_{n+1}),$$

- $\gamma_{n+1}$ is a positive random variable only depending on $(C_0, X_0, C_1, X_1, \ldots, C_n, X_n)$ (the past of the algorithm),
- $(\gamma_n)_n$ is non increasing, $\sum_n \gamma_n = \infty$, $\sum_n \gamma^2_n < \infty$ and $\sup_n \frac{\gamma_n}{\gamma_{n+I-1}} < \infty$,

and then check that these hypotheses are satisfied by $(\gamma_{n+1} = \frac{\gamma_n}{g(\sum_{j=1}^{I} C_n(j))})_{n \in \mathbb{N}}$.

$$\theta_{n+1}(i) = \frac{C_n(i)}{\sum_{j=1}^{I} C_n(j)} \times \frac{1 + \gamma_{n+1} \frac{\rho(\theta_n(i))}{\theta_n(i)} \mathbb{I}_{D_i}(X_{n+1})}{1 + \gamma_{n+1} \sum_{j=1}^{I} \rho(\theta_n(j)) \mathbb{I}_{D_j}(X_{n+1})}$$

$$= \theta_n(i) + \gamma_{n+1} \left(\rho(\theta_n(i)) \mathbb{I}_{D_i}(X_{n+1}) - \theta_n(i) \sum_{j=1}^{I} \rho(\theta_n(j)) \mathbb{I}_{D_j}(X_{n+1})\right) + O(\gamma^2_{n+1}).$$

$H_i(\theta_n, X_{n+1})$
Convergence of the Generalized Wang-Landau algorithm

\[ h(\theta) := \int_{\mathbb{R}^d} H(\theta, x) \pi_{\rho(\theta)}(x) d\lambda(x) = \left( \sum_{j=1}^{I} \frac{\theta_*(j)}{\rho(\theta(j))} \right)^{-1} (\theta_* - \theta). \]

- By considering a subsequence of \( (\min_{1 \leq i \leq I} \theta_n(i))_n \) along well-chosen stopping times \( (T_k)_{k \geq 1} \) such that \( X_{T_k} \) is in the stratum with smallest weight \( \theta_{T_k-1}(\cdot) \), we check the recurrence of the algorithm: there is a compact subset \( \mathcal{K} \) of the open subset \( \Theta = \{ \theta \in (\mathbb{R}^*)^I : \sum_{i=1}^{I} \theta(i) = 1 \} \) of \( \mathbb{R}^I \) such that \( (\theta_n)_n \) is infinitely often in \( \mathcal{K} \) \( \iff \limsup_{n \to \infty} \min_{1 \leq i \leq I} \theta_n(i) > 0 \).

- Introduce the Lyapunov function \( U(\theta) = \sum_{i=1}^{T} \theta_*(i) \ln(\theta_*(i)/\theta(i)) \) given by the relative entropy (Kullback-Leibler divergence) of the probability measure \( \theta \) on \( \{1, \ldots, I\} \) w.r.t. \( \theta_* \). Since \( \partial_{\theta(i)} U(\theta) = -\frac{\theta_*'(i)}{\theta(i)} \),

\[ \left( \sum_{j=1}^{I} \frac{\theta_*(j)}{\rho(\theta(j))} \right) \nabla U.h(\theta) = \left( \sum_{i=1}^{I} \frac{\theta_*(i)}{\theta(i)} \right)^{-1} \left( \sum_{i=1}^{I} \theta_*(i) \right) \]

\[ = 1 = \sum_{i=1}^{I} (2\theta_*(i) - \theta(i)) \]

\[ = - \sum_{i=1}^{I} \theta(i) \left( \frac{\theta_*(i)}{\theta(i)} - 1 \right)^2 \leq 0. \]
Convergence of the Generalized Wang-Landau algorithm

- Rewrite

\[ \theta_{n+1} = \theta_n + \gamma_{n+1} h(\theta_n) + \gamma_{n+1} R_{n+1} \]

and check using results by Fort, Moulines, Priouret (2012) on the dependence on \( \theta \) of \( \pi_\theta \) and the solution \( F_\theta \) to the Poisson equation \( F_\theta - P_{\rho(\theta)} F_\theta = H(., \theta) - h(\theta) \)

that \( \lim_{n \to \infty} \sup_{k \geq n} \left| \sum_{j=n}^{k} \gamma_j R_j \right| = 0. \)

- With \( \nabla U.h \leq 0, \mathcal{L} := \{ \theta \in \Theta : \nabla U.h(\theta) = 0 \} = \{ \theta^* \} \) and using Andrieu, Moulines, Priouret (2005), deduce stability: \( \lim_{n \to \infty} \inf_{1 \leq i \leq I} \theta_n(i) > 0 \) and a.s. convergence of \( (U(\theta_n))_n \) to the image \( \{ 0 \} \) of \( \mathcal{L} \) by \( U. \)

By the Pinsker-Csiszar-Kullback inequality,

\[ \sum_{i=1}^{I} |\theta_n(i) - \theta^*(i)| \leq \sqrt{2U(\theta_n)} \xrightarrow{n \to \infty} 0. \]
Is there a gain in such a self-tuned and partially biasing algorithm?

Figure: Left: level curves of the potential. Right: target density.

Make the metastability larger by increasing $\beta$. 
Case $\rho(t) = t^a$ for $a \in [0, 1)$

$$g(s) = (\ln(1 + s))^{\alpha/(1-\alpha)} \text{ for } \alpha \in (1/2, 1) \Rightarrow \gamma_n = o_{wp1}(1/n^\alpha)$$

Start from the left mode, measure the exit time $T$ i.e. time to reach $X_{n,1} > 1$

- $T \uparrow$ when $\beta \uparrow$
- for fixed $\beta$ and $a$: $T \downarrow$ when $\alpha \downarrow$.
- for fixed $\beta$ and $\alpha$: $T \downarrow$ when $a \uparrow$.
- Linear fit with a slope indep of $a$: $\ln T = c + (1 - \alpha)^{-1} \ln \beta$

Figure: Left: Exit times for $\alpha = 0.8$. Right: Exit times for $\alpha = 0.6$. 
Comparison to the Well-Tempered Metadynamics

\[ g(s) = s^{1-a} \Rightarrow \gamma_n = \mathcal{O}(1/n) \] and \[ \rho(t) = t^a \] for \( a \in (0, 1) \)

Figure: Left: Exit times for various values of \( a \). Right: Associated slopes, fitted by 2.43(1 – a).

Exit time \( T \)

- Linear fit: \( \ln T = c + 2.43(1-a)\beta \)
- For fixed \( \beta \): \( T \downarrow \) when \( a \uparrow \)
Efficiency Factor (EF) \( g(s) = \ln(1 + s)^{\alpha/(1-\alpha)} \), \( \alpha \in (1/2, 1) \), \( \rho(t) = t^a \), \( a \in [0, 1) \)

![Graph showing efficiency factors EF(a) for various values of \( \beta \).](image)

\[
EF(n) = \frac{\left( n^{-1} \sum_{k=1}^{n} \sum_{i=1}^{I} \theta_{\ast}^a(i) \mathbb{I}_{D_i}(X_k) \right)^2}{n^{-1} \sum_{k=1}^{n} \left( \sum_{i=1}^{I} \theta_{\ast}^a(i) \mathbb{I}_{D_i}(X_k) \right)^2} \in [0, 1], \quad (X_k)_k \text{ i.i.d. } \sim \pi_{\theta_{\ast}}
\]

\[
\lim_{n \to \infty} EF(n) = \left( \sum_{i=1}^{I} \theta_{\ast}^{1-a}(i) \right)^{-1} \left( \sum_{i=1}^{I} \theta_{\ast}^{1+a}(i) \right)^{-1} \uparrow \text{ when } a \downarrow \text{ for fixed } \beta.
\]
A convergent algorithm

- which estimates the free energy of $\pi$ by a Stochastic Approximation algorithm, where the stepsize sequence $\{\gamma_n, n \geq 0\}$ is tuned on the fly
- which provides an approximation of $\pi$ by a set of weighted points with a controlled discrepancy of the weights.
- which requires two design parameters $(\alpha, a)$ to be fixed by the user
  - a stepsize parameter $\alpha \in (1/2, 1]$, $\gamma_n = O(n^{-\alpha})$ as $n \to \infty$,
  - a biasing parameter $a \in [0, 1]$. 