Analysis and optimization of certain parallel Monte Carlo methods in the low temperature limit

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Outline

1. Problem of interest

2. Metastability and accelerated Monte Carlo

3. Performance measure

4. Large deviation properties of empirical measure of metastable diffusion

5. Optimality in two-well model and multi-well model

Problem of interest

RARE EVENT PROBABILITIES AND MCMC

Compute probability $\mu^\varepsilon(A)$ with respect to a Gibbs measure of the form

$$\mu^\varepsilon(dx) = e^{-V(x)/\varepsilon}dx \Big/ Z(\varepsilon),$$

where $V : \mathbb{R}^d \to \mathbb{R}$ is the potential of a complex physical system, ε is the temperature of the system, and A does not contain the global minimum of V.

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Well-known: $\mu^\varepsilon(dx)$ is the unique invariant distribution of the diffusion process $\{X(t)\}_t$ satisfying

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Markov Chain Monte Carlo (MCMC)

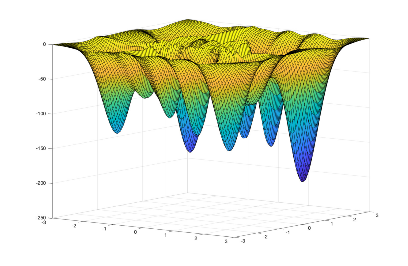
The empirical measure over a large time T:

$$\lambda^T(dx) = \frac{1}{T}\int_0^T \delta_{X(t)}(dx)dt \in \mathcal{P}(\mathbb{R}^d).$$

Use $\lambda^T(A)$ for some large T as an estimate of $\mu^{\varepsilon}(A)$.

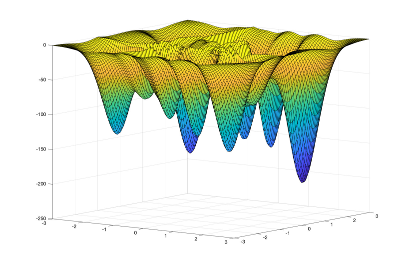
Metastability

EXPONENTIAL EXIT TIME



In general V contains many deep and shallow local minima.

Exponential exit time



In general V contains many deep and shallow local minima.

Exponential exit time: Mean transition time from one local minimum to another is roughly $\exp(h/\varepsilon)$ when the temperature ε is small, where h is the barrier height.

Parallel tempering (two temperatures)

Besides $\varepsilon_1 = \varepsilon$, introduce higher temperature $\varepsilon_2 = \varepsilon/\alpha$ with $\alpha \in (0,1)$.

$$dX_1 = -\nabla V(X_1)dt + \sqrt{2\varepsilon_1}dW_1$$
$$dX_2 = -\nabla V(X_2)dt + \sqrt{2\varepsilon_2}dW_2,$$

with W_1 and W_2 independent. Then allow "swaps" with rate

$$ag(x_1,x_2) = a\left(1 \wedge e^{-\left[\frac{V(x_1)}{\varepsilon_1}+\frac{V(x_2)}{\varepsilon_2}\right]+\left[\frac{V(x_2)}{\varepsilon_1}+\frac{V(x_1)}{\varepsilon_2}\right]}\right).$$

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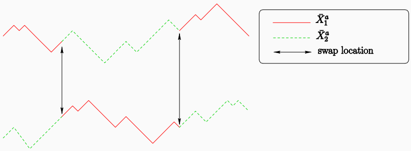
Particle swapped process: (X_1^a, X_2^a)



$\mu^{\varepsilon_1}(dx_1)\mu^{\varepsilon_2}(dx_2)$ is the unique invariant distribution of (X_1^a, X_2^a).

INFINITE SWAPPING PROCESS (TWO TEMPERATURES)

INS process *(limit process as swap rate $a \to \infty$)*:

$$dY_1 = -\nabla V(Y_1)dt + \sqrt{2\varepsilon_1 \rho(Y_1, Y_2) + 2\varepsilon_2 \rho(Y_2, Y_1)}dW_1$$
$$dY_2 = -\nabla V(Y_2)dt + \sqrt{2\varepsilon_2 \rho(Y_1, Y_2) + 2\varepsilon_1 \rho(Y_2, Y_1)}dW_2,$$

where

$$\rho(x_1, x_2) = e^{-\left[\frac{V(x_1)}{\varepsilon_1} + \frac{V(x_2)}{\varepsilon_2}\right]} \Big/ Z_\rho(x_1, x_2),$$
$$Z_\rho(x_1, x_2) = e^{-\left[\frac{V(x_1)}{\varepsilon_1} + \frac{V(x_2)}{\varepsilon_2}\right]} + e^{-\left[\frac{V(x_2)}{\varepsilon_1} + \frac{V(x_1)}{\varepsilon_2}\right]}.$$

The unique invariant distribution of (Y_1, Y_2) becomes $[\mu^{\varepsilon_1}(dx_1)\mu^{\varepsilon_2}(dx_2) + \mu^{\varepsilon_2}(dx_1)\mu^{\varepsilon_1}(dx_2)]/2$.

Weighted empirical measure:

$$\eta^T(dx) = \frac{1}{T}\int_0^T \left[\rho(Y_1, Y_2)\delta_{(Y_1,Y_2)} + \rho(Y_2, Y_1)\delta_{(Y_2,Y_1)}\right] dt,$$

Use $\eta^T(A \times \mathbb{R}^d)$ as an estimate of $\mu^\varepsilon(A)$.

K-TEMPERATURE INS ALGORITHM

K-temperature INS process $\{\boldsymbol{X}^{\varepsilon}(t)\}_{t\geq 0} = \{(X_1^{\varepsilon}(t), \ldots, X_K^{\varepsilon}(t))\}_{t\geq 0}$ for a given $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_K)$ with $1 = \alpha_1 \geq \alpha_2 \geq \cdots \geq \alpha_K$:

$$\begin{cases} dX_1^{\varepsilon} = -\nabla V\left(X_1^{\varepsilon}\right) dt + \sqrt{2\varepsilon}\sqrt{\rho_{11}^{\varepsilon}/\alpha_1 + \rho_{12}^{\varepsilon}/\alpha_2 + \cdots + \rho_{1K}^{\varepsilon}/\alpha_K} dW_1 \\ \vdots \\ dX_K^{\varepsilon} = -\nabla V\left(X_K^{\varepsilon}\right) dt + \sqrt{2\varepsilon}\sqrt{\rho_{K1}^{\varepsilon}/\alpha_1 + \rho_{K2}^{\varepsilon}/\alpha_2 + \cdots + \rho_{KK}^{\varepsilon}/\alpha_K} dW_K \end{cases},$$

where

$$\rho_{ij}^{\varepsilon} \doteq \sum_{\sigma:\sigma(j)=i} w^{\varepsilon}\left(\boldsymbol{x}_{\sigma}; \boldsymbol{\alpha}\right), \quad w^{\varepsilon}\left(\boldsymbol{x}; \boldsymbol{\alpha}\right) \doteq \frac{\exp[-\frac{1}{\varepsilon}\sum_{\ell=1}^{K}\alpha_\ell V\left(x_\ell\right)]}{\sum_{\sigma\in\Sigma_K}\exp[-\frac{1}{\varepsilon}\sum_{\ell=1}^{K}\alpha_\ell V(x_{\sigma(\ell)})]}.$$

INS estimator of $\mu^{\varepsilon}(A)$ is defined as

$$\theta_{\text{INS}}^{\varepsilon,T} \doteq \frac{1}{T}\int_0^T \sum_{\sigma\in\Sigma_K} w^{\varepsilon}\left(\boldsymbol{X}_{\sigma}^{\varepsilon}\left(t\right); \boldsymbol{\alpha}\right) 1_A(X_{\sigma(1)}^{\varepsilon}(t))dt.$$

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Question: How to choose $\boldsymbol{\alpha}$?

Performance measure

UNBIASEDNESS AND DECAY RATE OF VARIANCE

Time scale: Good estimation requires $T^\varepsilon = e^{\frac{1}{\varepsilon}c}$ for some $c > 0$.

DEFINITION

An estimator $\theta^{\varepsilon,T^\varepsilon}$ of $\mu^\varepsilon(A)$ is called **essentially unbiased** if there is $c_0 \in (0,\infty)$ such that

$$\liminf_{\varepsilon\to 0} -\varepsilon \log \left| E\theta^{\varepsilon,T^\varepsilon} - \mu^\varepsilon(A) \right| \geq \lim_{\varepsilon\to 0} -\varepsilon \log \mu^\varepsilon(A) + c_0.$$

DEFINITION

The decay rate of the variance (per unit time) of $\theta^{\varepsilon,T^\varepsilon}$ is defined as

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- Optimize decay rate among essentially unbiased estimators.
- Conflict between improving the decay rate and achieving essential unbiasedness is insignificant.

LD properties

Small-noise diffusion and quasipotential

Consider $\{X_t^\varepsilon\}_{0\le t\le T}$ satisfies

$$dX_t^\varepsilon = b(X_t^\varepsilon)dt + \sqrt{\varepsilon}\sigma(X_t^\varepsilon)dW_t, \quad X_0^\varepsilon = x.$$

Let $\{O_i\}_{i\in L}$ be all the equilibrium points of $\dot{x}_t = b(x_t)$ and $\{X_t^\varepsilon\}$ has an unique invariant distribution μ^ε satisfying

$$\lim_{\varepsilon\to 0} -\varepsilon \log \mu^\varepsilon(O_1) < \lim_{\varepsilon\to 0} -\varepsilon \log \mu^\varepsilon(O_i).$$

Under some conditions, $\{X_t^\varepsilon\}$ satisfies a large deviation principle with rate function I_T for any $T\in(0,\infty)$.

SMALL-NOISE DIFFUSION AND QUASIPOTENTIAL

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$$Q(x,y) \doteq \inf\left\{I_T(\phi) : \phi(0) = x, \phi(T) = y, T < \infty\right\}.$$

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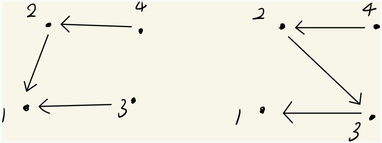
DEFINITION

Given a subset $W \subset L$, a directed graph consisting of arrows $i \to j$ $(i \in L\setminus W, j \in L, i \neq j)$ is called a W**-graph on** L if

1. every point $i \in L \setminus W$ is the initial point of exactly one arrow.
2. for any point $i \in L \setminus W$, there exists a sequence of arrows leading from i to some point in W.

W-GRAPHS

Example: $L = \{1, 2, 3, 4\}$ and $W = \{1\}$.



Denote the set of all W-graphs by $G(W)$.

DEFINITION

For all $i \in L$,

$$W(O_i) \doteq \min_{g \in G(i)} \left[\sum_{(m \to n) \in g} Q(O_m, O_n) \right]$$

and

$$W(O_1 \cup O_i) \doteq \min_{g \in G(1,i)} \left[\sum_{(m \to n) \in g} Q(O_m, O_n) \right].$$

Generalization of Freidlin-Wentzell

Freidlin-Wentzell proved that

$$\lim_{\varepsilon \to 0} -\varepsilon \log \mu^{\varepsilon}(B_{\delta}(x)) = W(x) - W(O_1),$$

where $W(x) \doteq \min_{i \in L}[W(O_i) + Q(O_i, x)]$.

Theorem (Dupuis and Wu, 2020)

Let $T^{\varepsilon} = e^{\frac{1}{\varepsilon}c}$ for some $c > h \vee w$. Given a continuous function $f : \mathbb{R}^d \to \mathbb{R}$ and any compact set $A \subset \mathbb{R}^d$,

$$\liminf_{\varepsilon \to 0} -\varepsilon \log \left| E\left(\frac{1}{T^{\varepsilon}} \int_0^{T^{\varepsilon}} e^{-\frac{1}{\varepsilon} f(X_t^{\varepsilon})} 1_A(X_t^{\varepsilon})\, dt \right) - \int_{\mathbb{R}^d} e^{-\frac{1}{\varepsilon} f(x)} 1_A(x)\, \mu^{\varepsilon}(dx) \right|$$
$$\geq \inf_{x \in A} [f(x) + W(x)] - W(O_1) + c - (h \vee w),$$

with $h \doteq \min_{i \in L \setminus \{1\}} Q(O_1, O_i)$ and $w \doteq W(O_1) - \min_{i \in L \setminus \{1\}} W(O_1 \cup O_i)$.

Decay rate of variance

Theorem (Dupuis and Wu, 2020)

Under the same conditions,

$$\liminf_{\varepsilon\to 0} -\varepsilon \log \left(T^{\varepsilon} \cdot \mathrm{Var}\left(\frac{1}{T^{\varepsilon}} \int_0^{T^{\varepsilon}} e^{-\frac{1}{\varepsilon} f(X_t^{\varepsilon})} 1_A\left(X_t^{\varepsilon}\right) dt \right) \right)$$

$$\geq \min_{i\in L} \left(R_i^{(1)} \wedge R_i^{(2)} \wedge R_i^{(3)} \right),$$

where

$$R_i^{(1)} \doteq \inf_{x\in A} \left[2f(x) + Q(O_i, x)\right] + W(O_i) - W(O_1),$$

$$R_1^{(2)} \doteq 2 \inf_{x\in A} \left[f(x) + Q(O_1, x)\right] - h,$$

and for $i \in L \setminus \{1\}$

$$R_i^{(2)} \doteq 2 \inf_{x\in A} \left[f(x) + Q(O_i, x)\right] + W(O_i) - 2W(O_1) + W(O_1 \cup O_i),$$

$$R_i^{(3)} \doteq 2 \inf_{x\in A} \left[f(x) + Q(O_i, x)\right] + 2W(O_i) - 2W(O_1) - w.$$

Optimality

Double well

Theorem (Dupuis and Wu, 2020)

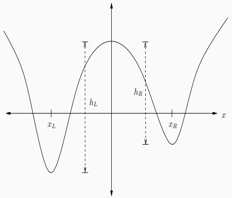
$\theta_{\mathrm{INS}}^{\varepsilon,T^{\varepsilon}}$ is an essentially unbiased estimator of $\mu^{\varepsilon}(A)$. Moreover,

$$\liminf_{\varepsilon\to 0} -\varepsilon \log\left(\mathrm{Var}\left(\theta_{\mathrm{INS}}^{\varepsilon,T^{\varepsilon}}\right)T^{\varepsilon}\right) \geq \begin{cases} r_1(\boldsymbol{\alpha}) \wedge r_3(\boldsymbol{\alpha}), & \text{if } A \subset (-\infty, 0] \\ r_1(\boldsymbol{\alpha}) \wedge r_2(\boldsymbol{\alpha}), & \text{if } A \subset [0, \infty) \end{cases},$$

where $r_3(\boldsymbol{\alpha}) \doteq 2V(A) - \alpha_K h_L$ with $V(A) \doteq \inf_{x\in A} V(x)$ and

$$r_1(\boldsymbol{\alpha}) \doteq \inf_{\boldsymbol{x}\in A\times\mathbb{R}^{K-1}} \left[2\sum_{\ell=1}^{K} \alpha_\ell V(x_\ell) - \min_{\sigma\in\Sigma_K}\left\{\sum_{\ell=1}^{K}\alpha_\ell V(x_{\sigma(\ell)})\right\}\right],$$

$$r_2(\boldsymbol{\alpha}) \doteq \min_{i\in\{2,\ldots,K+1\}}\left\{2V(A) + \left[\sum_{\ell=1}^{i-2}\alpha_{K-\ell+1} - \alpha_{K-i+2}\right](h_L - h_R)\right\} - \alpha_K h_R.$$



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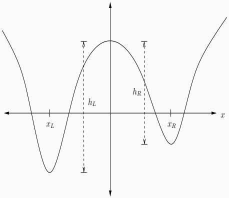

- Optimal $\boldsymbol{\alpha}^* = (1, 1/2, \ldots, (1/2)^{K-2}, \alpha^*_K)$, where α^*_K is determined by $V(A), h_L$ and h_R.

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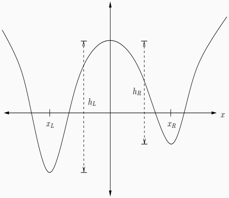

- Optimal $\boldsymbol{\alpha}^* = (1, 1/2, \dots, (1/2)^{K-2}, \alpha^*_K)$, where α^*_K is determined by $V(A), h_L$ and h_R.
- Supremum always $\geq 2V(A) - (1/2)^{K-2}V(A)$.

MULTI-WELL

THEOREM (DUPUIS AND WU, 2021)

There exists $B \in (0,\infty)$ such that the following hold. Consider any $\boldsymbol{\alpha}$ and let $T^{\varepsilon} = e^{\frac{1}{\varepsilon}c}$ for some $c > \alpha_K B$. Then $\theta_{\text{INS}}^{\varepsilon,T^{\varepsilon}}$ is essentially unbiased, and

$$\liminf_{\varepsilon\to 0} -\varepsilon \log \left(\text{Var}(\theta_{\text{INS}}^{\varepsilon,T^{\varepsilon}})T^{\varepsilon}\right) \geq r(\boldsymbol{\alpha}) - \alpha_K B,$$

where

$$r(\boldsymbol{\alpha}) \doteq \inf_{x\in A\times\mathbb{R}^{d(K-1)}} \left\{ 2\sum_{\ell=1}^{K} \alpha_\ell V(x_\ell) - \min_{\sigma\in\Sigma_K} \left\{ \sum_{\ell=1}^{K} \alpha_\ell V(x_{\sigma(\ell)}) \right\} \right\}.$$

THEOREM (DUPUIS AND WU, 2021)

For any closed set A, and any $\alpha_K \in (0,(1/2)^{K-1}]$,

$$\sup_{(\alpha_2,\ldots,\alpha_{K-1})\in[\alpha_K,1]^{K-2}} r(\alpha_1,\alpha_2,\cdots,\alpha_{K-1},\alpha_K) = (2+\alpha_K-(1/2)^{K-2})V(A).$$

The supremum is achieved at $(\alpha_1^*,\ldots,\alpha_{K-1}^*)$ with $\alpha_\ell^* = (1/2)^{\ell-1}$ for all ℓ.

SUMMARY

- "Metastability" present a particular challenge for the design of efficient Monte Carlo methods.
- As such, it is natural to use various asymptotic theories to understand issues of algorithm design.
- Have presented one use of large deviation ideas in the context of infinite swapping (and parallel tempering) algorithms to understand the mechanisms that produce variance reduction.
- INS process with a geometric sequence of temperatures explore landscape in a organized and meaningful way. (Ongoing work)

References

Infinite swapping as a limit of parallel tempering:

- ◇ "On the infinite swapping limit for parallel tempering", Dupuis, Liu, Plattner and Doll, *SIAM J. on MMS*, 10, 986–1022, 2012.

Large deviation estimates:

- ◇ "Large Deviation Properties of the Empirical Measure of a Metastable Small Noise Diffusion", Dupuis and **Wu**, *J Theo. Prob.*, 2020.

Analysis of INS algorithm:

- ◇ "Analysis and optimization of certain parallel Monte Carlo methods in the low temperature limit", Dupuis and **Wu**, submitted, 2021.

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