Advanced topics in Markov-chain Monte Carlo

Lecture 6: Sampling π (stationary distributions), computing π (Free energies) Part 1/2: Introduction

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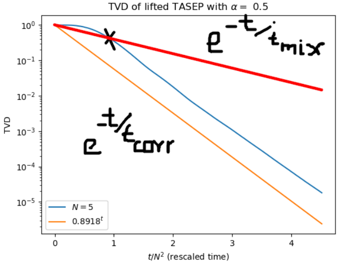
References

- D. A. Levin, Y. Peres, E. L. Wilmer, **Markov Chains and Mixing Times**, (American Mathematical Society, 2008),

Characteristic times in MCMC 1/2

- Correlation time: Time to move from one i ($\sim \pi$) to an independent j ($\sim \pi$).
- Mixing time: Time to reach a $j \sim \pi$ (to some precision) starting from $i \sim \pi^{\{0\}}$ with worst $\pi^{\{0\}}$.
- Cover time: Time to have seen all samples, starting from the worst initial sample x: $t_{\text{cov}} = \max_{x \in \Omega} \mathbb{E}\left[\tau_{\text{cov}}(x)\right]$ (with $\tau_{\text{cov}}(x)$ the time to have seen all $i \in \Omega$).

Characteristic times in MCMC 1/2



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Characteristic times in MCMC 2/2

Example (SSEP of N hard spheres on path graph $\mathcal{P}_{2N}$):

- Correlation time: $\propto N^3$.
- Mixing time: $\propto N^3 \log N$.
- Cover time: N^N.

Consequences:

1. Difficult to know normalization of π:
   - ... What is $Z = \sum_x \pi_x$? (Thermodynamic integration)
2. Difficult to know Ω:
   - ... What is $\min_x \pi_x$?
   - ... What is $\max_x \pi_x$? (Simulated annealing)
   - ... What is conductance?
3. Difficult to explore Ω:
   - Is $\Omega = \emptyset$?
   - Have we seen all of Ω? (Multicanonical MC)

Thermodynamic integration, simulated annealing, etc.

- “Regular” MCMC algorithm development
- “Lifted” MCMC algorithms (weeks 2-4)
- Meta: Thermodynamic integration, simulated annealing, sim. tempering, parallel tempering (weeks 6-7)

MCMC variant	π	P	Ω
“regular”	keep	change	keep
“lifted”	keep	keep	change
“meta”	change	keep	keep

- Mixtures of strategies possible.
- Sampling algorithms development *vs.* Metaheuristics.
- We will study metaheuristics for a single particle on the path graph $\mathcal{P}_n$