

Tutorial 8, Advanced MCMC

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1. Simulated tempering for the V-shaped stationary distribution

Last week (lecture 7—part 7.2), we discussed the simulated tempering algorithm, and even implemented it on our computers. We did not however compute mixing times, which is what we want to do here. In all the below versions, one move corresponds to one displacement followed (with probability ϵ) a replica move and, if necessary, a lifting move.

- (a) (DONE) Set up the simulated tempering algorithm for the case $k = 2$ (flat distribution and V-shaped distribution) on the path graph P_n as a function of n and of the switching probability ϵ .
- (b) (TODO) Numerically compute the conductance of this algorithm for the case $k = 2$ (flat distribution and V-shaped distribution) on the path graph P_n as a function of n and of the switching probability ϵ . Locate the bottleneck as a function of n and ϵ .
- (c) (TODO) Analytically compute the conductance for $k = 2$
- (d) (DONE) Set up the direction-lifted simulated tempering algorithm for this same case.
- (e) (TODO) Set up the transition matrices and compute the dominant and sub-dominant (left) eigenvalues both for the simulated tempering and for the direction-lifted simulated tempering.
- (f) (TODO) Compute the time-dependent TDV, and from there the mixing time of the reversible Metropolis algorithm on the path graph with the V-shaped stationary distribution as a function of n and of ϵ . Generalize to the direction-lifted Metropolis algorithm, if possible.

2. Event-driven MCMC

Here, we study a continuous-time lifted Markov chain in a time-driven and an event-driven formulation. We consider a single particle in a harmonic potential $U(x) = \frac{1}{2}x^2$. We set the inverse temperature to $\beta = 1$.

- (a) Implement the Metropolis algorithm for the single particle, using step sizes of your choosing. Compute the histogram of positions, and compare it to the Boltzmann distribution.
- (b) Implement the lifted “continuous-time” Metropolis algorithm for the single particle, with very small step size (say $\Delta_x = \pm 0.01$). If the particle move is rejected, perform a lifting move, and change the direction!
- (c) Implement the event-driven “continuous-time” Metropolis algorithm, and again check the distribution. Attention: Computing the histogram obliges you to stop the Markov process at fixed time steps.