

Monte Carlo Methods, Fall 2007, Courant Institute, NYU
Homework 5, Due December 34

1. Show that if a discrete time Markov chain satisfies detailed balance and $C(t)$ is the time t lag auto-covariance function in equilibrium, then $C(2t) \geq 0$ for all t .
2. We want to estimate

$$A = E \left[\int_0^1 X(t) dt \right],$$

over paths with $X(0) = 1$, $X(1) = 1$ and $dX = -X^2 dt + X dW$.

- (a) Given $\Delta t = 1/n$, suggest a sensible discrete approximation to the integral defining A and the SDE. Use this to create an n dimensional integral that approximates A . Let $F(\vec{x})$ be the probability density in this integral.
- (b) Suggest and implement a dynamic Monte Carlo strategy for sampling F that uses single site updates. These single site updates can be done using Metropolis, but you need to design a careful trial distribution that either is symmetric itself or whose asymmetry you can understand for the rejection step.
- (c) Suggest and implement a dynamic Monte Carlo strategy for sampling F that uses a global Langevin algorithm of the kind discussed on the previous homework. The time step for Langevin part will be related to, but not the same as, $\Delta t = 1/n$. Adjust the Langevin time step so the acceptance probability is somewhere near $1/2$.
- (d) Use your code from Homework 4 to estimate the auto-correlation time and create error bars for both of the dynamic samplers. Try to tune the samplers to reduce τ . Use this τ and an estimate of the static variance (which does not depend on the dynamic sampling strategy) to create error bars for both estimators.
- (e) For each of the samplers, plot the auto-correlation time (estimated) as a function of n and try to guess (from the plots) how τ depends on n for large n .
- (f) Which estimator is better for small Δt ? Be careful to compare the two approaches fairly by considering the amount of work per Monte Carlo step for each.
- (g) Check the correctness of the codes and algorithms in parts (b) and (c) by checking that they are consistent with each other. Do this by checking that they give \hat{A} values that are within each other's error bars and by checking that $X(1/2)$ has the same distribution (compare the histograms). Do this for $n = 4$ and $n = 100$, just in case a bug in the sampler is hard to see for small or large n .