Quiz: MCMC

STA414/2104 - Winter 2026

1. **Metropolis-Hastings Utility**

   Why is the Metropolis-Hastings (MH) algorithm often considered more practical than Rejection Sampling or Importance Sampling, particularly in high dimensions?

   (a) MH generates independent and identically distributed (i.i.d.) samples, which are statistically superior to the dependent samples from Rejection Sampling.

   (b) Rejection Sampling requires a proposal density $q(x)$ that globally approximates the target $p(x)$, which is difficult to find in high dimensions, MH allows for a local proposal $q(x'|x^{(t)})$ that does not need to look like $p(x)$.

   (c) MH eliminates the need to calculate the acceptance probability entirely, making the code faster to run.

   (d) MH guarantees convergence to the stationary distribution in a single step, whereas Rejection Sampling requires multiple steps.

   Correct Answer: (b)

   Rationale: Importance and rejection sampling work only if the proposal density $q(x)$ is similar to $p(x)$, and in high dimensions, it is hard to find such a q. The Metropolis-Hastings algorithm instead makes use of a proposal density q which depends on the current state $x^{(t)}$ (local). It is not necessary that this local proposal $q(x|x^{(t)})$ looks similar to the target $p(x)$.

2. **Detailed Balance**
Which of the following statements accurately describes the "Detailed Balance" condition?

(a) It is a necessary condition for stationarity: a Markov chain cannot have a stationary distribution unless it satisfies detailed balance.
(b) It implies that the transition matrix A must be symmetric (i.e., $A_{ij} = A_{ji}$).
(c) It is a sufficient condition for the existence of a stationary distribution.
(d) It requires that the Markov chain be irreducible and regular, guaranteeing that A^n has positive entries for all n.

Correct Answer: (c)
Rationale: The detailed balance equations are defined as $\pi_i A_{ij} = \pi_j A_{ji}$ *for all* i, j*. This means that the flow* $x \to x'$ *and* $x' \to x$ *are equally probable. If a Markov chain satisfies detailed balance with respect to distribution* π*, then* π *is a stationary distribution (Theorem).*

3. **Exact Hamiltonian Dynamics**
In the standard HMC algorithm, we use the Leap-frog integrator to approximate the Hamiltonian dynamics. Since this approximation introduces numerical errors, a Metropolis-Hastings acceptance step is required. Suppose we could instead simulate the Hamiltonian dynamics *exactly* (i.e., with zero numerical error). What would be the acceptance probability for any proposed state?

   (a) It would be exactly 1.
   (b) It would depend on the duration of the simulation T.
   (c) It would be approximately 0.5.
   (d) It would be 0, because the system would return exactly to the start.

Correct Answer: (a)
Rationale: Hamiltonian dynamics conserve the total energy (Hamiltonian), meaning $H(x, v) = H(x', v')$. *The acceptance probability in HMC is calculated as* $\min\{1, \exp(H(x, v) - H(x', v'))\}$. *If the simulation is exact, the difference in Hamiltonian is 0, so the acceptance probability becomes* $\min\{1, e^0\} = 1$.

4. $\hat{R}$
When using the $\hat{R}$ to diagnose convergence across multiple chains, which value indicates that the chains have likely mixed well?

(a) $\hat{R} \approx 0$
(b) $\hat{R} \approx 1$
(c) $\hat{R} > 1.5$
(d) $\hat{R} = n_{eff}$

Correct Answer: (b)
Rationale: The $\hat{R}$ coefficient compares the within-sequence variance W and the between-sequence variance B. It is defined such that if chains have not mixed well, $\hat{R}$ is larger than 1. Ideally, we want $\hat{R}$ to be near 1 (e.g., in the lecture example, a good mixing resulted in $\hat{R} = 1.005$).