MCMC Sampling Problems

ELG 5218 Uncertainty Evaluation in Engineering Measurements and Machine Learning

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Instructions

- Answer all questions. Show all steps for derivations.
- You may assume basic probability and calculus identities if clearly stated.
- When asked for intuition, use concise, precise explanations.

PART A: CONCEPTUAL QUESTIONS (Simple to Intermediate)

A1. Define a first-order Markov chain and stationary distribution.

Question. Provide:

(a) The definition of a first-order Markov chain.

(b) The definition of a stationary distribution for a Markov chain with kernel $P(\theta' \mid \theta)$.

Solution.

(a) A sequence $\{\theta_t\}_{t\geq 1}$ is a first-order Markov chain if, for all t,

$$P(\theta_{t+1} \mid \theta_t, \theta_{t-1}, \ldots, \theta_1) = P(\theta_{t+1} \mid \theta_t).$$ Just Depend on 1 Most Recent Previous state

That is, the future depends on the present state only, not on the full history.

(b) A distribution $\pi(\theta)$ is stationary for a Markov chain with transition kernel $P(\theta' \mid \theta)$ if applying one step of the chain leaves it unchanged:

$$\pi(\theta') = \int \pi(\theta) P(\theta' \mid \theta)\, d\theta.$$

If $\theta_0 \sim \pi$, then $\theta_1, \theta_2, \ldots$ all have distribution π.

A2. State the ergodicity conditions and their consequence.

Question. For a Markov chain with transition kernel $P(\theta' \mid \theta)$:

(a) Briefly define the concepts of irreducibility, aperiodicity, and positive recurrence.

(b) State the consequence of ergodicity for convergence to the stationary distribution.

Solution.

(a)

- *Irreducible:* From any state, there is a positive probability of reaching any other state (possibly in multiple steps).
- *Aperiodic:* The chain does not get trapped in cycles; the return times to a state do not all share a common period greater than 1.
- *Positive recurrent:* The expected return time to any state is finite.

(b) If a Markov chain is irreducible, aperiodic, and positive recurrent, it is ergodic. For an ergodic chain with stationary distribution π, we have

$$\lim_{t\to\infty} P(\theta_t \in A) = \int_A \pi(\theta)\, d\theta$$ Covered Area (in pdf) = Total Transition Possibilitiy

for any measurable set A, regardless of the initial distribution. In other words, the distribution of θ_t converges to π as $t \to \infty$.

A3. What is detailed balance and why is it useful in MCMC design?

Question. State the detailed balance condition and explain why it is convenient when constructing MCMC algorithms such as Metropolis–Hastings.

Solution.

Detailed balance with respect to $\pi(\theta)$ requires

$$\pi(\theta)P(\theta' \mid \theta) = \pi(\theta')P(\theta \mid \theta') \quad \text{for all } \theta, \theta'.$$

It implies that the flow of probability from θ to θ' equals the flow from θ' to θ. If detailed balance holds and $P(\cdot \mid \theta)$ is a proper kernel, then π is stationary:

$$\int \pi(\theta)P(\theta' \mid \theta)\, d\theta = \pi(\theta').$$

In MCMC design, detailed balance provides a simple sufficient condition: by constructing P to satisfy detailed balance with the target π, we guarantee that π will be stationary for the chain, without having to solve the stationary equation explicitly.

PART B: METROPOLIS–HASTINGS DERIVATIONS

B1. Derive the Metropolis–Hastings acceptance ratio and evidence cancellation.

Question. Let the target posterior be $\pi(\theta) = p(\theta \mid x)$, known up to a normalizing constant:

$$\pi(\theta) \propto \tilde{\pi}(\theta) = p(x \mid \theta)p(\theta).$$

Given a proposal density $q(\theta^* \mid \theta)$, the Metropolis–Hastings acceptance ratio is

$$r(\theta \to \theta^*) = \frac{\pi(\theta^*)q(\theta \mid \theta^*)}{\pi(\theta)q(\theta^* \mid \theta)}.$$

Show explicitly that the evidence term $p(x)$ cancels in this ratio.

Solution.

Write

$$\pi(\theta) = \frac{p(x \mid \theta)p(\theta)}{p(x)}.$$ Bayes' Theorem

Then the ratio becomes

$$r(\theta \to \theta^*) = \frac{\frac{p(x \mid \theta^*)p(\theta^*)}{p(x)}\, q(\theta \mid \theta^*)}{\frac{p(x \mid \theta)p(\theta)}{p(x)}\, q(\theta^* \mid \theta)}. \quad \text{Subs. into Convergence formula}$$

The evidence $p(x)$ appears both in numerator and denominator, so it cancels:

$$r(\theta \to \theta^*) = \frac{p(x \mid \theta^*)p(\theta^*)q(\theta \mid \theta^*)}{p(x \mid \theta)p(\theta)q(\theta^* \mid \theta)} = \frac{\tilde{\pi}(\theta^*)q(\theta \mid \theta^*)}{\tilde{\pi}(\theta)q(\theta^* \mid \theta)}.$$

Thus only the unnormalized posterior $\tilde{\pi}(\theta)$ is needed.

B2. Random-walk Metropolis tuning intuition.

Question. For a Gaussian random-walk Metropolis proposal

$$\theta^* = \theta + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2_{\text{prop}}),$$

explain qualitatively:

(a) What happens when σ_{prop} is too small?

(b) What happens when σ_{prop} is too large?

Solution.

(a) If σ_{prop} is too small, proposed moves θ^* are very close to the current state θ. Acceptance rates are high (often near 100%), but the chain explores the space slowly by tiny steps. This leads to high autocorrelation and low effective sample size per unit of computation.

(b) If σ_{prop} is too large, proposals jump far away from high-density regions. Many proposals land in low-posterior-density areas and are rejected. Acceptance rates become very low, and the chain often "sticks" for many iterations.

PART C: CONVERGENCE DIAGNOSTICS

C1. Autocorrelation and effective sample size (ESS).

Question. Let $\{\theta_t\}$ be a stationary MCMC chain for a scalar parameter θ, with lag-ℓ autocorrelation

$$\rho(\ell) = \text{Corr}(\theta_t, \theta_{t+\ell}).$$

Define:

(a) The integrated autocorrelation time τ.

(b) The effective sample size N_{eff} given a total of N iterations.

Solution.

(a) The integrated autocorrelation time is

$$\tau = 1 + 2\sum_{\ell=1}^{\infty} \rho(\ell),$$

assuming the sum converges.

(b) The effective sample size is

$$N_{\text{eff}} = \frac{N}{\tau}.$$

This is the approximate number of independent draws from the target that would yield the same Monte Carlo variance as the correlated MCMC samples.

C1. Gelman–Rubin $\hat{R}$ statistic derivation (scalar case).

Question. Suppose you run J independent chains, each of length L after burn-in, and obtain scalar draws $\theta_{j\ell}$, $j = 1, \ldots, J$, $\ell = 1, \ldots, L$. Define:

- Chain means: $\bar{\theta}_j = \frac{1}{L}\sum_{\ell=1}^{L} \theta_{j\ell}$.
- Grand mean: $\bar{\theta}_\cdot = \frac{1}{J}\sum_{j=1}^{J} \bar{\theta}_j$.
- Within-chain variances: $s_j^2 = \frac{1}{L-1}\sum_{\ell=1}^{L}(\theta_{j\ell} - \bar{\theta}_j)^2$.

Derive expressions for:

(a) Within-chain variance W.

(b) Between-chain variance B.

(c) The marginal variance estimate $\hat{V}^+ = \frac{L-1}{L}W + \frac{1}{L}B$.

(d) $\hat{R} = \sqrt{\hat{V}^+/W}$.

Solution.

(a) Within-chain variance:

$$W = \frac{1}{J}\sum_{j=1}^{J} s_j^2.$$

(b) Between-chain variance:

$$B = \frac{L}{J-1}\sum_{j=1}^{J}(\bar{\theta}_j - \bar{\theta}_\cdot)^2.$$

The factor L appears because $\bar{\theta}_j$ has variance roughly σ^2/L.

(c) Marginal variance estimate:

Within:
用自己lag推斷其他lags

$$\hat{V}^+ = \left(1 - \frac{1}{L}\right)W + \frac{1}{L}B = \frac{L-1}{L}W + \frac{1}{L}B.$$

between var:
只牽涉1個lag

(d) Potential scale reduction factor:

$$\hat{R} = \sqrt{\frac{\hat{V}^+}{W}}.$$

Values $\hat{R} \approx 1$ indicate convergence (between- and within-chain variances agree), whereas $\hat{R} > 1$ suggests that further sampling may reduce the variance.

C2. Interpreting trace plots and ACF.

Question. Describe, qualitatively, what you expect to see in:

(a) A trace plot of a well-mixed chain.

(b) The autocorrelation function (ACF) of a poorly mixed chain.

Solution.

(a) A well-mixed trace plot should look "hairy" and stationary: the chain moves quickly across the typical region of the posterior with no clear trends or drifts, and the variability appears stable over time.

(b) The ACF of a poorly mixed chain decays slowly: $\rho(\ell)$ remains large even for moderate lags (e.g., $\rho(10)$ high), indicating strong dependence between samples. In contrast, a well-mixed chain has rapidly decaying ACF, with $\rho(\ell)$ near zero for modest ℓ.

PART D: MODERN SAMPLERS (HMC, NUTS) AND PRACTICAL ISSUES

D1. Intuition behind Hamiltonian Monte Carlo (HMC).

Question. Provide a concise explanation of how HMC reduces random-walk behavior compared to random-walk Metropolis (RWM).

Solution.

HMC augments the parameter θ (position) with an auxiliary momentum variable p and defines a Hamiltonian dynamics system whose energy is related to the negative log posterior and a kinetic term. Starting from (θ, p), it simulates approximate Hamiltonian dynamics using gradient information $\nabla_\theta \log \pi(\theta)$ to follow trajectories that stay near constant energy. This produces distant proposals in parameter space that remain in high posterior-density regions, dramatically reducing back-and-forth "bumping" typical of random walks. A final Metropolis acceptance step corrects for numerical integration error, maintaining exactness.

D2. What problem does NUTS solve on top of HMC?

Question. Explain what key tuning parameter NUTS (No-U-Turn Sampler) eliminates compared to plain HMC, and how it does so conceptually.

Solution.

Plain HMC requires the user to choose the trajectory length (number of leapfrog steps) and step size. If trajectories are too short, the sampler behaves like a random walk; if they are too long, computation is wasted and trajectories may loop back. NUTS adaptively determines the trajectory length by expanding a binary tree of leapfrog steps forward and backward in time and stopping when it detects a "U-turn" (when further steps would start to retrace the path). Combined with step-size adaptation during warm-up, NUTS removes the need for manual tuning of trajectory length and often yields near-optimal exploration automatically.

PART E: OTHER PROBLEMS

E1. AR(1) Markov chain stationarity and convergence.

Consider the AR(1) process

$$x_{t+1} = \rho x_t + v_t, \quad v_t \sim \mathcal{N}(0, \sigma_v^2),$$

with $|\rho| < 1$ and x_0 arbitrary.

(a) Show that the stationary distribution is $\mathcal{N}(0, \sigma^2)$ with $\sigma^2 = \sigma_v^2/(1-\rho^2)$.

(b) Briefly explain why, regardless of x_0, the distribution of x_t converges to this stationary distribution.

Solution.
(a) For a stationary AR(1), $\mathbb{V}(x_{t+1}) = \mathbb{V}(x_t) = \sigma^2$. Using the recursion,

$$\mathbb{V}(x_{t+1}) = \rho^2 \mathbb{V}(x_t) + \mathbb{V}(v_t) = \rho^2 \sigma^2 + \sigma_v^2.$$

Setting $\mathbb{V}(x_{t+1}) = \mathbb{V}(x_t) = \sigma^2$, we get

$$\sigma^2 = \rho^2 \sigma^2 + \sigma_v^2 \quad \Rightarrow \quad \sigma^2(1-\rho^2) = \sigma_v^2 \quad \Rightarrow \quad \sigma^2 = \frac{\sigma_v^2}{1-\rho^2}.$$

The mean is zero because $\mathbb{E}[x_{t+1}] = \rho \mathbb{E}[x_t]$ and, in stationarity, the only finite solution is $\mathbb{E}[x_t] = 0$.

(b) The AR(1) with $|\rho| < 1$ defines a Gaussian Markov chain that is irreducible and aperiodic on $\mathbb{R}$, and the variance converges to σ^2 determined above. Explicitly solving the recursion,

$$x_t = \rho^t x_0 + \sum_{k=0}^{t-1} \rho^k v_{t-1-k},$$

the first term $\rho^t x_0$ converges to 0 as $t \to \infty$, and the second term converges in distribution to $\mathcal{N}(0, \sigma^2)$. Thus, regardless of x_0, the chain converges in distribution to the stationary $\mathcal{N}(0, \sigma^2)$.

E2. MCMC for a biased coin (NUTS vs random-walk MH).

You flip a coin $n = 100$ times and observe $k = 90$ heads. Assume a Beta(α, β) prior with $\alpha = 5, \beta = 3$, and denote the coin bias by $\theta \in (0, 1)$.

(a) Write down the posterior $p(\theta \mid k, n)$.

(b) Suppose you run NUTS in NumPyro for θ and obtain a posterior mean $\hat{\theta}_{\text{NUTS}} = 0.88$ with ESS per chain ≈ 3700 (out of 2500 samples per chain across 4 chains, grouped). Comment on this.

(c) You also run a simple random-walk MH on the logit scale with acceptance rate ≈ 0.70, ESS per chain ≈ 1200. Both have $\hat{R} \approx 1.00$. Compare the two samplers.

Solution.
(a) The likelihood is Binomial$(k \mid n, \theta)$, and the prior is Beta(α, β). The posterior is conjugate:

$$\theta \mid k, n \sim \text{Beta}(\alpha', \beta'), \quad \alpha' = \alpha + k = 95, \quad \beta' = \beta + n - k = 13.$$

So

$$p(\theta \mid k, n) = \text{Beta}(\theta \mid 95, 13).$$

(b) NUTS uses gradient-based proposals and adapts step sizes and trajectory lengths, giving very efficient exploration. An ESS per chain of ≈ 3700 (greater than the raw samples per chain due to grouping interpretation) indicates extremely low autocorrelation; effectively most samples are close to independent. The posterior mean of 0.88 is plausible for a Beta(95,13) posterior.

Mixing Well!

(c) Both samplers have $\hat{R} \approx 1.00$, so convergence is acceptable. However, NUTS yields a much larger ESS per chain, so the Monte Carlo standard error is much smaller for the same number of iterations. RWM, despite a decent acceptance rate (≈ 0.70), produces more correlated samples and thus lower ESS. NUTS is therefore clearly preferable in terms of sampling efficiency for this continuous, differentiable posterior.

E3. Single-chain convergence and ACF

You are given MCMC output for a scalar parameter θ from a single chain of length $N = 4000$ (after burn-in). The chain was generated by a random-walk Metropolis algorithm.

Summary diagnostics:

- Sample mean: $\hat{\theta} = 0.03$.
- Effective sample size (ESS): ESS ≈ 2660.
- Empirical autocorrelation function (ACF) for lags $\ell = 0, \ldots, 40$ (first few values):

$$\begin{aligned} \rho(0) &= 1.00, \\ \rho(1) &\approx 0.19, \\ \rho(2) &\approx 0.04, \\ \rho(3) &\approx 0.01, \\ \rho(\ell) &\approx 0 \quad \text{for } \ell \gtrsim 5. \end{aligned}$$

- A trace plot shows a stationary, "hairy" path around 0 with no visible trends.

Answer the following:

(a) Based on the trace and ACF, does the chain appear to have converged to its stationary distribution? Justify your answer.

(b) Comment on the mixing quality using the ACF and ESS.

(c) Would you recommend thinning this chain? Why or why not?

Solution

(a) The trace plot is stationary, with no visible drift or long-term trend, and it freely explores the apparent high-density region around 0. This is what we expect from a chain sampling its stationary distribution. The ACF decays quickly: $\rho(1) \approx 0.19$, $\rho(2) \approx 0.04$, and is essentially zero beyond a small number of lags. Rapid decay of autocorrelation is a strong indication that the chain has reached and is sampling from the stationary distribution. Thus there is no evidence of non-convergence.

(b) The ESS of about 2660 out of 4000 iterations indicates that a large fraction of the draws are information-equivalent to independent samples. This reflects very good mixing: autocorrelation is modest at lag 1 and negligible after a few lags, so the integrated autocorrelation time is small, directly leading to a large ESS. Consequently, Monte Carlo error for posterior summaries will be relatively small. standard error (the denominator)

(c) Thinning is not recommended. The chain already has a high ESS and quickly decaying ACF, so discarding intermediate draws would reduce the total information without substantially improving ESS per unit computation. Modern practice is to keep all post–burn-in draws and rely on ESS (and related diagnostics) to assess efficiency rather than thinning.

E4. Comparing chains via ACF and ESS

Two different MCMC algorithms (Algorithm G and Algorithm B) were used to sample from the same scalar posterior $p(\theta \mid x)$. Each produced a single chain of length $N = 4000$ after burn-in.

Diagnostics:

- Effective sample sizes:

$$\begin{aligned} \mathrm{ESS}_G &\approx 2660, \\ \mathrm{ESS}_B &\approx 128. \end{aligned}$$

- Empirical ACFs for lags 0–40 (selected values):
  - Algorithm G:

$$\begin{aligned} \rho_G(0) &= 1.00, \\ \rho_G(1) &\approx 0.19, \\ \rho_G(5) &\approx 0. \end{aligned}$$

  - Algorithm B:

$$\begin{aligned} \rho_B(0) &= 1.00, \\ \rho_B(1) &\approx 0.95, \\ \rho_B(10) &\approx 0.60, \\ \rho_B(20) &\approx 0.35, \\ \rho_B(40) &\approx 0.10. \end{aligned}$$

- Trace plots:
  - Algorithm G: rapid oscillations around the posterior bulk, no visible trend.
  - Algorithm B: very smooth, slowly drifting path; long stretches where the chain moves gradually in one direction.

Answer the following:

(a) Based on the ACFs and ESS, which chain mixes better? Explain in terms of autocorrelation and effective sample size.

(b) For Algorithm B, what can you conclude from the ACF plot about the correlation structure of the chain? How does this affect Monte Carlo error?

(c) Suppose both algorithms have similar posterior means and variances (i.e., no obvious bias). Which algorithm would you trust more for uncertainty quantification, and why?

Solution

(a) Algorithm G clearly mixes better. Its ACF decays quickly: by lag 5, $\rho_G(\ell)$ is essentially zero, indicating that samples become nearly independent after only a few steps. This leads to a large ESS of about 2660 out of 4000 iterations. In contrast, Algorithm B has very high autocorrelation: $\rho_B(1) \approx 0.95$, and even at lag 40 $\rho_B(40) \approx 0.10$, so dependence persists over many iterations. Consequently, its ESS is only about 128, meaning that only a small fraction of the 4000 draws contributes independent information.

(b) The ACF for Algorithm B decays slowly and remains substantially positive for many lags, indicating strong serial correlation and a long integrated autocorrelation time. Many of the draws are therefore almost duplicates in terms of information content. Because Monte Carlo standard error scales like $1/\sqrt{\text{ESS}}$, the high correlation and low ESS greatly increase Monte Carlo uncertainty for estimates based on Algorithm B.

(c) Even if both algorithms produce similar posterior means and variances, Algorithm G is preferable for uncertainty quantification. Its high ESS and rapidly decaying ACF imply much smaller Monte Carlo error for estimates such as posterior means, credible intervals, and tail probabilities. Algorithm B's low ESS means that credible intervals and other summaries will have much larger Monte Carlo noise and may require many more iterations to reach comparable precision. Thus Algorithm G is more reliable in practice.

E5. Metropolis–Hastings - Gamma proposal

For π the density of an inverse normal distribution with parameters $\theta_1 = 3/2$ and $\theta_2 = 2$,

$$\pi(x) \propto x^{-3/2} \exp\left(-\frac{3}{2}x - \frac{2}{x}\right) \mathbf{1}_{\{x>0\}},$$

write down and implement an independence Metropolis–Hastings sampler with a Gamma proposal with parameters $(\alpha, \beta) = (4/3, 1)$ and $(\alpha, \beta) = (0.5\sqrt{4/3}, 0.5)$.

Solution.
The unnormalized target density is

$$\tilde{\pi}(x) = x^{-3/2} \exp\left(-\frac{3}{2}x - \frac{2}{x}\right) \mathbf{1}_{\{x>0\}}.$$

For an independence Metropolis–Hastings algorithm with proposal $q(x) = \text{Ga}(\alpha, \beta)$ (shape–rate parameterization), the proposal density is

$$q(x) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} e^{-\beta x} \mathbf{1}_{\{x>0\}}.$$ GIVEN (Don't worry!)

Given the current state $X_t = x$, we draw a proposal $Y \sim q(\cdot)$ and accept it with probability

$$a(x, y) = \min\left\{1, \frac{\tilde{\pi}(y)q(x)}{\tilde{\pi}(x)q(y)}\right\} = \min\left\{1, \frac{y^{-3/2} \exp\left(-\frac{3}{2}y - 2/y\right) q(x)}{x^{-3/2} \exp\left(-\frac{3}{2}x - 2/x\right) q(y)}\right\}.$$

Using the explicit Gamma density and simplifying,

$$\frac{\tilde{\pi}(y)q(x)}{\tilde{\pi}(x)q(y)} = \left(\frac{x}{y}\right)^{\alpha+\frac{1}{2}} \exp\left\{\left(\beta - \frac{3}{2}\right)(x - y) + 2\left(\frac{1}{x} - \frac{1}{y}\right)\right\}.$$

Thus the acceptance probability is

$$a(x,y) = \min\left\{1, \left(\frac{x}{y}\right)^{\alpha+\frac{1}{2}} \exp\left[\left(\beta - \frac{3}{2}\right)(x-y) + 2\left(\frac{1}{x} - \frac{1}{y}\right)\right]\right\}.$$

For $(\alpha, \beta) = (4/3, 1)$ the rule is

$$a(x,y) = \min\left\{1, \left(\frac{x}{y}\right)^{\frac{11}{6}} \exp\left[-\frac{1}{2}(x-y) + 2\left(\frac{1}{x} - \frac{1}{y}\right)\right]\right\},$$

and for $(\alpha, \beta) = \left(0.5\sqrt{4/3}, 0.5\right)$ it is

$$a(x,y) = \min\left\{1, \left(\frac{x}{y}\right)^{0.5\sqrt{4/3}+\frac{1}{2}} \exp\left[-(x-y) + 2\left(\frac{1}{x} - \frac{1}{y}\right)\right]\right\}.$$

A pseudo–code implementation for either choice of (α, β) is:

```
Initialize x0 > 0.
For t = 0,...,T-1:
    Draw y ~ Gamma(alpha, beta).
    Compute
      logR = (alpha + 0.5)*(log(x_t) - log(y))
             + (beta - 1.5)*(x_t - y)
             + 2*(1/x_t - 1/y)
    Set a = min(1, exp(logR)).
    Draw u ~ Uniform(0,1).
    If u < a then set x_{t+1} = y else set x_{t+1} = x_t.
```

Prior belief

Log Posterior

This yields an independence Metropolis–Hastings chain with stationary distribution π.

E6. Metropolis–Hastings - Gaussian randow walk

Consider the non-standard target distribution

$$p(x) \propto \exp\left(-x^4 + 3x^2 - x\right), \qquad x \in \mathbb{R},$$

and a Gaussian random-walk proposal

$$q(x'|x) = \mathcal{N}(x, \sigma_q^2).$$

Tasks:

1. Implement the Metropolis–Hastings algorithm.
2. Compare acceptance rates for $\sigma_q \in \{0.1, 0.5, 1, 2\}$.
3. Use the rule of thumb that the optimal acceptance rate in 1D is about 0.234.
4. Estimate the mean and variance from the samples.

Solution.

The unnormalized target density is

$$\tilde{p}(x) = \exp\left(-x^4 + 3x^2 - x\right).$$

Because the proposal is symmetric, $q(x'|x) = q(x|x')$, the Metropolis–Hastings acceptance probability reduces to

$$a(x, x') = \min\left\{1, \frac{\tilde{p}(x')}{\tilde{p}(x)}\right\} = \min\left\{1, \exp\left[-x'^4 + 3x'^2 - x' + x^4 - 3x^2 + x\right]\right\}.$$

Equivalently, in log form,

$$\log r(x, x') = \left(-x'^4 + 3x'^2 - x'\right) - \left(-x^4 + 3x^2 - x\right), \qquad a(x, x') = \min\{1, \exp(\log r)\}.$$

An implementation for a given σ_q is:

```
Initialize x0 (e.g. x0 = 0).
For t = 0,...,T-1:
    Draw epsilon ~ N(0, sigma_q^2). Gaussian
    Set y = x_t + epsilon.
    Compute
      logR = (-y^4 + 3*y^2 - y) - (-x_t^4 + 3*x_t^2 - x_t).
    Set a = min(1, exp(logR)).
    Draw u ~ Uniform(0,1). Purely Random
    If u < a then set x_{t+1} = y else set x_{t+1} = x_t.  Accept if converged, else take previous state
```

To address item 2, run independent chains (or long segments of one chain) with $\sigma_q \in \{0.1, 0.5, 1, 2\}$, and record the empirical acceptance rate

$$\hat{\alpha} = \frac{\text{number of accepted proposals}}{\text{number of iterations}}.$$

Typically, very small σ_q such as 0.1 produces $\hat{\alpha}$ close to 1 but with slow mixing, whereas large σ_q such as 2 gives low $\hat{\alpha}$ and highly correlated samples. Values around 0.5–1 often yield acceptance rates near the heuristic target 0.234 with reasonable mixing.

For item 4, after a burn-in period of B iterations, use the remaining N samples $\{X_{B+1}, \ldots, X_{B+N}\}$ to estimate the mean and variance:

$$\hat{\mu} = \frac{1}{N}\sum_{i=1}^{N} X_{B+i}, \qquad \hat{\sigma}^2 = \frac{1}{N-1}\sum_{i=1}^{N}\left(X_{B+i} - \hat{\mu}\right)^2.$$