— Algorithm Metropolis Adjusted Langevin Algorithm (MALA)

Input: Target $f(x) \propto \exp(-V(x))$, initial distribution π_0, step-size $\epsilon > 0$, sample size N.

Define the Markov kernel

$$q_{\mathrm{LG}}(x, \cdot) := \mathcal{N}(x - \epsilon \nabla V(x), 2\epsilon I).$$

Run Metropolis Hastings with input f, π_0, q_{LG}, N.

Output: Sample $\{X^{(n)}\}_{n=1}^{N}$.

— Algorithm Parallel Tempering

Input: Inverse temperatures $\beta_1 = 1 > \cdots > \beta_K$, proposal Markov kernels $\{q_k(x, z)\}_{k=1}^{K}$, initializations $\{X_k^{(0)}\}_{k=1}^{K}$, sample size N.

for $n = 0, 1, \ldots, N-1$ **do**

  for $k = 1, \ldots, K$ **do**

    generate $\tilde{X}_k^{(n+1)}$ by doing a Metropolis Hastings step (including accept/reject) with current state $X_k^{(n)}$, proposal kernel q_k, and target f_{β_k}.

  end for

  Choose $\ell, m \in \{1, \ldots, K\}$ with $\ell \neq m$ uniformly at random.

  for $k \notin \{\ell, m\}$ **do**

    set $X_k^{(n+1)} = \tilde{X}_k^{(n+1)}$.

  end for

  Attempt a swap of states between the ℓ-th and the m-th chains:

$$(X_\ell^{(n+1)}, X_m^{(n+1)}) = \begin{cases} (\tilde{X}_m^{(n+1)}, \tilde{X}_\ell^{(n+1)}) & \text{with probability } a_{\ell,m}, \\ (\tilde{X}_\ell^{(n+1)}, \tilde{X}_m^{(n+1)}) & \text{with probability } 1 - a_{\ell,m}, \end{cases}$$

  where

$$a_{\ell,m} := \min\left\{1, \frac{f_{\beta_\ell}(\tilde{X}_m^{(n+1)}) f_{\beta_m}(\tilde{X}_\ell^{(n+1)})}{f_{\beta_m}(\tilde{X}_m^{(n+1)}) f_{\beta_\ell}(\tilde{X}_\ell^{(n+1)})}\right\}.$$

end for

Output: Sample = $\{X_1^{(n)}\}_{n=1}^{N}$.