Inference and Representation Project Proposal

Team Members:

- Genghis Luo kl4747@nyu.edu
- Jiasheng Ni jn2294@nyu.edu

Introduction:

Efficiently sampling from complex, high-dimensional probability distributions is a fundamental challenge in computational statistics, machine learning, and various applied scientific fields. Traditional Markov Chain Monte Carlo (MCMC) methods, such as the Random-Walk Metropolis algorithm, often suffer from slow convergence and poor scalability, particularly when exploring intricate posterior landscapes in high-dimensional settings. To address these limitations, the Hamiltonian Monte Carlo (HMC) method offers a powerful alternative by leveraging concepts from physics, specifically Hamiltonian dynamics, to guide the sampling process more effectively.

Hamiltonian Monte Carlo enhances the efficiency of MCMC sampling by introducing auxiliary momentum variables and simulating Hamiltonian dynamics over an extended phase space. This procedure generates proposals that traverse long distances in the target distribution with high acceptance rates, thereby mitigating the random walk behavior and autocorrelation issues inherent in conventional MCMC methods. The theoretical foundation of HMC is rooted in three key properties of Hamiltonian dynamics—**reversibility**, **volume preservation**, and **energy conservation**—which together ensure that the Markov chain maintains the desired stationary distribution.

This project aims to provide an insightful exploration of the theoretical underpinnings of Hamiltonian Monte Carlo, as well as to replicate and extend the numerical experiments discussed in seminal works by Neal (2011), Betancourt (2018), and Weare (lecture notes). Through these experiments, we intend to demonstrate the practical advantages and limitations of HMC in both low- and high-dimensional settings.

Objectives:

Specifically, the objectives of this project are twofold:

1. **Theoretical Exploration**: To develop a conceptual understanding of the mathematical principles underlying HMC, including the formulation of the Hamiltonian, the numerical implementation of Hamilton's equations using the Leapfrog integrator, and the justification of the Metropolis acceptance criterion.

2. **Numerical Validation & Application**: To replicate key numerical experiments from the literature, such as sampling from highly correlated low-dimensional Gaussian

distributions and high-dimensional target distributions, and to quantitatively evaluate the performance of HMC compared to traditional MCMC methods. These experiments will provide empirical insights into HMC's efficiency, acceptance rates, autocorrelation behavior, and scalability.

In detail, we will:

1. **Theoretical Exploration:**
   a. Why does HMC make sense? Why does it enhance sampling efficiency? How big is the improvement? More generally, what essentially differs HMC from traditional Monte Carlo methods?
   b. Understand the quantitative guarantee on HMC methods.
   c. What is the connection between HMC and Langevin Diffusion?
   d. Review on modern modifications by combining flow-matching methods with HMC to enhance efficiency and stability.

2. **Numerical Experiments:**
   a. Compare HMC and Random-Walk Metropolis (RWM) on a highly correlated 2D Gaussian distribution. To be specific, we will plot sample trajectories, autocorrelation of samples and adjust the parameters like effective sample size and acceptance rates.
   b. We will then generalize the 2D case to high-dimensional gaussian distribution for scalability test.