Vanilla HMC

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- Hamiltonian Monte Carlo (HMC) is an MCMC algorithm that leverages concepts from physics to propose new states in the Markov chain.
- It introduces auxiliary variable and simulates Hamiltonian dynamics to explore the target distribution more efficiently.
- In class we saw how MALA/Barker improved upon RW-Metropolis by using gradient information; HMC takes this further by simulating trajectories in the phase space.

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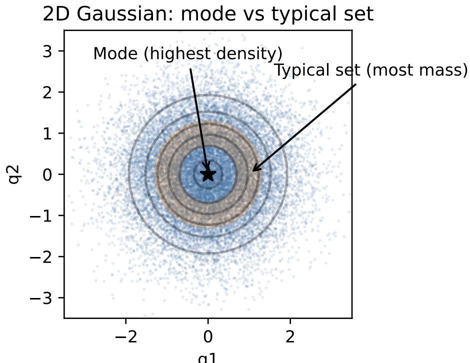
- In high-dimensional spaces it is not enough to explore regions around the modes.
- In high dimensions, probability mass concentrates on a thin shell away from modes
- Areas with lower density but massive volume $\rightarrow$ contains most probability mass
- So we need a method that makes proposals based on more than the local moves or local gradient at the current position.



Physical Interpretation

Neal, 2011

In two dimensions, we can visualize the dynamics as that of a frictionless puck that slides over a surface of varying height. The state of this system consists of the position of the puck, given by a 2D vector q*, and the momentum of the puck (its mass times its velocity), given by a 2D vector* p*.*

On a level part of the surface, the puck moves at a constant velocity. If it encounters a rising slope, the puck's momentum allows it to continue, with its kinetic energy $K(p)$ *decreasing and its potential energy* $U(q)$ *increasing, until the kinetic energy is zero, at which point it will slide back down (with kinetic energy increasing and potential energy decreasing)*

Hamiltonian Equation

Our target distribution is defined in terms of a potential energy function $U(q)$, which encodes the negative log probability of the target distribution $\pi(q)$ that we wish to sample from.

We extend the state space by introducing auxiliary variables and sample from π with density:

$$\pi(q, p) \propto \exp(-H(q, p)) = \exp(-U(q)) \exp(-K(p))$$

where $H(q, p)$ is the Hamiltonian function, representing the total energy of the system, given by the sum of kinetic and potential energy:

$$H(q, p) = U(q) + K(p) = U(q) + \frac{1}{2} p^T M^{-1} p$$

Note that marginalizing p recovers the target distribution $\pi(q)$.

Hamiltonian Dynamics

How to propose new states (q, p)? We simulate Hamiltonian dynamics to generate proposals that preserve the Hamiltonian (total energy) of the system. Exact Hamiltonian dynamics preserve both energy and volume; in discrete time, leapfrog approximately preserves energy but exactly preserves volume.

The dynamics of the system can be described by these equations,

$$\frac{dq}{dt} = \frac{\partial H}{\partial p} \quad \text{and} \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q}$$

which govern the time evolution of the position and momentum variables. How do we simulate these dynamics in discrete time? We use the Leapfrog integrator.

Leapfrog Integrator

To numerically simulate Hamiltonian dynamics, we use the leapfrog integrator, which is a symplectic method that preserves the volume in phase space and is time-reversible up to a momentum flip; that's why we often negate p at the end of the trajectory.

$$
\begin{aligned}
p\left(t+\frac{\varepsilon}{2}\right) &= p(t) - \frac{\varepsilon}{2}\nabla U(q(t)) \\
q(t+\varepsilon) &= q(t) + \varepsilon M^{-1} p\left(t+\frac{\varepsilon}{2}\right) \\
p(t+\varepsilon) &= p\left(t+\frac{\varepsilon}{2}\right) - \frac{\varepsilon}{2}\nabla U(q(t+\varepsilon))
\end{aligned}
$$

where ε is the step size.

Being symplectic means that this transformation preserves volume in phase space and that the Jacobian determinant of the transformation is equal to one and hence the Metropolis Acceptance ratio needs no volume correction factor.

Vanilla HMC Algorithm

Requires: Leapfrog integrator φ, step-size ε, number of steps L, current position q and positive definite matrix M.

1. **Energy lift**: given q, draw $p \sim N(0, M)$ - (random)
   This "lifts" our position into phase space by adding kinetic energy
2. **Hamilton flow**: propose $q^*, p^* = \varphi_\varepsilon^L(q, p)$ - (deterministic)
   Simulate dynamics for L steps using leapfrog integrator. Follow energy-conserving trajectory through phase space.
3. **Metropolis acceptance step** - (random)
   accept q^* with probability $\min\left\{1, \exp(H(q, p) - H(q^*, p^*))\right\}$
   Corrects for numerical errors in integration. No Jacobian term; leapfrog is volume-preserving

Note $H(q^*, -p^*) = H(q^*, p^*)$ because the K is even in p, so the minus is redundant.

Choosing parameters in HMC

Another story...

Step-size ε: optimal scaling

- Dimension dependence of stepsize:
  - RWM: $\mathcal{O}(d^{-1})$
  - MALA: $\mathcal{O}(d^{-1/3})$
  - HMC: $\mathcal{O}(d^{-1/4})$
- Optimal acceptance rates:
  - RWM: 0.234
  - MALA: 0.574
  - HMC: 0.651

Choose L **adaptively**: NUTS sampler