Computer Science

CSC 665-1: Advanced Topics in Probabilistic Graphical Models

Hamiltonian Monte Carlo (Addendum)

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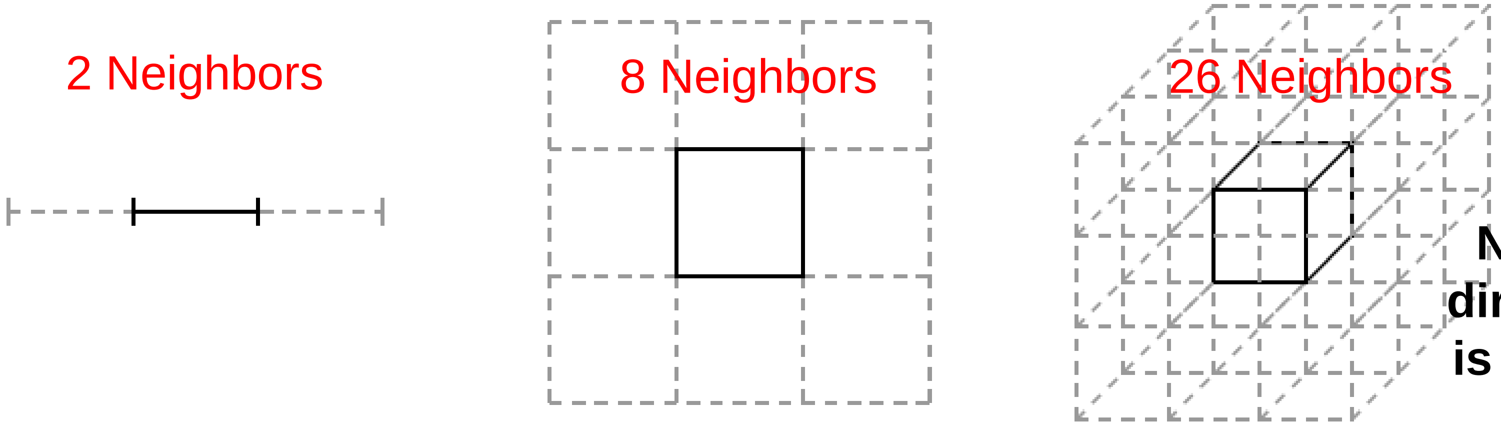
Images: From M. Betancourt, “A Conceptual Introduction to HMC”

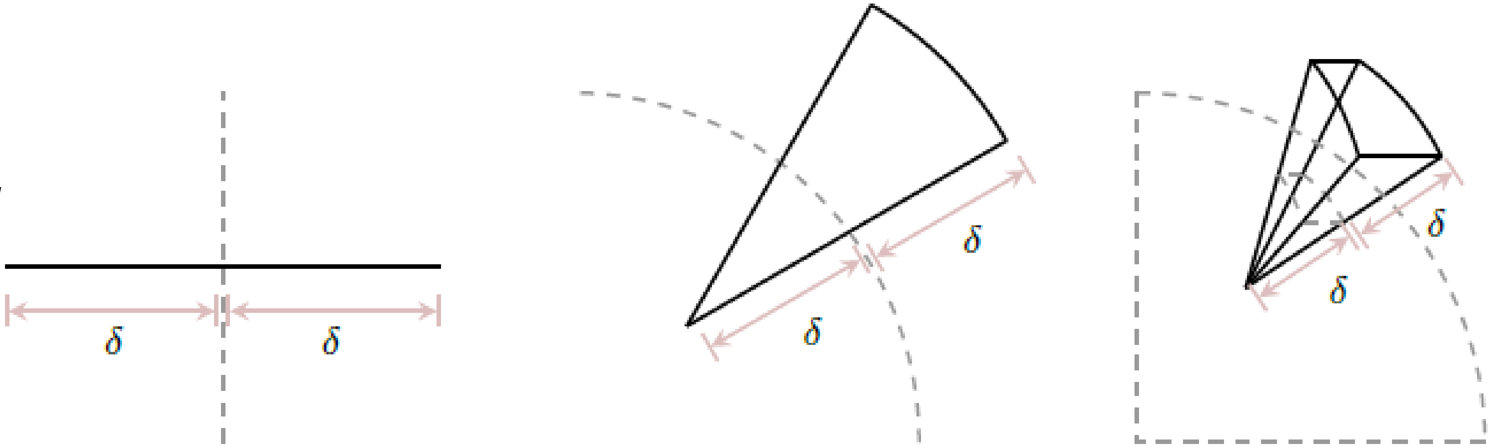
Volume vs. Dimension



Number of possible directions (neighbors) is 3^D-1, exponential in dimension

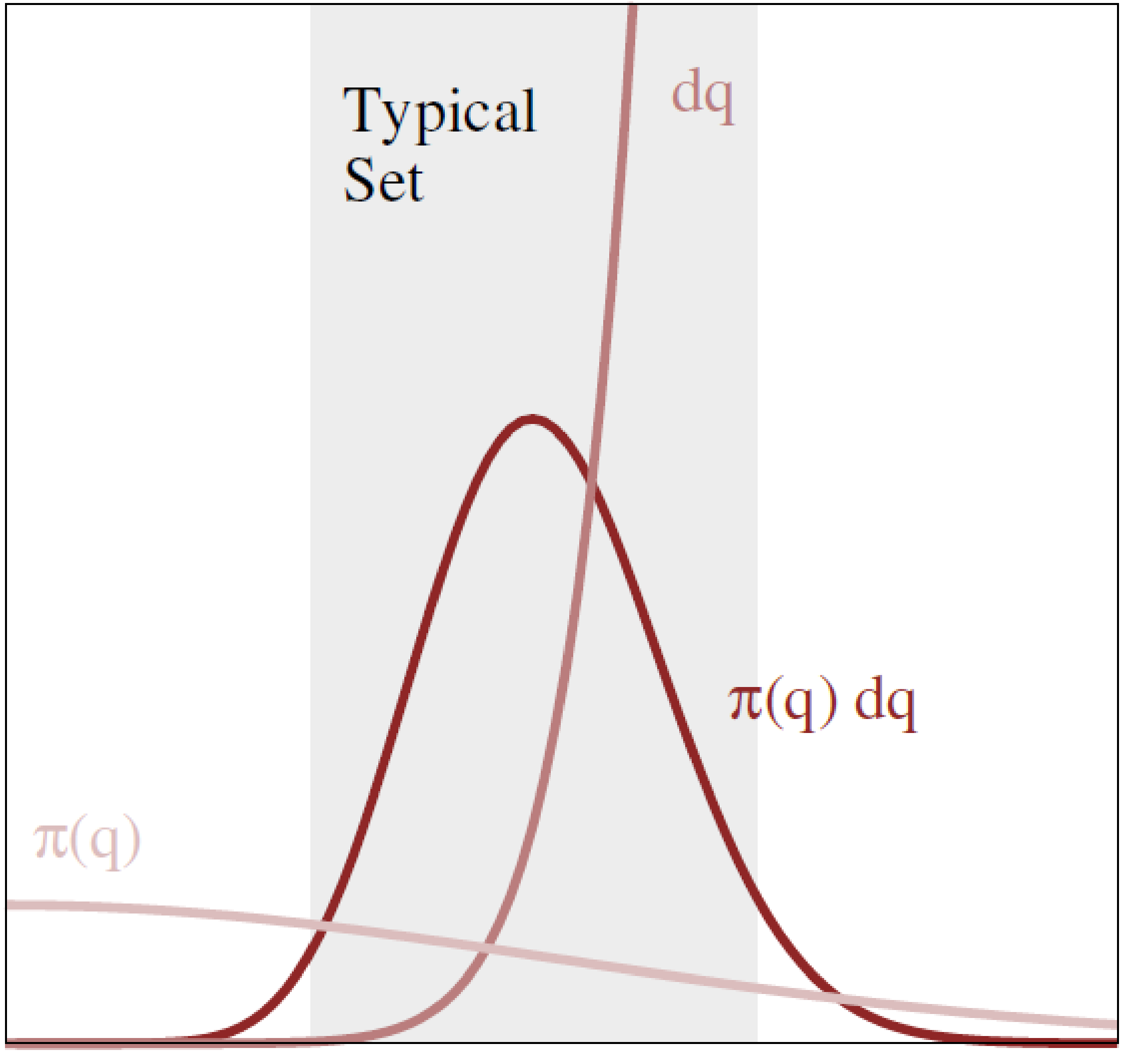
1D **2D** **3D**

Volume outside *shell* grows exponentially faster than volume inside



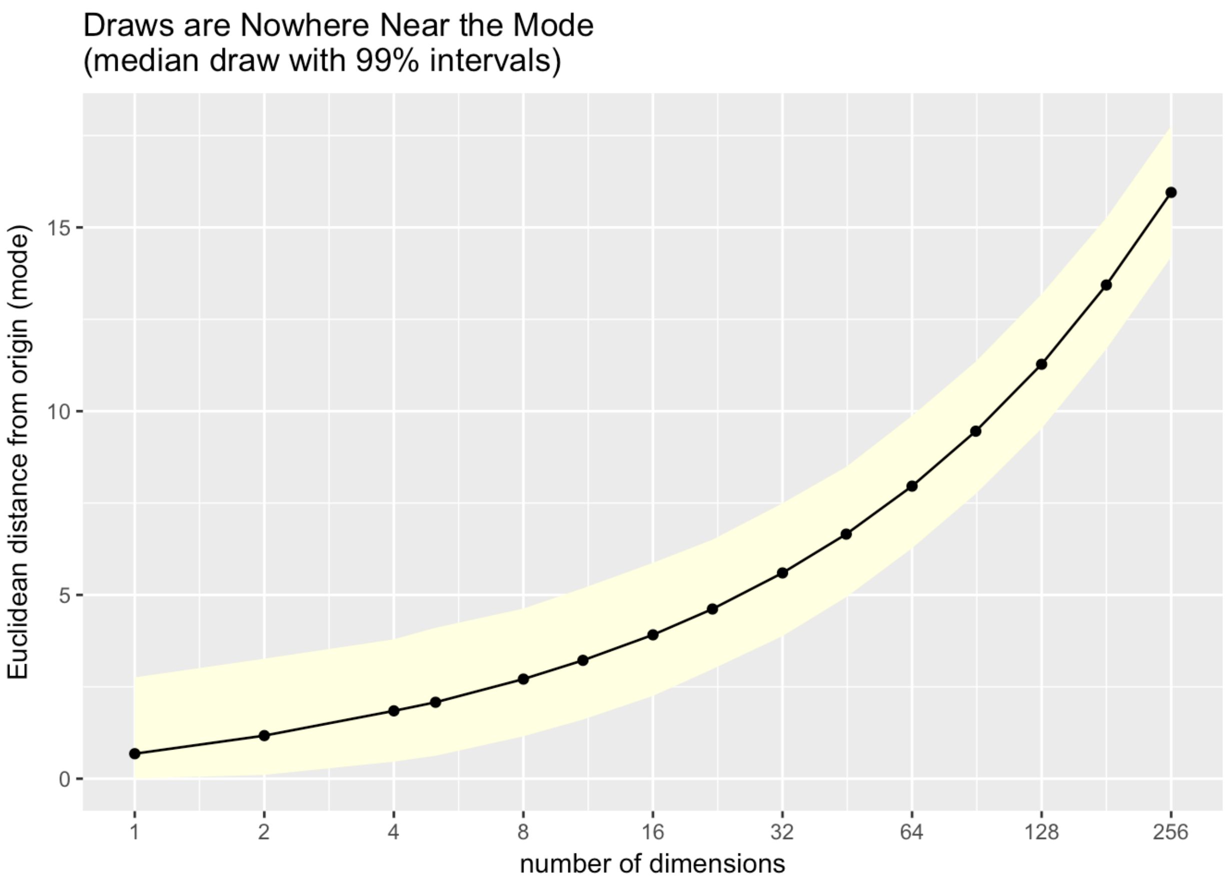
Volume containing mode becomes negligible as dim. increases

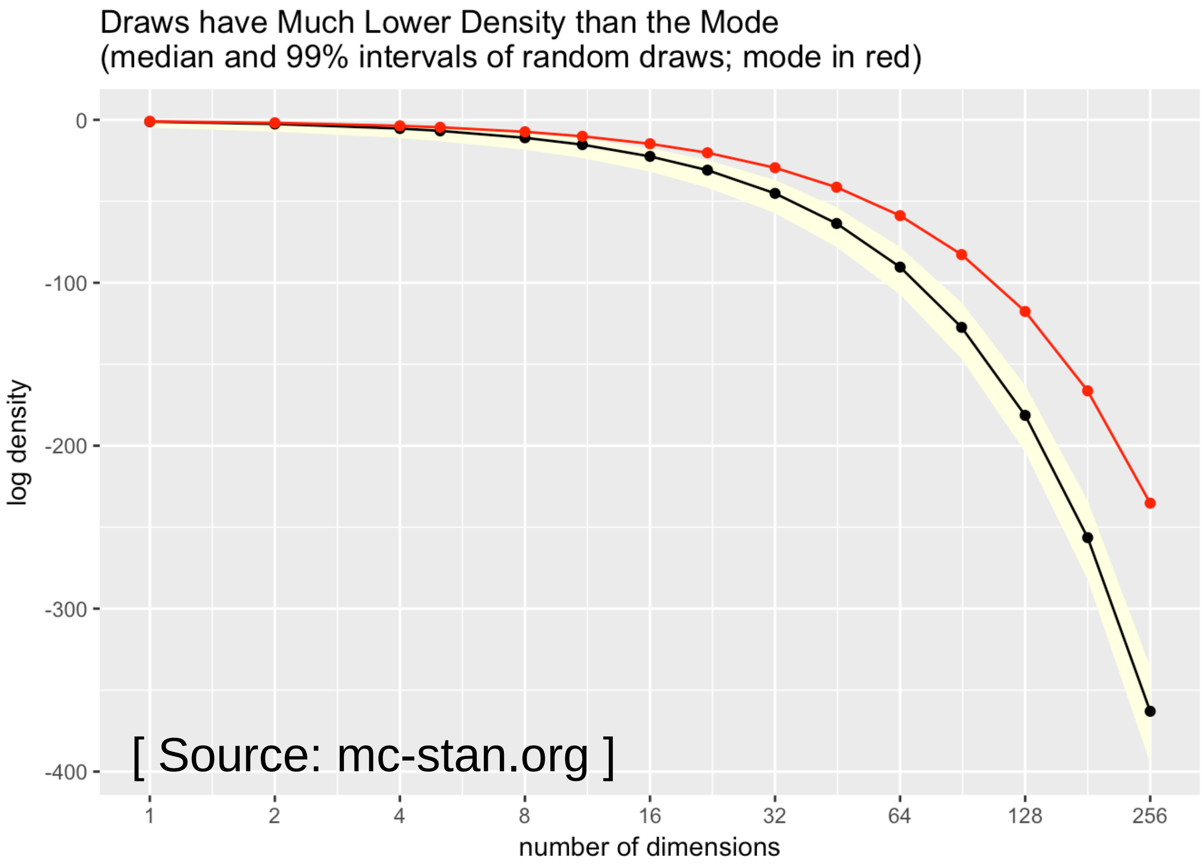
Intuition of Typical Set



Example: Gaussian

D i.i.d Gaussian RVs $y = (y_1, \ldots, y_D)^T \in \mathbb{R}^D: \quad y \sim \mathcal{N}(0, I)$





Squared distance is Chi-Squared RV: $\|y\|^2 \sim \chi^2(D)$

Weak Law of Large Numbers

Weak law of large numbers. Take x to be the average of N independent random variables $h_1, \ldots, h_N$, having common mean $\bar{h}$ and common variance σ_h^2: $x = \frac{1}{N}\sum_{n=1}^{N} h_n$. Then

$$P((x - \bar{h})^2 \geq \alpha) \leq \sigma_h^2/\alpha N. \tag{4.32}$$

Proof: obtained by showing that $\bar{x} = \bar{h}$ and that $\sigma_x^2 = \sigma_h^2/N$. $\square$

- Holds for any α and N large enough
- E.g. <u>on average</u> samples are similar to the mean

Asymptotic Equipartition Property (AEP)

- Applying LLN to estimate entropy we get:

$$\frac{1}{N}\sum_{n=1}^{N}\log_2\left(\frac{1}{p(x_n)}\right) \to H(X)$$

- Thus X *typically* belongs to a subset of size $2^{NH(X)}$ with each element having probability $p(x)$ near $2^{-NH(X)}$

- This is the called the *typical set* of elements with probability:

$$2^{-NH(X)-\epsilon} \leq p(x) \leq 2^{-NH(X)+\epsilon}$$

Example: Random Binary String

- Let $x = (x_1, \ldots, x_N)$ be N-length binary string
- Probability of r 1s and (N-r) 0s:

$$P(\mathbf{x}) = p_1^r (1 - p_1)^{N-r}$$

- Number of N-length strings with r 1s:

$$n(r) = \binom{N}{r}$$

- n(r) follows a Binomial distribution:

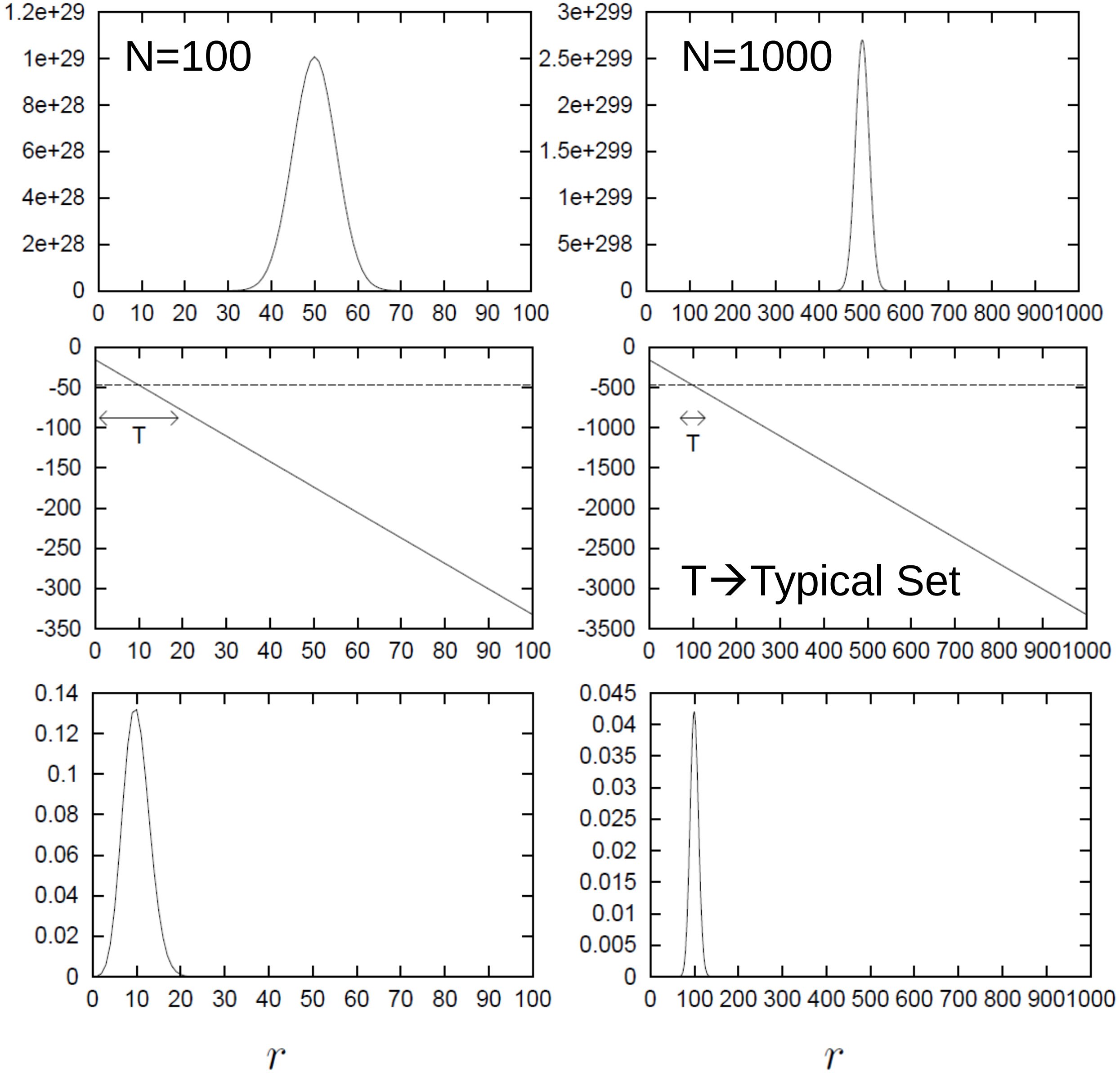
$$P(r) = \binom{N}{r} p_1^r (1 - p_1)^{N-r}$$

Example: Random Binary String

$$n(r) = \binom{N}{r}$$

$$\log_2 P(\mathbf{x})$$

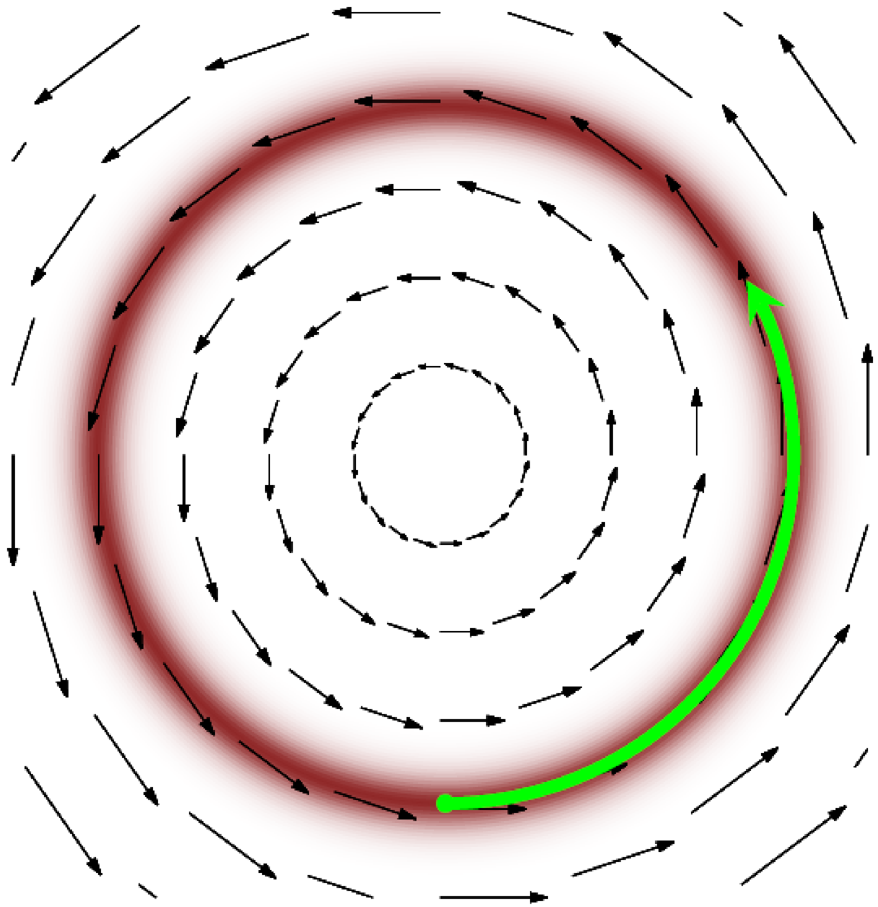
$$n(r)P(\mathbf{x}) = \binom{N}{r} p_1^r (1-p_1)^{N-r}$$



Most of the volume is concentrated away from the mean

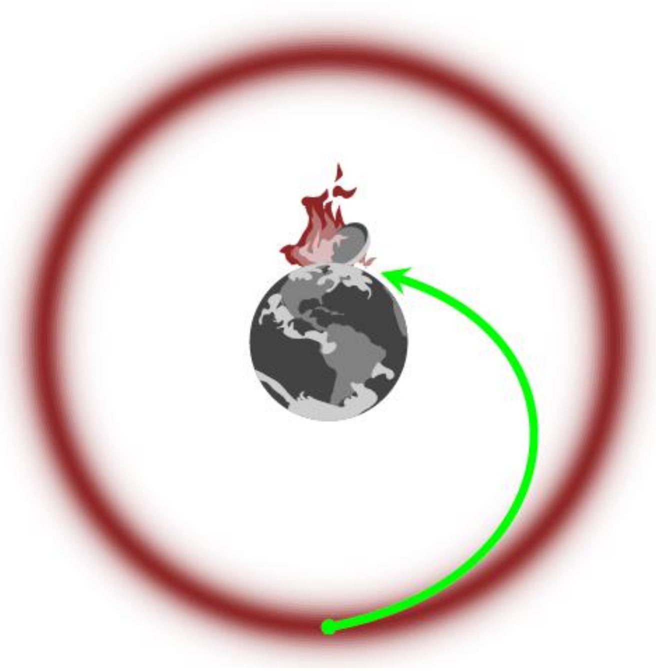
HMC Vector Field Intuition

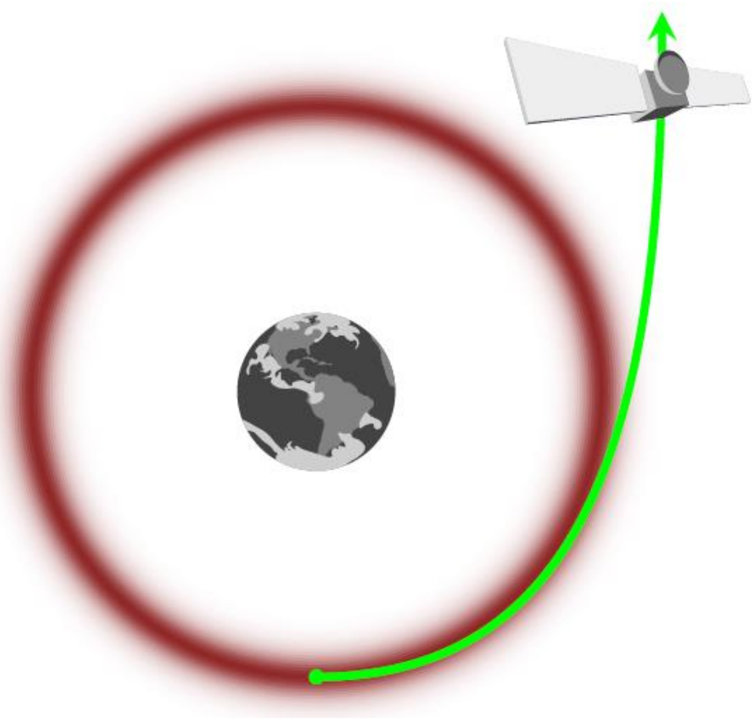
Ideally, MCMC dynamics should explore typical set efficiently

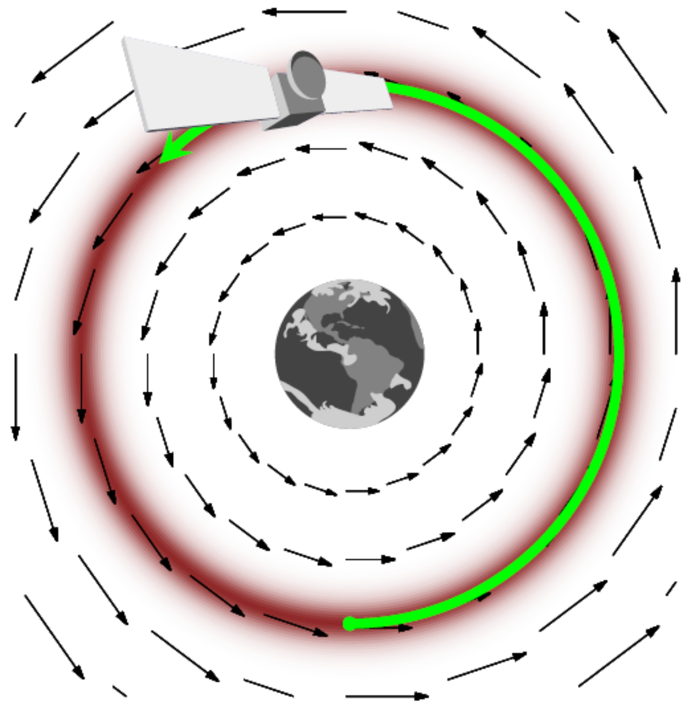


In theory, HMC aligns vector field with typical set

Conservative Dynamics Intuition

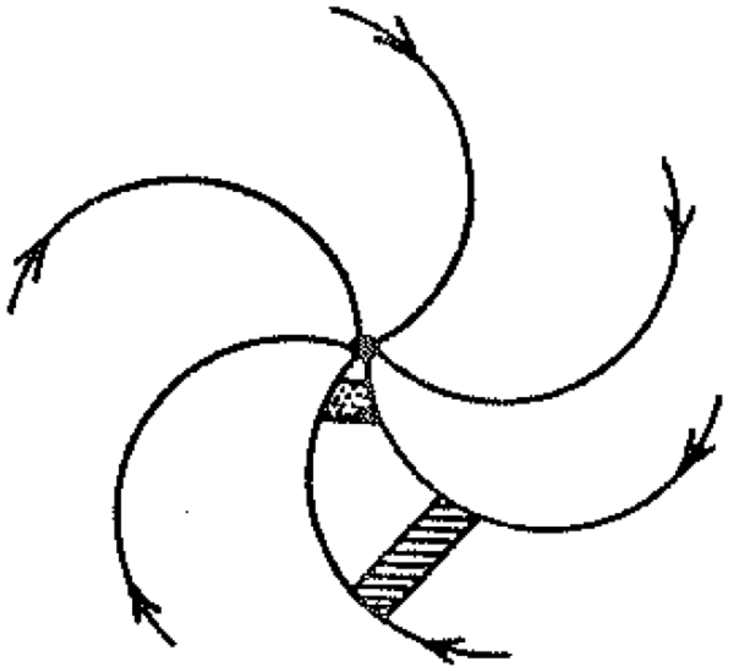




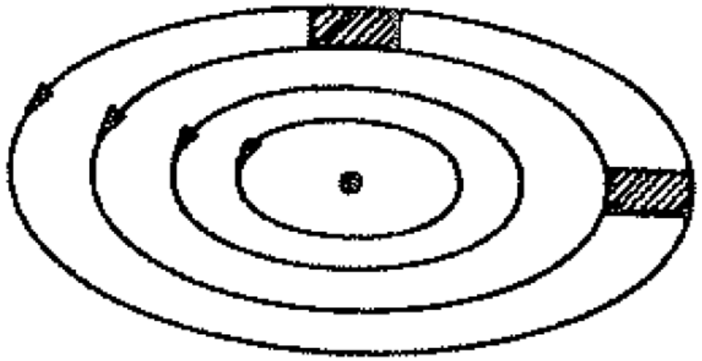


Attractive **Diffusion** **Conservative**

Volume Preservation



Dissipative System
(Volume Grows / Shrinks)



Conservative System
(Volume Preserved)

Conservative dynamics defined by volume preservation

Proof of Volume Preservation

- Recall Hamiltonian dynamics:

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \qquad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}$$

- Approximation of HMC transition for d=1 and time $\delta \approx 0$:

$$T_\delta(q,p) = \begin{bmatrix} q \\ p \end{bmatrix} + \delta \begin{bmatrix} dq/dt \\ dp/dt \end{bmatrix} + \text{ terms of order } \delta^2 \text{ or higher}$$

- Jacobian:

$$B_\delta = \begin{bmatrix} 1 + \delta\frac{\partial^2 H}{\partial q \partial p} & \delta\frac{\partial^2 H}{\partial p^2} \\ -\delta\frac{\partial^2 H}{\partial q^2} & 1 - \delta\frac{\partial^2 H}{\partial p \partial q} \end{bmatrix} + \text{ terms of order } \delta^2 \text{ or higher}$$

Proof of Volume Preservation (cont'd)

- Determinant of Jacobian equals volume:

$$\begin{aligned}\det(B_\delta) &= 1 + \delta\frac{\partial^2 H}{\partial q \partial p} - \delta\frac{\partial^2 H}{\partial p \partial q} + \text{terms of order } \delta^2 \text{ or higher} \\ &= 1 + \text{terms of order } \delta^2 \text{ or higher}\end{aligned}$$

- $\log\det(B_\delta) \approx 0$ since $\log(1+x) \approx x$ for x near zero
- Consider $\log\det(B_s)$ for s not close to zero
  - Set $\delta = s/n$ and apply T_δ n times

$$\begin{aligned}\log\det(B_s) &= \sum_{i=1}^{n} \log\det(B_\delta) = \sum_{i=1}^{n}\left\{\text{terms of order } 1/n^2 \text{ or smaller}\right\} \\ &= \text{terms of order } 1/n \text{ or smaller}\end{aligned}$$

As $n \to \infty$ we have $\log\det(B_s) \to 0$

Proof of Volume Preservation (cont'd)

- For d>1 each dxd submatrix (row j, col i) of Jacobian is:

$$B_\delta = \begin{bmatrix} I + \delta \left[\dfrac{\partial^2 H}{\partial q_j \partial p_i}\right] & \delta \left[\dfrac{\partial^2 H}{\partial p_j \partial p_i}\right] \\ \\ -\delta \left[\dfrac{\partial^2 H}{\partial q_j \partial q_i}\right] & I - \delta \left[\dfrac{\partial^2 H}{\partial p_j \partial q_i}\right] \end{bmatrix} + \text{ terms of order } \delta^2 \text{ or higher}$$

- Determinant is still 1 + higher order terms, remainder of argument holds