Hamiltonian Monte Carlo

Paper: A Conceptual Introduction to Hamiltonian Monte Carlo

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The Paper

A Conceptual Introduction to Hamiltonian Monte Carlo

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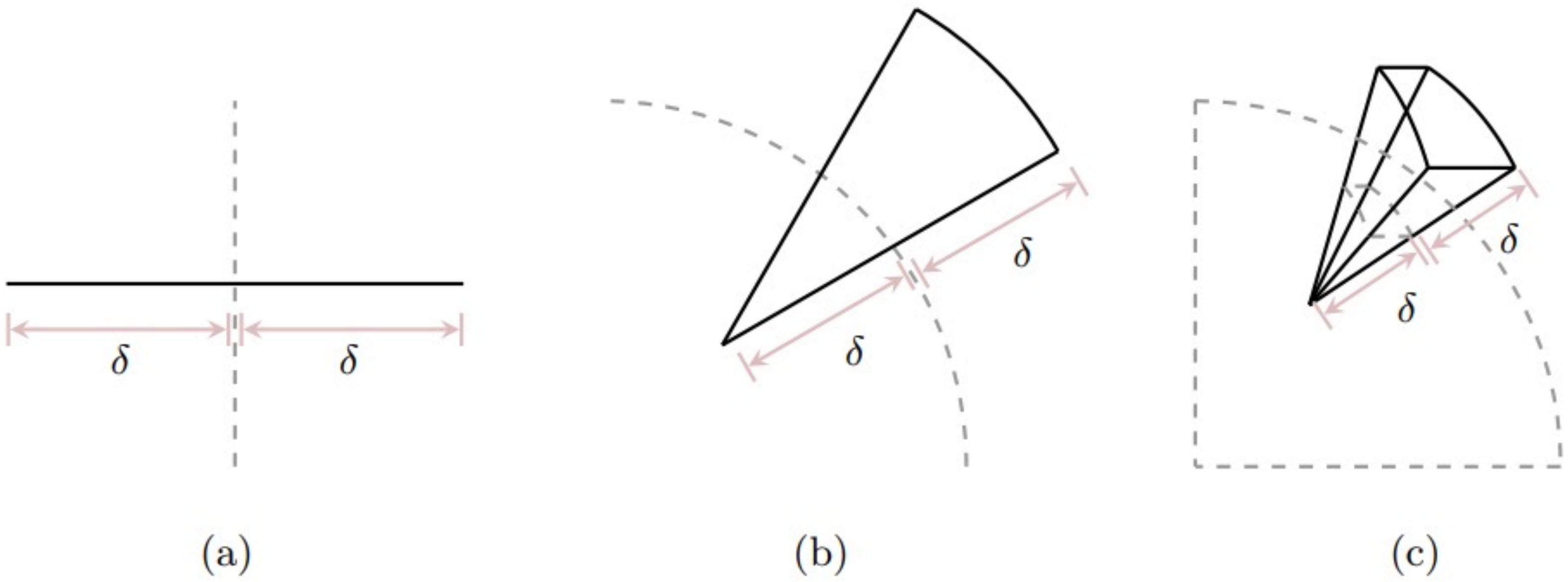
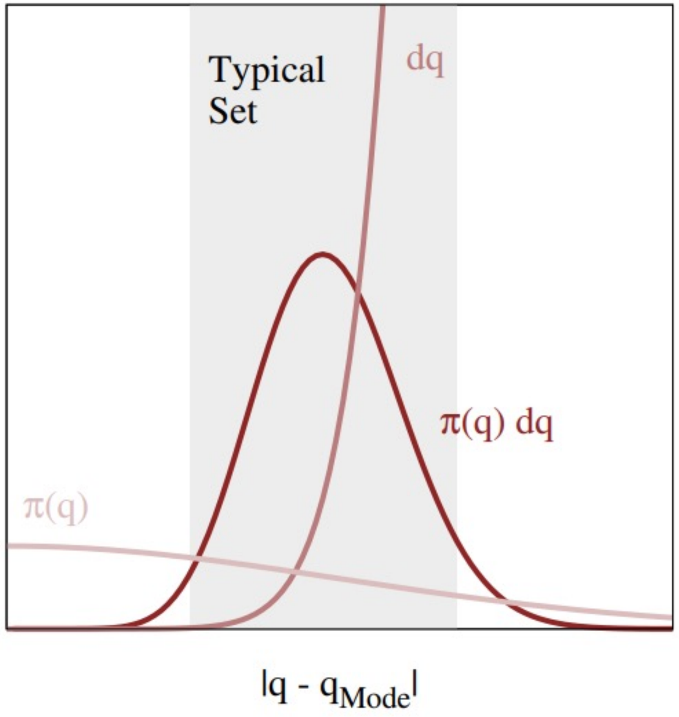
Abstract. Hamiltonian Monte Carlo has proven a remarkable empirical success, but only recently have we begun to develop a rigorous understanding of why it performs so well on difficult problems and how it is best applied in practice. Unfortunately, that understanding is confined within the mathematics of differential geometry which has limited its dissemination, especially to the applied communities for which it is particularly important.

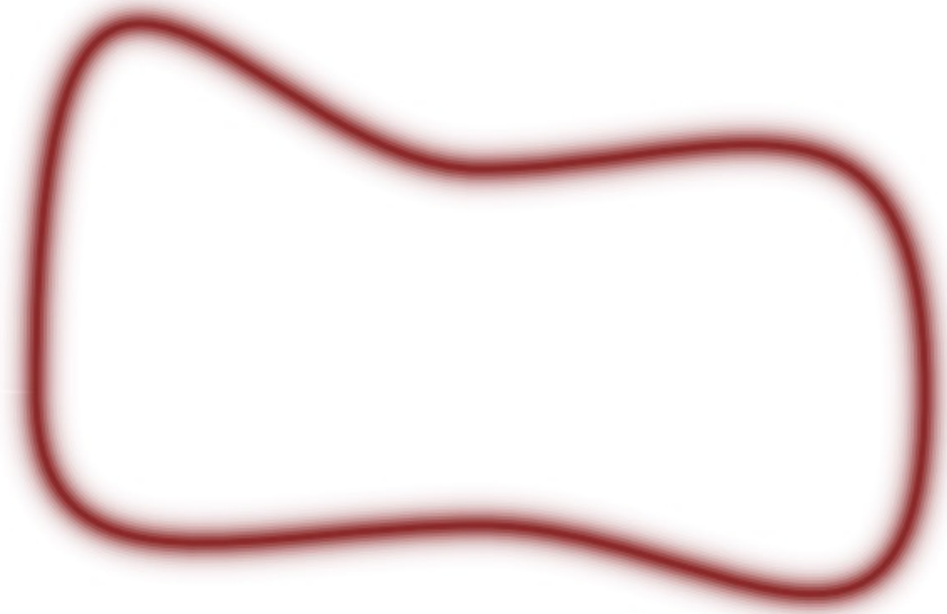
In this review I provide a comprehensive conceptual account of these theoretical foundations, focusing on developing a principled intuition behind the method and its optimal implementations rather of any exhaustive rigor. Whether a practitioner or a statistician, the dedicated reader will acquire a solid grasp of how Hamiltonian Monte Carlo works, when it succeeds, and, perhaps most importantly, when it fails.

The Typical Set

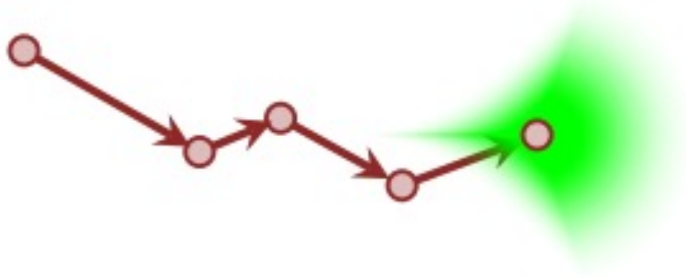


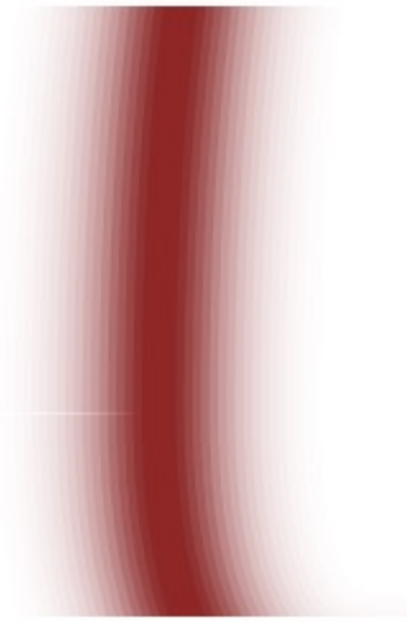
The Typical Set





Markov Chain Monte Carlo



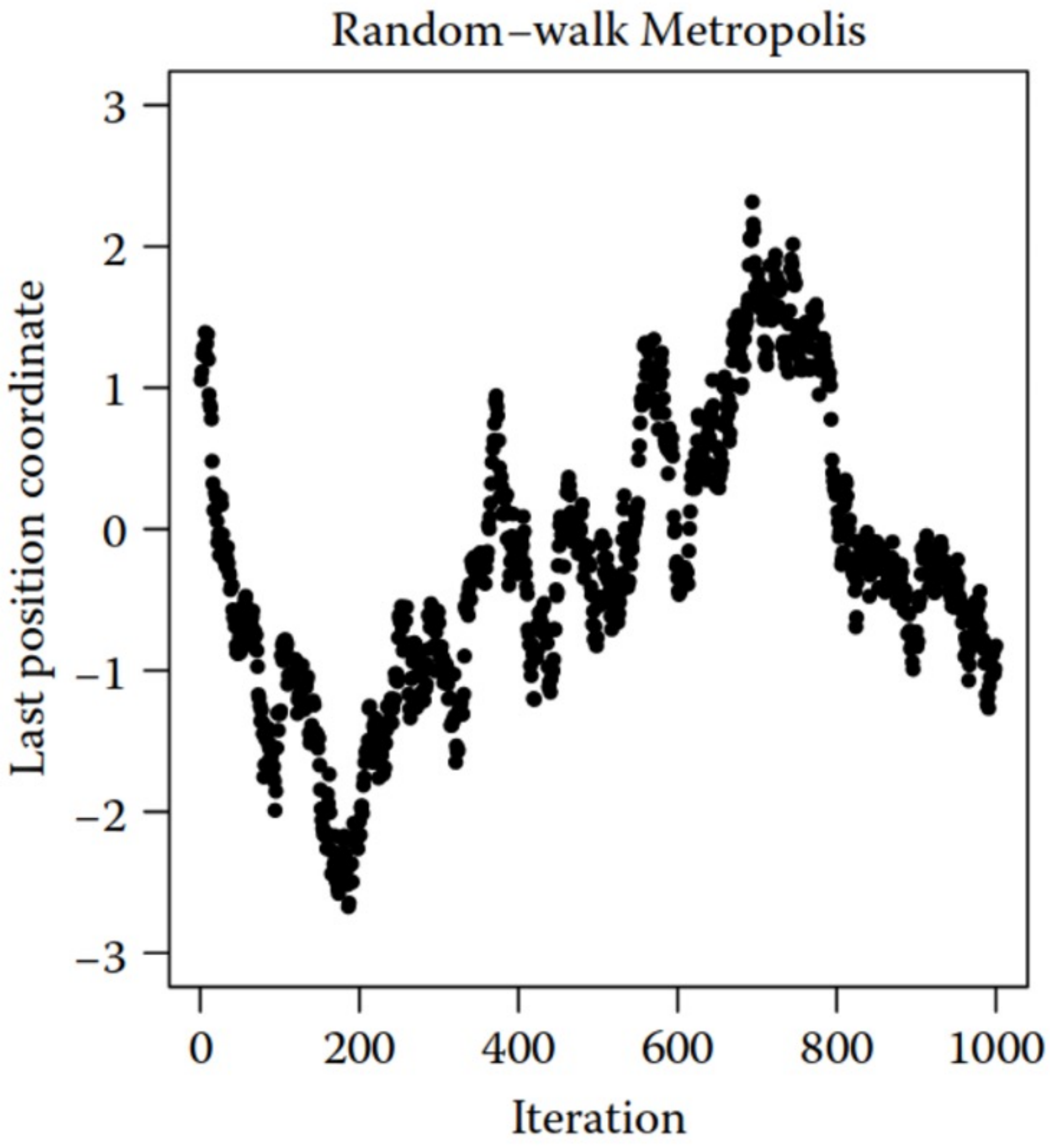


Metropolis-Hastings

$$a(q' \mid q) = \min\left(1, \frac{\mathbb{Q}(q \mid q')\,\pi(q')}{\mathbb{Q}(q' \mid q)\,\pi(q)}\right)$$

$$\mathbb{Q}(q' \mid q) = \mathcal{N}(q' \mid q, \Sigma)$$

$$a(q' \mid q) = \min\left(1, \frac{\pi(q')}{\pi(q)}\right)$$

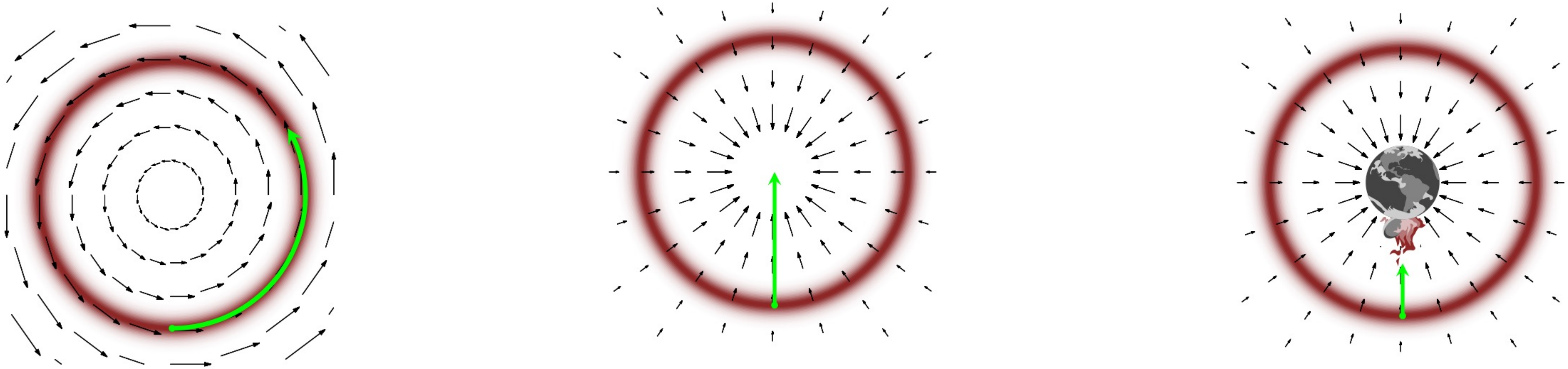


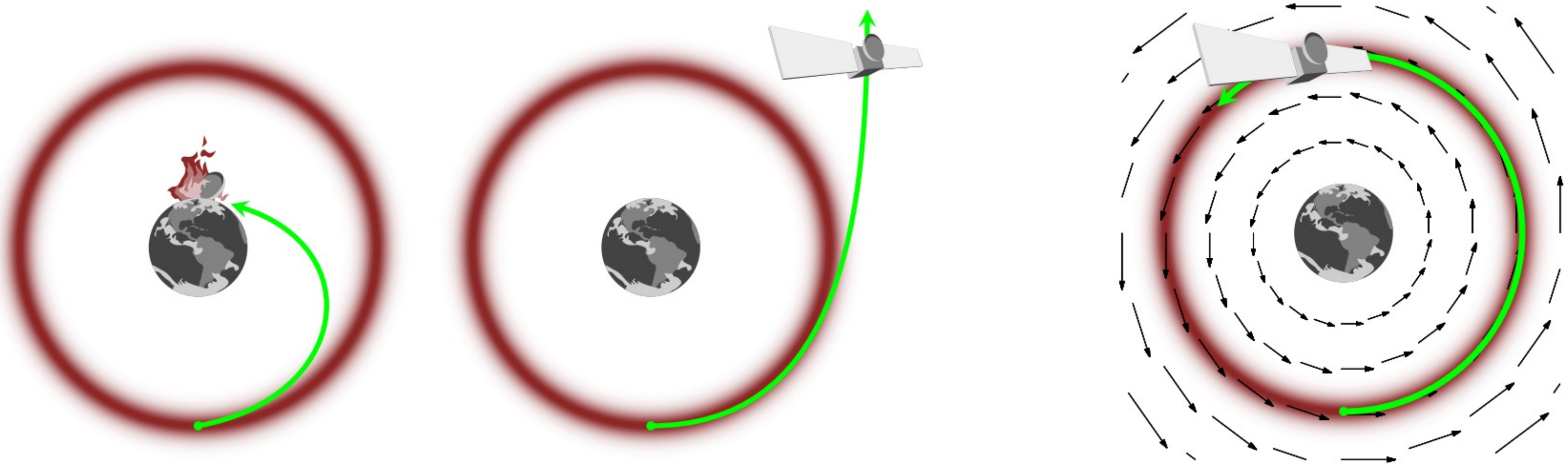
Lucas Mahler. “Randomized Algorithms - Using Randomness to Solve Increasingly Complex Problems - A Review”. In: (Dec. 2018)

Metropolis-Hastings in high dimensions

(a) (b)

Solution proposal - Hamiltonian Monte Carlo





(a) (b)

Solution proposal - Hamiltonian Monte Carlo

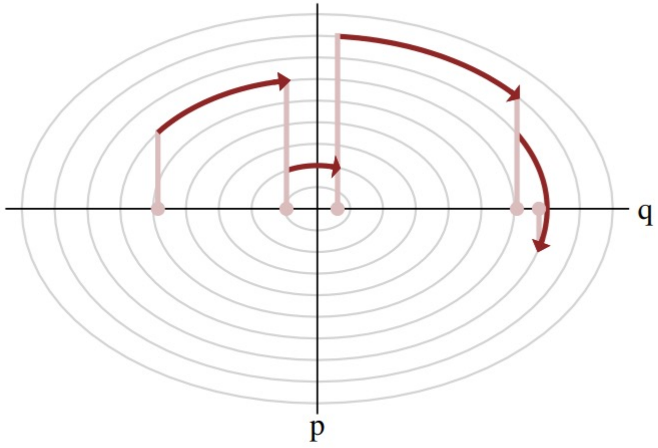
$$\pi(q,p) = \pi(p \mid q)\,\pi(q)$$

$$\pi(q,p) = e^{-H(q,p)}$$

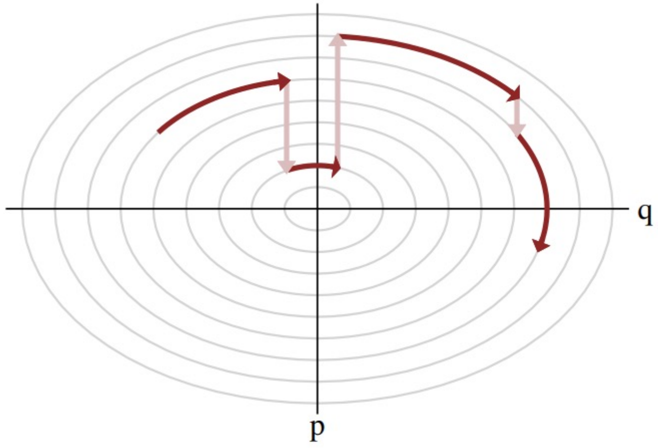
$$H(q,p) \equiv -\log \pi(q,p)$$

$$\begin{aligned} H(q,p) &= -\log \pi(p \mid q) - \log \pi(q) \\ &\equiv \quad K(p,q) \quad + V(q)\,. \end{aligned}$$

$$\begin{aligned} \frac{\mathrm{d}q}{\mathrm{d}t} &= +\frac{\partial H}{\partial p} = \frac{\partial K}{\partial p} \\ \frac{\mathrm{d}p}{\mathrm{d}t} &= -\frac{\partial H}{\partial q} = -\frac{\partial K}{\partial q} - \frac{\partial V}{\partial q} \end{aligned}$$

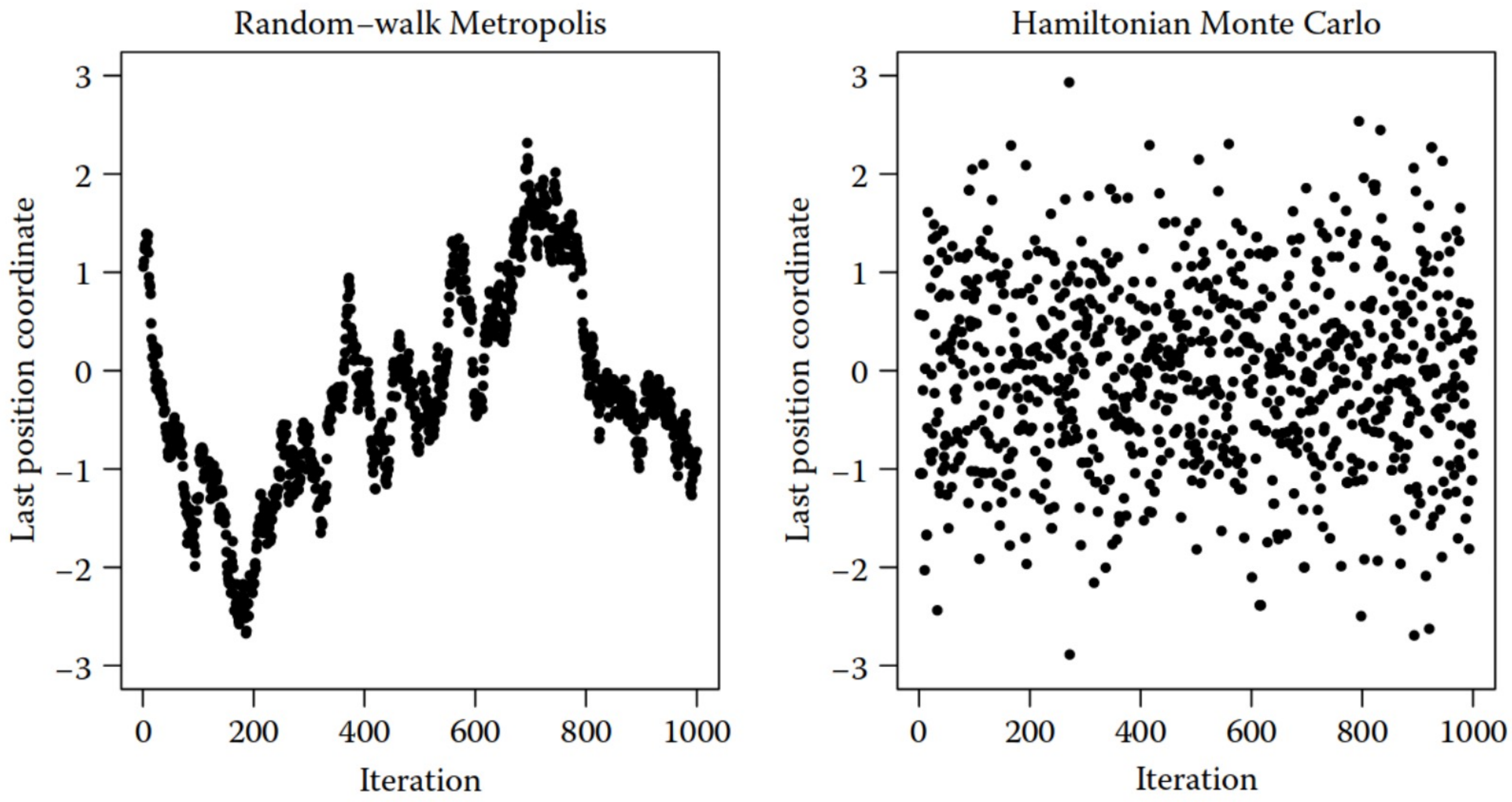


(a)



(b)

Solution proposal - Hamiltonian Monte Carlo



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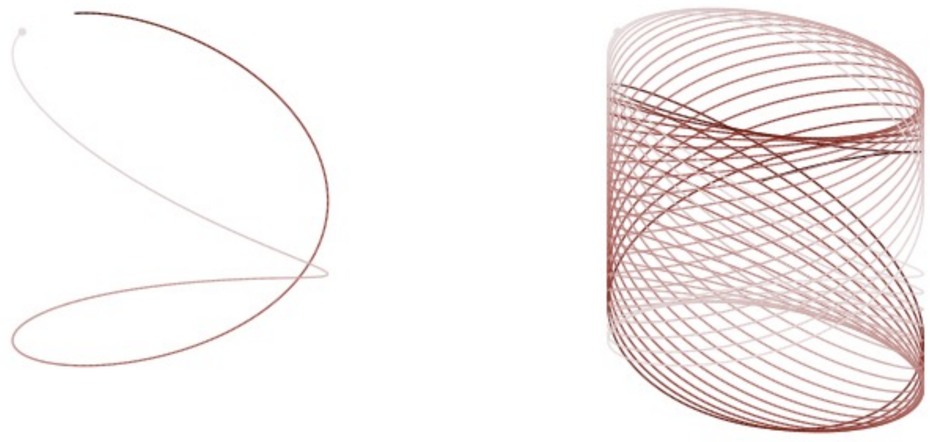
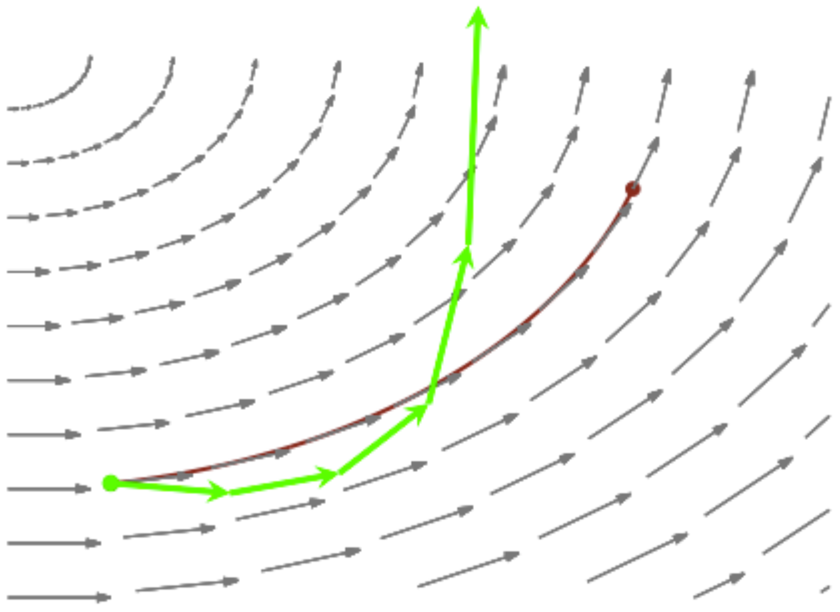
Tuning of Hamiltonian Monte Carlo

Integration time



(a) (b)

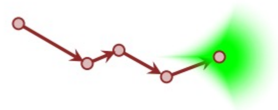
Step size

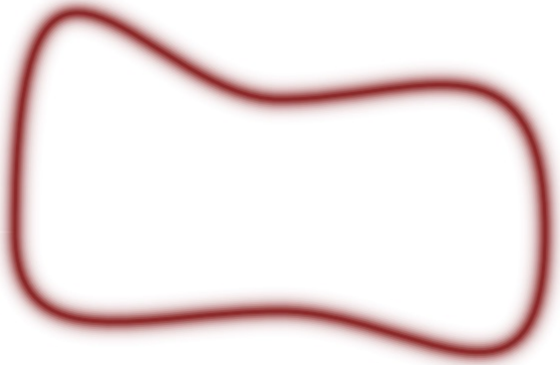


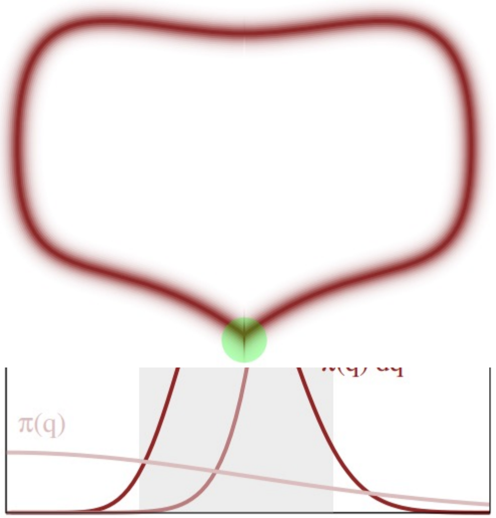
Conclusion

- Hamiltonian Monte Carlo is an efficient method of implementing high dimensional Markov Chain Monte Carlos
- The need to understand differential geometry makes the barrier of entry high
- The method is difficult to tune

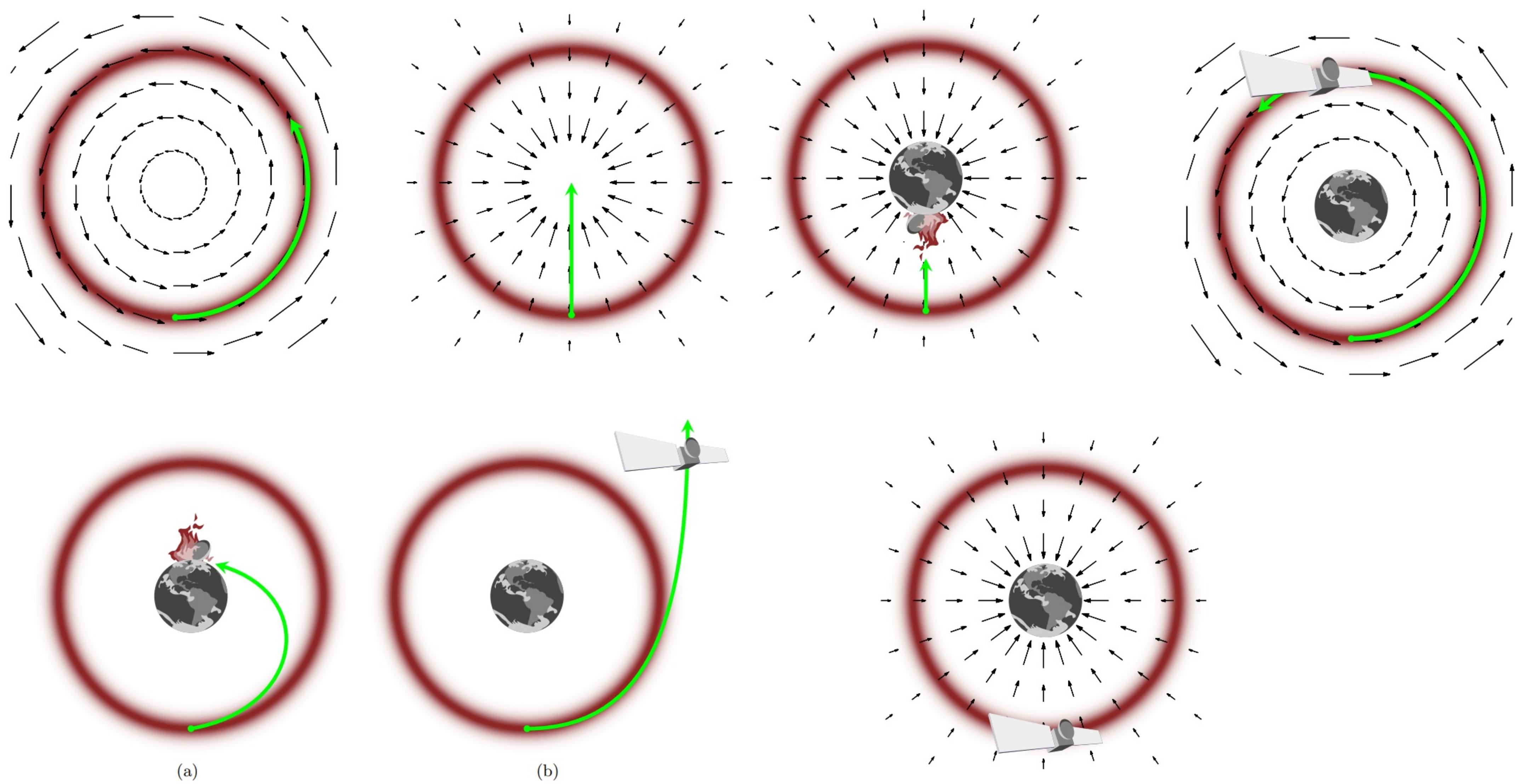
Thanks for listening

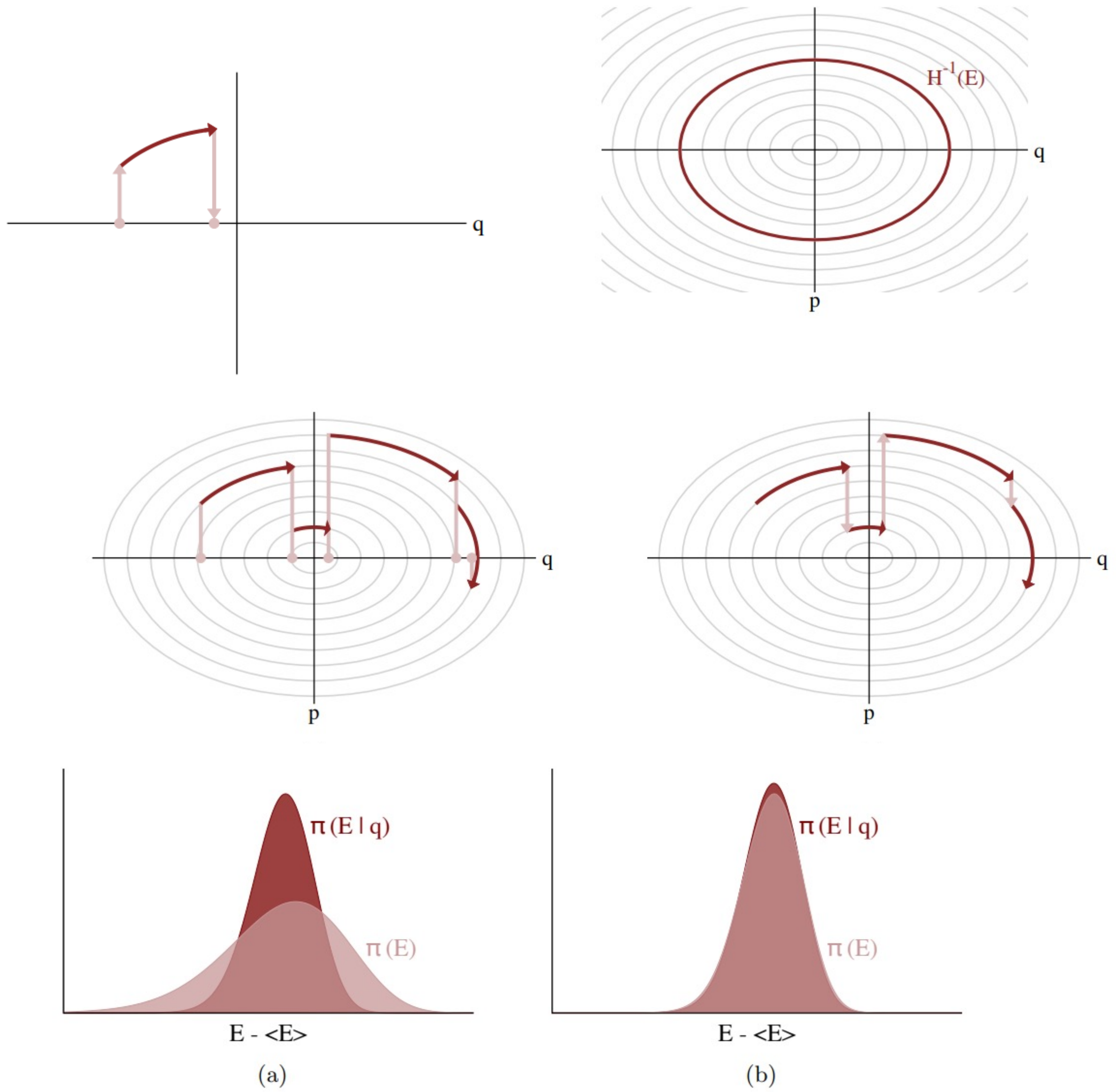


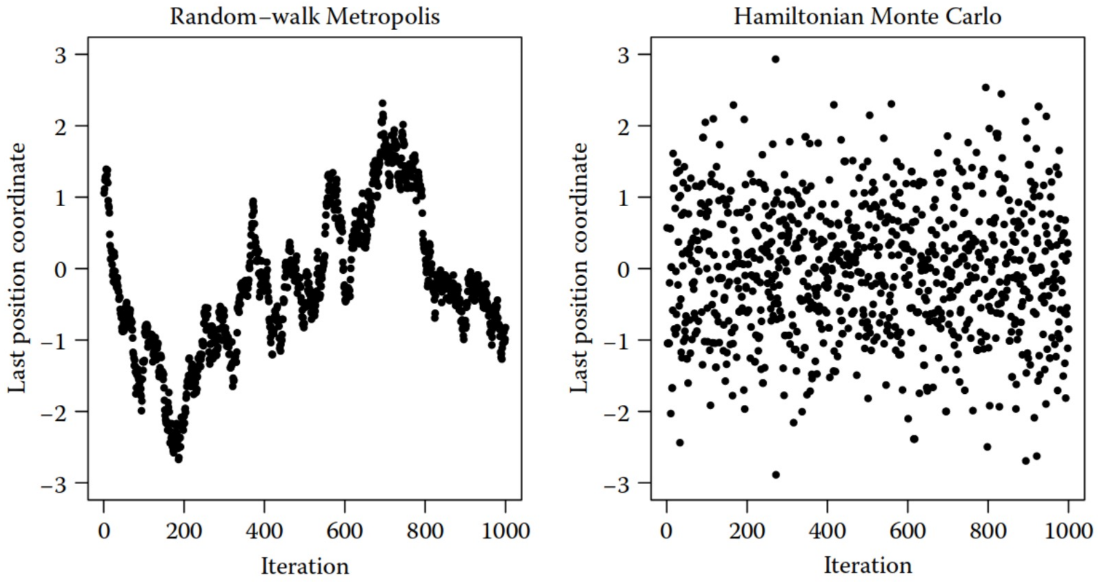




(a) (b)


(a)
(b)


q
H^-1(E)
q
p
q
p
q
p
π (E | q)
π (E)
E - <E>
π (E | q)
π (E)
E - <E>
(a)
(b)


Random–walk Metropolis
Hamiltonian Monte Carlo
Last position coordinate
Iteration
3
2
1
0
−1
−2
−3
0
200
400
600
800
1000