

# Hamiltonian Monte Carlo

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# Introdução

# Artigo 1

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## MCMC using Hamiltonian dynamics

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# 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.

## Fontes adicionais

- ▶ Ben Lambert - A Student's Guide to Bayesian Statistics
- ▶ Richard McElreath - Statistical Rethinking (2nd Ed.)

## Um pouco de história

- ▶ **Markov Chain Monte Carlo (MCMC)** originated with the classic paper of **Metropolis et al. (1953)**, where it was used to **simulate the distribution of states** for a system of idealized molecules.
- ▶ Not long after, **another approach to molecular simulation** was introduced (**Alder and Wainwright, 1959**), in which the motion of the molecules was deterministic, following Newton's laws of motion, which have an elegant formalization as **Hamiltonian dynamics**.
- ▶ In **1987**, a landmark paper by Duane, Kennedy, Pendleton, and Roweth **united the MCMC and molecular dynamics approaches**. They called their method "Hybrid Monte Carlo", which abbreviates to "HMC", but the phrase "**Hamiltonian Monte Carlo**", retaining the abbreviation, is more specific and descriptive

# Referências

(Neal 2011)

Neal, Radford. 2011. "MCMC Using Hamiltonian Dynamics." In. Chapman; Hall/CRC. <https://doi.org/10.1201/b10905-6>.