Lecture 27: Physics-informed deep neural networks

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The Metropolis algorithm

PREDICTIVE
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The Metropolis algorithm

$$p(x) = \frac{\pi(x)}{Z}$$ know this function ?

- **Initialize:** x_0
- For $n = 1, 2, \dots$
  - **Generate** candidate sample: $x' \sim q(x' | x_{n-1})$ proposal distribution
  - **Calculate** the *acceptance ratio*:
    $$a(x', x_{n-1}) = \max\left\{\frac{\pi(x')}{\pi(x_{n-1})}, 1\right\}$$
  - **Accept/Reject:**
    - Generate $u \sim U([0,1])$
    - If $u \le a$, then accept: $x_n \leftarrow x'$
    - If $u > a$, then reject: $x_n \leftarrow x_{n-1}$

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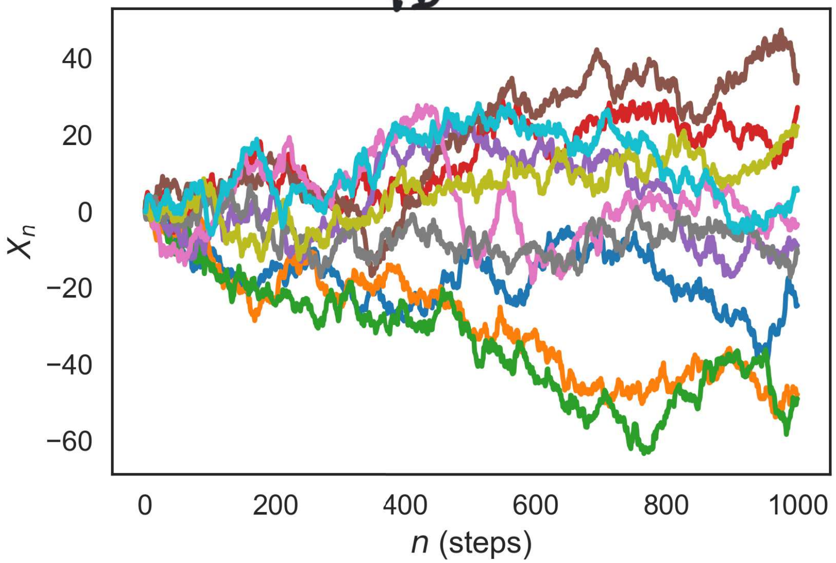
What are the restrictions on the Metropolis proposal?

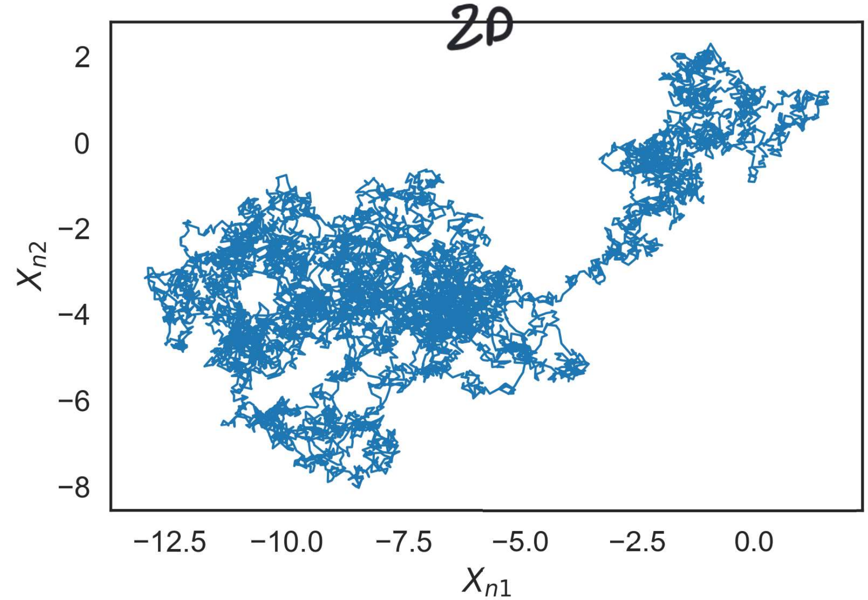
$$q(x' \mid x_{n-1}) = q(x_{n-1} \mid x')$$

The random walk proposal

1D



2D



$$q(x' \mid x_{n-1}) = \mathcal{N}(x' \mid x_{n-1}, \Sigma)$$

tunable parameter

Why does the Metropolis algorithm work?

- Intuitively: It constructs a series of samples that eventually come from the desired probability density.

- Math reason: It constructs a stationary, reversible, aperiodic, Harris recurrent Markov chain that leaves the desired probability density invariant.

- Metropolis is an example of a Markov Chain Monte Carlo (MCMC) algorithm.