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The leapfrog method is the original global leapfrog method (also known as the Leimkuhler leapfrog method) providing numerical Hamiltonian derivatives for leapfrog integration.

Metropolis-Adjusted

If the target distribution is not perfectly symmetric, the Metropolis-adjusted leapfrog method (also known as the Metropolis-adjusted Hamiltonian Monte Carlo method) is used. It uses the Metropolis-Hastings algorithm to adjust the leapfrog method. The target distribution is (ρ^*, θ^*) and the proposal distribution is $q(\theta | \theta^*)$. The acceptance probability is $\min(1, \frac{q(\theta^* | \theta)}{q(\theta | \theta^*)} \frac{\rho^*(\theta)}{\rho^*(\theta^*)})$.

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Algorithm

The Hamiltonian Monte Carlo algorithm consists of the following steps: 1. Initialize the parameters θ and the momentum p . 2. Generate a random number u from a uniform distribution. 3. Compute the Hamiltonian function $H(\theta, p)$ and its gradient. 4. Update the parameters θ and the momentum p using the leapfrog method. 5. Compute the acceptance probability α . 6. Accept or reject the proposed parameters θ and the momentum p using the Metropolis-Hastings algorithm.

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