Physics Recap - Energy

Kinetic energy - Energy an object has because it is in motion

Example: A drop of rain falling

Example: A wheel spinning.

Physics Recap - Energy

Potential Energy - Energy an object has stored as a result of its position.

Example: A person holding a coin above the ground. When the coin is dropped, the potential energy is converted to kinetic energy and the coin falls.

Example: The voltage measured across the terminals of a battery.

Physics Recap - Hamiltonian

$$H(q,p) = K + U$$

Q = position

P = Momentum (p = mv), where m = mass.

Physics Recap - Hamiltonian

H(q,p) = K + U

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q} \qquad \frac{dq}{dt} = \frac{\partial H}{\partial p}$$

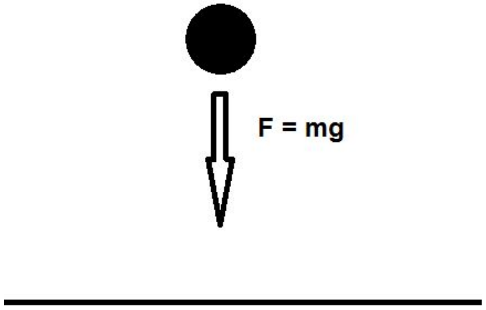
Physics Recap - Hamiltonian Example

Example: Object in free fall

$$H = K + U$$

$$H = \frac{1}{2}mv^2 + mgh$$

$$H = \frac{p^2}{2m} + mgq$$



Physics Recap - Hamiltonian Example

$$H = \frac{p^2}{2m} + mgq$$

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q} \qquad \frac{dq}{dt} = \frac{\partial H}{\partial p}$$

$$\frac{dp}{dt} = -mg \qquad \frac{dq}{dt} = \frac{p}{m}$$

Physics Recap - Hamiltonian Example

$$H = \frac{p^2}{2m} + mgq$$

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q} \qquad \frac{dq}{dt} = \frac{\partial H}{\partial p}$$

$$\frac{dp}{dt} = -mg \qquad \frac{dq}{dt} = \frac{p}{m}$$

$$\frac{d(mv)}{dt} = -mg \qquad v = \frac{p}{m}$$

$$ma = -mg \qquad v = \frac{mv}{m}$$

$$a = -g \qquad v = v$$

Which we already know!

Leapfrog Algorithm

Now we have $p(q,t)$ and $q(p,t)$.

Need to approximate with discrete timesteps.

Naive approach: $p(t+\varepsilon) = p(t) + (dp/dt) * \varepsilon$

$q(t+\varepsilon) = q(t) + (dq/dt) * \varepsilon$

Issues with convergence. p and q depend on each other

Leapfrog Algorithm

Leapfrog Algorithm:

$p(t+0.5\boldsymbol{\varepsilon}) = p(t) + (dp/dt)*0.5\varepsilon$

$q(t+\varepsilon) = q(t) + (dq/dt)*\varepsilon$

$p(t+\varepsilon) = p(t+0.5\varepsilon) + (dp/dt)*0.5\varepsilon$

Better convergence! Only one extra step is needed.

Hamiltonian Monte Carlo

Suppose we wish to sample from D dimensions$(q_1, q_2, \ldots, q_D)$

We can cleverly construct D addition dimensions$(p_1, p_2, \ldots, p_D)$

$$\pi(q,p) = \exp(-H(q,p))$$

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

$$H(q,p) = -\log(\pi(p|q)\pi(q))$$

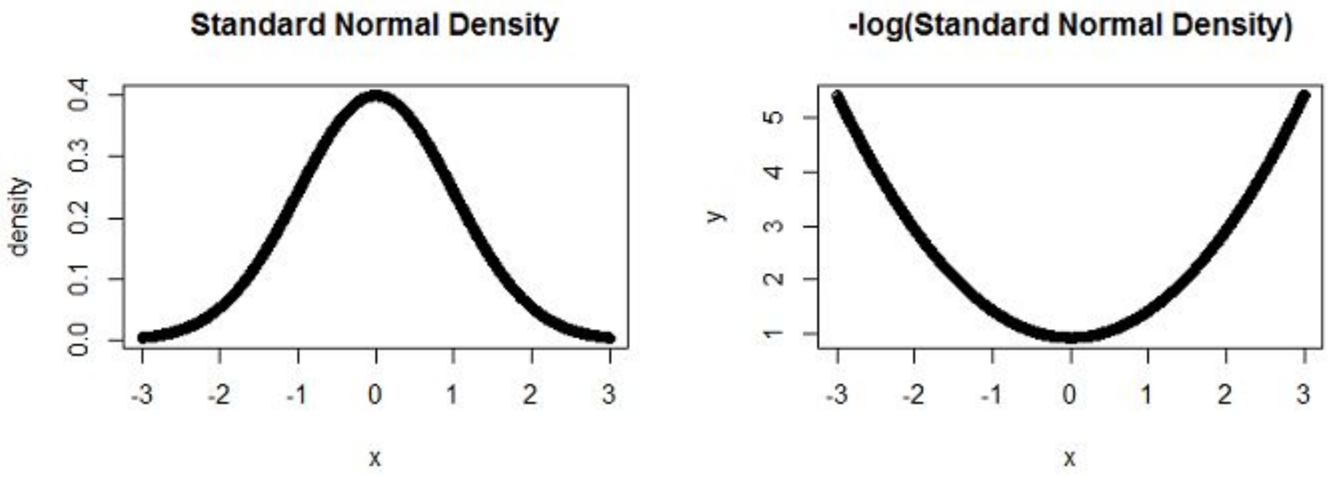
$$H(q,p) = -\log(\pi(p|q)) - \log(\pi(q))$$

$$H(q,p) = K(p,q) + U(q)$$

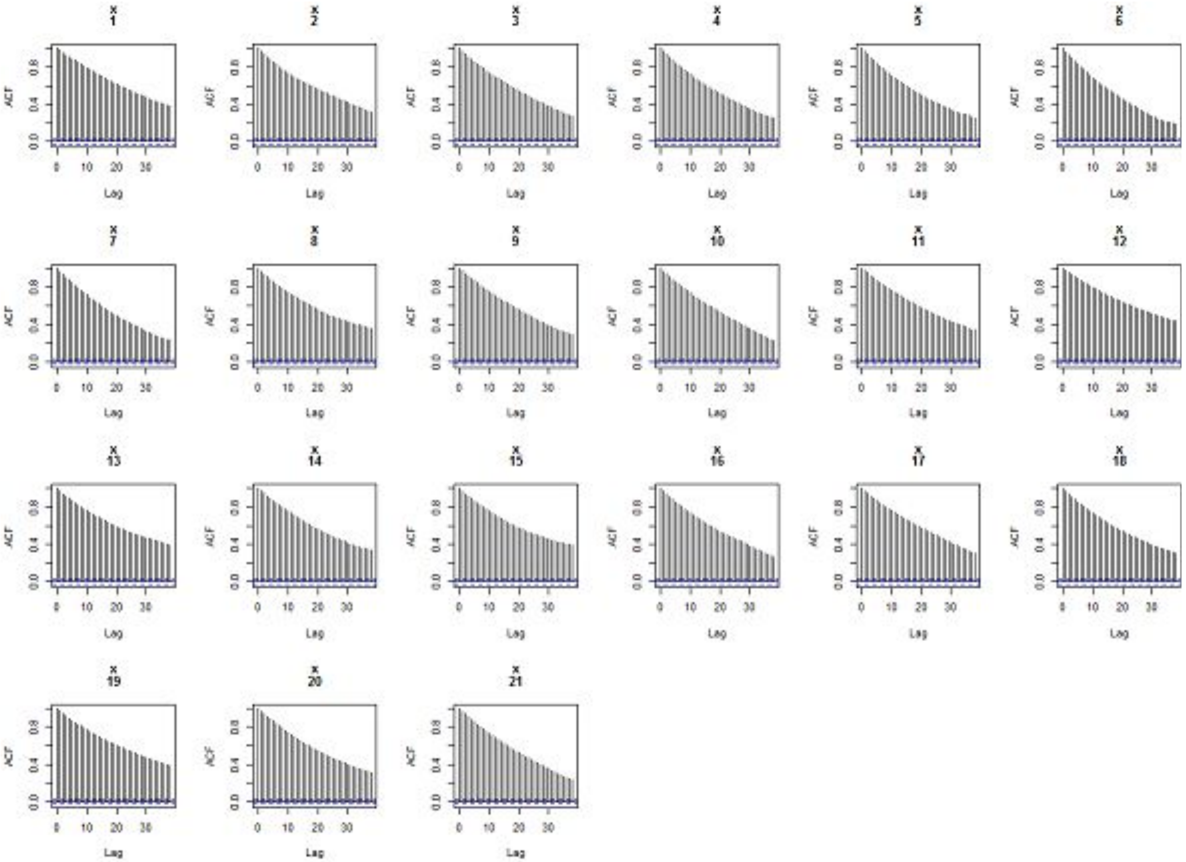
Hamiltonian Monte Carlo

Transform density into potential energy.

U = -log(f)



Autocorrelation: MH



Autocorrelation: HMC