John Vastola
10/17/18

Consider a Lagrangian

$$L = \sum_{j=1}^{N} \frac{(\dot{x}_j - f_j)^2}{2g_j^2} \tag{1}$$

which describes the least action trajectory for a stochastic system governed by the SDEs

$$\dot{x}_i = f_i + g_i \eta_i \ .$$

We want to derive Hamilton's equations and show that energy is conserved.

1 Deriving Hamilton's equations in one dimension

For simplicity's sake, let's look at things in one dimension first, where

$$L = \frac{(\dot{x} - f)^2}{2g^2}$$

The rub is that our canonical momentum p, defined in terms of the Lagrangian as

$$p := \frac{\partial L}{\partial \dot{x}} \ ,$$

will now depend on x, since for our Lagrangian we have

$$p(x) = \frac{\dot{x} - f(x)}{g(x)^2} \ .$$

Usually in Hamiltonian mechanics, we assume that we are working with velocity-independent potentials, allowing us to say that p is a function of $\dot{x}$ only. Sometimes we work with velocity-*dependent* potentials (for example, to describe a charged particle in a magnetic field), but those potentials are usually handled on a case by case basis.

How do we deal with the fact that momentum depends on x, in a possibly complicated way? The answer turns out to be surprisingly simple. We will just do what we normally do, but take the partial derivative of p with respect to x into account. For example:

$$\frac{dH}{dx} = \frac{\partial H}{\partial x} + \frac{\partial H}{\partial p}\frac{\partial p}{\partial x} \ .$$

Let's now derive our Hamilton's equations. Note that

$$\begin{aligned}
\frac{dH}{dx} &= \frac{d}{dx}\left[p\dot{x} - L\right] \\
&= \frac{\partial p}{\partial x}\dot{x} - \frac{dL}{dx} \\
&= \frac{\partial p}{\partial x}\dot{x} - \frac{\partial L}{\partial x} \\
&= \frac{\partial p}{\partial x}\dot{x} - \dot{p}
\end{aligned}$$

where we have used the Euler-Lagrange equation in the last step. On the other hand,

$$\begin{aligned}
\frac{\partial H}{\partial p} &= \frac{\partial}{\partial p}\left[\frac{g^2}{2}p^2 + fp\right] \\
&= g^2 p + f \\
&= \dot{x}
\end{aligned}$$

which means that

$$\begin{aligned}
\frac{dH}{dx} &= \frac{\partial H}{\partial x} + \frac{\partial H}{\partial p}\frac{\partial p}{\partial x} \\
&= \frac{\partial H}{\partial x} + \dot{x}\frac{\partial p}{\partial x}
\end{aligned}$$

Hence,

$$\begin{aligned}
\frac{\partial H}{\partial x} + \dot{x}\frac{\partial p}{\partial x} &= \frac{\partial p}{\partial x}\dot{x} - \dot{p} \\
\implies \quad \frac{\partial H}{\partial x} &= -\dot{p}
\end{aligned}$$

which means that our set of Hamilton's equations is the same as always:

$$\boxed{\begin{aligned}
\frac{\partial H}{\partial x} &= -\dot{p} \\
\frac{\partial H}{\partial p} &= \dot{x}
\end{aligned}}$$

(2a), (2b)

One must keep in mind what $\partial H/\partial x$ means: we are differentiating with respect to x *only as it appears explicitly in the Hamiltonian*, ignoring the fact that p depends on x. In this way, we can treat p and x independently in our Hamiltonian formulation.

2 Conservation of energy in one dimension

To show that an energy-like quantity is conserved, we need a few facts about the canonical momentum p. Note that

$$\dot{x} = g^2 p + f \implies \ddot{x} = g^2 \dot{p} + [2gg'p + f']\,\dot{x}$$

and that

$$\frac{\partial p}{\partial x} = -\frac{1}{g^2}\,[2gg'p + f']$$

so that

$$\ddot{x} = g^2\left[\dot{p} - \frac{\partial p}{\partial x}\dot{x}\right]$$

Also, note that

$$\frac{dH}{d\dot{x}} = \frac{d}{d\dot{x}}\,[p\dot{x} - L] = \frac{\partial p}{\partial \dot{x}}\dot{x} + p - \frac{\partial L}{\partial \dot{x}} = \frac{\dot{x}}{g^2} + p - p = \frac{\dot{x}}{g^2}$$

Finally, thinking of H as a function of x and $\dot{x}$ (which is a little easier, since x and $\dot{x}$ are genuinely independent variables):

$$\begin{aligned}
\frac{dH}{dt} &= \frac{\partial H}{\partial t} + \frac{dH}{dx}\dot{x} + \frac{dH}{d\dot{x}}\ddot{x} \\
&= \left[\frac{\partial H}{\partial x} + \frac{\partial H}{\partial p}\frac{\partial p}{\partial x}\right]\dot{x} + \frac{dH}{d\dot{x}}\ddot{x} \\
&= \left[-\dot{p} + \dot{x}\frac{\partial p}{\partial x}\right]\dot{x} + \frac{\dot{x}}{g^2}g^2\left[\dot{p} - \frac{\partial p}{\partial x}\dot{x}\right] \\
&= \left[-\dot{p} + \dot{x}\frac{\partial p}{\partial x}\right]\dot{x} + \dot{x}\left[\dot{p} - \frac{\partial p}{\partial x}\dot{x}\right] \\
&= 0
\end{aligned}$$

so the Hamiltonian is indeed conserved, as desired.

3 General results

The substance of our arguments for the general case completely matches the substance of our arguments for the one-dimensional case; still, we include the general result for completeness' sake.

Note that

$$\begin{aligned}
\frac{dH}{dx_i} &= \frac{d}{dx_i}\left[\sum_j p_j \dot{x}_j - L\right] \\
&= \sum_j \frac{\partial p_j}{\partial x_i}\dot{x}_j - \frac{dL}{dx_i} \\
&= \sum_j \frac{\partial p_j}{\partial x_i}\dot{x}_j - \frac{\partial L}{\partial x_i} \\
&= \sum_j \frac{\partial p_j}{\partial x_i}\dot{x}_j - \dot{p}_i
\end{aligned}$$

where we have used an Euler-Lagrange equation in the last step. On the other hand,

$$\begin{aligned}
\frac{\partial H}{\partial p_i} &= \frac{\partial}{\partial p_i}\left[\sum_j \frac{g_j^2}{2}p_j^2 + f_j p_j\right] \\
&= g_i^2 p_i + f_i \\
&= \dot{x}_i
\end{aligned}$$

which means that

$$\begin{aligned}
\frac{dH}{dx_i} &= \frac{\partial H}{\partial x_i} + \sum_j \frac{\partial H}{\partial p_j}\frac{\partial p_j}{\partial x_i} \\
&= \frac{\partial H}{\partial x_i} + \sum_j \dot{x}_j \frac{\partial p_j}{\partial x_i}
\end{aligned}$$

Hence,

$$\begin{aligned}
\frac{\partial H}{\partial x_i} + \sum_j \dot{x}_j \frac{\partial p_j}{\partial x_i} &= \sum_j \frac{\partial p_j}{\partial x_i}\dot{x}_j - \dot{p}_i \\
\Longrightarrow \quad \frac{\partial H}{\partial x_i} &= -\dot{p}_i
\end{aligned}$$

which means that our set of Hamilton's equations is just:

$$\boxed{\begin{aligned}
\frac{\partial H}{\partial x_i} &= -\dot{p}_i \qquad (3a) \\
\frac{\partial H}{\partial p_i} &= \dot{x}_i \qquad (3b)
\end{aligned}}$$

for $i = 1, 2, ..., N$.

Now for the conservation of energy. Note,

$$\dot{x}_i = g_i^2 p_i + f_i \implies \ddot{x}_i = g_i^2 \dot{p}_i + \sum_j \left[2g_i \frac{\partial g_i}{\partial x_j} p_i + \frac{\partial f_i}{\partial x_j} \right] \dot{x}_j$$

and that

$$\frac{\partial p_i}{\partial x_j} = -\frac{1}{g_i^2} \left[2g_i \frac{\partial g_i}{\partial x_j} p_i + \frac{\partial f_i}{\partial x_j} \right]$$

so that

$$\ddot{x}_i = g_i^2 \left[\dot{p}_i - \sum_j \frac{\partial p_i}{\partial x_j} \dot{x}_j \right]$$

Also, note that

$$\frac{dH}{d\dot{x}_i} = \frac{d}{d\dot{x}_i} \left[\sum_j p_j \dot{x}_j - L \right] = \sum_j \frac{\partial p_j}{\partial \dot{x}_i} \dot{x}_j + p_i - \frac{\partial L}{\partial \dot{x}_i} = \frac{\dot{x}_i}{g_i^2} + p_i - p_i = \frac{\dot{x}_i}{g_i^2}$$

Finally:

$$\begin{aligned}
\frac{dH}{dt} &= \frac{\partial H}{\partial t} + \sum_i \frac{dH}{dx_i} \dot{x}_i + \frac{dH}{d\dot{x}_i} \ddot{x}_i \\
&= \sum_i \left[\frac{\partial H}{\partial x_i} + \sum_j \dot{x}_j \frac{\partial p_j}{\partial x_i} \right] \dot{x}_i + \frac{dH}{d\dot{x}_i} \ddot{x}_i \\
&= \sum_i \left[-\dot{p}_i + \sum_j \dot{x}_j \frac{\partial p_j}{\partial x_i} \right] \dot{x}_i + \frac{\dot{x}_i}{g_i^2} g_i^2 \left[\dot{p}_i - \sum_j \frac{\partial p_i}{\partial x_j} \dot{x}_j \right] \\
&= \sum_i \left[-\dot{p}_i + \sum_j \dot{x}_j \frac{\partial p_j}{\partial x_i} \right] \dot{x}_i + \dot{x}_i \left[\dot{p}_i - \sum_j \frac{\partial p_i}{\partial x_j} \dot{x}_j \right] \\
&= \sum_i \sum_j \dot{x}_j \frac{\partial p_j}{\partial x_i} \dot{x}_i - \sum_i \sum_j \dot{x}_i \frac{\partial p_i}{\partial x_j} \dot{x}_j \\
&= \sum_i \sum_j \dot{x}_i \frac{\partial p_i}{\partial x_j} \dot{x}_j - \sum_i \sum_j \dot{x}_i \frac{\partial p_i}{\partial x_j} \dot{x}_j \\
&= 0
\end{aligned}$$

where we have relabeled the sum on the left to get our result (this is allowed, since both sums go from 1 to N and are independent). Hence, as desired, the Hamiltonian is conserved, even in the general case.

4 Usefulness of energy for studying transitions between attractors

Consider the general case, and let $x = (x_1, x_2, ..., x_N)$. If $y = (y_1, y_2, ..., y_N)$ is an attractor, it is true that $f_1(y) = f_2(y) = \cdots = f_N(y) = 0$. Hence, if the least action path goes through at least one attractor y, the energy E satisfies

$$E = H(y) = \sum_j \frac{g_j(y)^2}{2} p_j(y, \dot{y})^2 + f_j(y) p_j(y, \dot{y}) = \sum_j \frac{g_j(y)^2}{2} p_j(y, \dot{y})^2 \ .$$

In particular, suppose that we are interested in the least action path *between* two attractors y_0 (where the cell starts) and y_f (where the cell ends). Then it is true that

$$\sum_j \frac{g_j(y_0)^2}{2} p_j(y_0, \dot{y_0})^2 = \sum_j \frac{g_j(y_f)^2}{2} p_j(y_f, \dot{y_f})^2 \ .$$

Because

$$p_i(x, \dot{x}) = \frac{\dot{x}_i - f_i(x)}{g_i(x)^2} \ ,$$

we can rewrite this condition in terms of the velocities as

$$\sum_j \frac{\dot{y_{i0}}^2}{2 g_i(y_0)^2} = \sum_j \frac{\dot{y_{if}}^2}{2 g_j(y_f)^2} \ .$$

For example, if we have a two-dimensional system following a cell with coordinates $z = (x, y)$, with noise provided by functions $g_1 = \sigma_x x$ and $g_2 = \sigma_y y$, then for a transition between two attractors (x_0, y_0) and (x_f, y_f) we will have

$$\frac{\dot{x_0}^2}{2\sigma_x^2 x_0^2} + \frac{\dot{y_0}^2}{2\sigma_y^2 y_0^2} = \frac{\dot{x_f}^2}{2\sigma_x^2 x_f^2} + \frac{\dot{y_f}^2}{2\sigma_y^2 y_f^2} \ .$$