The principle of least action (Hamilton's variational principle)

By now we have become familiar with two formulations (or approaches) of classical mechaniss: the Newton formulation and the Lagrangian formulation. Both of them yield some differential equations of motions by solving which we can find the trajectories (or paths) that describe the state of our mechanical system at any given moment of time. The number of the (independent) equations of motion is equal to the number of degrees of freedom, which can be large if our system consists of many constituents/particles. It turns out (and this is remarkable!) that all those Lagrange equations of motions can be derived from a simple principle called the Hamilton's principle of least (or stationary) action. It can be stated as follows:

The motion of a mechanical system between time t_1 and t_2 is such that the integral

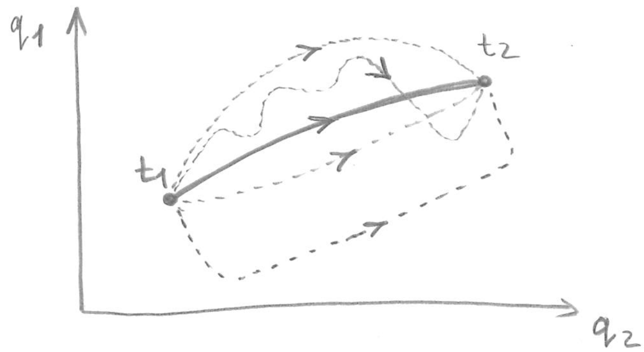
$$S = \int_{t_1}^{t_2} L(q_1, \ldots q_2, \dot{q}_1, \ldots \dot{q}_n, t)\, dt$$

has a stationary value for the actual path of the motion.

Here $L = T - V$ is the Lagrange function of the system (which depends on generalized coordinates q_k and generalized velocities $\dot{q}_k$; it may also have explicit dependence on time). The quantity S is called action.

Essentially the action integral takes the least possible value for any sufficiently short segment of the path. For

the entire path the integral must have an extremum.
The principle of least action can be used as the basic postulate of mechanics rather than Newton's laws of motion.



← of all physicaly possible paths the nature chooses the one that extremizes the action

When we vary the path of the system (in the corresponding n-dimensional configuration space, where n is the number of degrees of freedom) the extremum condition can be expressed as

$$\delta S = 0 \qquad \text{or} \qquad \delta \int_{t_1}^{t_2} L \, dt = 0$$

Before seeing how Lagrange's equations emerge from the principle of least action we must learn the basic concepts of the variational calculus.

Elements of the Calculus of Variation

A function is a rule (or correspondence), which associates a number (real or complex) with another number. In other words, it takes a number as input and excretes another number as output:

$$x_1 \xrightarrow{f(x_1)} f_1$$
$$x_2 \xrightarrow{f(x_2)} f_2$$
$$x_3 \xrightarrow{f(x_3)} f_3$$
$$\vdots$$

Of course we can also have functions that take vectors and excrete other vectors (and the number of components in the output vector could differ from the number of components of the input vector)

A functional is somewhat different from a function. It associates a number with a function. That is, it takes a function as input and excretes a number:

$$f_1(x) \xrightarrow{F[f_1(x)]} F_1$$
$$f_2(x) \xrightarrow{F[f_2(x)]} F_2$$
$$f_3(x) \xrightarrow{F[f_3(x)]} F_3$$
$$\vdots$$

The above definition of a functional can be well described as "a function of a function"

Here are some examples of functionals

1) $$F[f(x)] = \int_{x_1}^{x_2} f(x)\, dx$$

2) $$F[f(x,y)] = \int_{x_1}^{x_2} \int_{y_1}^{y_2} f(x,y)\, dx\, dy$$

3) $F_w[f(x)] = \int_{x_1}^{x_2} f(x)\, w(x)\, dx$ $\quad$ $w(x)$ - fixed weight function

4) $F[f(x)] = f(x_0)$ $\leftarrow$ a rule that associates a function with the values of that function at some particular point x_0 within interval $[x_1, x_2]$

or, alternatively

$$F_\delta[f(x)] = \int_{x_1}^{x_2} \delta(x-x_0) f(x)\, dx$$

In general a functional can itself be a function of a variable, i.e. may depend on some parameter in its definition, for example the upper limit of the integral or the point x_0 in example 4)

It should be noted that in physics functionals are most often appear as integrals.

Functionals can be linear as in example 1):

$$F[\alpha f(x) + \beta g(x)] = \alpha F[f(x)] + \beta F[g(x)]$$

or nonlinear, such as

$$F[f(x)] = \int_{x_1}^{x_2} \left(f(x)\right)^{5/3} dx$$

or

$$F_w[f_1(x), f_2(x)] = \int_a^b \int_a^b f_1(x_1)\, W(x_1, x_2)\, f_2(x_2)\, dx_1\, dx_2$$

The action integral in classical mechanics is a nonlinear functional

$$S[q(t)] = \int_{t_1}^{t_2} L(q(t), \dot{q}(t), t)\, dt$$

because $\dot{q}$ usually appears nonlinearly (e.g. as a square) in the Lagrange function.

Oftentimes we do not really need the complete knowledge of functional $F[f]$. Rather it is the behavior of F in the vicinity of the function f_0, which makes F extremal, is of the actual interest.

How do we find extrema of function $f(x)$? We send the independent variable x to $x+dx$ and demand that the change (variation) of f is zero to first order in dx:

$$df = 0$$

$$f(x+dx) = f(x) + f'(x)\,dx + \frac{1}{2} f''(x)\,(dx)^2 + \dots$$

$$df \equiv f(x+dx) - f(x) = f'(x)\,dx + O(dx^2)$$

the extrema occur at those points x^* for which

$$f'(x^*) = 0$$

In a somewhat similar way, to find extrema of functinal $F[f]$ we send the function

$$f(x) \longrightarrow f(x) + \delta f(x)$$

where $\delta f(x)$ is an arbitrary (yet very small in magnitude) variation of function f. We then demand that the change (variation) of F, which we can denote δF, vanishes up to first order in δf.

Often the variation $\delta f(x)$ must satisfy certain boundary conditions. For instance, if our $F[f]$ only operates on functions which take specific values at a pair of endpoints, i.e. $f(x_1) = \alpha$ & $f(x_2) = \beta$, we must allow only such functions in our functional. This requires that $\delta f(x_1) = \delta f(x_2) = 0$

Note that a variation of any function f by an infinitesimal but arbitrary amount can without any loss of generality be represented in the form

$$\delta f(x) = \varepsilon \eta(x)$$

where ε is an infinitesimal number and $\eta(x)$ is an arbitrary (and not necessarily small) function. In the case of several independent variables it is also true:

$$\delta f(x, y, \dots) = \varepsilon \eta(x, y, \dots)$$

In order to explore extrema of functionals we have to introduce a generalization of the derivative – the functional derivative. It can be defined as the variation δF of the functional $F[f]$, which results from variation of f by δf,

$$\delta F = F[f + \delta f] - F[f]$$

The technique we can use to evaluate δF is a Maclaurin expansion of $F[f+\delta f] = F[f+\varepsilon\eta]$ in powers of δf, respectively of ε. The functional $F[f+\varepsilon\eta]$ is now an ordinary function of parameter ε. Therefore we can expand $F[f+\varepsilon\eta]$ in powers of ε:

$$F[f+\varepsilon\eta] = F[f] + \left.\frac{dF[f+\varepsilon\eta]}{d\varepsilon}\right|_{\varepsilon=0} \varepsilon + \frac{1}{2!} \left.\frac{d^2F[f+\varepsilon\eta]}{d\varepsilon^2}\right|_{\varepsilon=0} \varepsilon^2 + \dots$$

The series can be finite or infinite. In the latter case it has to be assumed that $F(\varepsilon)$ is differentiable any number of times

The derivatives with respect to ε now have to be related to the functional derivatives. The definition of the functional derivative (sometimes called variational derivative) is

$$\left.\frac{dF[f+\varepsilon\eta]}{d\varepsilon}\right|_{\varepsilon=0} = \int \underbrace{\frac{\delta F[f(x)]}{\delta f(x)}}_{\text{functional derivative}} \eta(x)\, dx \qquad (*)$$

Our definition certainly implies that the left-hand side can be represented in the form of a linear functional that appears on the right-hand side. In general this is not guaranteed, but we will not go into into depths here.

In a similar way we can define higher order functional derivatives, e.g

$$\left.\frac{d^2F[f+\varepsilon\eta]}{d\varepsilon^2}\right|_{\varepsilon=0} = \iint \frac{\delta^2 F[f]}{\delta f(x_1)\,\delta f(x_2)} \eta(x_1)\,\eta(x_2)\,dx_1\,dx_2$$

These derivatives constitute the kernel of the Maclaurin expansion of F in terms of the variation $\delta f(x) = \varepsilon\eta(x)$:

$$F[f+\varepsilon\eta] = \sum_{n=0}^{N} \frac{1}{n!} \int \frac{\delta^n F[f]}{\delta f(x_1)\ldots\delta f(x_n)} \delta f(x_1)\ldots\delta f(x_n)\, dx_1 \ldots dx_n$$

(N can be finite or infinite depending on the functional)

Let us consider some examples

1) $F_\delta[f] = \int_{x_1}^{x_2} \delta(x-x_0)\, f(x)\, dx$

by looking at formula $(*)$ above we can immediately see that

$$\frac{\delta F_\delta}{\delta f(x)} = \delta(x-x_0) \qquad \text{as } \eta(x) \text{ can vary arbitrarily.}$$

We can also recast it as a very useful formula given that $F_\delta[f] = f(x_0)$:

$$\frac{\delta F_\delta}{\delta f(x)} = \frac{\delta f(x_0)}{\delta f(x)} = \delta(x - x_0)$$

All higher order functional derivatives of F_δ vanish.

2) $$F[f] = \int \delta(x - x_0) f^\alpha(x)\, dx \qquad \alpha = \text{const}$$

or

$$F[f] = f^\alpha(x_0)$$

The variation of F can be evaluated by Maclaurin expansion :

$$\delta f^\alpha(x_0) = \int \delta(x - x_0) \left\{ (f(x) + \varepsilon\eta(x))^\alpha - f^\alpha(x) \right\} dx =$$

$$= \int \delta(x - x_0) \left\{ \alpha f^{\alpha-1}(x)\, \varepsilon\eta(x) + \frac{\alpha(\alpha-1)}{2} f^{\alpha-2}(x)\, \varepsilon^2 \eta^2(x) + \dots \right\} dx$$

So we see that

$$\frac{\delta F}{\delta f} = \frac{\delta f^\alpha(x_0)}{\delta f(x)} = \delta(x - x_0)\, \alpha f^{\alpha-1}(x)$$

Moreover, by reusing the last expression we could show

$$\frac{\delta^2 f^\alpha(x_0)}{\delta f(x_1) \delta f(x_2)} = \delta(x_1 - x_0)\, \delta(x_2 - x_0)\, \alpha(\alpha - 1) f^{\alpha-2}(x)$$

3) $$F[f] = \int (f(x))^{5/3} dx$$

Here we can write variation δF in the form of a binomial expansion :

$$\delta F = \int \left\{ (f(x) + \varepsilon\eta(x))^{5/3} - f^{5/3}(x) \right\} dx$$

$$(f+\varepsilon\eta)^{5/3} - f^{5/3} = f^{5/3}\left(1+\frac{\varepsilon\eta}{f}\right)^{5/3} - f^{5/3}$$

$$= f^{5/3}\sum_{k=0}^{\infty}\binom{5/3}{k} 1^{5/3-k}\left(\frac{\varepsilon\eta}{f}\right)^{k}$$

(recall that $(a+b)^s = \sum_{k=0}^{\infty}\binom{s}{k} a^{s-k} b^k$ where $\binom{s}{k} = \frac{(s)_k}{k!} =$

$= \frac{s(s-1)\ldots(s-k+1)}{k!}$)

so in our case we have

$$\delta F = \int f^{5/3}(x)\sum_{k=1}^{\infty}\binom{5/3}{k}\left(\frac{\varepsilon\eta(x)}{f(x)}\right)^{k} dx$$

then we immediately relate

$$\frac{\delta F}{\delta f(x)} = f^{5/3}(x)\cdot\frac{5/3}{1!}\,\frac{1}{f(x)} = \frac{5}{3} f^{2/3}(x)$$