Very brief introduction to Functionals

Function : a mathematical relation which maps one (or more) numbers (known as variables) into one number (the value of the function). Notation: $f(x, y, z, ...)$.

Example: if $f(x) = 3x$ then $x = 1 \rightarrow f = 3$, $x = 2 \rightarrow f = 6$, etc.

Functional : a mathematical relation which maps one (or more) **functions** into one number. Notation $F[f, g, h...]$.

Example: $F[f] = \int_0^1 dx f^2(x)$. If $f(x) = x \rightarrow F = 1/3$, if $f(x) = 1 \rightarrow F = 1$, etc. Some care must be taken that the argument functions are well-behaved mathematically.

Example: $F[f, g] = \int_0^\infty dx(f(x)/g(x) - x^3 g(x))$. As long as the integrand is well-behaved, we can find a value for F given any $f(x)$ and $g(x)$.

Action is a functional depending on the generalized coordinates. For instance, assume that we have just one degree of freedom, and suppose that we know that $\mathcal{L}(q, \dot{q}, t) = 3\dot{q}^2 + 4q$ (we will learn next how to find the Lagrangian for any given mechanical system). Hamilton's principle tells us that the true trajectory $q(t)$ is the one function $q(t)$ which minimizes $S = \int_{t_1}^{t_2} dt\mathcal{L}$ and also satisfies the boundary conditions $q(t_1) = q_1$ and $q(t_2) = q_2$.

How can we find this function? One (terrible) way is to try various possibilities, and see which works best. For instance, we could try a linear function $q(t) = at + b$. Our trial function must satisfy the boundary conditions. The only linear function that does is $q(t) = q_1 + q_2(t - t_1)/(t_2 - t_1)$. For simplicity, let's assume that we have $t_1 = 0$, $q_1 = 0$, $t_2 = 1$, $q_2 = 1$ (in some proper units), in which case $q(t) = t$. For this "guess", we have $\dot{q} = 1$ and therefore

$$S = \int_0^1 dt\,(3 + 4t) = 5$$

But we could also try a quadratic function, $q(t) = a + bt + ct^2$. This satisfies the boundary conditions if $a = 0$ and $b + c = 1$, so the most general form for such a trial function is $q(t) = bt + (1 - b)t^2$. Then $\dot{q} = b + 2(1 - b)t$ and we find

$$S(b) = \int_0^1 dt\left(3(b + 2(1 - b)t)^2 + 4(bt + (1 - b)t^2)\right) = \frac{16}{3} - \frac{4}{3}b + b^2$$

Remember that we're trying to find the minimum possible value, which is obtained when $dS/db = 0$, $d^2S/db^2 > 0 \rightarrow b = 2/3 \rightarrow S_{min} = 44/9$. In other words, the choice $q(t) = 2/3t + 1/3t^2$ is better than $q(t) = t$, since it leads to a lower value for the action. But now you see the problem with this approach: we could try third order polynomials, fourth order polynomials and so on and so forth. But we could also try exponentials, square roots, logarithmic dependencies ... Besides the fact that this problem would occupy the rest of our lives, we could never be quite sure that there isn't a better function that would lead to an even lower value for S!

So let us learn how to solve this problem nicely and painlessly.

Extremum of a functional

We know that a **function** reaches an extremum value when its derivative is zero. In other words, if x_0 is the value for which $f(x_0)$ has an extremum (min. or max. value), then for any small variation δx we have $f(x_0 + \delta x) - f(x) = \delta x \frac{df}{dx} = 0$ (see definition of derivative).

For **functionals**, the situation is very similar. An extremum is given by the function f if, for any small variation δf, we have $\delta F = F[f + \delta f] - F[f] = 0$ (here, we assume that any term proportional to $(\delta f)^2$, $(\delta f)^3$ etc is vanishingly small). This means that to first order, small variations in the argument f do not change the value of the functional, F, if we are at an extremum.

Example: **Q** for what expression of $f(x)$ does the functional $F[f] = \int_0^1 (3f^2(x) - xf(x))$ take an extremum value?

A: Keeping only terms up to δf, we find:

$$F[f + \delta f] = \int_0^1 \left[3(f^2 + 2f\delta f + ...) - x(f + \delta f)\right] dx$$

and therefore

$$F[f + \delta f) - F[f] = \int_0^1 \delta f(x)\,[6f(x) - x]\, dx$$

This quantity is zero for any small variation δf if and only if $6f(x) - x = 0 \to f(x) = x/6$.

Euler equations

Assume that we have a functional of the following particular form (single degree of freedom):

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

and we want to find the condition for an extremum which satisfies the condition $q(t_1) = q_1$, $q(t_2) = q_2$. The function $\mathcal{L}$ is assumed to be known.

We proceed in the same way: we consider a small variation $\delta q(t)$ of the function $q(t)$. Then, the function $\dot{q}(t)$ will vary by the amount $\frac{d}{dt}\delta q(t)$. Since the boundary condition must be satisfied by all functions $q(t)$ considered (and therefore, in particular, by $q + \delta q$), it follows that we can only use small variations $\delta q(t)$ for which $\delta q(t_1) = \delta q(t_2) = 0$.

Then,

$$S[q + \delta q] - S[q] = \int_{t_1}^{t_2} dt \left[\mathcal{L}(q + \delta q, \dot{q} + \frac{d}{dt}\delta q, t) - \mathcal{L}(q, \dot{q}, t)\right] = \int_{t_1}^{t_2} dt \left[\frac{\partial \mathcal{L}}{\partial q}\delta q + \frac{\partial \mathcal{L}}{\partial \dot{q}}\frac{d}{dt}\delta q\right]$$

We have now to integrate the second term by parts, since we need the dependence on δq, not on its time derivative. We have:

$$\int_{t_1}^{t_2} dt \frac{\partial \mathcal{L}}{\partial \dot{q}}\frac{d}{dt}\delta q = \frac{\partial \mathcal{L}}{\partial \dot{q}}\delta q(t)|_{t_1}^{t_2} - \int_{t_1}^{t_2} dt \left(\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}}\right)\delta q(t) = -\int_{t_1}^{t_2} dt \left(\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}}\right)\delta q(t)$$

since $\delta q(t_1) = \delta q(t_2) = 0$.

Collecting the terms, we finally find that:

$$S[q + \delta q] - S[q] = \int_{t_1}^{t_2} dt \left(\frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}}\right)\delta q(t)$$

It follows that the extremum is reached when

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}} - \frac{\partial \mathcal{L}}{\partial q} = 0$$

This is the famous **Euler-Lagrange equation**. If there are $s > 1$ degrees of freedom, one can follow the same procedure and show that the extremum of the action is reached when the Euler-Lagrange equations:

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_i} - \frac{\partial \mathcal{L}}{\partial q_i} = 0$$

are satisfied for all $i = 1, 2, ..., s$ generalized coordinates.

In Lagrangian formalism, the Euler-Lagrange equations provide the equations of motion of the system (the equivalent of Newton's second law).

Observations

A. We now understand why we require that $\mathcal{L}$ is a function of $q, \dot{q}$ and t only. If we added higher order derivatives, such as $\ddot{q}$, ... , then we would have third or higher order derivatives of the generalized coordinates appearing in the Euler-Lagrange equations. We know (from Newtonian mechanics, based on experimental evidence), that the equations of motion involve only accelerations, speeds and coordinates (plus time), and therefore this implies that $\mathcal{L}$ can be a function of only $q, \dot{q}$ and t.

B. Dynamics is invariant to a scaling of the Lagrangian by an overall factor. This will change the action by the same overall constant, but the Euler-Lagrange equations are unaffected and therefore the dynamics is the same. We will make a particular convention on choosing a "magnitude" for the Lagrangians, but this scaling property is quite useful, as we will learn later.

C. Dynamics is invariant if we add the total time derivative of any well-behaved function of $f(q,t)$ to the Lagrangian, i.e. $\mathcal{L}' = \mathcal{L} + df(q,t)/dt$. (f should not depend on higher order derivatives of q since that would imply that the new Lagrangian depends on $\ddot{q}$ or higher derivatives – see A). This can be demonstrated from Hamilton's principle directly, since such a change implies a change in the total action

$$S' = \int_{t_1}^{t_2} dt\mathcal{L}(q, \dot{q}, t) + \int_{t_1}^{t_2} dt\frac{df(q,t)}{dt} = S + f(q,t)|_{t_1}^{t_2} = S + f(q_2, t_2) - f(q_1, t_1)$$

Since the initial and final points are fixed, all that happened is that we added an overall constant to the action. This will not change the extremum condition, and therefore the dynamics of the system is unchanged. The invariance can be shown directly on the Euler-Lagrange equations as well.

Before continuing with Lagrangian mechanics, it is useful to point out such "optimization problems" can be used to solve a variety of problems outside mechanics.

Optimization problems

These are problems in which one tries to find a solution which provides an extremum for some global condition. One can think, for instance, of economic problems, where one wants to maximize profit from investing certain amounts of money in certain stocks over time, when the financial markets have a certain evolution, etc.

Here, we will consider a few simpler examples.

Example 1. What is the path that provides the shortest distance between two points?

Solution: Let us assume (with no loss in generality) that the two points are in the $z = 0$ plane and that they have coordinates (x_1, y_1) and (x_2, y_2). Let $y(x)$ be a path that links the two points. It follows that $y(x)$ must satisfy the condition $y(x_1) = y_1$ and $y(x_2) = y_2$ (see Fig. 1).

For the infinitesimal interval between $[x, x + dx]$, the length of the path is $ds = \sqrt{dx^2 + dy^2} = dx\sqrt{1 + (dy/dx)^2}$. It follows that the total length of the path must be

$$L[y] = \int_{x_1}^{x_2} dx\sqrt{1 + \left(\frac{dy}{dx}\right)^2}$$

We already know the solution which minimizes this problem. If we look at the Euler-Lagrange equation, here we have the same type of functional, if we equate $L \to S$, $y \to q$, $x \to t$ and therefore $\dot{y} = dy/dx \to dq/dt = \dot{q}$ and the function $\mathcal{L}(y, \dot{y}, x) = \sqrt{1+\dot{y}^2}$. With these notations, the Euler-Lagrange equation is

$$\frac{d}{dx}\frac{\partial \mathcal{L}}{\partial \dot{y}} - \frac{\partial \mathcal{L}}{\partial y} = 0$$

Since $\mathcal{L}$ has no explicit dependence on y, it follows that $\frac{\partial \mathcal{L}}{\partial y} = 0$, while $\frac{\partial \mathcal{L}}{\partial \dot{y}} = \dot{y}/\sqrt{1+\dot{y}^2}$. Then, we must have:

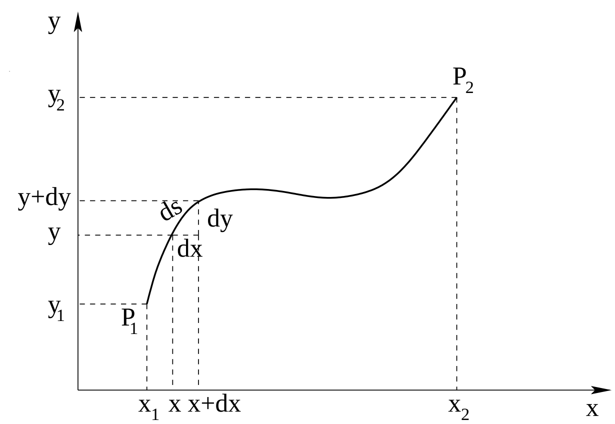

Fig 1. Figure for problem 1.

$$0 = \frac{d}{dx}\frac{\dot{y}}{\sqrt{1+\dot{y}^2}} \to \frac{\dot{y}}{\sqrt{1+\dot{y}^2}} = const \to \dot{y} = const \to y(x) = \alpha x + \beta.$$

The unknowns constants α and β are given by the conditions $y(x_1) = y_1$ and $y(x_2) = y_2$, leading to the final solution

$$y(x) = \frac{(y_2 - y_1)}{x_2 - x_1}x + \frac{y_2 x_1 - y_1 x_2}{x_2 - x_1}$$

In other words, the path minimizing the total distance is the straight line between the points.

Example 2. This is a famous problem in the history of physics, called the "brachistochrone", and solved by Bernoulli in 1696: consider a particle that starts at rest from $x = 0$ and height $z = 0$ and moves in the plane $y = 0$ to a lower position $x = d$, $z = h$ (see Fig. 2). If the particle moves in the gravitational field of the Earth, what must be the shape of the curve $z(x)$ such that the **time** needed for the particle to move between the two points is minimized?

Solution As already discussed in Example 1, the length of the path as the particle moves between $[z, z+dz]$ is $ds = \sqrt{dx^2 + dz^2} = dz\sqrt{1+\dot{x}^2}$, where we now use the shorthand notation $\dot{x} = dx/dz$.

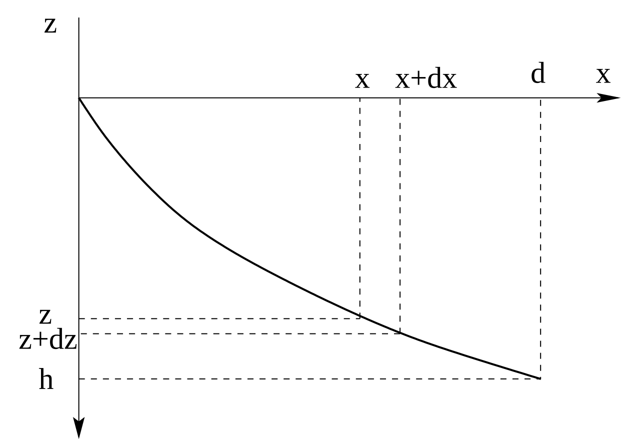

Fig 2. Figure for problem 2.

The time dt needed to move along the length ds is given by $dt = ds/v(z)$, where $v(z)$ is the speed of the particle when its height is z (we know that the speed is always tangential to the path). From the conservation of energy we have $mv^2/2 - mgz = ct$, where the constant is found to be zero from the initial conditions $v = 0$ for $x = z = 0$. Then

$$v(z) = \sqrt{2gz}$$

(the speed is a positive number, so the $-\sqrt{2gz}$ solution is physically unacceptable), and we find the total time to move from $z = 0$ to $z = h$ to be

$$T[z] = \int_0^h dz \frac{\sqrt{1+\dot{x}^2}}{\sqrt{2gz}}$$

We use again the Euler-Lagrange equation to find the solution $x(z)$ which minimizes this functional. In this case, $\mathcal{L}(x, \dot{x}, z) = \sqrt{1+\dot{x}^2}/\sqrt{2gz}$ and therefore

$$\frac{\partial \mathcal{L}}{\partial \dot{x}} = \frac{\dot{x}}{\sqrt{1+\dot{x}^2}\sqrt{2gz}}$$

while

$$\frac{\partial \mathcal{L}}{\partial x} = 0$$

Then, the E-L equation becomes:

$$\frac{d}{dz}\frac{\partial \mathcal{L}}{\partial \dot{x}} - \frac{\partial \mathcal{L}}{\partial x} = 0 \rightarrow \frac{d}{dz}\left(\frac{\dot{x}}{\sqrt{1+\dot{x}^2}\sqrt{2gz}}\right) = 0 \rightarrow \frac{\dot{x}}{\sqrt{1+\dot{x}^2}\sqrt{2gz}} = c_1$$

where c_1 is a constant. We can now square this to find

$$\frac{\dot{x}^2}{(1+\dot{x}^2)(2gz)} = c_1^2 \rightarrow \dot{x} = \frac{dx}{dz} = \sqrt{\frac{2gzc_1^2}{1-2gzc_1^2}}$$

Now, we integrate from the initial point $x = 0, z = 0$ to some point on the curve (x, z) to find:

$$x = \int_0^z dz \sqrt{\frac{2gzc_1^2}{1-2gzc_1^2}}$$

We know that the expression under the square root must be positive, because x is certainly a real number. It follows that $1 > 2gzc_1^2 > 0$, and so we make the substitution:

$$2gzc_1^2 = \sin^2\frac{\theta}{2} \rightarrow 1 - 2gzc_1^2 = \cos^2\frac{\theta}{2} \rightarrow \sqrt{\frac{2gzc_1^2}{1-2gzc_1^2}} = \frac{\sin\frac{\theta}{2}}{\cos\frac{\theta}{2}}$$

(the factor of 2 turns out to be convenient at the end, otherwise one could certainly choose just $\sin^2\theta$ in the substitution. We could also choose $\cos^2$, but $\sin^2$ is more convenient since it follows that for $z = 0 \rightarrow \theta = 0$, which is nice). Taking the variation, we also find:

$$2gc_1^2 dz = \sin\frac{\theta}{2}\cos\frac{\theta}{2}d\theta$$

We use the angle θ to parameterize the solution. We already know that

$$z = \frac{1}{2gc_1^2}\sin^2\frac{\theta}{2} = \frac{1}{4gc_1^2}(1-\cos\theta)$$

and

$$x = \int_0^\theta \frac{d\theta \sin\frac{\theta}{2}\cos\frac{\theta}{2}}{2gc_1^2}\frac{\sin\frac{\theta}{2}}{\cos\frac{\theta}{2}} = ... = \frac{1}{4gc_1^2}(\theta - \sin\theta)$$

Since both x and z are distances, let us use a new constant $a = \frac{1}{4gc_1^2}$ which must be some length, to be determined from the condition that for $x = d$, $z = h$. The solution is then:

$$x = a(\theta - \sin\theta)$$

$$z = a(1 - \cos\theta)$$

Finding a as a function of d and h is rather ugly (one must solve the problem numerically). However, this solution has a very nice geometrical interpretation, shown in Fig. 3. Assume that P is a point on the circumference of a wheel of radius a. Then, the curve described by P as the wheel rotates (without sliding) an angle θ is precisely the brachistochrone. Such a curve is called a "cycloid". If you wish to see one experimentally, attach a small light on the wheel of a bike, and watch the curve it generates as the bike moves at night.

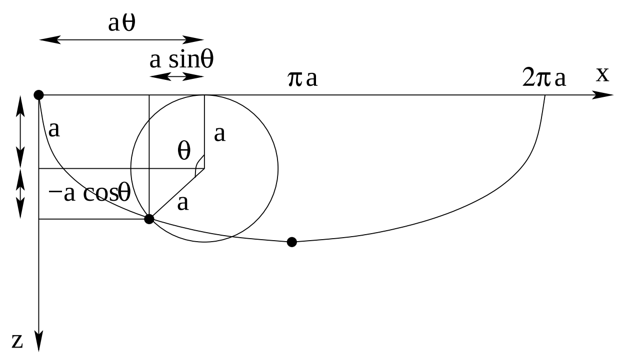

Fig 3. Figure for problem 2.

There are many more such examples, such as Fermat's principle in optics, the geodesics, etc – and, of course, all the Lagrangian mechanics we will be dealing with in the rest of this course. However, it is important to point out that there is a more general class of optimization problems, which involve additional constraints. The only constraints for the problems we considered are that the solution starts and ends at given points. However, there may be more general constraints. For instance, consider the following problem: we want to find the shape of the planar geometrical closed curve with the largest possible total area $\mathcal{A}$, for a fixed perimeter L. If this shape was a circle, than its radius is $2\pi r = L \to r = L/(2\pi)$, and therefore the corresponding area is $\mathcal{A} = \pi r^2 = L^2/(4\pi)$. If the shape is a square, then $L = 4a \to a = L/4$, and therefore $\mathcal{A} = a^2 = L^2/16$. This is smaller than the area of the corresponding circle, so clearly the answer is not the square. But maybe it is a parallelogram, or a hexagon, or some other unusual planar shape? It turns out that the extremum is given by the circle.

The constraint that the total perimeter L be fixed is a global constraint (it depends on the shape of the entire curve, not only its initial and final points), and therefore must be imposed in a different way than we imposed the boundary constraints. The technique to do this is well established, and involves the so-called "Lagrange multipliers". The main idea is that for each new such constraint, one must add a new term to the total functional. This new term is multiplied by an unknown constant (called a Lagrange multiplier), and is chosen in a specific way to enforce the desired constraint. Then, one finds the Euler-Lagrange equations for this more complicated functional, and the values of the Lagrange multipliers are found from the constraints.

This might sound complicated, but it is really quite simple. However, since we will not deal with such problems in the rest of the course, we will not study this technique here. Physics students are guaranteed to learn this technique in other courses.