Chapter 4: Functionals and the action principle

1 Introduction

In this chapter, I summarise, very briefly, the matter covered in the classes on functionals and the action principle. The importance of the principle is difficult to exaggerate, since it occupies a central position in physics today. But first, we need to define a functional.

2 Functional

Let us begin with things simple. We are familiar with mappings in the set theoretical sense: Let $\mathcal{A}$ and $\mathcal{B}$ be two sets. We have a mapping, or a function, from $\mathcal{A}$ to $\mathcal{B}$ if, for every element $A \in \mathcal{A}_1$, there is an element $b \in \mathcal{B}$ associated with it. That is, we write $f : a \to b$, or simply, $b = f(a)$.

We recognise two classes of mappings. The first one is one-to-one (injective) where each a goes to a distinct b. Example: $x \to \exp(x)$. In such a case, an inverse mapping is defined. In our example, it is the logarithm.

We are more interested in the case when the mapping is *not* injective. Consider the following simple examples, all of which involve only real numbers:

1. The most well known function $f(x) = x^2$ where $\pm x$ have the same image.

2. The mapping from the set of integers : $f(n) = 0$ if n is even, and $f(n) = 1$ when n is odd. That is, f is the positive remainder term when we divide an integer by 2.

3. Finally, the mapping of all nonzero real numbers, defined by: $f(x) = \frac{x}{|x|}$. All the positive numbers map to a single number $+1$, and the negative real numbers map to -1.

In example 1, a finite number of elements (2 to be precise) map to the same number. In example 2, an infinite number of them map to the same number, but they are still discrete. They are countable. But in the last example, a continuous set has a single number as its image. The last example is your first example of a functional!

So we now define a functional formally. If a continuous set maps to a number, then that number is called the functional. In other words, If all the elements that map to a given number form a continuous set, then b is called the functional associated with the set.

We are all familiar with continuous sets. In example 3 above, the two sets were negative and positive real numbers respectively. It does not require much effort to imagine higher dimensional sets: area segments in a plane, or regions in three dimensions. Consider the following examples.

1. The set $\mathcal{A}$ is the set of all points in a plane except those that lie on the x and y axes. We can then map each quadrant to an integer.

2. Indicator functions: Let R be the set of all points lying inside and on a closed loop in a plane. Let S be the region outside it. We then define the indicator function of R to be $I(P) = 1$ if $P \in R$ and $I(P) = 0$ if $P \in S$.

So functionals are abundant and natural. Even more familiar examples are what we discussed in the class: (i) length of a curve, (ii) area within a closed curve of a given perimeter, (iii) Mass of a body which has a position dependent density, so on and so forth.

We employ a sepcial notation to distinguish functionals from other functions. Let S be a continuous set. Then the functional of the set is written as $F[S]$. Let us again give some illustrations.

1. Let the collection of points $y = f(x)$ denote a curve extending between two end points x_1, x_2. Its length L is a functional and is written as $L = F[f(x)]$. For this reason, functionals are called functions of functions. As discussed in the class, F is given by the expression

$$F[f] = \int_{x_1}^{x_2} \left\{ dy(x)^2 + dx^2 \right\}^{\frac{1}{2}} \equiv \int_{x_1}^{x_2} \left\{ 1 + \left(\frac{dy}{dx} \right)^2 \right\}^{\frac{1}{2}} \mathrm{dx} \tag{1}$$

   We see that F is a property of the entire function.

2. One more example involving areas. Let C be a closed loop, enclosing the origin. At any angle θ let its distance from the origin be $r(\theta)$. Then the area enclosed within the loop is a functional of the loop. Its form will be

$$F = \int_0^{2\pi} r(\theta) \mathrm{d}r \mathrm{d}\theta \tag{2}$$

3 Linear continuous functional

We are not interested in any kind of functional, but in those that have some nice properties. The first property is linearity.

3.1 Linear functionals

Definition: Let f_1, f_2 be two functions. Let Ff_1 and Ff_2 be the corresponding functionals. We say that F is linear if,

- $F[kf] = kF[f]$, k a number
- $F[f_1 + f_2] = F[f_1] + F[f_2]$. It is assumed, of course, that the sum of the functions is well defined.

As ususal, some examples:

1. Overlap with a fixed $h(x)$ given by $F_h[f] = \int h(x)f(x)\mathrm{dx}$
2. Convolution given by $F_h[f] = \int h(x-y)f(y)\mathrm{dxdy}$

3.2 Continuous functionals

These are the most important class of functionals. For, without them, we cannot even initiate a study of calculus of variatons, on which the action principle rests.

I give a heuristic (hand waving) description. Consider a thread of length l. If it lies on the floor, the distance d, between its ends, can vary between 0 and l. This depends on the curve made by the thread, and we get l only when it is fully stretched in one direction. Two curves made by the thread can be transformed to each other by continuously alteration. Accordingly, we see that the functional $F[C] = d$ also varies continuously as we change the curve. This is an example of a continuoud functional.

Thus let $\{f(x;p)\}$ be a family of functions characterised by a set of k continuous parameters $\{p_1, p_2, \cdots, p_k\}$[1]. We say that that a functional is continuous if $F[f(x;p_1,p_2,\cdots,p_k)] \equiv \phi(p_1,p_2,\cdots,p_k)$ is a continuous function of the parameters.

In fact, we may demand more of functionals. That ϕ be differentiable too, as many times as required.

We are now in a position to state the variational problem involving functionals.

4 Extremal functionals

The first task is to impose a condition on the functionals (continuous sets, more precisely). For example, we may ask:

1. Of all the closed loops of a fixed perimeter, which of them encloses the largest area?
2. Of all the curves connecting two points in a plane, which of them has the shortest length?
3. Consider curves in a plane connecting two points P_1, P_2. Which of them generates a surface of minimum surface area when the curve is rotated about, say, y axis?
4. A thin rope of uniform mass density is hung between two points in a vertical plane. What would be that shape of the rope for which its centre of mass is at its lowest position?

[1] That is to say, as p vary continuously, we move among the curves smoothly.

We could add many more examples, but you realise that each of them involves the extremization of a family of functionals. In other words, we look for extrema (maxima or minima) of the function $\phi(p)$ defined above. To make this operational, we must define the functional derivative carefully.

4.1 Functional derivative

We need to build two notations. One of them is familar to you. That is dx. What does it tell us? Let $\mathcal{C}_1$ be a curve defined by $y = f_1(x)$. The notation dx means that you make a small displacement along the curve. On the other hand, let $\mathcal{C}_2$ be another curve very close to $\mathcal{C}$, defined by $y = f_2(x)$. A stricter definition, if you need , is the following. Choose any number, however small, $\epsilon > 0$. Demand that at every point x, $|f_2(x) - f_1(x)| \equiv |h(x)| < 0$. In this manner we can generate a curve as close to another as possible.

We are interested in the change that accrues in F when we move by $h(x)$, from f_1 to f_2. We now need a second notation. We denote, δx, the dispacement *away from* the curve, to reach a point on the other curve. The figure below illustrates it.

Do note the following: To move from a point on $\mathcal{C}_1$ to a neighbouring point on $\mathcal{C}_2$, we could adopt several equivalent procedures. The first consists of a single displacement δx . The second involves a δx followed by a dx along $\mathcal{C}_2$. The third one interchanges the order. We move by dx along $\mathcal{C}_1$ and then make a displacement δx to $\mathcal{C}_2$. Loosely speaking the operations commute, in the infinitesmal sense (and not in magnitude).

Keeping in mind our aim, I shall employ the following notation. The parameter that characterises the continuous set will be denoted by t, time for us. The functional is an integral of a function f which depends on generalised coordinates, q_i and generalised velocities $\dot{q}_i$. These are, of course, functions of time. In addition to this implicit dependence, f can also have explicit time dependence[2]. In short, we write the functional as

$$F[f(q_i, \dot{q}_, t)] = \int_{t_i}^{t_f} dt f(q_i, \dot{q}_, t) \tag{3}$$

You have concrete examples in Eq 1 and 2.

Our aim is to derive differential equations for the coordinates q_i as a function of time by extremising F. Note: The equation that emerges after extremization then automatically determines $\dot{q}_i$, after solving the differential equation with boundary conditions. But the extremal configuration will itself be obtained by varying both $q_i, \dot{q}_i$ independently. This should be borne in mind clearly.

Once this is settled, we can now vary the functional F. So starting from Eq 3, we write

$$\delta F = \int_{t_i}^{t_f} dt \Big\{ \frac{\partial f(q_i, \dot{q}_, t)}{\partial q_i} \delta q_i + \frac{\partial f(q_i, \dot{q}_i, t)}{\partial \dot{q}_i} \delta \dot{q}_i \Big\} \tag{4}$$

[2]More generally, books will denote the parameter by x, the place of q_i will be taken by functions $y_i(x)$ and similarly, $\dot{q}_i \rightarrow \frac{dy_i}{dx} \equiv y_i'$.

Summation over all the i values is implicit. We vary $q_i, \dot{q}_i$ independently (but infinitesmally) for all times except at the initial and final times. Why? because we are asking for a solution for the equation when we specify initial and final configurations, i.e., coordinates[3].

Let a specific configuration be the extrema. Then, by principles of calculus, δF around that configuration must vanish. So we demand that in Eq 4, $\delta F = 0$. To proceed further, we remember the interchangeability of δ and d. So we write

$$\delta \dot{q}_i = \frac{d}{dt}\delta q_i \tag{5}$$

in the second term of Eq 4, and integrate it by parts. So we write,

$$\frac{\partial f(q_i, \dot{q}, t)}{\partial \dot{q}_i}\frac{d}{dt}\delta q_i = \frac{d}{dt}\left\{\frac{\partial f(q_i, \dot{q}_i, t)}{\partial \dot{q}_i}\delta q_i\right\} - \frac{d}{dt}\left\{\frac{\partial f(q_i, \dot{q}, t)}{\partial \dot{q}_i}\right\}\delta q_i \tag{6}$$

Plugging it is Eq 4, we see that the first term in Eq 6 is a total derivative and, on integration, gives

$$\left\{\frac{\partial f(q_i, \dot{q}_i, t)}{\partial \dot{q}_i}\delta q_i\right\}\Bigg|_{t_i}^{t_f} \equiv 0 \tag{7}$$

since we *do not* vary the end points. The RHS in Eq 6 is called the boundary term. Finally, we get the equation

$$\delta F = \int_{t_i}^{t_f} dt \delta q_i \left[\frac{d}{dt}\left\{\frac{\partial f}{\partial \dot{q}_i}\right\} - \frac{\partial f}{\partial q_i}\right] = 0 \tag{8}$$

Pay attention to the integration variable. Here, each of δq_i, though infinitesmal, are arbitrary. The limits of the integration are also free. Hence, the only was that Eq 8 is satisfied is if the integrand itself vanishes. We conclude

$$\boxed{\frac{d}{dt}\left\{\frac{\partial f}{\partial \dot{q}_i}\right\} - \frac{\partial f}{\partial q_i} = 0;\ i = 1, \cdots, n} \tag{9}$$

This is a set of n differential equations and they are known as Euler equations in calculus of variations. But notice that the Lagrange equations which we derived from D'Alembert's principle for conservative forces has exactly the same form if we choose the Lagranagian, $L = T - V$ to be the function f. The functional itself is, then, given a special name – the action, and is usually denoted by teh symbol S.

Thus, we may state the action principle by rewriting the equations above with the replacements $F \to S$, $f \to L$. The equations are now called Euler Lagarnge equations.

$$\boxed{\frac{d}{dt}\left\{\frac{\partial L}{\partial \dot{q}_i}\right\} - \frac{\partial L}{\partial q_i} = 0;\ i = 1, \cdots, n} \tag{10}$$

[3]This is equivalent to specifying initial coordinates and initial momenta, as you know.

In generalised coordinates, the kinetic energy is a function of $q_i, \dot{q}_i$. The potential energy depends only on q_i. In the Newtonian case that we are discussing, it is also quadratic (actually bilinear) in velocities. So we may write

$$T = \sum_{i,k=1}^{n} m_{ik}(q)\dot{q}_i\dot{q}_k \tag{11}$$

where the symmetric coefficients m_{ik} depend only on the coordinates. It is a simple exercise for you to check that with this form, the Euler Lagrange equations become a set of n coupled second order differential equations in the coordinates. These are Newton's force equations for generalised coordinates.

There are a number of problems in problem set 2. Work them out. One exercise may be stated here.

Problem: What are the conditions on the symmetric matrix m_{ik}?. Hint: Kinetic energy is always positive unless the velocities vanish.