8 Variational Calculus

In this part of the course, we consider the energetics governing the shape of water droplets, soap films, bending beams etc. For systems with a few degrees of freedom (e.g., particle mechanics) you are used to the idea of solving equations of the form

$$\frac{d^2x}{dt^2} = -\frac{dU(x)}{dx}, \tag{175}$$

where $U(x)$ is an energy function. You will recall that the basic idea to understanding this type of equation is to first find the fixed points (the places where the force on the particle is zero) and then understand their stability. By piecing the trajectories that go into and out of the fixed points together you arrive at a complete description of how the system works, even if you can't calculate everything.

We now want to figure out how to think about solving such problems in continuous systems. In this case the state of the system is described not by discrete variables x_i but by functions $f_i(x)$. A good example of the difference is to consider a mass-spring system. If there are n masses connected by springs then we would want to know $x_i(t)$, the position of the ith mass. The limit of infinitely many small masses connected by small springs is an elastic rod, in which case we would want to know $h(x,t)$, the displacement of the rod at a given position x and time t. To develop techniques for continuous systems we consider an energy functional $U[f(x)]$, which is a function of a function. Several sorts of difficulties arise (mathematical and otherwise) when one tries to think about physical problems described by this energy using the same notions as those for finite dimensional dynamical systems. We will start by considering some simple problems.

8.1 What is the shortest path between two points?

It will come as no great surprise that it is a straight line, but lets show this to be the case. In 2D there is some function $h(x)$ that is the path between two points x_1 and x_2 (think of

$h(x)$ as the height above the x-axis). The length of the path is given by the functional

$$L[h] = \int_{x_1}^{x_2} dx \sqrt{1 + \left(\frac{dh}{dx}\right)^2}. \tag{176}$$

Now consider an alternate path $h(x)+\delta h(x)$ which is only slightly different from the previous path considered. The length of this path is

$$L[h + \delta h] = \int_{x_1}^{x_2} dx \sqrt{1 + \left(\frac{d}{dx}(h + \delta h)\right)^2}. \tag{177}$$

Taylor-expanding the integrand for small δh and keeping only terms of linear order in $\delta h' = d\delta h/dx$, we find

$$L[h + \delta h] - L[h] \simeq \int_{x_1}^{x_2} dx \frac{h' \delta h'}{\sqrt{1 + h'^2}}. \tag{178}$$

Integrating by parts gives

$$L[h + \delta h] - L[h] \simeq \left[\frac{h'}{\sqrt{1 + h'^2}} \delta h\right]_{x_1}^{x_2} - \int_{x_1}^{x_2} dx \left(\frac{h'}{\sqrt{1 + h'^2}}\right)' \delta h. \tag{179}$$

The first term on the right hand side is identically zero, as we require δh to be zero at either end (since we know our starting and ending point). Otherwise, for our path to be a minimum we require δL to be zero for arbitrary δh. If this were not the case we could always choose a δh and $-\delta h$ to increase or decrease the path length. Thus $h(x)$ must satisfy

$$\left(\frac{h'}{\sqrt{1 + h'^2}}\right)' = 0, \tag{180}$$

the solution of which is a straight line (check this for yourself). By analogy with systems containing few degrees of freedom we say that this solution satisfies the condition $\delta L/\delta h$=0.

8.2 Functional differentiation

We now generalize the example from the previous section by defining a formal functional derivative. To this end consider a general functional $I[f]$ of some function $f(x)$. A functionals is, by definition, a map that assigns a number to a function $f(x)$. Basic examples are the delta-functional $\Delta_{x_0}[f] := f(x_0)$, which is related to the delta function by

$$\Delta_{x_0}[f] = \int_{-\infty}^{\infty} dx\ \delta(x - x_0) f(x) = f(x_0), \tag{181a}$$

or integrals

$$J[f] = \int_{-\infty}^{\infty} dx\, f(x)\, c(x). \tag{181b}$$

A functional I is called *linear*, if it satisfies

$$I[af + bg] = aI[f] + bI[g] \tag{182}$$

for arbitrary numbers a, b and functions f, g. Obviously, both examples in Eq. (181) are linear. Typical examples of nonlinear functionals are action functionals, such as

$$S[x,\dot{x}] = \int_0^t ds\ \left[\frac{m}{2}\dot{x}(s)^2 - V(x(s))\right], \tag{183}$$

where, for example, $V(x) = kx^2/2$ for the harmonic oscillator.

Given some functional $I[f]$, we can define its point-wise *functional derivative* by

$$\frac{\delta I[f]}{\delta f(y)} = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\left\{I[f(x)+\epsilon\delta(x-y)] - I[f(x)]\right\} \tag{184}$$

If I is linear, this simplifies to

$$\frac{\delta I[f]}{\delta f(y)} = I[\delta(x-y)], \tag{185}$$

yielding, for example,

$$\frac{\delta \Delta_{x_0}[f]}{\delta f(y)} = \int dx\ \delta(x-x_0)\delta(x-y) = \delta(x_0-y_0) \tag{186a}$$

and

$$\frac{\delta J[f]}{\delta f(y)} = \int dx\,\delta(x-y)c(x) = c(y). \tag{186b}$$

Similar to ordinary derivatives, functional derivatives are linear[7]

$$\frac{\delta}{\delta f}\left\{aF[f]+bG[f]\right\} = a\frac{\delta F}{\delta f} + b\frac{\delta G}{\delta f}\ , \qquad a,b\in\mathbb{R}, \tag{187a}$$

satisfy the product rule

$$\frac{\delta}{\delta f}\left\{F[f]G[f]\right\} = \frac{\delta F}{\delta f}G[f] + F\frac{\delta G}{\delta f} \tag{187b}$$

as well as *two* chain rules

$$\frac{\delta}{\delta f}(F[g(f)]) = \frac{\delta(F[g(f)])}{\delta g}\frac{dg(x)}{df(x)} \tag{187c}$$

$$\frac{\delta}{\delta f}g(F[f]) = \frac{dg(F[f])}{dF}\frac{\delta(F[f])}{\delta f} \tag{187d}$$

As a nice little exercise, you can use the above properties to prove that the exponential functional

$$F[f] = e^{\int dx\ f(x)c(x)} \tag{188}$$

satisfies the *functional differential equation*

$$\frac{\delta F[f]}{\delta f(y)} = c(y)\,F[f]. \tag{189}$$

[7]See, e.g., Appendix A in Parr & Young, *Density-Functional Theory of Atoms and Molecules* (1989, Oxford University Press)

8.3 Euler-Lagrange equations

In practice, relevant functionals typically not just depend on a function but also on its derivatives, see Eq. (183). For instance, let us assume we are looking for a twice differentiable function $Y(x)$, satisfying the boundary conditions $Y(x_1) = y_1$, $Y(x_2) = y_2$ and minimizing the integral

$$I[Y] = \int_{x_1}^{x_2} f(x, Y, Y')dx. \tag{190}$$

What is the differential equation satisfied by $Y(x)$? To answer this question, we compute the functional derivative

$$\begin{aligned}
\frac{\delta I[Y]}{\delta Y} &= \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left\{ I[Y(x) + \epsilon\delta(x-y)] - I[Y(x)] \right\} \\
&= \int_{x_1}^{x_2} \left[\frac{\partial f}{\partial Y} \delta(x-y) + \frac{\partial f}{\partial Y'} \delta'(x-y) \right] dx \\
&= \int_{x_1}^{x_2} \left[\frac{\partial f}{\partial Y} - \frac{d}{dx} \frac{\partial f}{\partial Y'} \right] \delta(x-y)dx.
\end{aligned} \tag{191}$$

Equating this to zero, yields the Euler-Lagrange equations

$$0 = \frac{\partial f}{\partial Y} - \frac{d}{dx} \frac{\partial f}{\partial Y'} \tag{192}$$

It should be noted that the condition $\delta I/\delta Y = 0$ alone is not a sufficient condition for a minimum. In fact, the relation might even indicate a maximum. It is often possible, however, to convince oneself that no maximum exists for the integral (e.g., the distance along a smooth path can be made as long as we like), and that our solution is a minimum. To be rigorous, however, one should also consider the possibility that the minimum is merely a local minimum, or perhaps the relation $\delta I/\delta Y = 0$ indicates a point of inflexion.

It is easy to check that Eq. (192) yields the Newton equations

$$m\ddot{x} = -V'(x), \tag{193}$$

when applied to the action functional (183). Similarly, the Euler-Lagrange equations for the shortest-path integral (176) just give the ODE (180).

8.4 Brachistochrone

In June 1696, Johann Bernoulli set the following problem: Given two points A and B in a vertical plane, find the path from A to B that takes the shortest time for a particle moving under gravity without friction. This proposal marked the real beginning of general interest in the calculus of variations. (The term 'brachistochrone' derives from the Greek *brachistos* meaning shortest and *chronos* meaning time.)

If the particle starts with zero initial speed at height h_0, energy conservation requires $mv^2/2 = mg(h_0 - h(x))$, where v is particle speed, h_0 is the original height of the particle and $h(x)$ is the height of the particle at position x. Thus

$$v = \sqrt{2g(h_0 - h(x))}. \tag{194}$$

By definition $v = ds/dt$ so that the time taken to go from A to B is

$$\int_A^B dt = \int_A^B \frac{ds}{\sqrt{2g[h_0 - h(x)]}}. \tag{195}$$

We know that $ds = \sqrt{1 + h'^2}$, so that the time taken is

$$T[h] = \int_A^B dx \sqrt{\frac{1 + h'^2}{2g(h_0 - h)}}. \tag{196}$$

The integrand

$$f = \sqrt{\frac{1 + h'^2}{2g(h_0 - h)}} \tag{197}$$

determines the time of descent. We can insert f directly into the Euler-Lagrange equation (192) to obtain the ODE that governs the shortest-time solution. Here, we shall pursue a slightly different approach by starting from the readily verifiable identity

$$\frac{d}{dx}\left(h' \frac{\partial f}{\partial h'} - f\right) = 0, \tag{198}$$

which integrates to

$$h' \frac{\partial f}{\partial h'} - f = C, \tag{199}$$

with some constant C. Substituting for f we obtain explicitly

$$\frac{h'^2}{\sqrt{(h_0 - h)(1 + h'^2)}} - \sqrt{\frac{1 + h'^2}{h_0 - h}} = C. \tag{200}$$

Solving this for h' and integrating both sides of the expression, we obtain

$$x = \int dh \frac{\sqrt{h_0 - h}}{\sqrt{2a - (h_0 - h)}}, \tag{201}$$

where $C = (2a)^{-\frac{1}{2}}$. To evaluate this integral we substitute $h_0 - h = 2a \sin^2 \frac{\theta}{2}$ and obtain

$$x = 2a \int \sin^2 \frac{\theta}{2} d\theta + x_0 = a(\theta - \sin\theta) + x_0. \tag{202}$$

We have thus found a parametric representation for the desired curve of most rapid descent:

$$x = x_0 + a(\theta - \sin\theta), \qquad h = h_0 - a(1 - \cos\theta). \tag{203}$$

These are the equations of a cycloid generated by the motion of a fixed point on the circumference of a circle of radius a, which rolls on the negative side of the given line $h = h_0$. By adjustments of the arbitrary constants, a and x_0 it is always possible to construct one and only one cycloid of which one arch contains the two points between which the brachistochrone is required to extend. Moreover, this arc renders the time of descent an absolute minimum compared with all other arcs.

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