CALCULUS OF VARIATIONS

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Contents

1.	Introduction: Stationary values of integrals	1
2.	The Euler–Lagrange equation	5
3.	Classical examples and basic theorems	9
4.	Extension to many dependent variables and Hamilton's principle	14
5.	More examples in dynamics and geometry	17
6.	Generalization to several independent variables and to higher derivatives	21
7.	Extremals subject to an integral constraint	24
8.	Application to Sturm-Liouville equations	27

1. Introduction: Stationary values of integrals

This course on the calculus of variations is a doorway to modern applied mathematics and theoretical physics that also connects with the analysis of PDEs and numerical analysis. For examination purposes you can treat it as a comparatively self-contained topic, but that is not its only purpose. The central point of the course is to show how abstract and non-obvious ideas can play a part in solving concrete problems. For example, the reformulation of Newton's laws into Hamilton's Principle will be taken much further in Part B Classical Mechanics.

As mathematics, Euler, Lagrange, and Hamilton played notable rôles in developing the calculus of variations in the $18^{\rm th}$ and $19^{\rm th}$ centuries. Although stimulated by physics, they created quite new ideas in mathematics which turned out to be vital in the $20^{\rm th}$ century formulation of quantum mechanics, special and general relativity, the rigorous theory of partial differential equations, and the finite element method in numerical analysis.

First, let us recall a basic principle from calculus about how we can look for maxima or minima of functions of one variable:

Principle (Maxima are stationary points). Let f(x) be a 'nice' function. Then the maxima and minima of f occur when f'(x) = 0.

('Nice' can mean continuously differentiable in the principle above, but we will deliberately not try to classify precisely what sort of pathological exceptions might occur in this

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course, typically assuming that we are only interested in sufficiently smooth functions for us to not have to worry about justifying differentiation.)

The Calculus of Variations is a set of techniques where instead of looking for the maxima/minima of a function of one variable, you look at a functional (a function of functions), and you want to choose the function which minimises the functional. Such problems appear all the time in physics.

Example 1 (Shortest path between two points). Given points (x_1, y_1) and (x_2, y_2) , what is the shortest length path between them?

By rotating the plane (which leaves distances unchanged) we may assume that $y_1 = y_2$.

Let us imagine that the path is given by a suitably nice (continuously differentiable) function y(x). Then the length of the path is given by

$$I[y] = \int_{x_1}^{x_2} \sqrt{1 + y'(x)^2} \, \mathrm{d}x.$$

This defines I[y] as a functional that assigns a real number, the length of the path, to each continuously differentiable function y.

The only constraints that we have on y are that $y(x_1) = y(x_2) = y_1$. Since $y'(x)^2 \ge 0$, the integral is minimised when

$$y'(x) = 0,$$

so the straight line path minimises the distance.

(It is intuitively reasonable that any path can be approximated by a smooth path arbitrarily well, and so it suffices to just consider smooth paths. Again, this is not the point of this course, and so we will often assume that we can restrict ourselves to sufficiently well-behaved functions without rigorous justification.)

Notice that we have deduced a *local* rule about what happens at one point from a *global* criterion — variation over *all possible paths*. This is the basic idea of the calculus of variations that we shall generalise considerably and apply to a wide range of problems.

One of the simplest ideas in physics is that light travels in straight lines. This observation gains much greater power when put in the following way: light travels in a straight line because a straight line is the shortest distance between two points. This may sound a trivial reformulation but it remains one of the basic ideas in Einstein's general theory of relativity.

Example 2 (Biatholon problem). A person is travelling from point A to point B. They first need to cross a field (running at speed c_1) and then cross a river (swimming at speed c_2). What path should they follow to get from A to B fastest? Clearly the biathlete should run in as straight line from A to P on the edge of the river, and then swim in a straight line from P to B, since straight lines minimise distance. (If $c_1 \geq c_2$ then consider the last point P at which the athlete is on the field; the fastest way to get from A to P is running in a straight line in the field. After this point they must just swim from P to B, and the fastest route is to swim in a straight line.)

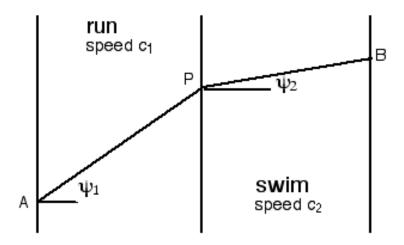


FIGURE 1. The biathlon problem

Let $A = (x_A, y_A)$, $B = (x_B, y_B)$ and $P = (x_P, y_P)$. We want to choose y_P to minimise the total time. At the optimum value of y_P we have

$$\frac{\mathrm{d}}{\mathrm{d}y_P} \left(\frac{\sqrt{(x_A - x_P)^2 + (y_A - y_P)^2}}{c_1} + \frac{\sqrt{(x_B - x_P)^2 + (y_B - y_P)^2}}{c_2} \right) = 0,$$

which implies

$$\frac{(y_A - y_P)}{c_1 \sqrt{(x_A - x_P)^2 + (y_A - y_P)^2}} = \frac{(y_P - y_B)}{c_2 \sqrt{(x_B - x_P)^2 + (y_B - y_P)^2}}.$$

The optimum position of P is such that the angles ψ_1, ψ_2 satisfy:

$$\frac{\sin \psi_1}{c_1} = \frac{\sin \psi_2}{c_2}.$$

You may recognise (1) as *Snell's Law* governing the refraction of light in its passage from one medium to another, provided that the observed *refractive index* of the medium is identified with the inverse of speed. Fermat observed that Snell's Law follows from such a least-time principle, although it was not until the 20th century that such a principle could be understood in terms of quantum physics.

We can now solve a slightly more general problem. Suppose that someone is running on a muddy field that occupies the region x > 0 at a speed c(x), where c(x) is some smooth function that depends only on the x coordinate. Equivalently, we have an optical medium with a continuously varying refractive index proportional to $(c(x))^{-1}$. What then is the shortest-time path from one point to another?

We can consider this in the following way. Divide up the muddy field into strips of thickness δx , so that in the strip from x to $x + \delta x$, the speed is a constant given by c(x).

Then repeatedly applying Snell's law from equation (1), it must be true that

(2)
$$\frac{\sin(\psi(x))}{c(x)}$$
 is a constant along the path.

Now take the limit as $\delta x \to 0$, and this law will remain true.

1.1. A bit of elementary calculus: The angle $\psi = \psi(x)$ that the path makes to the x-axis is such that $\tan \psi = dy/dx = y'(x)$. We also have arc-length s defined by $ds^2 = dx^2 + dy^2$. Putting these together gives

$$\sin \psi = \frac{y'}{\sqrt{1 + y'^2}} = \frac{dy}{ds}, \quad \cos \psi = \frac{1}{\sqrt{1 + y'^2}} = \frac{dx}{ds}.$$

It is also useful to derive from these that

$$\kappa = \frac{\mathrm{d}\psi}{\mathrm{d}s} = \frac{y''}{(1+y'^2)^{3/2}}$$

where κ is the *curvature* of the path, defined in a way that is invariant under rotation of the axes.

Example 3 (Shortest path on a 'muddy field'). As an example of special interest, take the case where c(x) is linear in x, in fact suppose c(x) = x. Then we have

(3)
$$\frac{\sin \psi(x)}{x} = constant.$$

So we can translate the statement of Snell's law into a statement that the function y(x) is a solution of

$$\frac{y'}{\sqrt{1+y'^2}} = Ax.$$

If A = 0 this gives the lines y = constant, and for $A \neq 0$, we obtain

(5)
$$x^2 + (y - y_0)^2 = A^{-2}.$$

This is the equation of a circle with centre $(0, y_0)$ on the line x = 0. This completely solves the problem of finding the runner's shortest-time path between any two points on the field. We shall return later to this remarkable geometrical fact.

Clearly we could now consider the even more general problem that arises when c = c(x, y). Instead, we will take a different point of view. We reformulate the problem we have been studying in the following much more general terms.

We will think of the time taken to cover the path as a *functional* of the path taken. That is, it is a function on the space of possible paths, which are themselves functions, that assigns a real number to each path.

Specifically, in the problem we have been considering, we can define a functional I[y] for functions y = y(x) by:

(6)
$$I[y] = \int_{a}^{b} \frac{\sqrt{1 + y'(x)^2}}{c(x)} dx,$$

and then we ask for the least value of I[y] as y(x) varies over all possible paths. The function y(x) that achieves this least value is called an *extremal*.

In this case it is obvious that we are looking at minimum values of an integral, but in general this is too restrictive. We use the term $stationary\ value$. This will mean that (in a sense to be defined) the first derivative of I[y] vanishes. It will allow for a range of possibilities: a minimum, or maximum, or something equivalent to saddles, or more complicated situations in which higher derivatives also vanish.

We now regard this as a special case of a far more general problem in which we look for stationary values of

(7)
$$I[y] = \int_a^b F(x, y(x), y'(x)) dx,$$

for a fixed function F(x, u, v) of three independent arguments. For simplicity, we write this as $I[y] = \int_a^b F(x, y, y') dx$ when we substitute u = y(x) and v = y'(x).

The remarkable discovery (due principally to Euler and Lagrange) is that there is a *single method* that deals with all such questions. It can be extensively generalised to many dimensions, many derivatives, and to include constraints.

Even more remarkably, problems that don't look at all like least-time problems can usefully be reformulated in this way. Dynamical systems have trajectories which can be considered as being solutions to such stationary-value problems, not of shortest distance or shortest time but of *least action*, as will be explained later. One reason that this is a very useful description of physical problems is that the concept of the stationary value is independent of the coordinates used to describe it.

Theoretical physics today is rooted in the idea of stationary values of functionals of fields. The current Standard Model of particles and forces is defined by writing down a least action principle, as also are string and superstring theories. So part of the motivation for this course comes from the deepest properties of the physical world, properties which only come to light through the transforming power of creative mathematics.

2. The Euler-Lagrange equation

We now consider the general problem of finding the function y(x) that gives a stationary value to the functional

(8)
$$I[y] = \int_a^b F(x, y, y') dx.$$

As in the proof of Picard's theorem for a second-order equation (or first-order system) in Differential Equations 1, we sometimes treat F as a function of three independent arguments x, u, v, and sometimes as a function of x alone by putting u = y(x) and v = y'(x). For example, the chain rule gives

(9)
$$\frac{\mathrm{d}}{\mathrm{d}x}F(x,y(x),y'(x)) = \frac{\partial F}{\partial x} + \frac{\partial F}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}x} + \frac{\partial F}{\partial y'}\frac{\mathrm{d}^2y}{\mathrm{d}x^2} = \frac{\partial F}{\partial x} + y'\frac{\partial F}{\partial y} + y''\frac{\partial F}{\partial y'},$$

where $\partial F/\partial y'$ means the partial derivative of F(x, u, v) with respect to its third argument v evaluated at u = y(x) and v = y'(x).

From a completely rigorous point of view, we would have to specify the exact (huge) class of functions y(x) over which the functional is taken (differentiable, differentiable with continuous derivative, differentiable to every order?), and we would also need some concept of what it means to vary a function to a 'nearby' function, by putting a metric or at least a topology on the class of functions.

In this course we will take a more elementary point of view and assume that all the functions we use have sufficient differentiability for the problem in hand. We will typically state results for smooth (infinitely differentiable) functions, since most situations in the real world are smooth (or can be approximated arbitrarily well by smooth functions).

The one point that we will make rigorous, to help justify this rather cavalier approach, is the idea of a "bump function".

Lemma 2.1 (Bump function). There exists a function B(x) with the following properties:

- (1) B(x) is infinitely differentiable,
- (2) B(x) = 0 unless $x \in [0, 1]$,
- (3) $0 < B(x) \le 1$ if $x \in (0,1)$.

Proof (sketch, non-examinable). Let B(x) be the function

$$B(x) = \begin{cases} 0, & x \le 0, \\ \exp(-x^{-1}(1-x)^{-1}), & 0 < x < 1, \\ 0, & x \ge 1. \end{cases}$$

Then for all positive integers n, the n^{th} derivative $B^{(n)}(x) \to 0$ as $x \downarrow 0$ or $x \uparrow 1$, since the exponential decay dominates the polynomial growth, so B is infinitely differentiable at 0 and 1, and hence infinitely differentiable everywhere in [0,1]. Moreover, $0 \le B(x) \le 1$, and B(x) > 0 if and only if $x \in (0,1)$.

These bump functions are very similar to the "test functions" met in Part A Integral Transforms, with the additional property that they always take non-negative values. The example we use is the same, except its support is [0,1] rather than [-1,1]. (The support of a function is the closure of the set of points on which the function takes nonzero values.)

By considering B((x-a)/(b-a)) we can define a "bump function" whose support is any closed interval [a,b], and by scaling we can assume it takes the value 1 (its maximum) at the midpoint.

A function can thus always be varied within any interval, by adding on a bump function, without changing its differentiability. This is true whatever the degree of differentiability we required of the original function.

Lemma 2.2 (The fundamental lemma in the calculus of variations). Let y(x) be a continuous function on [a, b] such that

(10)
$$\int_{a}^{b} y(x)\eta(x) \, \mathrm{d}x = 0,$$

for every smooth function $\eta(x)$ with $\eta(a) = \eta(b) = 0$. Then y(x) = 0 for all $x \in [a, b]$.

Proof. For a proof by contradiction, suppose that $y(x_0) \neq 0$ for some $x_0 \in (a, b)$. W.L.O.G assume that $y(x_0) > 0$. Since y is continuous, we must have y(x) > 0 everywhere on some interval [c, d] containing x_0 with a < c < d < b. Now consider a bump function $\beta(x)$ with support [c, d]. By assumption,

$$\int_{a}^{b} y(x)\beta(x)\mathrm{d}x = 0,$$

but since $\beta(x) = 0$ unless $x \in [c, d]$, this implies

$$\int_{c}^{d} y(x)\beta(x)\mathrm{d}x = 0,$$

which is impossible as $y(x)\beta(x)$ is strictly positive and continuous on (c,d). This gives a contradiction, and so we must have that y(x) = 0 for all $x \in (a,b)$. Moreover, y is continuous, so y(x) = 0 at the endpoints x = a and x = b too.

For a fixed function y, we can treat the left-hand side of (10) as defining a linear functional from smooth functions η to the real numbers,

$$\eta \mapsto \int_a^b y(x)\eta(x) \, \mathrm{d}x.$$

Equivalently, y defines a regular distribution in the terminology of Part A Integral Transforms, Lemma 2.2 says that if this distribution is identically zero, i.e. it maps all smooth functions η to the value zero, and y is continuous (not just locally integrable) then y(x) = 0 for all $x \in [a, b]$.

The following lemma is an extension of lemma 2.2 that will be useful later.

Lemma 2.3 (An extension of the fundamental lemma). Let y(x) be a continuous function on [a, b] and c_1, c_2 constants such that

(11)
$$c_1 \eta(a) + c_2 \eta(b) + \int_a^b y(x) \eta(x) dx = 0$$

for every smooth function $\eta(x)$. Then $c_1 = c_2 = 0$ and y(x) = 0 for $x \in [a, b]$.

Proof. The set of every smooth function $\eta(x)$ includes the subset of smooth functions $\eta(x)$ that satisfy $\eta(a) = \eta(b) = 0$. For this subset, the left-hand side of (11) becomes

$$\int_{a}^{b} y(x)\eta(x)\mathrm{d}x = 0.$$

Lemma 2.2 implies that y(x) = 0 for all $x \in [a, b]$. Having established this, and returning to the unrestricted set of all smooth functions $\eta(x)$, the left-hand side of (11) becomes

$$c_1\eta(a) + c_2\eta(b) = 0.$$

Choosing functions η satisfying $\eta(a)=1,\ \eta(b)=0,$ and vice versa, establishes that $c_1=c_2=0.$

Now we embark on the analysis of the stationary values of the functional I[y]. We might be tempted to try to vary y(x) by some infinitesimal function $\epsilon(x)$, but there are uncountably many possible functions and this can lead to many difficulties. To avoid needing to worry about these many possibilities, we instead focus on a single one-parameter family of variations. We fix a function $\eta(x)$, and consider

$$(12) y(x) + \alpha \eta(x),$$

where α is a real parameter. This allows us to consider

(13)
$$I[y + \alpha \eta] = \int_a^b F(x, y + \alpha \eta, y' + \alpha \eta') \, \mathrm{d}x.$$

Specifically, we have the following lemma.

Lemma 2.4 (Minimisers give stationary values). Let y(x) be a minimiser for I[y], and $\eta(x)$ a smooth function. Then we have that

(14)
$$\frac{\mathrm{d}}{\mathrm{d}\alpha}I[y+\alpha\eta]\Big|_{\alpha=0}=0.$$

Proof. This is just the standard calculus criterion for minima in disguise. If y(x) is a minimiser of I then $I[y + \alpha \eta] \ge I[y]$ for all α in the neighbourhood of zero, so $f(\alpha) = I[y + \alpha \eta]$ attains a minimum at $\alpha = 0$. Thus f'(0) = 0, which is the result (14)

Lemma 2.5 (Constrained minimisers give stationary values). Let y(x) be a minimiser for I[y] subject to the constraint $y(a) = c_1$ and $y(b) = c_2$, and $\eta(x)$ a smooth function with $\eta(a) = \eta(b) = 0$. Then we have that

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}I[y+\alpha\eta]\Big|_{\alpha=0}=0.$$

Proof. This is the same as the previous proof, noting that if $\eta(a) = \eta(b) = 0$ then $y + \alpha \eta$ still satisfies the constraints $y(a) = c_1$ and $y(b) = c_2$.

Theorem 2.6 (Euler–Lagrange equation for natural boundary conditions). Let I[y] be the functional

$$I[y] := \int_a^b F(x, y, y') \, \mathrm{d}x$$

for some smooth function F. Then the minimisers y(x) of I satisfy

(15)
$$\frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial F}{\partial y'} - \frac{\partial F}{\partial y} = 0,$$

and

(16)
$$\frac{\partial F}{\partial y'}\bigg|_{x=a} = \frac{\partial F}{\partial y'}\bigg|_{x=b} = 0.$$

Proof. Let y = y(x) be a minimiser of I[y], and $\eta = \eta(x)$ a smooth function. By Lemma 2.4, we have that

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}I[y+\alpha\eta]\Big|_{\alpha=0}=0.$$

By applying the chain rule, we can write

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}I[y+\alpha\eta]\Big|_{\alpha=0} = \int_a^b \Big(\eta(x)\frac{\partial}{\partial y}F(x,y,y') + \eta'(x)\frac{\partial}{\partial y'}F(x,y,y')\Big)\mathrm{d}x.$$

(Here by $\frac{\partial}{\partial y'}F(x,y,y')$ we mean $F_3(x,y,y')$, where the function F_3 is defined by $F_3(x,y,z) = \frac{\partial}{\partial z}F(x,y,z)$.)

The next key step is an integration by parts to eliminate $\eta'(x)$. First note that:

$$\frac{\mathrm{d}}{\mathrm{d}x} \left(\eta \frac{\partial}{\partial y'} F(x, y, y') \right) = \eta' \frac{\partial}{\partial y'} F(x, y, y') + \eta \frac{\mathrm{d}}{\mathrm{d}x} \frac{\partial}{\partial y'} F(x, y, y'),$$

so

$$\int_{a}^{b} \eta'(x) \frac{\partial}{\partial y'} F(x, y, y') dx = \left[\eta \frac{\partial}{\partial y'} F(x, y, y') \right]_{a}^{b} - \int_{a}^{b} \eta(x) \frac{\mathrm{d}}{\mathrm{d}x} \frac{\partial}{\partial y'} F(x, y, y') \mathrm{d}x.$$

Here d/dx represents a total derivative, acting on every appearance of x, whether explicit or implicit in y and y'.

Hence

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}I[y+\alpha\eta]\Big|_{\alpha=0} = \left[\eta\frac{\partial F}{\partial y'}\right]_a^b + \int_a^b \eta(x)\left(\frac{\partial F}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial F}{\partial y'}\right)\mathrm{d}x.$$

Now, for y to be an extremal, the LHS of this equation must vanish for every choice of η . Hence the RHS must vanish for all $\eta(x)$. But then Lemma 2.3 implies that

$$\frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial F}{\partial y'} - \frac{\partial F}{\partial y} = 0,$$

and

$$\left. \frac{\partial F}{\partial y'} \right|_{x=a} = \left. \frac{\partial F}{\partial y'} \right|_{x=b} = 0.$$

as required.

Theorem 2.7 (Euler–Lagrange equation for fixed endpoint boundary conditions). Let I[y] be the functional

$$I[y] = \int_a^b F(x, y, y') \, \mathrm{d}x$$

for some smooth function F. Then the minimisers y(x) of I with $y(a) = c_1$ and $y(b) = c_2$ satisfy

(17)
$$\frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial F}{\partial y'} - \frac{\partial F}{\partial y} = 0.$$

Proof. This is essentially the same as the previous proof, but by Lemma 2.5 we only consider functions η satisfying $\eta(a) = \eta(b) = 0$. For all such functions we find that

$$0 = \frac{\mathrm{d}}{\mathrm{d}\alpha} I[y + \alpha \eta] \Big|_{\alpha=0} = \left[\eta \frac{\partial F}{\partial y'} \right]_a^b + \int_a^b \eta(x) \left(\frac{\partial F}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x} \frac{\partial F}{\partial y'} \right) \mathrm{d}x$$
$$= \int_a^b \eta(x) \left(\frac{\partial F}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x} \frac{\partial F}{\partial y'} \right) \mathrm{d}x.$$

The term $[\eta \frac{\partial F}{\partial y'}]_a^b$ vanishes since $\eta(a) = \eta(b) = 0$. Now, by Lemma 2.2 we see that we must have

$$\frac{\partial F}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x} \frac{\partial F}{\partial y'} = 0,$$

as required.

Note: Remember that finding *extremals* and *stationary* values does not mean the same thing as locating maxima or minima. It will need some further piece of information to determine whether an extremal is a (local) maximum, or (local) minimum, or neither of these. However, maxima and minima must be extremals.

3. Classical examples and basic theorems

We first recall the two examples we saw before, now from the point of view of the Euler–Lagrange equations.

Example 4 (Shortest distance on the Euclidean plane). Minimizing the distance of a path y = y(x) between (x_1, y_1) and (x_2, y_2) is equivalent to minimizing $I[y] = \int_a^b F(x, y, y') dx$ subject to $y(x_1) = y_1$, $y(x_2) = y_2$, where F is given by

(18)
$$F(x, y, y') = \sqrt{1 + y'^2}.$$

Since $\partial F/\partial y = 0$, the Euler-Lagrange equation becomes

(19)
$$\frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial F}{\partial y'} = \frac{\mathrm{d}}{\mathrm{d}x}\frac{y'}{\sqrt{1+y'^2}} = 0,$$

so $y'/\sqrt{1+y'^2}$ is constant. This expression is a monotonic increasing of y', so y' itself is constant, and hence the solution is a straight line.

Example 5 (Shortest paths on the 'muddy field'). Next, we can verify the circular paths found for the 'muddy field' problem in chapter 1. We now take

(20)
$$F(x, y, y') = \frac{\sqrt{1 + y'^2}}{x}.$$

The Euler-Lagrange equation is

(21)
$$\frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial F}{\partial y'} = \frac{\mathrm{d}}{\mathrm{d}x}\frac{y'}{x\sqrt{1+y'^2}} = \frac{\partial F}{\partial y} = 0$$

and this immediately allows one integral to be done, leaving

(22)
$$\frac{y'}{x\sqrt{1+y'^2}} = c.$$

This is just a rearrangement of equation (4) that we derived earlier by generalizing Snell's Law. To remind you, the solutions are (arcs of) circles with centres on the y-axis. Again, there are both fixed point and natural boundary conditions to consider. You can check that these all give solutions that make sense.

3.1. An 'ignorable coordinate'. Each of these problems simplified from a second-order ODE to a first-order ODE because the particular F(x, y, y') had no explicit dependence on y, i.e. $\partial F/\partial y = 0$. This turns out to be of enormous importance, especially in applications to mathematical physics. The dependent variable y is said to be *ignorable* in this situation. We can state a general theorem:

Theorem 3.1 (Special case of Euler-Lagrange equation). Let F(x, u, v) be a smooth function such that

$$\frac{\partial}{\partial u}F(x,u,v) = 0.$$

Let y = y(x) be a minimiser for the functional

$$I[y] := \int_a^b F(x, y, y') dx.$$

Then $\partial F/\partial y'$ is a constant.

Proof. This result follows immediately from writing the Euler–Lagrange equation as

$$\frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial F}{\partial y'} = \frac{\partial F}{\partial y} = 0.$$

3.2. The same problem from a different standpoint. If we consider the problem of finding stationary values of the functional I[y] that comes from taking

(23)
$$F(x, y, y') = \frac{\sqrt{1 + y'^2}}{y},$$

the geometrical interpretation tells us immediately that the extremals must be (arcs of) circles with centre on the x-axis. However, this is not immediately obvious if we write down the Euler-Lagrange equation:

(24)
$$\frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{y'}{y\sqrt{1+y'^2}} \right) + \frac{\sqrt{1+y'^2}}{y^2} = 0.$$

This is a complicated-looking second-order ODE. However, there is another general result that holds when F has no explicit dependence on x. This is Beltrami's identity. It is also of great importance.

Theorem 3.2 (Beltrami's identity). Let F(x, u, v) be a smooth function such that

$$\frac{\partial}{\partial x}F(x,u,v) = 0.$$

Let y = y(x) be a minimiser of $I[y] = \int_a^b F(x, y, y') dx$. Then we have

(25)
$$\frac{\mathrm{d}}{\mathrm{d}x} \left(y' \frac{\partial F}{\partial y'} - F \right) = 0,$$

and so

(26)
$$H = y' \frac{\partial F}{\partial y'} - F = constant.$$

Proof. For a general function F(x, y, y'), the chain rule gives

$$\frac{\mathrm{d}}{\mathrm{d}x}F(x,y,y') = \frac{\partial}{\partial x}F(x,y,y') + y'\frac{\partial}{\partial y}F(x,y,y') + y''\frac{\partial}{\partial y'}F(x,y,y').$$

The total derivative d/dx on the left-hand side includes the implicit dependence of F(x, y, y') on x via y and y' treated as functions of x.

For the particular case with $\partial F(x, u, v)/\partial x = 0$, we have

$$\frac{\mathrm{d}}{\mathrm{d}x}F(x,y,y') = 0 + y'\frac{\partial}{\partial y}F(x,y,y') + y''\frac{\partial}{\partial y'}F(x,y,y').$$

Eliminating $\partial F/\partial y$ using the Euler-Lagrange equation gives

$$\frac{\mathrm{d}}{\mathrm{d}x}F(x,y,y') = y'\frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial F}{\partial y'} + y''\frac{\partial}{\partial y'}F(x,y,y') = \frac{\mathrm{d}}{\mathrm{d}x}\left(y'\frac{\partial}{\partial y'}F(x,y,y')\right),$$

which proves the result.

Alternative proof. Although the preceding proof is easy, it does not give any idea of why this first integral should exist. The following argument shows the reason: it is really just a special case of an ignorable coordinate. We simply exchange the roles of x and y and think of extremal curve as a function x(y) instead of a function y(x). (This is a very natural idea for the particular problem that inspired this result.) Writing x' for dx/dy, so that $y' = (x')^{-1}$, the integral

(27)
$$\int_{a}^{b} F(x, y, y') dx, \quad y(a) = c, \ y(b) = d,$$

becomes

(28)
$$\int_{c}^{d} F(x, y, (x')^{-1}) x' \, dy, \quad x(c) = a, \ x(d) = b.$$

Now x is the ignorable coordinate, so the Euler-Lagrange equation becomes

$$\frac{\partial}{\partial x'} \left(F(x, y, (x')^{-1}) x' \right) = \text{constant.}$$

After taking care over the partial derivatives here, i.e. remembering how expressions like $(\partial/\partial y') F(x, y, y')$ are properly defined, this yields

$$-(x')^{-2}F_3(x, y, (x')^{-1})x' + F(x, y, (x')^{-1}) = \text{constant},$$

where $F_3(x, u, v) = \partial_v F(x, u, v)$ is the partial derivative of F with respect to its last argument. Using $(x')^{-1} = y'$ gives

$$-y'F_3(x, y, y') + F(x, y, y') = \text{constant},$$

which is equivalent to the Beltrami identity.

Applied to the 'muddy field' problem, we deduce that

(29)
$$H = \frac{-1}{y\sqrt{1+y'^2}} = \text{constant.}$$

It is straightforward to perform the remaining integral to recover the circular paths.

In this case, however, there are no solutions satisfying the natural boundary conditions. This agrees with the fact that there is no minimum or maximum value for the integral between x = a and x = b. It can take any real positive value, and the infimum 0 cannot be attained.

We shall come back to such shortest-path problems, or more generally the problems of *geodesics*, in chapter 5. It will turn out that the 'muddy field' is actually a way of representing the mathematical concept of the *hyperbolic plane*.

Example 6 (Brachistochrone). Find the curve that allows a smoothly falling particle released from rest at one point to reach a given lower point, not immediately below the upper point, in the shortest time.

This is the most famous example of a stationary integral problem, originally solved by Newton, J. Bernoulli and others in the 17th century. The answer is not at all intuitive.

See http://mathworld.wolfram.com/BrachistochroneProblem.html

This needs some first-year mechanics to obtain the relevant F(x, y, y'). In this problem we use x for horizontal distance and y for distance moved downwards. (This is purely for the sake of being able to start at the origin and yet avoid expressions like $\sqrt{-y}$.) We assume that gravity exerts a constant downward acceleration of magnitude g.

Explicitly, suppose the particle is released from (x,y) = (0,0) at t = 0, and then follows a curve y = y(x) which reaches (x,y) = (a,h), so that h is the height lost, and a the horizontal distance traversed. Using the initial conditions, and conservation of energy, we know that at each point in the motion along the curve y = y(x),

$$E = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) - mgy = 0.$$

Solving for \dot{x}^2 gives

$$\dot{x}^2 = \frac{2gy}{1 + y'^2}$$

where y' = dy/dx, and so

$$\mathrm{d}t = \frac{1}{\sqrt{2g}} \frac{\sqrt{1 + y'^2}}{\sqrt{y}} \, \mathrm{d}x.$$

The total travel time T is given, as a functional of the curve y(x), by

(30)
$$T[y] = \frac{1}{\sqrt{2g}} \int_0^a \frac{\sqrt{1+y'^2}}{\sqrt{y}} \, \mathrm{d}x.$$

We want the curve y(x) that minimises T[y], subject to the fixed-end boundary conditions of passing through (0,0) and (a,h). This can also be interpreted as solving the quickest path problem for a 'muddy field' with speed proportional to \sqrt{y} .

We could easily write down the Euler-Lagrange equations, but it is more efficient to take a short cut and use the Beltrami identity since F(x, y, y') depends only on y and y'. This tells us that

(31)
$$\sqrt{y}\sqrt{1+y'^2} = \sqrt{2c},$$

for some constant 2c. To solve, make the substitution $y = 2c\sin^2(\phi/2)$ to derive

$$\frac{\mathrm{d}x}{\mathrm{d}\phi} = 2c\sin^2(\phi/2) = c(1-\cos\phi),$$

and hence (using the initial condition)

(32)
$$x = c(\phi - \sin \phi), \quad y = c(1 - \cos \phi).$$

This is the parametric form of a **cycloid**. This is the same curve that is traced out by a point on the rim of a wheel rolling in a direction parallel to the x-axis.

See http://mathworld.wolfram.com/Cycloid.html for pictures.

The ratio of a to h fixes the arc of the cycloid that solves the problem. If $a/h = \pi/2$, the cycloid is followed to its lowest point, at $\phi = \pi$, with $c = a/\pi$; if $a/h < \pi/2$ then it is a smaller segment of the cycloid, with c chosen to fit, and so on.

It is worth filling in some more details. One finds that $\dot{\phi}$ is constant, namely $\sqrt{g/c}$, so the time taken to reach the point with parameter ϕ is just $\sqrt{c/g}\,\phi$. Suppose the horizontal distance a is given, and we ask for the path which reaches it fastest, over all possible h. The time is given by $\sqrt{c/g}\,\phi$, where c is given implicitly by the relation $a=c(\phi-\sin\phi)$. So finding the fastest way of reaching a is equivalent to minimising $\phi/\sqrt{\phi-\sin\phi}$. One may check that this is given by $\phi=\pi$. This verifies what we obtain much more easily from taking the natural boundary condition y'=0 at x=a. This selects the cycloid which arrives at x=a at its lowest point, i.e. where $\phi=\pi$.

Example 7 (Soap film). Consider a surface obtained by revolving the curve y = y(x) around the x-axis, between the values $x = x_1$ and $x = x_2$. What curve gives the minimum area?

The problem is to find a minimum area, but as it is the area of a surface of revolution, this reduces to finding a curve. This can be visualised as a soap film suspended between two circular wires at x_1, x_2 , given that the film will establish an equilibrium with a minimum area due to surface tension (see Part A Fluids and Waves).

The functional A[y] to be minimised is thus

(33)
$$A[y] = 2\pi \int_{x_1}^{x_2} y\sqrt{1 + y'^2} \, \mathrm{d}x.$$

The integrand does not depend explicitly on x, so the Beltrami identity gives us a first integral:

$$\frac{y}{\sqrt{1+y'^2}} = c.$$

The solutions are

$$(34) y = c \cosh\left(\frac{x - x_0}{c}\right).$$

Filling in the details and then fitting the initial conditions is a rather fiddly business that is left as an exercise.

The cosh curve will turn up again in connection with another problem — finding the shape taken by a hanging chain. It is called the *catenary* because of this connection, and the surface we have discovered is the *catenoid*. It plays a major rôle in the geometry of surfaces.

Example 8 (A typical second order ODE problem). Suppose

(35)
$$F(x,y,y') = \frac{1}{2}y'^2 - \frac{1}{2}y^2 + y f(x), \quad y(0) = 0 = y(1).$$

Then $\frac{\partial F}{\partial y'} = y', \frac{\partial F}{\partial y} = -y + f$, and the Euler-Lagrange equation is

(36)
$$y'' + y - f(x) = 0.$$

In this case we don't have any helping hand from an ignorable coordinate or Beltrami's identity. However, we recognise the second-order ODE as the type of equation studied intensively in Differential Equations 2. With these boundary conditions it can be solved using a Green's function.

In this course we shall not pursue the solutions of such equations any further; actually, we are more interested in a different question. Can we translate the differential equations we have met before into a problem of finding extremals?

4. Extension to many dependent variables and Hamilton's principle

In this section we explore the application of the calculus of variations to classical mechanics.

First we need a modest generalization to allow more than one dependent variable. For this it is convenient to change our notation, since in mechanical applications it is usually *time* that is the one independent variable. The many dependent variables represent the spatial coordinates of the mechanical system. So we think first about q(t) and $F(t, q, \dot{q})$ instead of y(x) and F(x, y, y'), where q is a typical spatial coordinate and t is time. There is a reason for using q rather than x as the dependent variable; we do not want to be restricted to Cartesian coordinates as use of the letter x might wrongly suggest. The variable q might be angle or radial distance, for instance. We then make a generalization to

 $q_1(t), q_2(t), \dots, q_n(t)$ and functions $F(t, q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n)$. Thus we consider stationary values of the functional

(37)
$$I[q_1, \dots, q_n] = \int_a^b F(t, q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n) dt.$$

Theorem 4.1. Let F be a smooth function, and

$$I[q_1, \dots, q_n] := \int_a^b F(t, q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n) dt.$$

Then the minimisers $q_1 = q_1(t), \ldots, q_n = q_n(t)$ of I satisfy

(38)
$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial F}{\partial \dot{q}_i} - \frac{\partial F}{\partial q_i} = 0, \text{ for } i = 1, \dots, n$$

and the natural boundary conditions

(39)
$$\left[\frac{\partial F}{\partial \dot{q}_i}\right]_a^b = 0, \text{ for } i = 1, \dots, n.$$

The minimisers of I subject to the constraints $q_i(a) = c_{1,i}$ and $q_i(b) = c_{2,i}$ satisfy (38) but not necessarily (39).

Proof sketch. The method of finding these is the same as in the simplest case; we choose an index i and a test function η_i , and temporarily fix q_j for $j \neq i$ but vary q_i with $q_i(t) \to q_i(t) + \alpha \eta_i(t)$. Since we have temporarily fixed q_j for $j \neq i$, the functional I is precisely the form of the cases already considered. The Euler-Lagrange equation gives

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial F}{\partial \dot{q}_i} - \frac{\partial F}{\partial q_i} = 0,$$

with natural boundary condition

$$\left[\eta_i \frac{\partial F}{\partial \dot{q}_i}\right]_a^b = 0.$$

Doing this for each index i in turn gives the result.

We have two important special cases:

1) An 'ignorable coordinate' that arises when some variable q_i does not appear in F,

(40)
$$\frac{\partial F}{\partial q_i} = 0 \text{ implies } \frac{\partial F}{\partial \dot{q}_i} \text{ is a constant.}$$

2) The generalisation of the Beltrami identity that arises when F is independent of t,

(41)
$$\frac{\partial F}{\partial t} = 0 \text{ implies } H = \sum_{i=1}^{n} \dot{q}_{i} \frac{\partial F}{\partial \dot{q}_{i}} - F \text{ is a constant.}$$

4.1. **Hamilton's Principle.** The following statement sums up why classical mechanics can be reformulated in terms of extremal problems and solved by the calculus of variations.

Definition 1. A constraint in a mechanical system is called **workless** if there is no friction, so the constraint does no work.

A constraint is called **holonomic** if it is of the form $\phi(q_i, t) = 0$, where the q_i are some set of coordinates. Specifically, the constraints do not involve the velocities \dot{q}_i .

A force is called **conservative** if it is the gradient of a potential V.

Principle (Hamilton's Principle). If a mechanical system is subject only to holonomic, workless constraints and all forces are conservative, then the motion according to Newton's laws is an extremal of the integral

(42)
$$I[q] = \int L(q_i, \dot{q}_i, t) dt,$$

where the coordinates q_i are arbitrary but unconstrained, and L = T - V = KineticEnergy - Potential Energy of the system as expressed in those coordinates. L is called the Lagrangian.

This is Hamilton's Principle, also referred to as the *principle of least action*, where the integral I[q] is called the *action*.

In this course, we shall take it as given, not proved, that it correctly encodes physical laws. (In the Part B Classical Mechanics course it will be shown that it is equivalent to Newton's laws.)

Note that I[q] has the dimensions of energy \times time. Action is a technical term for a physical quantity with these dimensions. It turns out to be the most fundamental physical quantity (and in particular Planck's constant is a quantum of action.)

Example 9 (Motion in free space without any forces). The simplest example is just given by taking $L = T = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2)$. The Euler-Lagrange equations are just

$$\ddot{x} = \ddot{y} = \ddot{z} = 0,$$

i.e. Newton's laws of motion for a free particle.

Example 10 (Motion in free space subject to a conservative force with potential). The next simplest example arises from $L = T - V = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - m\psi(x,y,z)$ for motion in free space subject only to a conservative force with potential ψ (typically, Newtonian gravity.) The Euler-Lagrange equations then become

$$\ddot{x} = -\frac{\partial \psi}{\partial x}, \quad \ddot{y} = -\frac{\partial \psi}{\partial y}, \quad \ddot{z} = -\frac{\partial \psi}{\partial z}.$$

The value of the reformulation as a stationary integral often emerges more clearly if we make a change of coordinates. For orbit problems, with $\psi = -k/r$, the use of Cartesian x, y, z is valid but not very helpful. Since the Lagrangian formalism does not mind which coordinates we use, it is more convenient to use spherical polars instead.

Example 11 (Orbit problems with potential $\psi = -k/r$). In polar coordinates (r, ϕ, θ) for motion in free space with potential $\psi = -k/r$ we have

$$L = T - V = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\dot{\phi}^2) + \frac{km}{r}.$$

The θ -equation is:

$$\frac{\mathrm{d}}{\mathrm{d}t}(r^2\dot{\theta}) - r^2\sin\theta\cos\theta\dot{\phi}^2 = 0,$$

which is solved by $\theta \equiv \pi/2$, i.e. by paths always in the equatorial plane. Restricting our attention to such paths, the remaining equations become

$$\ddot{r} - r\dot{\phi}^2 + \frac{k}{r^2} = 0,$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(r^2\dot{\phi}) = 0.$$

The same equations were obtained following a longer argument in Prelims Dynamics. The ϕ -equation obviously integrates to

$$r^2\dot{\phi} = h$$
.

It is very important to note that the simplicity of this step arises directly from the fact that ϕ never appears in L; it is an ignorable coordinate. The conservation of angular momentum is an immediate consequence of this ignorable coordinate in this Lagrangian formulation using Hamilton's Principle

The energy conservation statement can be equally easily derived; it is the equivalent of the Beltrami identity. By the remarks above, the fact that L has no explicit dependence on t implies that

(44)
$$H = \sum_{i=1}^{n} \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L$$

remains constant along the path.

It is immediate to see from the original form of L (before the specialisation to equatorial paths) that in this case H is just T + V, i.e. total energy. For equatorial paths we reduce to

(45)
$$\frac{1}{2}(\dot{r}^2 + r^2\dot{\phi}^2) - \frac{k}{r} = E,$$

and hence now we have reduced the whole problem to a single integration, with its well known conic solutions.

The two simplifying theorems we have used, that of ignorable coordinates and Beltrami's identity, point to a deep feature of physical theory. There is a direct connection between the concepts of *symmetry* (i.e. invariance under a group of transformations) and *conservation laws*.

Independence of angle ϕ means that the action is invariant under $\phi \to \phi + \alpha$, and this fact is equivalent to the conservation of angular momentum. In a problem where x is ignorable, i.e. the action is invariant under $x \to x + \alpha$, the corresponding momentum in the x-direction is conserved. And when t can be replaced by $t + \alpha$, we have a conserved energy.

Notice that angle \times angular momentum, length \times momentum, and time \times energy, all have the dimensions of action. This conjugacy becomes fundamental in quantum mechanics, and is the basis of the famous Heisenberg Uncertainty Principle.

The Euler–Lagrange equations must remain the same in form under change of coordinates, because the concept of being stationary doesn't depend on which coordinates are used to describe the question. On a technical level this means that we can write down T and V using any coordinates we like, without any chain-rule transformation of variables.

We shall just look at a few examples to illustrate this simplicity.

5. More examples in dynamics and geometry

So far we have not made use of the new freedom to impose holonomic constraints.

A typical problem studied in Prelims Dynamics is where a particle moves smoothly on a surface of revolution, say the paraboloid $az = x^2 + y^2$. Let's derive the equations of motion from Hamilton's Principle.

Example 12 (Movement on a paraboloid). At any time the position of the particle may be given as $(\sqrt{az}\cos\theta, \sqrt{az}\sin\theta, z)$. That is, we have used the holonomic constraint provided by the smooth surface to eliminate one of the three spatial dimensions and reduce the space to that of two dimensions. Here we have used z, θ as the two coordinates needed, but in principle we could have used whatever we liked. It's a good idea, however, to use the angle θ as one coordinate because θ turns out to be ignorable in L, and so gives rise to an easy first integral. To be concrete, the Lagrangian in z and θ coordinates is

$$L = T - V = \frac{1}{2} \left\{ \left(1 + \frac{a}{4z} \right) \dot{z}^2 + az \dot{\theta}^2 \right\} - gz.$$

The Lagrangian has no explicit dependence on θ , i.e. θ is ignorable, so $\dot{\theta} = h/z$ for some constant h. Moreover, L has no explicit dependence on t, and L is quadratic in the generalised velocities \dot{z} and $\dot{\theta}$, so T+V is conserved. All the results in the Prelims treatment are immediately derived without any dotting and wedging of vectors to eliminate the reaction force.

Prelims questions do sometimes ask for the reaction force (e.g. to determine when a particle will lose contact with a surface) and if this is needed then a further step is required to deduce it from the acceleration of the particle. But in many contexts we are not concerned with the reaction force at all, so nothing is lost by eliminating it from the analysis altogether.

Example 13 (A particle on a rotating wire). A question on the 2010 Mods¹ Paper C involves a particle moving smoothly along a straight wire that is inclined at an angle β to the vertical, and rotating with constant angular velocity ω about a vertical axis. There is a similar question on the current Dynamics sheet 5.

Working directly from Newton's second law, as in Prelims, one needs to eliminate the normal reaction force by dotting Newton's second law with a vector tangent to the wire. Using Hamilton's Principle we can ignore the normal reaction and go directly to the Lagrangian L = T - V. The particle is at position

$$\mathbf{x} = (z \tan \beta \cos \omega t, z \tan \beta \sin \omega t, z),$$

relative to an inertial frame. The particle's mass is irrelevant, and can be set to unity, so the particles' kinetic and potential energies become

$$T = \frac{1}{2}|\dot{\mathbf{x}}|^2 = \frac{1}{2}\{(z\omega\tan\beta)^2 + (\dot{z}\sec\beta)^2\}, \quad V = gz.$$

There is just one generalised coordinate, z, and so just one Euler-Lagrange equation. This immediately gives the equation of motion,

$$\ddot{z} - \omega^2 \sin^2 \beta z = -g \cos^2 \beta.$$

as asked for in the question. The Mods question also asked whether E = T + V is conserved, which it is not. A torque must be applied, and hence work must be done, to keep the rod rotating at a constant angular velocity ω .

¹The exams at the end of the first year were called Moderations ("Mods") until 2013, when they became Prelims. The original question can be found in the past papers archive.

The Lagrangian method does better. It constructs a Hamiltonian H that is conserved, but is not equal to the total energy,

$$H = \dot{z}\frac{\partial L}{\partial \dot{z}} - L = \frac{1}{2}\{(\dot{z}\sec\beta)^2 - (z\omega\tan\beta)^2\} + gz.$$

The Hamiltonian differs from T+V because T is not a homogeneous quadratic polynomial in the velocities. The kinetic energy T contains a contribution from z^2 as well as from \dot{z}^2 .

Now we are free to consider more general problems that would not be easy to solve using the methods from Prelims Dynamics.

Example 14 (Movement on a general surface without forces). Suppose we have a particle moving on a quite general surface embedded in three dimensions. (In what follows, we shall assume this constraint of contact with the surface without worrying about how it could be physically realised without the particle ever losing contact. For a mental picture, you might consider a spacecraft whose exterior surface is in the form of a double layer; the particle moves between these two layers so that the normal reaction can point either inwards or outwards.)

Hamilton's Principle leads us immediately to a Lagrangian for this motion: it is simply the kinetic energy T for motion constrained to lie on the surface. Explicitly, suppose the surface is parametrised by (u,v), so that its points are specified by $\mathbf{x}(u,v) = (x(u,v),y(u,v),z(u,v))$. Then writing L in terms of the coordinates (u,v), we have:

$$L = T = \frac{m}{2}(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) = \frac{m}{2}(E(u, v)\dot{u}^2 + 2F(u, v)\dot{u}\dot{v} + G(u, v)\dot{v}^2)$$

where

$$E(u, v) = \mathbf{x}_u \cdot \mathbf{x}_u, F(u, v) = \mathbf{x}_u \cdot \mathbf{x}_v, G(u, v) = \mathbf{x}_v \cdot \mathbf{x}_v$$

We can now write down the Euler-Lagrange equations, thus in principle determining the entire motion. In general these second-order differential equations for u and v will not be easy to solve, but a simplifying feature is that the path taken by the particle is a geodesic on the surface — a stationary value of arc-length.

To show this, note first that a Lagrangian L of a purely 'kinetic energy' form, (i.e. quadratic in the velocities \dot{q}_i , and with no explicit dependence on t) has a special property: by the Beltrami identity the value of L is itself a constant of the motion.

The kinetic energy is also positive-definite. Suppose that f is some strictly increasing function on the positive real numbers, and consider the stationary value problem for f(L). The Euler-Lagrange equations will be

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial f(L)}{\partial \dot{q}_i} - \frac{\partial f(L)}{\partial q_i} = 0$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(f'(L) \frac{\partial L}{\partial \dot{q}_i} \right) - f'(L) \frac{\partial L}{\partial q_i} = 0$$

$$f''(L) \frac{\mathrm{d}L}{\mathrm{d}t} \frac{\partial L}{\partial \dot{q}_i} + f'(L) \left(\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} \right) = 0$$

but as dL/dt = 0 and $f'(L) \neq 0$ this reduces to the Euler-Lagrange equations for L.

Taking f(L) to be \sqrt{L} tells us that

$$\int \sqrt{E(u,v)\dot{u}^2 + 2F(u,v)\dot{u}\dot{v} + G(u,v)\dot{v}^2} \,dt$$

generates the same Euler-Lagrange equations. But this is simply the arc-length for a trajectory on the surface, defining a geodesic where it is stationary.

If we wish we can eliminate the time variable t and write the integral as

$$\int \sqrt{E(u,v) + 2F(u,v)v_u + G(u,v)v_u^2} \, du$$

where now v = v(u) is being considered as defining the curve on the surface. This is of the same form as we studied earlier.

So in the absence of forces, a particle simply takes the shortest path (at least in the sense of a local minimum) it can, consistent with geometrical constraints. In this case, least action actually coincides with shortest distance. This is a generalization of Newton's second law.

5.1. More geodesics.

Example 15 (Circular cylinder). Take the surface to be the circular cylinder of radius 1 and axis along the z-axis. It is then given by

$$\mathbf{x}(u,v) = (\cos u, \sin u, v).$$

We then calculate $\mathbf{x}_u = (-\sin u, \cos u, 0), \mathbf{x}_v = (0, 0, 1),$ so that E = G = 1, F = 0. The Lagrangian is just the kinetic energy,

$$L(u, v, \dot{u}, \dot{v}) = \frac{1}{2}(\dot{u}^2 + \dot{v}^2),$$

so the geodesics are given by

$$\ddot{u} = \ddot{v} = 0$$
.

Tjese are straight lines in the (u, v) coordinates. The same conclusion comes equally easily from finding the geodesics as curves of stationary arc-length. The method above gives $v_{uu} = 0$, i.e. v = au + b, as the equation of the geodesics. (Note that paths on the cylinder illustrate very clearly that a local minimum of path-length is not at all the same thing as the global minimum.)

Why is this so simple? The point is that although the cylinder has been given as a curved surface in \mathbb{R}^3 , it is in fact intrinsically flat, as is intuitively obvious: the surface can be unwrapped without any stretching and laid out on a Euclidean plane. The proper word for this is that it is isometric to the plane. Under such an isometry, the geodesics are unchanged, since they are defined intrinsically.

It is worth noting that the concept of geodesic on a surface is much more general than this. There is no need to restrict to surfaces as defined by an embedding in an ambient three-dimensional space. The metric can be given abstractly (in fact we did this with our 'speed' functions in the opening lecture). Also, there is no need to restrict attention to geodesics on surfaces; we could equally well study geodesics in spaces of any number of dimensions.

In physics, this is a most important idea in the development of Einstein's general theory of relativity. In this theory, gravity becomes a part of the four-dimensional space-time geometry, not a force, and the orbits of free fall under gravity (including light rays) must be geodesics in the resulting space; the four-dimensional space is not thought of as embedded in anything bigger.

In pure mathematics, the study of geodesics is a vital part of Geometry and something you could pursue in the B course Geometry of Surfaces.

6. Generalization to several independent variables and to higher derivatives

6.1. Several independent variables. Suppose that instead of considering the stationary values of functionals of a curve y(x), we go up one dimension and consider the variation of surfaces z(x, y). Thus we define the functional

$$I[z] = \int \int_{R} F(x, y, z, z_x, z_y) dx dy,$$

where R is some region in the (x, y)-plane, and z_x, z_y are the partial derivatives of z(x, y) with respect to x and y.

For example, $F(x, y, z, z_x, z_y) = \sqrt{1 + z_x^2 + z_y^2}$ would give the area of the surface, and so allow the investigation of minimal surfaces in generality (not restricted to surfaces of revolution).

The method, as always, is to vary the dependent variable along a one-dimensional path:

$$z(x,y) \rightarrow z(x,y) + \alpha \eta(x,y),$$

to obtain

$$\frac{\mathrm{d}I}{\mathrm{d}\alpha}\bigg|_{\alpha=0} = \iint_R \left(\eta \frac{\partial F}{\partial z} + \eta_x \frac{\partial F}{\partial z_x} + \eta_y \frac{\partial F}{\partial z_y}\right) \,\mathrm{d}x \,\mathrm{d}y.$$

We can eliminate η_x and η_y using the divergence theorem (or Green's theorem since we are in 2D)

$$\frac{\mathrm{d}I}{\mathrm{d}\alpha}\bigg|_{\alpha=0} = \iint_{R} \left\{ \eta \frac{\partial F}{\partial z} + \frac{\partial}{\partial x} \left(\eta \frac{\partial F}{\partial z_{x}} \right) - \eta \frac{\partial}{\partial x} \frac{\partial F}{\partial z_{x}} + \frac{\partial}{\partial y} \left(\eta \frac{\partial F}{\partial z_{y}} \right) - \eta \frac{\partial}{\partial y} \frac{\partial F}{\partial z_{y}} \right\} \, \mathrm{d}x \, \mathrm{d}y, \\
= \int_{\partial R} \eta \left(\frac{\partial F}{\partial z_{x}} n_{x} + \frac{\partial F}{\partial z_{y}} n_{y} \right) \, \mathrm{d}s + \iint_{R} \eta \left\{ \frac{\partial F}{\partial z} - \frac{\partial}{\partial x} \frac{\partial F}{\partial z_{x}} - \frac{\partial}{\partial y} \frac{\partial F}{\partial z_{y}} \right\} \, \mathrm{d}x \, \mathrm{d}y,$$

where $\mathbf{n} = (n_x, n_y)$ is the outward-pointing normal vector on the boundary curve ∂R with arc length s.

In the case of fixed boundary conditions, $\eta=0$ on ∂R , the integral over ∂R vanishes, so we obtain:

$$\frac{\mathrm{d}I}{\mathrm{d}\alpha}\bigg|_{\alpha=0} = \iint_R \eta \left(\frac{\partial F}{\partial z} - \frac{\partial}{\partial x} \frac{\partial F}{\partial z_x} - \frac{\partial}{\partial y} \frac{\partial F}{\partial z_y} \right) \, \mathrm{d}x \, \mathrm{d}y.$$

We conclude that the Euler-Lagrange equation, which must hold at all points in R, is

$$\frac{\partial}{\partial x}\frac{\partial F}{\partial z_x} + \frac{\partial}{\partial y}\frac{\partial F}{\partial z_y} - \frac{\partial F}{\partial z} = 0.$$

Further generalization, to n rather than 2 independent variables, is immediate. The result is the following theorem.

Theorem 6.1. Let F be a smooth function, and I the functional

$$I[u] = \int_{R} F(x_1, \dots, x_n, u, u_1, \dots, u_n) dx_1 \dots dx_n,$$

an integral over a region $R \subseteq \mathbb{R}^n$, for smooth functions $u = u(x_1, x_2 \dots x_n)$ where we write u_i for $\partial u/\partial x_i$. Then the minimisers of I[u], subject to fixed boundary conditions on ∂R , satisfy the Euler-Lagrange equation

$$\sum_{i=1}^{n} \frac{\partial}{\partial x_i} \frac{\partial F}{\partial u_i} - \frac{\partial F}{\partial u} = 0.$$

Note: In the above theorem we need to assume that not only u, but also the region R, is sufficiently 'nice' for the statement to hold.

We can write the Euler–Lagrange equation more compactly as

(46)
$$\nabla \cdot \left(\frac{\partial F}{\partial \nabla u}\right) - \frac{\partial F}{\partial u} = 0,$$

by introducing the notation

(47)
$$\frac{\partial F}{\partial \nabla u} = \left(\frac{\partial F}{\partial u_1}, \frac{\partial F}{\partial u_2}, \dots, \frac{\partial F}{\partial u_n}\right)$$

for the vector of partial derivatives of F with respect to u_1, u_2, \ldots, u_n .

Example 16 (Reformulation of Laplace's equation). A simple and beautiful example of this is the case where

$$F = \frac{1}{2}|\nabla u|^2 = \frac{1}{2}\sum_{i=1}^n u_i^2$$

in which case the Euler-Lagrange equation is just

$$0 = \sum_{i=1}^{n} \frac{\partial}{\partial x_i} \frac{\partial F}{\partial u_i} - \frac{\partial F}{\partial u} = \sum_{i=1}^{n} \frac{\partial}{\partial x_i} u_i = \nabla^2 u,$$

i.e. the Laplace equation or its n-dimensional generalization. This indicates that Laplacian or wave-equation problems can readily be reformulated in a variational form — an idea which is fundamental both o modern quantum field theory, and also to the numerical solution of elliptic equations using the finite element method.

6.2. **Higher derivatives.** Suppose now we wish to find stationary values for

$$I[y] = \int_a^b F(x, y, y', y'') dx.$$

Varying y(x) as before, we find

$$\frac{\mathrm{d}I}{\mathrm{d}\alpha}\bigg|_{\alpha=0} = \int_a^b \left(\eta \frac{\partial F}{\partial y} + \eta' \frac{\partial F}{\partial y'} + \eta'' \frac{\partial F}{\partial y''}\right) \,\mathrm{d}x.$$

Integrating by parts twice, we find

$$\frac{\mathrm{d}I}{\mathrm{d}\alpha}\bigg|_{\alpha=0} = \left[\eta\left(\frac{\partial F}{\partial y'} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial F}{\partial y''}\right) + \eta'\frac{\partial F}{\partial y''}\right]_{a}^{b} + \int_{a}^{b} \eta\left(\frac{\partial F}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial F}{\partial y'} + \frac{\mathrm{d}^{2}}{\mathrm{d}x^{2}}\frac{\partial F}{\partial y''}\right) \mathrm{d}x.$$

Thus we now have, as a necessary condition for a stationary solution, the satisfaction of the Euler–Lagrange equation

$$\frac{\partial F}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x} \frac{\partial F}{\partial y'} + \frac{\mathrm{d}^2}{\mathrm{d}x^2} \frac{\partial F}{\partial y''} = 0.$$

This is a fourth-order differential equation, requiring four constants of integration. These must come from a suitable selection of end-point conditions (now on both y and y'), and natural boundary conditions

$$\frac{\partial F}{\partial y'} - \frac{\mathrm{d}}{\mathrm{d}x} \frac{\partial F}{\partial y''} = 0, \quad \frac{\partial F}{\partial y''} = 0.$$

Example 17 (A diving board). We shall study a problem which gives a picture of how the calculus of variations can solve practical problems of optimisation such as arise in engineering and economics.

We consider the functional

$$E[y] = \int_0^L (\frac{1}{2}K(y'')^2 + \rho gy) \, dx,$$

which can be considered as the total energy of an elastic beam of horizontal length L, clamped at x=0 so that it has y=0,y'=0 there, but free at x=L and bending under its weight. (We assume that y is suitably small, so that this functional is a reasonable approximation to the physical situation.) The beam will settle in an equilibrium where the total energy is minimised, and so the calculus of variations gives a method to find the shape of the beam.

The Euler-Lagrange equation is

$$Ky'''' + \rho g = 0$$

and the four boundary conditions are supplied by y(0) = y'(0) = 0 at one end, and then the natural boundary conditions y''(L) = y'''(L) = 0 at the other. This clearly specifies a quartic polynomial, and satisfaction of the boundary conditions gives

$$y(x) = -\frac{\rho g}{24K}(x^4 - 4Lx^3 + 6L^2x^2).$$

Note that in this situation, the free end of the board will droop to height $y = -\rho g L^4/(8K)$. Imagine a swimmer in the pool putting a hand to the free end and fixing it at height $y = -\rho g L^4/(8K) + h$. Clearly, if h = 0 no force is required at all. But for $h \neq 0$ a force will be required. We can evaluate this force by extending the analysis.

First, solve the stationary problem again but now for the fixed-end condition $y(L) = -\rho g L^4/(8K) + h$. To shorten the expressions, write $w = \rho g/K$ in what follows. We find, straightforwardly, that now

$$y(x) = -\frac{w}{24}(x^4 - 4Lx^3 + 6L^2x^2) + \frac{h}{2L^4}(-Lx^3 + 3L^2x^2).$$

Clearly the energy functional E[y] can now be considered as a function of h. It will take the least value when h=0. If the free end is raised, the energy will increase, and this can only come from the work done, which is given by $\int F(h) dh$, where F(h) is the force needed to keep $y(L) = -w/(8L^4) + h$. Thus F(h) = E'(h).

This is easily calculated and is $3hK/L^3$.

Returning to the situation where the end x = L is free, we can apply the same ideas to find the forces being applied at x = 0 in order to maintain the constraints. In this case

24 PAUL DELLAR

it is even easier to see that the upward force to maintain y(0) = 0 is just the total weight ρgL of the board; slightly less obvious is that a torque of moment $\frac{1}{2}\rho gL^2$ is applied by the clamp to maintain the condition y'(0) = 0. In this case, the work done is the integral of torque with respect to angle, rather than the integral of force with respect to displacement as above.

You will already be familiar with this idea of a *force* being associated with a constraint, since it is just the idea of a normal reaction that you had in Prelims mechanics.

But suppose the functional is something that measures not energy but cost. Then the elements of the problem, including the constraints, take on an *economic* interpretation. You could imagine this diving-board curve as representing the effect of a company buying a hospital and changing a policy of stable employment to one of running down the work force. (The independent variable x is now time, and y measures the size of the work force.) How can it pursue this policy at least cost? Suppose that its cost functional is given by the same elements as appeared in the diving-board functional: the wages, proportional to y, and the cost in administrative disruption, strikes, etc. from making swingeing cuts, modelled as proportional to $(y'')^2$. The solution with natural boundary conditions will represent the ideal situation (from the point of view of the company, of course, not that of the patients!) at the end of a period. If a government regulator imposes a constraint, of dictating what the workforce level must be at that point, that constraint is naturally associated with a price: it is what it will be worth the company paying to persuade the regulator to reduce the imposed quota by one unit. In the Optimisation course, using linear programming, you met the idea that prices are dual variables associated with constraints, and this is a another example of it.

7. Extremals subject to an integral constraint

The problem addressed in this section is that of how to find a stationary value of an integral

$$I[y] = \int_a^b F(x, y, y') \, \mathrm{d}x,$$

subject to an integral constraint

$$J[y] = \int_a^b G(x, y, y') \, \mathrm{d}x = C.$$

We can do this using the method of Lagrange multipliers from Prelims. Suppose η_1 and η_2 are two linearly-independent test functions, and consider the variation

$$y \to y + \alpha_1 \eta_1 + \alpha_2 \eta_2$$

where α_1 and α_2 are real parameters. For fixed η_1 and η_2 this determines two functions of α_1 and α_2 ,

$$\hat{I}(\alpha_1, \alpha_2) = I[y + \alpha_1 \eta_1 + \alpha_2 \eta_2], \quad \hat{J}(\alpha_1, \alpha_2) = J[y + \alpha_1 \eta_1 + \alpha_2 \eta_2].$$

We know from Prelims that the problem of finding a stationary value of $\hat{I}(\alpha_1, \alpha_2)$ subject to $\hat{J}(\alpha_1, \alpha_2) = C$ is equivalent to finding a stationary value of $\hat{I}(\alpha_1, \alpha_2) - \lambda \hat{J}(\alpha_1, \alpha_2)$.

Since this holds for all linearly-independent pairs η_1 and η_2 , and indeed for variations of the form

$$y \to y + \sum_{i=1}^{n} \alpha_i \eta_i$$

for n real parameters α_i and linearly-independent test functions η_i , it seems reasonable to suppose that we can find a stationary value of I[y], constrained by J[y] = C, by looking for stationary values of

$$I[y] - \lambda J[y].$$

Hence y must satisfy the Euler-Lagrange equation

$$\frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{\partial}{\partial y'} (F - \lambda G) \right) - \frac{\partial}{\partial y} (F - \lambda G) = 0,$$

for some constant λ . Moreover, y must satisfy the corresponding fixed end point or natural boundary conditions, where the natural boundary conditions are now

$$\frac{\partial}{\partial y'}(F - \lambda G) = 0$$
 at $x = a$ and $x = b$

Let us record this as a useful theorem.

Theorem 7.1. Let F, G be two smooth functions, and

$$I[y] := \int_a^b F(x, y, y') dx, \qquad J[y] := \int_a^b G(x, y, y') dx.$$

then any smooth stationary value of I[y] subject to the constraint J[y] = C satisfies

$$\frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{\partial}{\partial y'} (F - \lambda G) \right) - \frac{\partial}{\partial y} (F - \lambda G) = 0,$$

for some constant λ .

A freely hanging chain — the catenary:

We can use this method to find the shape taken by an idealised hanging chain of constant density, supported only at its two ends. Assume that the chain falls on a curve described by y = y(x), with fixed endpoints y = b at $x = \pm a$. It is subject to the constraint that its total length is fixed:

$$J[y] = \int_a^a \sqrt{1 + y'^2} \, \mathrm{d}x = \ell,$$

with $\ell > 2a$. Its equilibrium is then determined by minimising its gravitational potential energy, which is

$$I[y] = g\rho \int_{-a}^{a} y \sqrt{1 + y'^2} \, \mathrm{d}x.$$

Applying the Lagrange multiplier method, and absorbing ρg into the λ , gives

$$F - \lambda G = (y - \lambda)\sqrt{1 + y'^2}.$$

This has no explicit x-dependence, so Beltrami's identity gives a first integral:

$$(y - \lambda) = c\sqrt{1 + y'^2}.$$

Substituting $y = \lambda + c \cosh u$ readily gives the solution

$$y = \lambda + c \cosh\left(\frac{x - x_0}{c}\right).$$

Fitting the constants c, λ , x_0 to the given data a, b, ℓ is left as an exercise.

Dido's Problem:

Another classical problem of this nature is the simplest example of an *isoperimetric* problem. On the Euclidean plane, given a fixed length as a perimeter, what is the largest area that can be enclosed by it? (The answer is given by taking a circle.) We will consider a slightly different version of this problem, in which the area is on one side of a given straight line, w.l.o.g the x-axis. Then the answer is given by taking the boundary to be a circular arc. You will find this described as 'Dido's problem', since it can somewhat fancifully be considered as arising in the Aeneid. Dido (better known for inspiring Purcell's famous Lament) supposedly fixed the boundaries of Carthage by this criterion. The line y=0 represents the Mediterranean coastline.

See http://mathworld.wolfram.com/DidosProblem.html

For this problem, we could take F = y and $G = \sqrt{1 + y'^2}$, where the boundary curve is taken to be y = y(x), but it is actually better to represent the boundary curve in parametric form as (x(t), y(t)), where t is an arbitrary parameter. We this consider the extremals of

$$\int \left(y\dot{x} - \lambda\sqrt{\dot{x}^2 + \dot{y}^2}\right) dt.$$

The Euler–Lagrange equations are

(48)
$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{-\lambda \dot{y}}{\sqrt{\dot{x}^2 + \dot{y}^2}} \right) = \dot{x}, \quad \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{-\lambda \dot{x}}{\sqrt{\dot{x}^2 + \dot{y}^2}} \right) = -\dot{y},$$

SO

(49)
$$\frac{-\lambda \dot{y}}{\sqrt{\dot{x}^2 + \dot{y}^2}} = (x - a), \quad \frac{-\lambda \dot{x}}{\sqrt{\dot{x}^2 + \dot{y}^2}} = -(y - b).$$

Eliminating λ gives

$$(x-a)\dot{x} + (y-b)\dot{y} = 0,$$

which integrates to give

$$(x-a)^2 + (y-b)^2 = c^2,$$

so the curves must be circles.

For the original Dido problem we are interested in the case of a fixed boundary condition y(t) = 0 at each end, and a natural boundary condition for x(t) at each end (that is, we are taking the extremals over all possible x, given y = 0.) The natural boundary condition for x is $y - \lambda \dot{x}/\sqrt{\dot{x}^2 + \dot{y}^2} = 0$, and since y = 0, this means $\dot{x} = 0$. The derivative $\mathrm{d}y/\mathrm{d}x$ is infinite here, which is why the y(x) formulation is not appropriate. The centre of the circle must thus be on y = 0, and the stationary area, given the constraint, will be bounded by a semi-circle, as expected.

These are the same semi-circles as we have met in the problem of the quickest paths on the muddy field (more formally, geodesics on the hyperbolic plane). This can be seen more directly if we proceed slightly differently. The second equation in (48) can be written

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\lambda \dot{x}}{\sqrt{\dot{x}^2 + \dot{y}^2}} - y \right) = 0, \quad \text{so } \frac{\lambda \dot{x}}{\sqrt{\dot{x}^2 + \dot{y}^2}} - y = \text{constant.}$$

When the boundary conditions $y = 0, \dot{x} = 0$ are imposed, this constant must be 0, and so

$$y\sqrt{1+y'^2} = \lambda.$$

This is the same equation that arises for the quickest-path problem, at (29), and so has the same semi-circle solutions.

This feature extends to the more general land enclosure problem where a varying value h(y) is attached to the land and the objective is to secure the greatest total value for a given length of border. In this case, the problem is given by taking F = H(y) and $G = \sqrt{1 + y'^2}$, where $H(y) = \int_0^y h(u) du$. For the case of natural boundary conditions, the resulting equation is

$$H(y)\sqrt{1+y'^2} = \lambda,$$

which you can check is the same equation as arises from the problem of finding the quickest path on the muddy field when the speed of movement is H(y).

Thus if $h(y) = 1/\sqrt{y}$, so $H(y) = 2\sqrt{y}$, we recover equation (31) from the Brachistochrone problem, so the solution is a cycloid.

Constraints and prices again

We now have another example of where a constraint can be thought of as defining a *price*. How much more I can we get if we change the constraint J = C to $J = C + \delta C$? Write I(C) for the stationary value of I, given the constraint J = C. Then we find that

(50)
$$\lambda = \frac{\mathrm{d}I(C)}{\mathrm{d}C},$$

giving a nice interpretation of the λ .

For a proof of this, recall that the solution $I - \lambda J$ is stationary, i.e. is unchanged, to first order, when the extremal y is changed to any $y + \delta y$ consistent with the boundary conditions. Suppose we choose the particular δy which makes $y + \delta y$ the extremal for the problem where the constraint $J = C + \delta C$ is imposed. Then we have

$$I(C) - \lambda C = I(C + \delta C) - \lambda (C + \delta C)$$

to first order. Subtracting and taking $\delta C \to 0$, we recover the relation.

Thus, in Dido's problem the value of λ in the solution indicates the value (in extra area gained) of increasing the length of the rope which defines the perimeter. We have thus solved an extra problem: how much money Dido should be willing to pay for additional rope.

Specifically, in this problem, we have for perimeter of length L, a stationary area $I(L) = L^2/(2\pi)$, and so $dI/dL = L/\pi$, which is just the radius of the circle. It is easy to check that this is indeed the value of λ .

8. Application to Sturm-Liouville equations

8.1. Some motivation from quantum mechanics. In quantum mechanics, the state of a physical system depends not on the motion of point particles but of wave functions. These are actually complex-valued, but for the purpose of this discussion we can give a simplified picture with real functions. The simplest situation is for a single particle confined to a one-dimensional finite interval [0,1]. Whilst a point particle could simply remain at rest in this interval, and have zero kinetic energy, the wave-function $\psi(x)$ has an kinetic energy associated with (half) the integrated square of its derivative: $\int_0^1 \{\psi'(x)\}^2 dx$. So far this might look something like the kinetic energy of a fluid, but there is a subtlety which makes a wave-function completely different from a classical fluid. The energy is actually determined by the ratio

$$\frac{\int_0^1 \{\psi'(x)\}^2 dx}{\int_0^1 \{\psi(x)\}^2 dx}$$

so that multiplying $\psi(x)$ by a constant makes no difference. The energy is a functional of the *shape* of the ψ , not of its scale. In particular, $\psi \equiv 0$ makes no sense in this ratio, so there is no obvious analogue of a particle at rest. Instead, the question of the *least value* taken by this ratio emerges, and it is far from intuitively clear. In fact, for functions such that $\psi(0) = 0 = \psi(1)$, the answer is π^2 , as we shall show, and the existence of such a non-zero *ground-state energy* is a typical feature of quantum systems in much more general settings.

We need a formalism that will handle this problem, but also the more general problems that arise when the energy functional is not so simple, and the geometry of the space not just a simple interval. Clearly, the theory of stationary integrals, subject to an integral constraint, provides just this formalism. The ratio problem as described above can be restated as the problem of finding a minimum for $\int_0^1 \{\psi'(x)\}^2 dx$ subject to the constraint that $\int_0^1 \{\psi(x)\}^2 dx = 1$.

Thus the ratio of interest can be identified with the value taken by the Lagrange multiplier λ in the solution. If we look at this in the light of the preceding discussion, we see that the relationship of I[y] to J[y] is very simple in this case: it is simply linear, $I = \lambda J$, with λ interpretable as a constant price. But what is new in this situation is that for the first time we are taking seriously the fact that there are many local extrema, in fact a countable infinity of them, and we are studying how they inter-relate.

The inter-relation of the extrema is naturally expressed by seeing that λ also takes on a further meaning as the *eigenvalue* of an differential operator.

8.2. **The Sturm–Liouville equation.** The differential operators we are concerned with are just the same as you may have met in Differential Equations 2, but written in a slightly different way. The standard *Sturm–Liouville form* is

$$(p(x)y')' + q(x)y = -\lambda r(x)y$$
 for $a \le x \le b$,

with boundary conditions which will be specified below. Here p, q, r are taken to have continuous derivatives, and we shall assume that $p \ge 0$ and r > 0.

This is the Euler–Lagrange equation for the variational problem of finding stationary values of

$$I[y] = \int_a^b (p(y')^2 - qy^2) dx,$$

subject to

$$J[y] = \int_a^b ry^2 dx = \text{ constant.}$$

We can now note the boundary conditions that are consistent with this interpretation: we have the usual choice between fixed and natural boundary conditions at each end, so that either

$$y(a) = 0 \text{ or } p(a)y'(a) = 0,$$

and similarly at b.

- 8.3. **Examples.** 1. If $p \equiv 1, q \equiv 0, r \equiv 1$, we regain the motivating example that began this section. But now we can solve it: the allowed values of λ are just the sequence $\lambda_n = n^2 \pi^2$, and the corresponding $y_n(x)$ are (proportional to) $\sin(n\pi x)$.
- 2. If $p(x) = 1 x^2$, $q \equiv 0$, $r \equiv 1$, we have Legendre's equation on [-1, 1]. With natural boundary conditions, the solutions are the Legendre polynomials $P_n(x)$, as met in the course Differential Equations 2.

3. If p(x) = x, $q(x) = -k^2/x$, r(x) = x, we obtain the equation

$$(xy')' - \frac{k^2}{x}y = -\lambda xy$$

which is equivalent to

$$y'' + \frac{1}{x}y' - \frac{k^2}{x^2}y = -\lambda y$$

also recognisable from Differential Equations 2 as Bessel's equation of order k. This has solutions vanishing at x=0 of form $J_k(\lambda x)$ for k>0. A fuller treatment would bring in the solutions to Bessel's equation that diverge at x=0, but in the simplest situation, when boundary conditions y=0 at x=0 and x=a are imposed, there will be a discrete spectrum of λ_n such that $J_k(\lambda_n x)$ vanishes at x=0 and x=a.

8.4. **Eigenfunction expansions.** The idea of Sturm-Liouville theory is to generalise the Fourier analysis that is naturally associated with the first example. You may have met Sturm-Liouville theory in Differential Equations 2. The time-independent Schrödinger equation in a bounded domain from Part A Quantum Theory is a special case of a Sturm-Liouville problem with p(x) taken to be a constant.

From Prelims Fourier Series and PDEs, you know how to expand a general function in terms of sines and cosines, making use of their completeness and orthogonality properties. It turns out that these properties are not unique to the trigonometrical functions. They can be regarded as following from their emergence as solutions to a Sturm-Liouville ODE, and any other Sturm-Liouville equation will give rise to another set of functions with these completeness and orthogonality properties. That is, there is in general, for any Sturm-Liouville equation, a sequence of eigenfunctions $y_n(x)$ with completeness and orthogonality properties, such that a general function can usefully be expanded as $\sum_n c_n y_n$, as in Differential Equations 2.

The proper statement and proof of this lies beyond this course (remember that even for Fourier theory the question of completeness is subtle, with great attention being needed for points of discontinuity.) However, we can show how the vital orthogonality properties emerge directly from this formulation.

Suppose, for a (p,q,r) Sturm-Liouville system, we have two solutions y_n, y_m with the corresponding $\lambda_n \neq \lambda_m$.

We will first verify that λ_n , the eigenvalue associated with the eigenfunction y_n , is equal to the quotient $I[y_n]/J[y_n]$ and so to the Lagrange multiplier in the integral formulation. We have

$$(p(x)y_n')' + q(x)y_n = -\lambda_n r(x)y_n$$

so multiplying by y_n and integrating,

$$\int_a^b (p(x)y_n')'y_n + q(x)y_n^2 dx = -\lambda_n \int_a^b r(x)y_n^2 dx$$

SO

$$\int_{a}^{b} \frac{\mathrm{d}}{\mathrm{d}x} (py'_{n}y_{n}) \, \mathrm{d}x - \int_{a}^{b} (p(x){y'}_{n}^{2} - q(x)y_{n}^{2}) \, \mathrm{d}x = -\lambda_{n} \int_{a}^{b} r(x)y_{n}^{2} \, \mathrm{d}x$$

i.e.

(51)
$$[py'_n y_n]_a^b - I[y_n] = -\lambda_n J[y_n].$$

But the boundary term vanishes because a we either have $y_n(a) = 0$ or we have $p(a)y'_n(a) = 0$, and similarly at b. Hence $I[y_n] = \lambda_n J[y_n]$ as required.

Now we shall show that y_m, y_n are orthogonal, in the sense that

$$\int_{a}^{b} r y_n y_m \mathrm{d}x = 0.$$

We have that

$$(p(x)y_n')' + q(x)y_n = -\lambda_n r(x)y_n$$

$$(p(x)y_m')' + q(x)y_m = -\lambda_m r(x)y_m$$

Multiplying the first by y_m , the second by y_n , subtracting, and integrating from a to b gives

$$\int_a^b (y_m(py_n')' - y_n(py_m')') dx = -(\lambda_n - \lambda_m) \int_a^b r(x) y_m y_n dx$$

. The LHS can be exactly integrated to

$$[p(y_m y'_n - y_n y'_m)]_a^b$$

and thus vanishes by the boundary conditions. At a, we either have $y_m(a) = 0 = y_n(a)$ or we have $p(a)y_m'(a) = 0 = p(a)y_n'(a)$, and similarly at b. Thus the RHS vanishes, and since $\lambda_m - \lambda_n \neq 0$ by assumption, the orthogonality follows.

This argument is the same as that used in the Algebra course where the general definition of an inner product is discussed. We have in effect defined an inner product structure on a space of functions by using r(x) as the weight function. We can then define an orthonormal set of basis functions y_n , with respect to this inner product, by choosing the scale such that

$$J[y_n] = \int_a^b r(x) \{y_n(x)\}^2 dx = 1.$$

8.5. Rayleigh—Ritz approximation. Throughout the course we have emphasised that the variational formalism is a two-way street. Our theory allows the solution, via differential equations, of notable problems involving extremals. On the other hand, it can be used profitably to reformulate problems to do with differential equations in terms of stationary integrals. In the context of Sturm—Liouville equations, the spectrum eigenvalues can be usefully investigated by calculating the integrals I[y] and J[y]. In particular, trying out any y whatever gives an upper bound for the lowest eigenvalue λ_1 .

Thus, returning to the original example of

$$\frac{\int_0^1 \{\psi'(x)\}^2 dx}{\int_0^1 \{\psi(x)\}^2 dx},$$

we can try the simplest possible y satisfying the boundary conditions, y = x(1 - x), and calculate

$$Q = \frac{\int_0^1 (2x - 1)^2 dx}{\int_0^1 x^2 (1 - x)^2 dx} = 10,$$

so that $\lambda_1 \leq 10$. This is a good approximation to $\lambda_1 = \pi^2$.

This process can be refined. Clearly, this approximation could be improved by optimising the trial y over a set of parameters. Hence we arrive at a good approximation \tilde{y}_1 to y_1 . Then, the next eigenvalue could be estimated by optimising over another class of trial functions, all orthogonal to \tilde{y}_1 . This gives an estimate of λ_2 and y_2 , and so on.

There is a reason why the approximation of eigenvalues is good; if the trial function \tilde{y}_1 is correct to $O(\epsilon)$, the eigenvalue λ_1 will be good to $O(\epsilon^2)$. For if

$$\tilde{y}_1 = y_1 + \sum_{n=2}^{\infty} c_n y_n,$$

where each c_n is of $O(\epsilon)$, then $Q[\tilde{y}_1]$ differs from λ_1 by $O(\epsilon^2)$ because

$$I[\tilde{y}_1] = \lambda_1 + \sum_{n=2}^{\infty} \lambda_n |c_n|^2, \quad J[\tilde{y}_1] = 1 + \sum_{n=2}^{\infty} |c_n|^2.$$

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