Chapter 1

Variational Methods

1.1 Stationary Values of Functions

Recall Taylor's Theorem for a function $f(\mathbf{x})$ in three dimensions with a displacement $\delta\mathbf{x} = (\delta x, \delta y, \delta z)$:

$$f(\mathbf{x}+\delta\mathbf{x}) = f(\mathbf{x}) + \frac{\partial f}{\partial x}\,\delta x + \frac{\partial f}{\partial y}\,\delta y + \frac{\partial f}{\partial z}\,\delta z + \text{higher order terms}$$

so that

$$\delta f = f(\mathbf{x}+\delta\mathbf{x}) - f(\mathbf{x}) = \frac{\partial f}{\partial x}\,\delta x + \frac{\partial f}{\partial y}\,\delta y + \frac{\partial f}{\partial z}\,\delta z + \cdots$$

$$= \nabla f \,.\, \delta\mathbf{x} + \cdots .$$

In the limit $|\delta\mathbf{x}| \to 0$ we write

$$\boxed{\mathrm{d}f = \nabla f \,.\, \mathrm{d}\mathbf{x}.}$$

This result is true in any number n of dimensions.

At an extremum (a maximum or minimum) f must be stationary, i.e. the first variation $\mathrm{d}f$ must vanish *for all* possible directions of $\mathrm{d}\mathbf{x}$. This can only happen if $\nabla f = \mathbf{0}$ there.

Note that if we try to find the extrema of f by solving $\nabla f = \mathbf{0}$, we may also find other stationary points of f which are neither maxima nor minima, for instance saddle points. (This is the same difficulty as in one dimension, where a stationary point may be a point of inflection rather than a maximum or minimum.)

If we need to find the extrema of f in a *bounded* region – for instance, within a two-dimensional unit square – then not only must we solve $\nabla f = \mathbf{0}$ but we must also compare the resulting values of f with those on the boundary of the square. It is quite possible for the maximum value to occur on the boundary without that point being a stationary one.

Constrained stationary values

Suppose that we wish to find the extrema of $f(\mathbf{x})$ subject to a constraint of the form $g(\mathbf{x}) = c$, where c is some constant. In this case, the first variation $\mathrm{d}f$ must still vanish, but now not all possible directions for $\mathrm{d}\mathbf{x}$ are allowed: only those which lie in the surface defined by $g(\mathbf{x}) = c$. Hence, since $\mathrm{d}f = \nabla f \boldsymbol{.} \mathrm{d}\mathbf{x}$, the vector ∇f must lie perpendicular to the surface.

But recall that the normal to a surface of the form $g(\mathbf{x}) = c$ is in the direction ∇g. Hence ∇f must be parallel to ∇g, i.e., $\nabla f = \lambda \nabla g$ for some scalar λ.

This gives us the method of *Lagrange's undetermined multiplier*: solve the n equations

$$\boxed{\nabla(f - \lambda g) = \mathbf{0}}$$

for $\mathbf{x}$ together with the single constraint equation

$$g(\mathbf{x}) = c.$$

The resulting values of $\mathbf{x}$ give the stationary points of f subject to the constraint. Note that while solving the total of $n+1$ equations it is usually possible to eliminate λ without ever finding its value; hence the moniker "undetermined".

If there are two constraints $g(\mathbf{x}) = c$ *and* $h(\mathbf{x}) = k$, then we need a multiplier for each constraint, and we solve

$$\nabla(f - \lambda g - \mu h) = \mathbf{0}$$

together with the two constraints. The extension to higher numbers of constraints is straightforward.

1.2 Functionals

Let $y(x)$ be a function of x in some interval $a < x < b$, and consider the definite integral

$$F = \int_a^b \left(\{y(x)\}^2 + y'(x) y''(x) \right) \mathrm{d}x.$$

F is clearly independent of x; instead it depends only on the *function* $y(x)$. F is a simple example of a *functional*, and to show the dependence on y we normally denote it $F[y]$.

We can think of functionals as an extension of the concept of a function of many variables – e.g. $g(x_1, x_2, \ldots, x_n)$, a function of n variables – to a function of an infinite number of variables, because F depends on every single value that y takes in the range $a < x < b$.

We shall be concerned in this chapter with functionals of the form

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

where f depends *only* on x and the value of y and its first derivative at x. However, the theory can be extended to more general functionals (for example, with functions $f(x, y, y', y'', y''', \dots)$ which depend on higher derivatives, or double integrals with two independent variables x_1 and x_2 instead of just x).

1.3 Variational Principles

Functionals are useful because many laws of physics and of physical chemistry can be recast as statements that some functional $F[y]$ is minimised.

For example, a heavy chain suspended between two fixed points hangs in equilibrium in such a way that its total gravitational potential energy (which can be expressed as a functional) is minimised. A mechanical system of heavy elastic strings minimises the total potential energy, both elastic and gravitational. Similar principles apply when electric fields and charged particles are present (we include the electrostatic potential energy) and when chemical reactions take place (we include the chemical potential energy).

Two fundamental examples of such *variational principles* are due to Fermat and Hamilton.

Fermat's Principle

Consider a light ray passing through a medium of variable refractive index $\mu(\mathbf{r})$. The path it takes between two fixed points A and B is such as to minimise the optical path length

$$\boxed{\int_A^B \mu(\mathbf{r})\,\mathrm{d}l,}$$

where $\mathrm{d}l$ is the length of a path element.

Strictly speaking, Fermat's principle only applies in the *geometrical optics approximation*; i.e., when the wavelength of the light is small compared with the physical dimensions of the optical system, so that light may be regarded as rays. This is true for a telescope, but not for Young's slits: when the geometrical optics approximation fails to hold, diffraction occurs.

For example, consider air above a hot surface, say a tarmac road on a hot day. The air is hotter near the road and cooler above, so that μ is smaller closer to the road surface. A light ray travelling from a car to an observer minimises the optical path length by staying

close to the road, and so bends appropriately. The light seems to the observer to come from a low angle, leading to a virtual image (and hence to the "mirage" effect).

Hamilton's Principle of Least Action

Consider a mechanical system with kinetic energy T and potential energy V which is in some given configuration at time t_1 and some other configuration at time t_2. Define the *Lagrangian* of the system by

$$\boxed{\mathscr{L} = T - V,}$$

and define the *action* to be

$$\boxed{\mathscr{S} = \int_{t_1}^{t_2} \mathscr{L}\,\mathrm{d}t}$$

(a functional which depends on the way the system moves). Hamilton's principle states that the actual motion of the system is such as to minimise the action.

1.4 The Calculus of Variations

How do we find the function $y(x)$ which minimises, or more generally makes stationary, our archetypal functional

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

with fixed values of y at the end-points (viz. fixed $y(a)$ and $y(b)$)?

We consider changing y to some "nearby" function $y(x) + \delta y(x)$, and calculate the corresponding change δF in F (to first order in δy). Then F is stationary when $\delta F = 0$ for all possible small variations δy.

Note that a more "natural" notation would be to write $\mathrm{d}F$ rather than δF, since we will consider only the first-order change and ignore terms which are second order in δy. However, the notation δ is traditional in this context.

Now

$$\begin{aligned}
\delta F &= F[y+\delta y] - F[y] \\
&= \int_a^b f(x, y+\delta y, y'+(\delta y)')\,\mathrm{d}x - \int_a^b f(x,y,y')\,\mathrm{d}x \\
&= \int_a^b \left\{ f(x,y,y') + \frac{\partial f}{\partial y}\,\delta y + \frac{\partial f}{\partial y'}(\delta y)' \right\} \mathrm{d}x - \int_a^b f(x,y,y')\,\mathrm{d}x \\
&\qquad\qquad \text{[using a Taylor expansion to first order]} \\
&= \int_a^b \left\{ \frac{\partial f}{\partial y}\,\delta y + \frac{\partial f}{\partial y'}(\delta y)' \right\} \mathrm{d}x \\
&= \left[\frac{\partial f}{\partial y'}\,\delta y \right]_a^b + \int_a^b \left\{ \frac{\partial f}{\partial y}\,\delta y - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y'} \right) \delta y \right\} \mathrm{d}x \\
&\qquad\qquad \text{[integrating by parts]} \\
&= \int_a^b \left\{ \frac{\partial f}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y'} \right) \right\} \delta y\,\mathrm{d}x
\end{aligned}$$

since $\delta y = 0$ at $x = a$, b (because $y(x)$ is fixed there). It is clear that $\delta F = 0$ for all possible small variations $\delta y(x)$ if and only if

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y'} \right) = \frac{\partial f}{\partial y}.}$$

This is *Euler's equation.*

Notation

$\partial f/\partial y'$ looks strange because it means "differentiate with respect to y', keeping x and y constant", and it seems impossible for y' to change if y does not. But $\partial/\partial y$ and $\partial/\partial y'$ in Euler's equation are just formal derivatives (as though y and y' were unconnected) and in practice it is easy to do straightforward "ordinary" partial differentiation.

Example: if $f(x, y, y') = x(y'^2 - y^2)$ then

$$\frac{\partial f}{\partial y} = -2xy, \qquad \frac{\partial f}{\partial y'} = 2xy'.$$

Note however that $\mathrm{d}/\mathrm{d}x$ and $\partial/\partial x$ mean very different things: $\partial/\partial x$ means "keep y and y' constant" whereas $\mathrm{d}/\mathrm{d}x$ is a so-called "full derivative", so that y and y' are differentiated with respect to x as well.

Continuing with the above example,

$$\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y'}\right) = 2y',$$

but

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y'}\right) = \frac{\mathrm{d}}{\mathrm{d}x}(2xy') = 2y' + 2xy''.$$

Hence Euler's equation for this example is

$$2y' + 2xy'' = -2xy$$

or

$$y'' + \frac{1}{x}\,y' + y = 0$$

(Bessel's equation of order 0, incidentally).

Several Dependent Variables

What if, instead of just one dependent variable $y(x)$, we have n dependent variables $y_1(x)$, $y_2(x)$, …, $y_n(x)$, so that our functional is

$$F[y_1, \ldots, y_n] = \int_a^b f(x, y_1, \ldots, y_n, y_1', \ldots, y_n')\,\mathrm{d}x\,?$$

In this case, Euler's equation applies to each $y_i(x)$ independently, so that

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y_i'}\right) = \frac{\partial f}{\partial y_i}$$

for $i = 1, \ldots, n$.

The proof is very similar to before:

$$\begin{aligned}
\delta F &= \int_a^b \left\{ \frac{\partial f}{\partial y_1}\,\delta y_1 + \cdots + \frac{\partial f}{\partial y_n}\,\delta y_n + \frac{\partial f}{\partial y_1'}(\delta y_1)' + \cdots + \frac{\partial f}{\partial y_n'}(\delta y_n)' \right\} \mathrm{d}x \\
&= \int_a^b \sum_{i=1}^{n} \left\{ \frac{\partial f}{\partial y_i}\,\delta y_i + \frac{\partial f}{\partial y_i'}(\delta y_i)' \right\} \mathrm{d}x \\
&= \sum_{i=1}^{n} \int_a^b \left\{ \frac{\partial f}{\partial y_i} - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y_i'}\right) \right\} \delta y_i\,\mathrm{d}x
\end{aligned}$$

using the same manipulations (Taylor expansion and integration by parts). It is now clear that we can only have $\delta F = 0$ for *all* possible variations of *all* the $y_i(x)$ if Euler's equation applies to each and every one of the y_i at the same time.

1.5 A First Integral

In some cases, it is possible to find a first integral (i.e., a constant of the motion) of Euler's equation. Consider

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \frac{\partial f}{\partial x} + y'\frac{\partial f}{\partial y} + y''\frac{\partial f}{\partial y'}$$

(calculating $\frac{\mathrm{d}}{\mathrm{d}x} f\big(x, y(x), y'(x)\big)$ using the chain rule). Using Euler's equation,

$$\begin{aligned}\frac{\mathrm{d}f}{\mathrm{d}x} &= \frac{\partial f}{\partial x} + y'\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y'}\right) + y''\frac{\partial f}{\partial y'} \\ &= \frac{\partial f}{\partial x} + \frac{\mathrm{d}}{\mathrm{d}x}\left(y'\frac{\partial f}{\partial y'}\right)\end{aligned}$$

[product rule]

so that

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(f - y'\frac{\partial f}{\partial y'}\right) = \frac{\partial f}{\partial x}.$$

Hence, **if f has no explicit x-dependence**, so that $\partial f/\partial x = 0$, we immediately deduce that

$$\boxed{f - y'\frac{\partial f}{\partial y'} = \text{constant}.}$$

(Note that "f has no explicit x-dependence" means that x does not itself appear in the expression for f, even though y and y' implicitly depend on x; so $f = y'^2 - y^2$ has no explicit x-dependence while $f = x(y'^2 - y^2)$ does.)

If there are n dependent variables $y_1(x)$, …, $y_n(x)$, then the first integral above is easily generalised to

$$f - \sum_{i=1}^{n} y_i' \frac{\partial f}{\partial y_i'} = \text{constant}$$

if f has no explicit x-dependence.

1.6 Applications of Euler's Equation

Geodesics

A *geodesic* is the shortest path on a given surface between two specified points A and B. We will illustrate the use of Euler's equation with a trivial example: geodesics on the Euclidean plane.

The total length of a path from (x_1, y_1) to (x_2, y_2) along the path $y(x)$ is given by

$$L = \int_A^B \mathrm{d}l = \int_A^B \sqrt{\mathrm{d}x^2 + \mathrm{d}y^2}$$

$$= \int_A^B \sqrt{1 + \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2}\,\mathrm{d}x = \int_{x_1}^{x_2} \sqrt{1 + y'^2}\,\mathrm{d}x.$$

Note that we assume that $y(x)$ is single-valued, i.e., the path does not curve back on itself.

We wish to minimise L over all possible paths $y(x)$ with the end-points held fixed, so that $y(x_1) = y_1$ and $y(x_2) = y_2$ for all paths. This is precisely our archetypal variational problem with

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

and hence

$$\frac{\partial f}{\partial y} = 0, \qquad \frac{\partial f}{\partial y'} = \frac{y'}{\sqrt{1 + y'^2}}.$$

The Euler equation is therefore

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{y'}{\sqrt{1 + y'^2}}\right) = 0 \qquad \Longrightarrow \qquad \frac{y'}{\sqrt{1 + y'^2}} = k, \qquad \text{a constant.}$$

So $y'^2 = k^2/(1 - k^2)$. It is clear that $k \neq \pm 1$, so y' is a constant, m say. Hence the solutions of Euler's equation are the functions

$$y = mx + c$$

(where m and c are constants) – i.e., straight lines! To find the particular values of m and c required in this case we now substitute in the boundary conditions $y(x_1) = y_1$, $y(x_2) = y_2$.

It is important to note two similarities with the technique of minimising a function $f(\mathbf{x})$ by solving $\nabla f = \mathbf{0}$.

Firstly, we have not shown that this straight line does indeed produce a minimum of L: we have shown only that L is stationary for this choice, so it might be a maximum or even some kind of "point of inflection". It is usually easy to confirm that we have the correct solution by inspection – in this case it

is obviously a minimum. (There is no equivalent of the one-dimensional test $f''(x) > 0$ for functionals, or at least not one which is simple enough to be of any use.)

Secondly, assuming that we have indeed found a minimum, we have shown only that it is a *local* minimum, not a *global* one. That is, we have shown only that "nearby" paths have greater length. Once again, however, we usually confirm that we have the correct solution by inspection. Compare this difficulty with the equivalent problem for functions, illustrated by the graph below.

An alternative method of solution for this simple geodesic problem is to note that $f(x, y, y') = \sqrt{1 + y'^2}$ has no explicit x-dependence, so we can use the first integral:

$$\text{const.} = f - y'\frac{\partial f}{\partial y'} = \sqrt{1 + y'^2} - y'\frac{y'}{\sqrt{1 + y'^2}}$$

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

i.e., y' is constant (as before).

The Brachistochrone

A bead slides down a frictionless wire, starting from rest at a point A. What shape must the wire have for the bead to reach some lower point B in the shortest time? (A similar device was used in some early clock mechanisms.)

Using conservation of energy, $\frac{1}{2}mv^2 = mgy$, i.e., $v = \sqrt{2gy}$. Also $\mathrm{d}l = v\,\mathrm{d}t$, so

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

The time taken to reach B is therefore

$$T[y] = \frac{1}{\sqrt{2g}} \int_0^{x_B} \sqrt{\frac{1+y'^2}{y}}\, \mathrm{d}x$$

and we wish to minimise this, subject to $y(0) = 0$, $y(x_B) = y_B$. We note that the integrand has no explicit x-dependence, so we use the first integral

$$\begin{aligned}
\text{const.} &= \sqrt{\frac{1+y'^2}{y}} - y' \frac{\partial}{\partial y'} \sqrt{\frac{1+y'^2}{y}} \\
&= \sqrt{\frac{1+y'^2}{y}} - \frac{y'^2}{\sqrt{y}\sqrt{1+y'^2}} \\
&= \frac{1}{\sqrt{y}\sqrt{1+y'^2}}.
\end{aligned}$$

Hence $y(1+y'^2) = c$, say, a constant, so that

$$y' = \sqrt{\frac{c-y}{y}} \qquad \text{or} \qquad \sqrt{\frac{y}{c-y}}\, \mathrm{d}y = \mathrm{d}x.$$

Substitute $y = c\sin^2\theta$; then

$$\begin{aligned}
\mathrm{d}x &= 2c \sqrt{\frac{\sin^2\theta}{1-\sin^2\theta}}\, \sin\theta\cos\theta\, \mathrm{d}\theta \\
&= 2c\sin^2\theta\, \mathrm{d}\theta \\
&= c(1-\cos 2\theta)\, \mathrm{d}\theta.
\end{aligned}$$

Using the initial condition that when $y = 0$ (i.e., $\theta = 0$), $x = 0$, we obtain

$$\begin{aligned}
x &= c(\theta - \tfrac{1}{2}\sin 2\theta), \\
y &= c\sin^2\theta
\end{aligned}$$

which is an inverted *cycloid*. The constant c is found by applying the other condition, $y = y_B$ when $x = x_B$.

Note that strictly speaking we should have said that $y' = \pm\sqrt{(c-y)/y}$ above. Taking the negative root instead of the positive one would have lead to

$$x = -c(\theta - \tfrac{1}{2}\sin 2\theta),$$

$$y = c\sin^2\theta,$$

which is exactly the same curve but parameterised in the opposite direction. It is rarely worth spending much time worrying about such intricacies as they invariably lead to the same effective result.

Light and Sound

Consider light rays travelling through a medium with refractive index inversely proportional to $\sqrt{z}$ where z is the height. By Fermat's principle, we must minimise

$$\int \frac{\mathrm{d}l}{\sqrt{z}}.$$

This is *exactly* the same variational problem as for the Brachistochrone, so we conclude that light rays will follow the path of a cycloid.

More realistically, consider sound waves in air. Sound waves obey a principle similar to Fermat's: except at very long wavelengths, they travel in such a way as to minimise the time taken to travel from A to B,

$$\int_A^B \frac{\mathrm{d}l}{c},$$

where c is the (variable) speed of sound (comparable to $1/\mu$ for light). Consider a situation where the absolute temperature T of the air is linearly related to the height z, so that $T = \alpha z + T_0$ for some temperature T_0 at ground level. Since the speed of sound is proportional to the square root of the absolute temperature, we have $c \propto \sqrt{\alpha z + T_0} = \sqrt{Z}$ say. This leads once again to the Brachistochrone problem (for Z rather than z), and we conclude that sound waves follow paths $z(x)$ which are parts of cycloids, scaled vertically by a factor $1/\alpha$ (check this as an exercise).

1.7 Hamilton's Principle in Mechanical Problems

Hamilton's principle can be used to solve many complicated problems in rigid-body mechanics. Consider a mechanical system whose configuration can be described by a number of so-called *generalised coordinates* $q_1, q_2, \ldots, q_n$. Examples:

- A particle with position vector $\mathbf{r} = (x_1, x_2, x_3)$ moving through space. Here we can simply let $q_1 = x_1$, $q_2 = x_2$ and $q_3 = x_3$: there are three generalised coordinates.

- A pendulum swinging in a vertical plane: here there is only one generalised coordinate, $q_1 = \theta$, the angle to the vertical.
- A rigid body (say a top) spinning on its axis on a smooth plane. This requires five generalised coordinates: two to describe the position of the point of contact on the plane, one for the angle of the axis to the vertical, one for the rotation of the axis about the vertical, and one for the rotation of the top about its own axis.

The Lagrangian $\mathscr{L} = T - V$ is a function of t, $q_1, \ldots, q_n$ and $\dot{q}_1, \ldots, \dot{q}_n$, so

$$\mathscr{S} = \int \mathscr{L}\big(t, q_1(t), \ldots, q_n(t), \dot{q}_1(t), \ldots, \dot{q}_n(t)\big)\,\mathrm{d}t.$$

This is a functional with n dependent variables $q_i(t)$, so we can use Euler's equation (with t playing the role of x, and $q_i(t)$ playing the role of $y_i(x)$) for each of the q_i independently:

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathscr{L}}{\partial \dot{q}_i}\right) = \frac{\partial \mathscr{L}}{\partial q_i}}$$

for each i. In this context these equations are known as the Euler–Lagrange equations.

In the case when $\mathscr{L}$ has **no explicit time-dependence**, the first integral (from §1.5) gives us that

$$\boxed{\mathscr{L} - \sum_{i=1}^{n} \dot{q}_i \frac{\partial \mathscr{L}}{\partial \dot{q}_i} = \text{constant}.}$$

It is frequently the case that T is a homogeneous quadratic in the $\dot{q}_i$, i.e., it is of the form

$$\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(q_1, \ldots, q_n)\,\dot{q}_i\dot{q}_j$$

where the coefficients a_{ij} do not depend on any of the "generalised velocities" $\dot{q}_i$ or on t, and V also does not depend on the velocities or time so that $V = V(q_1, \ldots, q_n)$. Then it can be shown that

$$\mathscr{L} - \sum_{i=1}^{n} \dot{q}_i \frac{\partial \mathscr{L}}{\partial \dot{q}_i} = (T - V) - 2T = -(T + V),$$

i.e., the total energy $E = T + V$ is conserved when there is no explicit time-dependence. This fails however when the external forces vary with time or when the potential is velocity-dependent, e.g., for motion in a magnetic field.

A Particle in a Conservative Force Field

Here

$$\mathscr{L} = \tfrac{1}{2}m(\dot{x}_1^2 + \dot{x}_2^2 + \dot{x}_3^2) - V(x_1, x_2, x_3);$$

hence the Euler–Lagrange equations are

$$\frac{\mathrm{d}}{\mathrm{d}t}(m\dot{x}_1) = -\frac{\partial V}{\partial x_1}, \quad \frac{\mathrm{d}}{\mathrm{d}t}(m\dot{x}_2) = -\frac{\partial V}{\partial x_2}, \quad \frac{\mathrm{d}}{\mathrm{d}t}(m\dot{x}_3) = -\frac{\partial V}{\partial x_3},$$

or in vector notation

$$\frac{\mathrm{d}}{\mathrm{d}t}(m\dot{\mathbf{r}}) = -\nabla V,$$

i.e., $\mathbf{F} = m\mathbf{a}$ where $\mathbf{F} = -\nabla V$ is the force and $\mathbf{a} = \ddot{\mathbf{r}}$ is the acceleration.

Two Interacting Particles

Consider a Lagrangian

$$\mathscr{L} = \tfrac{1}{2}m_1|\dot{\mathbf{r}}_1|^2 + \tfrac{1}{2}m_2|\dot{\mathbf{r}}_2|^2 - V(\mathbf{r}_1 - \mathbf{r}_2),$$

where the only force is a conservative one between two particles with masses m_1 and m_2 at $\mathbf{r}_1$ and $\mathbf{r}_2$ respectively, and depends only on their (vector) separation.

We could use the six Cartesian coordinates of the particles as generalised coordinates; but instead define

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2,$$

the relative position vector, and

$$\mathbf{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{M},$$

the position vector of the centre of mass, where $M = m_1 + m_2$ is the total mass. Now

$$|\dot{\mathbf{r}}_1|^2 = \left|\dot{\mathbf{R}} + \frac{m_2}{M}\,\dot{\mathbf{r}}\right|^2 = \left(\dot{\mathbf{R}} + \frac{m_2}{M}\,\dot{\mathbf{r}}\right)\mathbf{.}\left(\dot{\mathbf{R}} + \frac{m_2}{M}\,\dot{\mathbf{r}}\right) = |\dot{\mathbf{R}}|^2 + \frac{m_2^2}{M^2}\,|\dot{\mathbf{r}}|^2 + \frac{2m_2}{M}\,\dot{\mathbf{R}}\mathbf{.}\dot{\mathbf{r}}$$

and similarly

$$|\dot{\mathbf{r}}_2|^2 = |\dot{\mathbf{R}}|^2 + \frac{m_1^2}{M^2}\,|\dot{\mathbf{r}}|^2 - \frac{2m_1}{M}\,\dot{\mathbf{R}}\mathbf{.}\dot{\mathbf{r}}.$$

Let $\mathbf{r} = (x_1, x_2, x_3)$, $\mathbf{R} = (X_1, X_2, X_3)$, and use these as generalised coordinates. Then

$$\begin{aligned}\mathscr{L} &= \tfrac{1}{2}M|\dot{\mathbf{R}}|^2 + \frac{m_1m_2}{2M}\,|\dot{\mathbf{r}}|^2 - V(\mathbf{r}) \\ &= \tfrac{1}{2}M(\dot{X}_1^2 + \dot{X}_2^2 + \dot{X}_3^2) + \frac{m_1m_2}{2M}(\dot{x}_1^2 + \dot{x}_2^2 + \dot{x}_3^2) - V(x_1, x_2, x_3).\end{aligned}$$

The Euler–Lagrange equation for X_i is therefore

$$\frac{\mathrm{d}}{\mathrm{d}t}(M\dot{X}_i) = 0,$$

i.e., $\ddot{\mathbf{R}} = \mathbf{0}$ (the centre of mass moves with constant velocity); and for x_i is

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{m_1 m_2}{M}\,\dot{x}_i\right) = -\frac{\partial V}{\partial x_i},$$

i.e., $\mu\ddot{\mathbf{r}} = -\nabla V$ where μ is the *reduced mass* $m_1 m_2/(m_1 + m_2)$ (the relative position vector behaves like a particle of mass μ).

Note that the kinetic energy T is a homogeneous quadratic in the $\dot{X}_i$ and $\dot{x}_i$; that V does not depend on the $\dot{X}_i$ and $\dot{x}_i$; and that $\mathscr{L}$ has no explicit t-dependence. We can deduce immediately that the total energy $E = T + V$ is conserved.

1.8 The Calculus of Variations with Constraint

In §1.1 we studied constrained variation of functions of several variables. The extension of this method to functionals (i.e., functions of an infinite number of variables) is straightforward: to find the stationary values of a functional $F[y]$ subject to $G[y] = c$, we instead find the stationary values of $F[y] - \lambda G[y]$, i.e., find the function y which solves $\delta(F - \lambda G) = 0$, and then eliminate λ using $G[y] = c$.

1.9 The Variational Principle for Sturm–Liouville Equations

We shall show in this section that the following three problems are equivalent:

(i) Find the eigenvalues λ and eigenfunctions $y(x)$ which solve the Sturm–Liouville problem

$$\boxed{-\frac{\mathrm{d}}{\mathrm{d}x}\big(p(x)y'\big) + q(x)y = \lambda w(x)y}$$

in $a < x < b$, where neither p nor w vanish in the interval.

(ii) Find the functions $y(x)$ for which

$$\boxed{F[y] = \int_a^b (py'^2 + qy^2)\,\mathrm{d}x}$$

is stationary subject to $G[y] = 1$ where

$$\boxed{G[y] = \int_a^b wy^2\,\mathrm{d}x.}$$

The eigenvalues of the equivalent Sturm–Liouville problem in (i) are then given by the values of $F[y]$.

(iii) Find the functions $y(x)$ for which

$$\boxed{\Lambda[y] = \frac{F[y]}{G[y]}}$$

is stationary; the eigenvalues of the equivalent Sturm–Liouville problem are then given by the values of $\Lambda[y]$.

Hence Sturm–Liouville problems can be reformulated as variational problems.

Note the similarity between (iii) and the stationary property of the eigenvalues of a symmetric matrix (recall that it is possible to find the eigenvalues of a symmetric matrix A by finding the stationary values of $\mathbf{a}^T A\mathbf{a}/\mathbf{a}^T\mathbf{a}$ over all possible vectors $\mathbf{a}$). The two facts are in fact closely related.

To show that (ii) is equivalent to (i), consider

$$\delta(F - \lambda G) = \delta \int_a^b (py'^2 + qy^2 - \lambda w y^2)\,\mathrm{d}x.$$

Using Euler's equation, $F - \lambda G$ is stationary when

$$\frac{\mathrm{d}}{\mathrm{d}x}(2py') = 2qy - 2\lambda w y,$$

i.e.,

$$-\frac{\mathrm{d}}{\mathrm{d}x}(py') + qy = \lambda w y,$$

which is the required Sturm–Liouville problem: note that the Lagrange multiplier of the variational problem is the same as the eigenvalue of the Sturm–Liouville problem.

Furthermore, multiplying the Sturm–Liouville equation by y and integrating, we obtain

$$\int_a^b \left(-y\frac{\mathrm{d}}{\mathrm{d}x}(py') + qy^2\right)\mathrm{d}x = \lambda \int_a^b wy^2\,\mathrm{d}x = \lambda G[y] = \lambda$$

using the constraint. Hence

$$\begin{aligned}
\lambda &= \int_a^b \left(-y\frac{\mathrm{d}}{\mathrm{d}x}(py') + qy^2\right)\mathrm{d}x \\
&= [-ypy']_a^b + \int_a^b (py'^2 + qy^2)\,\mathrm{d}x \\
&\qquad\qquad \text{[integrating by parts]} \\
&= \int_a^b (py'^2 + qy^2)\,\mathrm{d}x = F[y],
\end{aligned}$$

using "appropriate" boundary conditions. This proves that the stationary values of $F[y]$ give the eigenvalues.

There are two ways of showing that (ii) is equivalent to (iii).

The first, informal way is to note that multiplying y by some constant α say does not in fact change the value of $\Lambda[y]$. This implies that when finding the stationary values of Λ we can *choose* to normalise y so that $G[y] = 1$, in which case Λ is just equal to $F[y]$. So finding the stationary values of Λ is equivalent to finding the stationary values of F subject to $G = 1$.

The second, formal way is to calculate

$$\begin{aligned}\delta\Lambda &= \frac{F+\delta F}{G+\delta G} - \frac{F}{G} \\ &= \frac{F+\delta F}{G}\left(1 - \frac{\delta G}{G}\right) - \frac{F}{G} \\ &\qquad\qquad \text{[using a Taylor expansion for } (1+\delta G/G)^{-1} \text{ to first order]} \\ &= \frac{\delta F}{G} - \frac{F\,\delta G}{G^2}\end{aligned}$$

(again to first order). Hence $\delta\Lambda = 0$ if and only if $\delta F = (F/G)\,\delta G$; that is, Λ is stationary if and only if

$$\delta F - \Lambda\,\delta G = 0.$$

But this is just the same problem as (ii); so finding the stationary values of Λ is the same as finding the stationary values of F subject to $G = 1$.

In the usual case that $p(x)$, $q(x)$ and $w(x)$ are all positive, we have that $\Lambda[y] \geq 0$. Hence all the eigenvalues must be non-negative, and there must be a smallest eigenvalue λ_0; Λ takes the value λ_0 when $y = y_0$, the corresponding eigenfunction. But what is the absolute minimum value of Λ over all functions $y(x)$? If it were some value $\mu < \lambda_0$, then μ would be a stationary (minimum) value of Λ and would therefore be an eigenvalue, contradicting the statement that λ_0 is the smallest eigenvalue. Hence $\Lambda[y] \geq \lambda_0$ for *any* function $y(x)$.

As an example, consider the simple harmonic oscillator

$$-y'' + x^2 y = \lambda y$$

subject to $y \to 0$ as $|x| \to \infty$. This is an important example as it is a good model for many physical oscillating systems. For instance, the Schrödinger equation for a diatomic molecule has approximately this form, where λ is proportional to the quantum mechanical energy level E; we would like to know the ground state energy, i.e., the eigenfunction with the lowest eigenvalue λ.

Here $p(x) = 1$, $q(x) = x^2$ and $w(x) = 1$, so

$$\Lambda[y] = \frac{\int_{-\infty}^{\infty} (y'^2 + x^2 y^2)\,\mathrm{d}x}{\int_{-\infty}^{\infty} y^2\,\mathrm{d}x}.$$

We can solve this Sturm–Liouville problem exactly: the lowest eigenvalue turns out to be $\lambda_0 = 1$ with corresponding eigenfunction $y_0 = \exp(-\frac{1}{2}x^2)$. But suppose instead that we didn't know this; we can use the above facts about Λ to try to guess at the value of λ_0. Let us use a trial function

$$y_{\text{trial}} = \exp(-\tfrac{1}{2}\alpha x^2),$$

where α is a positive constant (in order to satisfy the boundary conditions). Then

$$\Lambda[y_{\text{trial}}] = \frac{(\alpha^2+1)\int_{-\infty}^{\infty} x^2 \exp(-\alpha x^2)\,\mathrm{d}x}{\int_{-\infty}^{\infty} \exp(-\alpha x^2)\,\mathrm{d}x}.$$

We recall that $\int_{-\infty}^{\infty} \exp(-\alpha x^2)\,\mathrm{d}x = \sqrt{\pi/\alpha}$ and $\int_{-\infty}^{\infty} x^2 \exp(-\alpha x^2)\,\mathrm{d}x = \frac{1}{2}\sqrt{\pi/\alpha^3}$ (by integration by parts). Hence $\Lambda[y_{\text{trial}}] = (\alpha^2+1)/2\alpha$.

We know that $\Lambda[y_{\text{trial}}]$, for any α, cannot be less than λ_0. The smallest value of $(\alpha^2+1)/2\alpha$ is 1, when $\alpha = 1$; we conclude that $\lambda_0 \le 1$, which gives us an upper bound on the lowest eigenvalue.

In fact this method has given us the *exact* eigenvalue and eigenfunction; but that is an accident caused by the fact that this is a particularly simple example!

The Rayleigh–Ritz Method

The Rayleigh–Ritz method is a systematic way of estimating the eigenvalues, and in particular the lowest eigenvalue, of a Sturm–Liouville problem. The first step is to reformulate the problem as the variational principle that $\Lambda[y]$, the *Rayleigh quotient*, is stationary. Secondly, using whatever clues are available (for example, symmetry considerations or general theorems such as "the ground state wavefunction has no nodes") we make an "educated guess" $y_{\text{trial}}(x)$ at the true eigenfunction $y_0(x)$ with lowest eigenvalue λ_0. It is preferable for y_{trial} to contain a number of adjustable parameters (e.g., α in the example above).

We can now find $\Lambda[y_{\text{trial}}]$, which will depend on these adjustable parameters. We calculate the minimum value $\Lambda_{\min}$ of Λ with respect to all the adjustable parameters; we can then state that the lowest eigenvalue $\lambda_0 \le \Lambda_{\min}$. If the trial function was a reasonable guess then $\Lambda_{\min}$ should actually be a good approximation to λ_0.

If we wish, we can improve the approximation by introducing more adjustable parameters.

The fact that $\Lambda[y]$ is stationary with respect to variations in the function y means that if y_{trial} is close to the true eigenfunction y_0 (say within $O(\varepsilon)$ of it) then the final calculated value $\Lambda_{\min}$ will be a very good approximation to λ_0 (within $O(\varepsilon^2)$ in fact). If the inclusion

of further adjustable parameters fails to significantly improve the approximation then we can be reasonably sure that the approximation is a good one.

Note that if the trial function happens to include the exact solution y_0 as a special case of the adjustable parameters, then the Rayleigh–Ritz method will find both y_0 and λ_0 *exactly*. This is what happened in the example above.

An alternative to calculating $\Lambda[y_{\text{trial}}]$ and minimising it with respect to the adjustable parameters is to calculate $F[y_{\text{trial}}]$ and $G[y_{\text{trial}}]$, and to minimise F subject to $G = 1$. These procedures are equivalent, as we showed at the start of this section.

Higher eigenvalues [non-examinable]

Once we have found a good approximation $y_{0\,\text{trial}}$ to y_0, we can proceed to find approximations to the higher eigenvalues $\lambda_1, \lambda_2, \ldots$. Just as λ_0 is the absolute minimum of $\Lambda[y]$ over all possible functions y, so λ_1 is the absolute minimum of $\Lambda[y]$ over functions which are constrained to be orthogonal to y_0. (Recall that y_1 is orthogonal to y_0 in the sense that $\int_a^b w y_0 y_1 \,\mathrm{d}x = 0$.) Hence, to estimate λ_1 we proceed as before but choose our new trial function $y_{1\,\text{trial}}$ in such a way that it is orthogonal to our previous best approximation $y_{0\,\text{trial}}$.

This process can be continued to higher and higher eigenvalues but of course becomes less and less accurate.
