Calculus of variations

Energy Minimization

Introduction

we will focus on two key techniques that can be exploited in problems where a minimisation is necessary such as energy minimisation. The two methods are i) the calculus of variations and ii) Lagrange multipliers to explore various problems. By combining these two, we can tackle many problems that would not be possible using conventional techniques. In particular, these are very powerful when we wish to minimise integrals under certain fixed constraints

The calculus of variations

The calculus of variations came about due to a mathematical challenge in 1697. During those days it was customary to try and flush out your mathematical rivals by setting challenging problems for them to solve. Johann Bernouilli, one of the Bernouilli mathematics clan, posed the *Brachristochrone* problem:

Given two points A and B, with B below A, what is the curve of fastest descent? i.e. what path will carry a frictionless body from A to B in the smallest amount of time?

To solve this problem, we first need to write down an expression for the total amount of time it takes to get from A to B along a given path. From conservation of energy:

$$\frac{1}{2}mv^2 = mgh \tag{4.1}$$

so the velocity v of the particle at a height h is given by:

$$v = \sqrt{2gh}. \tag{4.2}$$

Consider a curve $y(x)$ between A and B, as shown in figure **??**. The local angle from horizontal of the curve is θ. Then

$$\frac{dx}{dt} = v\cos\theta, \quad \frac{dy}{dx} = -\tan\theta. \tag{4.3}$$

The total travel time is given by

$$T = \int_{x_A}^{x_B} \frac{dx}{v\cos\theta} = \int_{x_A}^{x_B} \frac{\sqrt{1+y'^2}}{\sqrt{2gy}}dx \tag{4.4}$$

where x_A and x_B are the x-coordinates of the points A,B, and we have used the results of equation (4.3) to obtain the second equality.

Thus we have reduced the original question to the problem of: What is the path $y(x)$ that minimises the integral $T = \int f(x, y, y')dx$?

The 1d Euler-Lagrange equation

We solve this problem by deriving the Euler-Lagrange equations. In calculus, you learn that you find a minimum of a function $f(x)$ by solving the equation $df/dx = 0$. We can generalise this to minimising integrals: If we make a small perturbation to the path $y(x) \to y + \delta y$, we find the minimum by requiring that the resulting change $\delta T = 0$:

$$T + \delta T = \int_{x_A}^{x_B} f(x, y + \delta y, y' + \delta y')dx \tag{4.5}$$

Thus

$$\delta T = \int_{x_A}^{x_B} \left[f(x, y + \delta y, y' + \delta y') - f(x, y, y')\right] dx = 0 \tag{4.6}$$

and from Taylor expanding f,

$$\delta T = \int_{x_A}^{x_B} \left[\frac{\partial f}{\partial y}\delta y + \frac{\partial f}{\partial y'}\delta y'\right] dx = 0. \tag{4.7}$$

We integrate by parts (noticing that $\delta y' = d(\delta y)/dx$) to obtain:

$$\left[\delta y \frac{\partial f}{\partial y'}\right]_{x_A}^{x_B} + \int_{x_A}^{x_B} \delta y \left[\frac{\partial f}{\partial y} - \frac{d}{dx}\left(\frac{\partial f}{\partial y'}\right)\right] dx = 0. \tag{4.8}$$

If the path is fixed at $y(x_A)$, and $y(x_B)$, then $\delta y(x_A) = \delta y(x_B) = 0$, and we can throw away the first term. Then provided f is sufficiently smooth, the only way that the integral can always be 0 is if

$$\frac{\partial f}{\partial y} - \frac{d}{dx}\left(\frac{\partial f}{\partial y'}\right) = 0. \tag{4.9}$$

This is the well-known Euler-Lagrange equation that you will probably have encountered before. WARNING: it is not always the case that we can throw away the first term in equation 4.8. We will come across some examples later where we need to worry about the extra term.

In your first problem sheet, you'll use the Euler-Lagrange equation to prove the Beltrami identity: When $\partial f/\partial x = 0$,

$$f - y'\frac{\partial f}{\partial y'} = C, \tag{4.10}$$

where C is a constant.

We can use this result in the brachristochrone time equation (4.4) to obtain

$$\frac{1}{\sqrt{1+y'^2}\sqrt{2gy}} = C \tag{4.11}$$

or

$$\frac{dy}{dx} = \sqrt{\frac{c_0 - y}{y}}. \tag{4.12}$$

We can solve this numerically to find the final solution - an inverted cycloid generated by a circle of diameter c_0.

Higher order Euler-Lagrange equations

You can also derive Euler-Lagrange equations for higher order problems. In the first problem sheet, you'll also prove that if we minimise:

$$\int_{x_A}^{x_B} f(x, y, y', y'')dx \tag{4.13}$$

then

$$\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y'} + \frac{d^2}{dx^2}\frac{\partial f}{\partial y''} = 0, \tag{4.14}$$

provided certain boundary conditions are met (which you should state).

Later, we will also return to derive Euler-Lagrange equations for the case when we need to minimise volume or area integrals rather than line integrals like those above.

Lagrange multipliers

The second important technique that we will use is the Lagrange multipliers. This is a useful way to find minima or maxima of functions subject to a constraint. For example:

Minimise $f(x, y)$ *subject to the constraint* $g(x, y) = c$.

The solution technique is illustrated in Figure **??**. $g(x, y)$ gives some curve in the (x, y) plane. If we plot $f(x, y)$ as we move along this curve, there will be a minimum at some point, (x_0, y_0). Here, f does not change in the direction tangent to the curve $g(x, y) = c$ so ∇f must point in the normal direction $\mathbf{n}$, so $\nabla f \propto \mathbf{n}$. Note that

$$\mathbf{n} \propto \nabla(g(x, y) - c), \tag{4.15}$$

so $\nabla f \propto \nabla(g(x, y) - c)$, or

$$\nabla f - \lambda \nabla(g - c) = 0, \tag{4.16}$$

where λ is the Lagrange multiplier.

Interestingly, we shall see that the Lagrange multiplier often turns out to be an important variable. For instance, when we calculate the shape of a droplet on a flat surface, the Lagrange multiplier will give the pressure inside of the droplet.

Quick example

What shape should a rectangular box be in order to minimise its surface area for a given volume ratio?

Let x, y, z be the lengths of the sides of the box. Then we have the volume constraint $V = xyz$. We want to minimise the surface area $A = 2(xy + yz + xz)$, so from the equation (4.16)

$$\frac{\partial}{\partial x}\left[2(xy + yz + xz) - \lambda(xyz - V)\right] = 0 \tag{4.17}$$

$$\frac{\partial}{\partial y}\left[2(xy + yz + xz) - \lambda(xyz - V)\right] = 0 \tag{4.18}$$

$$\frac{\partial}{\partial z}\left[2(xy + yz + xz) - \lambda(xyz - V)\right] = 0 \tag{4.19}$$

and we find

$$2(y + z) - \lambda yz = 0, \quad 2(x + z) - \lambda xz = 0, \quad 2(x + y) - \lambda xy = 0. \tag{4.20}$$

From symmetry, we guess that there is a solution $x = y = z$ and find that $\lambda = 4/x$. Finally, we also need to check that this is a minimum solution - I leave this to you to satisfy yourself.

Combining Lagrange multipliers with the Calculus of Variations

The power of Lagrange multipliers and the Calculus of Variations can really be seen when we combine the two techniques together. Often (especially when minimising energy problems), we need to find the minimum of an integral subject to a constraint. For example, we wish to minimise

$$E = \int_a^b f(x, y, y')dx \tag{4.21}$$

subject to

$$\int_a^b g(x, y, y')dx = C. \tag{4.22}$$

Using the natural extension of equation (4.16), this problem is equivalent to minimising

$$\int_a^b (f(x, y, y') - \lambda g(x, y, y'))dx. \tag{4.23}$$

Where λ is a Lagrange multiplier. This can be solved using the Euler-Lagrange equations,

Energy minimisation

The principle of minimum total potential energy is one of the fundamental laws governing the physical behaviour of everything in the world around us. It is a consequence of the 2nd law of thermodynamics, and essentially says that any body or structure will deform or move to a position that minimises its total potential energy. The lost energy will be dissipated as heat.

For example, if you stand on a tightrope, it will stretch to lower your gravitational potential energy. This simultaneously increases the rope's stored elastic energy. The principle of minimum total potential energy then says that the final position is the point where the elastic energy + gravitational potential energy is minimised. Obviously if you fall off you will minimise your potential energy even more.

This principle is very useful for deriving the governing equations of complex (and simple) systems. You will be used to deriving equations of systems in equilibrium by considering force balance at points, but we shall see that we cannot use this approach for some systems. In fact, even in simple situations, it is more rigorous to derive the governing equations from minimising energy; analytical mechanicians will not consider equations valid unless they can be derived in this way (and this can cause strife).

Example: Mass on a spring

As a simple example, consider putting a mass M on a linear spring of stiffness k. If the initial length of the spring is x_0, and it stretches to a length x then its elastic energy is $\frac{1}{2}k(x-x_0)^2$. The gravitational potential energy of the mass is Mgz, where z is its height.

We hang the mass on the spring. Then the total potential energy is

$$E = Mgz + \frac{1}{2}k(z-z_0)^2 \tag{4.24}$$

where z_0 is the initial position of the end of the spring before the mass is placed on it.

We minimise E by setting $dE/dz = 0$ to find $Mg + k(z-z_0) = 0$. This is the usual force-balance equation that you would normally write down straight away. Note that in this case, a big advantage is that we do not have to do the usual head scratching about getting the signs right.

The case above was for a simple, linear-elastic spring, but in real life springs are not always linear elastic! A material like rubber needs to be treated using a special model. This means that it has a more complex strain energy function, and we cannot just write down the simple force balance. The strain energy of a Neo-Hookean solid (a good model for rubber) that is stretched uniaxially is:

$$E_{el} = C\left[\left(\frac{l}{l_0}\right)^2 + 2\frac{l_0}{l}\right], \tag{4.25}$$

where l is the length of the rubber spring, and l_0 and C are constants.

We can find the equilibrium length of the spring by minimising the elastic potential energy E_{el} to find that $l = l_0$ when there is no force on the spring. Then you can hang a weight on the spring to obtain its equilibrium position. First we write down the energy

$$E = C\left[\left(\frac{z}{l_0}\right)^2 + 2\frac{l_0}{z}\right] + Mg(h - z). \tag{4.26}$$

note we have flipped z to point downwards here for simplicity,

Then we minimise to obtain the equilibrium equation:

$$2C\left(\frac{z}{l_0^2} - \frac{l_0}{z^2}\right) = Mg. \tag{4.27}$$

We can analyse this expression asymptotically to see that rubber initially behaves like a linear spring which gets softer for large deformation.

Surface tension and capillary statics

we'll look at phenomena in liquids when surface tension is important. Surface tension is important in a wide variety of situations, in particular at lengthscales below the capillary length $l_c = \sqrt{\gamma/\rho g}$, where γ is surface tension and ρ is the density of the liquid (for water, $l_c \sim 3$mm). Here, we'll concentrate on capillary statics - i.e. the shape of liquids in equilibrium.

What is surface tension?

Liquids consist of molecules tightly packed together and interacting with one another through an attractive force (this is why gases condense to form liquids when the molecules are slowed down by cooling). A molecule in the bulk of a liquid is therefore happy in the sense that it feels these attractive interactions from all directions. A molecule at the liquid surface, however, is unhappy because it has attractive interactions with only half as many neighbours as the bulk molecule. This unhappiness corresponds to an excess potential energy of the liquid that is proportional to the surface area, A:

$$E_{cap} = \gamma A. \tag{4.28}$$

γ represents the excess potential energy per unit area of surface, and is known as either the *surface energy* or the *surface tension*. The value of γ depends on the liquid, but for most pure liquids, $\gamma \sim 2 \times 10^{-2}\mathrm{J/m^2}$. This is because in liquids, the thermal energy of a molecule must be comparable in size to the attractive energy with its neighbours. If the thermal energy is much greater, then molecules will easily escape from the liquid and become a gas. If the thermal energy is too small, molecules will get locked into place and form a crystal lattice. The thermal energy of a molecule is $k_B T = 4 \times 10^{-21}$J at room temperature. The attractive interaction $\sim \gamma a^2$. Thus $\gamma \sim k_B T/a^2$. Most molecules are of a similar size ($a \sim 0.5$nm), hence why surface tension is always roughly the same magnitude. Liquid metals are an exception with surface tensions about 20 times higher than usual.

Force vs energy interpretation

A common source of confusion is: should we think about surface tension as a force or an energy? Let's do a simple thought experiment. We consider a bath of water that has constant volume, and ignore gravity effects. Originally the surface area is vanishingly small, and we apply a constant force F to pull open a larger area. If we extend the surface area to be $A = xt$, where t is the thickness of the bath in the y-direction, then the total surface energy is $E_{cap} = \gamma A$. The work done by the force (which you can think of as reducing the potential energy of the system) is $E_F = -Fx$. Thus the total potential energy of the system is

$$E_{cap} + E_F = \gamma x t - F x \tag{4.29}$$

minimising this with respect to x, we find that $\gamma = F/t$. i.e. there is a force of size γ per unit length of the contact line that is trying to pull back along the surface.

Thus for a liquid, surface tension can equivalently be thought of as a force per unit length, or an excess potential energy per unit area.

The shape of a small droplet on a surface

Firstly, let's consider the shape of a small droplet on a flat surface, as shown in figure **??**. For the moment we'll ignore gravity, and use our experience which tells us that small droplets always want to form spherical caps (you can prove this rigorously using energy minimisation if you would like!). There are three separate interfaces: the solid/liquid, solid/vapour and liquid/vapour interfaces, and each of these has a surface energy. Let's call these $\gamma_{sl}, \gamma_{sv}, \gamma_{lv}$ respectively.

We assume that the droplet forms a spherical cap of height h, contact radius a and radius of curvature r. Then, from wikipedia, we have that the curved area of the spherical cap is $\pi(a^2 + h^2)$ and its volume is $V = \frac{\pi h}{6}(3a^2 + h^2)$. Thus the total potential energy of the system is

$$E = \pi(a^2 + h^2)\gamma_{lv} + \pi a^2(\gamma_{sl} - \gamma_{sv}) + E_0, \tag{4.30}$$

where E_0 is a constant equal to the total area of the flat, bare surface multiplied by γ_{sv}.

We need to minimise this subject to a constant total volume of the droplet, so we minimise

$$U = \pi(a^2 + h^2)\gamma_{lv} + \pi a^2(\gamma_{sl} - \gamma_{sv}) - \lambda\left(\frac{\pi h}{6}(3a^2 + h^2) - V\right). \tag{4.31}$$

First, $\partial U/\partial a$ gives

$$\gamma_{lv} + \gamma_{sl} - \gamma_{sv} = \frac{\lambda h}{2}. \tag{4.32}$$

Then $\partial U/\partial h$ gives (after some manipulation)

$$\frac{2h^2\gamma_{lv}}{a^2 + h^2} = \frac{\lambda h}{2}. \tag{4.33}$$

Combining these, and noting that $2h^2/(a^2 + h^2) = (1 - \cos\theta)$, where θ is the contact angle of the droplet, we obtain Young's law:

$$\gamma_{lv}\cos\theta + \gamma_{sl} - \gamma_{sv} = 0. \tag{4.34}$$

This is illustrated in figure **??**. Amazingly, it says that the contact angle of a droplet is independent of the droplet size. We have proven Young's law for the simple case of a droplet on a flat surface. However, this result also applies to more general surfaces: in equilibrium the contact angle of a droplet always takes the value given by equation (4.34).

If you recall, we mentioned earlier that the Lagrange multiplier often takes an important value. I leave it as a challenge to you to show that here $\lambda = 2\gamma_{lv}/R$, the Laplace pressure inside the droplet (R is the radius of curvature of the spherical cap).

The meniscus equation

Now let's consider the shape of a liquid in a tank with a wall at $x = 0$, as shown in figure **??**. We want to be able to predict what is the shape of the meniscus against the tank wall.

The energy can be split into three parts: the gravitational potential energy of the liquid, the surface energy of the free surface, and the surface energy of the walls. We first calculate the gravitational potential energy.

Consider a parcel of fluid at height z, as shown in figure **??**. Its energy is $mg = (\rho dxdz)gz$. Thus if the height of the free surface is $h(x)$

$$E_g = \int_0^X \int_0^{h(x)} \rho gz dz dx = \int_0^X \rho g\frac{h^2}{2}dx \tag{4.35}$$

The surface energy of the free surface is

$$E_{\gamma_{lv}} = \gamma_{lv} \int_0^X \sqrt{1+h'^2}dx, \tag{4.36}$$

while the free energy of the wall at $x=0$ is

$$E_{wall} = (\gamma_{sl} - \gamma_{sv})h(0) + E_0 \tag{4.37}$$

Thus we need to minimise the total potential energy

$$E = \int_0^X \left[\rho g \frac{h^2}{2} + \gamma_{lv}\sqrt{1+h'^2}\right] dx + (\gamma_{sl} - \gamma_{sv})h(0) + E_0 \tag{4.38}$$

The last term poses a small problem, as if $h(0)$ is not fixed, we can no longer immediately use the Euler-Lagrange technique as before. However, we can still solve this by making use of the extra term in equation (4.8) that we normally ignore.

Let $h \to h + \delta h$, as usual, and write the integrand as $f(x, h, h')$. Then from equation (4.8)

$$\delta E = \left[\delta h \frac{\partial f}{\partial h'}\right]_0^X + \int_0^X \delta h \left[\frac{\partial f}{\partial h} - \frac{d}{dx}\left(\frac{\partial f}{\partial h'}\right)\right] dx + (\gamma_{sl} - \gamma_{sv})\delta h(0) = 0. \tag{4.39}$$

The only way we can ensure that the energy is minimised for all δh is if we have two conditions: firstly the standard Euler-Lagrange result:

$$\frac{\partial f}{\partial h} - \frac{d}{dx}\left(\frac{\partial f}{\partial h'}\right) = 0 \tag{4.40}$$

and secondly (assuming that $\delta h(X) = 0$) the boundary condition

$$-\frac{\partial f}{\partial h'}(0) + (\gamma_{sl} - \gamma_{sv}) = 0. \tag{4.41}$$

In the problems, you'll show that the equation for the free surface reduces to

$$\frac{\rho g h^2}{2} + \frac{\gamma_{lv}}{\sqrt{1+h'^2}} = \gamma_{lv} \tag{4.42}$$

while the boundary condition means that the contact angle of the liquid must satisfy Young's law.

References and further readings

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