Contour integration. Lagrange multipliers

In this final session we discuss two unrelated topics, suggested by the class. The first of these is integration in the complex plane and its exploitation in the evaluation of definite integrals. In discussing this topic we will go over functions of a complex variable in more detail than we have done until now and add a couple of neat tricks to your mathematical tool kit. Lagrange multipliers provide us with a systematic method for attacking problems of maximisation and minimisation subject to constraints

We will start by reminding ourselves of the basic material that has been covered in previous sessions. The concept of differentiation in the complex domain leads us to define regular and analytic functions. We then focus our attention on non-regular behaviour: singularities, multiple values and discontinuities. These are the simple properties we will identify and exploit again and again in subsequent applications, so its worth going over them informally and in some detail. With these preliminaries under our belts we move on to a detailed discussion of integration in the complex plane. This serves two purposes: it introduces useful, and quite strikingly neat, methods for evaluating integrals and, perhaps more importantly, provides us with a testbed where we can identify, apply and appreciate the properties of functions of a complex variable. This will provide a raft of examples for your entertainment; if you like twiddling formulae into submission these can be great fun. (If not, do not worry as long as you get the basic ideas on board.) The basic aim here is to get a working familiarity with the behaviour of simple functions in the complex plane; this is best done by example and practice.

<u>Complex numbers</u>

Real and imaginary parts, modulus and argument (phase):

$$\begin{aligned} z &= x + iy \\ &= |z|\exp(i\ \mathrm{Arg}\ (z)) \\ |z| &= \sqrt{x^2 + y^2} \\ \mathrm{Arg}(z) &= \tan^{-1}\left(\frac{y}{x}\right) \end{aligned} \tag{1}$$

De Moivre's theorem; rotations in the Argand plane

$$\begin{aligned} &\exp(i\theta) = \cos\theta + i\sin\theta \\ &\exp(i\pi/2) = i, \quad \exp(i\pi) = -1, \quad \exp(3i\pi/2) = -i \\ &\exp(2ni\pi) = 1 \end{aligned} \tag{2}$$

Functions of a complex variable

$$f(z) = F(x, y) = u(x, y) + iv(x, y); \quad u, v, x, y \text{ are real} \tag{3}$$

Differentiation and the Cauchy Reimann conditions

$$\begin{aligned} &\frac{df(z)}{dz} = \lim_{\Delta z \to 0} \frac{f(z + \Delta z) - f(z)}{\Delta z}, \text{ independent of the phase of } \Delta z \\ &\frac{\partial u(x, y)}{\partial x} = \frac{\partial v(x, y)}{\partial y}; \quad \frac{\partial v(x, y)}{\partial x} = -\frac{\partial u(x, y)}{\partial y} \end{aligned} \tag{4}$$

Note that, as they are necessarily real, $|z|$ and $\mathrm{Arg}(z)$ are not differentiable; they do not satisfy the Cauchy Reimann conditions.

Regular and analytic functions

A function is said to be analytic in a domain D of the Argand plane if it is single valued and differentiable at every point in that domain, save possibly for a finite number of exceptional points. The exceptional points are called singular points, or singularities, of the function. If the function has no singularities in D it is said to be regular. (The considerably grander term holomorphic is also used.)

Types of singular behaviour

The least interesting of these is a removable singularity; an infinite extra bit is plonked down at one point, on top of an otherwise smooth variation than can be represented by a Taylor series i.e. if, in the region of the singular point z_0, *f* is represented by

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z - z_0)^n \quad z \neq z_0 \tag{5}$$

then

$$a_n = 0; \quad n \leq -1. \tag{6}$$

If, however,

$$a_n = 0; \quad n \leq -1 - m \tag{7}$$

the singularity is referred to as a pole of order *m* (which is taken to be a positive integer) In the vicinity of z_0 we can write

$$f(z) = \frac{\phi(z)}{(z - z_0)^m} \tag{8}$$

where ϕ is regular. So, if *f* has a pole of order *m* at z_0, its reciprocal has a *m*ple zero at that point. The coefficient a_{-1} is particularly important, and is referred to as the residue of the function *f* at z_0.

An altogether more spectacular singular behaviour is encountered if the Taylor-Laurent expansion of $f(z)$ does not terminate and establish a pole. This presents us with an isolated essential singularity, which is also a isolated essential singularity of $1/f(z)$. An example is $\exp(1/z)$, which has an isolated essential singularity at the origin. (As the transformation $z \to 1/z$ maps infinity onto the origin we also say that exp(*z*) has an isolated essential singularity at infinity; other singular behaviours at infinity can be analysed in much the same way) The variation in an analytic function in the vicinity of an isolated essential singularity is amazing; it can be shown that in every neighbourhood of an isolated essential singularity there exists a point at which the function attains any given value, with at most one exception (e.g. zero in the case of $\exp(1/z)$). (This is known as Picard's theorem). In the main, though, we shall concern ourselves with poles.

Multiple valued functions and cuts in the complex plane.

One of the more diverting consequences of the introduction of negative numbers is that it allows every positive real number to have two square roots; if we confine our attention to real numbers, the square root of a negative number is not defined. When we plot numbers out on a log scale, we never actually reach the negative numbers. These observations alert us to the multivalued character of many functions of a complex variable. Thus if we represent a complex number in its polar form

$$z = r\exp(i\phi) \tag{9}$$

we can increment its phase by an integer multiple of 2π and still arrive at the same *z*. When we form the square root of z we find the two values

$$z^{1/2} = \sqrt{r}\exp(i\phi/2), \quad \sqrt{r}\exp(i\phi/2 + i\pi). \tag{10}$$

Similarly a complex number will have three distinct cube roots and so on; these roots are multiple valued. When we form the more general surd z^{μ}, where μ is not a rational number, we can keep on circling round the origin, generating as many values as we like. The logarithm of a complex number also has an infinite number of values, obtained by adding successive integer multiples of 2πi. However, our definition of an analytic function requires it to be single valued. How can we tame these commonly occurring functions? One way is to make the Argand plane into something altogether more complicated. Thus the square root function can be accommodated on a surface consisting of two sheets. Going round the origin once takes you from one sheet to the other; a second circuit around the origin takes you back onto the original sheet. These remarkable constructs, which can consist of an infinite number of connected sheets if you are considering the logarithmic function for example, are known as Reimann surfaces. A more brutal and straightforward approach is to cut the complex plane, so that the functions are single valued on the resulting surface, but show a discontinuity across the cut. So, if we cut the complex plane from 0 to ∞ along the real axis, the surd z^{α} is single valued on the surface but has a discontinuity of $|z|^{\alpha}(1-\exp(2\pi\alpha i))$ across the cut. Similarly the function $\sqrt{1-z^2}$ can be rendered single valued by cutting the complex plane from -1 to +1 along the real axis. We will get plenty of chance to try out this trick in subsequent applications.

Complex integration and Cauchy's theorem.

We have already mentioned in an earlier session that integration can be carried out along a path in the complex plane and that, if the integrand is differentiable along the path, the Cauchy Reimann conditions ensure that value the integral takes depends only on the end points of this path.

$$\begin{aligned}\int_C f(z)dz &= \int_C (u(x,y)+iv(x,y))(dx+idy) = \int_C (u(x,y)dx) - v(x,y)dy) + i\int_C (v(x,y)dx + u(x,y)dy)\\ &= \int_C (Q(x,y)dx) + P(x,y)dy); \quad P = u + iv, Q = iu - v\end{aligned} \tag{11}$$

So we might expect the integral to vanish if it is taken round a closed path, on and inside of which the function is suitably well behaved. This is the substance of Cauchy's theorem, which states that:

'If *f*(*z*) is an analytic function continuous within and on the simple closed rectifiable curve *C*, and if $f'(z)$ exists at each point within *C*, then

$$\int_C f(z)dz = 0 \text{.'} \tag{12}$$

To prove Cauchy's theorem at this level of generality is rather difficult; if we firm up the conditions on *f* to its derivative $f'(z)$ existing and being continuous everywhere inside and on *C*, then it follows straightaway from Stoke's theorem (familiar from vector calculus). As you may recall, this expresses a line integral of a vector field around a closed path in terms of the surface integral of the curl of that vector field. Specialised to a line integral in a plane Stoke's theorem tells us that

$$\int_C (Qdx + Pdy) = \iint_D dxdy\left(\frac{\partial P}{\partial x} - \frac{\partial Q}{\partial y}\right). \tag{13}$$

D is the domain contained within the close curve *C*; the Cauchy Reimann conditions ensure that the integrand in the surface term vanishes.

What happens if the curve *c* encloses a pole at z_0? The conditions for Cauchy's theorem to hold are vitiated at that point; we can nonetheless shrink the contour of integration down to a tiny circle around z_0 without changing the value of the integral. Substituting the Taylor Laurent expansion gives

$$\begin{aligned}\int_C f(z)dz &= i\rho\int_0^{2\pi} \exp(i\theta)\sum_{n=-m}^{\infty} a_n\rho^n \exp(in\theta)d\theta; z - z_0 = \rho\exp(i\theta) \\ &= 2\pi i a_{-1}\end{aligned} \tag{14}$$

$$\text{as} \int_0^{2\pi} \exp(im\theta) = 2\pi\delta_{m,0}$$

So the value of the integral is determined by the residue of the pole contained within the contour; if the integrand has several poles within *C*, you merely add up the residues.
Variants on Cauchy's theorem, that you might like to show are, at least, credible, are

$$\begin{aligned} f(z_0) &= \frac{1}{2\pi i}\int_C \frac{f(z)}{z - z_0}dz \\ f^{(n)}(z) &= \frac{n!}{2\pi i}\int_C \frac{f(z)}{(z - z_0)^{n+1}}dz \end{aligned} \tag{15}$$

Expanding the denominator in the first of these, and subsequent term by term integration gives us a new slant on Taylor's theorem

$$f\left(z_0+\delta\right)=\frac{1}{2\pi i}\int_C \frac{f(z)}{\left(z-z_0-\delta\right)}dz=\frac{1}{2\pi i}\int_C \frac{f(z)}{\left(z-z_0\right)\left(1-\delta/\left(z-z_0\right)\right)}dz$$

$$=\sum_{n=0}^{\infty}\delta^n \frac{1}{2\pi i}\int_C \frac{f(z)}{\left(z-z_0\right)^{n+1}}dz \qquad (16)$$

$$==\sum_{n=0}^{\infty}\delta^n \frac{f^{(n)}\left(z_0\right)}{n!}$$

As it stands this is just formula twiddling. Copson's book 'An introduction to the theory of functions of a complex variable' (OUP, 1970) fills in the rigorous detail without getting too carried away, and is well worth a look if you are interested.

Some applications to the evaluation of integrals

Most of the art in the use of Cauchy's theorem to evaluate definite integrals resides in the choice of the contour of integration. Banging out the residues is just a matter of algebraic brute force. (Mathematica has an inbuilt routine called, perhaps not surprisingly, `Residue`, that does all the hard work for you.) Let's start off with an example where the choice of contour is obvious. This can be done relatively easily using A level tricks (you might like to have a go); the contour integral approach, when it is applicable, is fairly systematic and user friendly.

$$\int_0^{2\pi}\frac{d\theta}{a-b\sin\theta}, \quad |a|>|b| \qquad (17)$$

Here we set $z=\exp(i\theta)$; the path of integration is identified as the unit circle centred on the origin in the complex plane. We see that the denominator is a quadratic in z, which we can solve to find the first order poles in the integrand. Only one of these lies within the contour of integration and so makes a contribution. Don't forget the $2\pi i$.

$$\int_0^{2\pi}\frac{d\theta}{a-b\sin\theta}=2i\int_0^{2\pi}\frac{\exp(i\theta)d\theta}{2ia\exp(i\theta)-b\exp(2i\theta)+b}$$

$$=2\int_C \frac{dz}{2iaz-bz^2+b}$$

$$=-\frac{2}{b}\int_C \frac{dz}{z^2-2iaz/b-1} \qquad (18)$$

$$=-\frac{2}{b}\int_C \frac{dz}{\left(z-z_+\right)\left(z-z_-\right)}; \quad z_\pm=i\left(\frac{a}{b}\pm\sqrt{\frac{a^2}{b^2}-1}\right)$$

$$=\frac{2\pi i}{b}\frac{2}{z_+-z_-}$$

A final bit of tidying up gives us the answer $2\pi\big/\sqrt{a^2-b^2}$.

A slightly more complicated strategy requires us to identify the required range of integration as part of a closed contour, the contribution from the remainder of which we can either evaluate explicitly or, more usually, set equal to zero. The first example of this technique is an old friend

$$\int_{-\infty}^{\infty} \frac{dx}{a^2 + x^2} \quad . \tag{19}$$

To do this we consider

$$\int_C \frac{dz}{z^2 + a^2} \tag{20}$$

We note that the integrand has simple poles at $z = \pm ia$. We take the contour from -*R* to *R* along the real axis then back along a semi-circle of radius *R* in the upper half plane. This 'catches' the pole at *ia*. On the semi-circular bit the integrand is basically going like $1/R^2$; the angular integral around the upper half plane gives a contribution that is consequently of the order of $1/R$ and vanishes as *R* gets bigger. This basically gives us

$$\int_{-\infty}^{\infty} \frac{dx}{a^2 + x^2} = 2\pi i \frac{1}{2ia} = \frac{\pi}{a} . \tag{21}$$

You can carry on like this till the cows come home; most of the problem in applications of this sort is in the evaluation of the residue. This is basically down to low cunning, though a 'churning it out' formula does exist. You might like to prove that, if $f(z)$ has a pole of order *m* at z_0, its residue is given by

$$\frac{1}{(m-1)!} \left(\frac{d}{dz} \right)^{m-1} \left((z - z_0)^m f(z) \right) \Big|_{z=z_0} \quad . \tag{22}$$

A second order pole arises when you use this method to evaluate

$$\int_{-\infty}^{\infty} \frac{dx}{\left(a^2 + x^2\right)^2} \tag{23}$$

while two simple poles contribute to the evaluation of

$$\int_{-\infty}^{\infty} \frac{dx}{\left(a^4 + x^4\right)} . \tag{24}$$

You might like to fill in the details here.

The next level of subtlety is demanded by a harmonically oscillating term in the integrand. To get some idea of what we expect in this case we look at a simple Fourier transform pair. If we take the function

$$\begin{aligned}\phi(t) &= 0; \quad t < 0 \\ &= \exp(-at), t \geq 0\end{aligned} \tag{25}$$

and take its Fourier transform we get

$$\tilde{\phi}(\omega) = \int_{-\infty}^{\infty} \phi(t)\exp(-i\omega t)dt = \frac{1}{a + i\omega}. \tag{26}$$

The original function is recovered on Fourier inversion. Thus we have

$$\frac{1}{2\pi i}\int_{-\infty}^{\infty} d\omega \frac{\exp(i\omega t)}{\omega - ia} = \begin{cases} 0; & t < 0 \\ \exp(-at), & t \geq 0 \end{cases}. \tag{27}$$

We have tarted up our Fourier inversion integral to make it look a bit more Cauchy like. Can we get this result directly from Cauchy's theorem? Obviously there's a simple pole in the upper half of the complex ω plane. How do we decide on our contour of integration? First up we go from -*R* to *R* along the real axis. Now we must close the contour. Let us say that ,for the moment, *t* is greater than zero. If we close in the upper half plane the exponential term behaves like

$$\exp(it(p + iq)) = \exp(-qt)\exp(ipt) \quad -\infty < p = \Re(\omega) < \infty \quad 0 < q = \Im(\omega) < \infty \tag{28}$$

Consequently the contribution from the semi circular path in the upper half plane will get negligibly small. (Copson gives a full discussion of this analysis, it is called Jordan's lemma in the books) Thus we can evaluate the integral by closing in this way, capturing the contribution from the pole at *ia*. If *t* is less than zero the contribution from closing the path in the upper half plane is doesn't fall off to zero; we would be much better advised to close in the lower half plane, which contains no poles. So, for negative *t*, the integral vanishes in line with our 'model' Fourier calculation. Once you have got the hang of this closing in the upper or lower half plane, depending on whether *t* is positive or negative, this type of integral is not too bad. We also see here the germ of the technique of introducing causality into the analysis. The lack of any poles in the lower half plane is a manifestation of there being no signal prior to *t* zero.

Now let's do something a little more complicated:

$$\int_{0}^{\infty} \frac{\cos(kx)}{x^2 + a^2}dx = \frac{1}{2}\int_{-\infty}^{\infty} \frac{\exp(ikx)}{x^2 + a^2}dx \tag{29}$$

We note the simple poles at $z = \pm ia$; we close in the upper or lower half plane, depending on whether *k* is greater or less than 0. Note that, in closing in the lower half plane, we will get a contribution of **minus** $2\pi i$ times the residue of the pole (why?) All told it comes to

$$\int_{0}^{\infty} \frac{\cos(kx)}{x^2 + a^2}dx = \frac{\pi}{2a}\exp(-|k|a) \tag{30}$$

Once more the contour integral technique introduces a function with non-analytic behaviour; this calculation has an interpretation in terms of a Lorentzian power spectrum corresponding to an exponentially decaying acf. All sorts of definite integrals can be constructed using this trick.

So far we have considered integrands whose poles lie well off the real axis and are captured quite unambiguously when we close the contour in a suitable fashion. We have come across principal value integrals in an earlier (the third) session. Cauchy's theorem helps us evaluate these things quite nicely. Consider

$$P\int_{-\infty}^{\infty} F(x)\frac{dx}{x-x_0} \tag{31}$$

where $F(z)$ has no poles in the upper half plane, and falls off for large z. We take our contour along the real axis, hopping over the pole at x_0 in a tiny semi-circle, then closing in the uhp. The only contribution to the integral is from the indented semi-circle, amounting to $\pi i F(x_0)$ (i.e. half that you get when going round the full circle.) As we have seen earlier on, for a function to be differentiable in the complex plane it must have both real and imaginary parts. In a physical context these real and imaginary parts might specify the resistive and reactive parts of an impedance or the dielectric and conductive responses to an applied electric field. There is an intimate relationship between the real and imaginary parts of such a function when evaluated for a real argument. Thus if $F(x,y) = U(x,y) + iV(x,y)$ we have from Cauchy's integral formula

$$U(x,0) + iV(x,0) = \frac{1}{\pi i} P\int_{-\infty}^{\infty} \frac{U(x',0) + iV(x',0)}{x'-x} dx' \tag{32}$$

which, on equating real and imaginary parts, gives us

$$\begin{aligned} U(x,0) &= \frac{1}{\pi} P\int_{-\infty}^{\infty} \frac{V(x',0)}{x'-x} dx' \\ V(x,0) &= -\frac{1}{\pi} P\int_{-\infty}^{\infty} \frac{U(x',0)}{x'-x} dx' \end{aligned} \tag{33}$$

If, as is frequently the case, U and V are respectively even and odd functions of x on the real axis,we find that

$$U(x,0) = \frac{2}{\pi} P\int_0^{\infty} \frac{x'V(x',0)}{x'^2 - x^2} dx' \quad V(x,0) = -\frac{2x}{\pi} P\int_0^{\infty} \frac{U(x',0)}{x'^2 - x^2} dx' \tag{34}$$

These are known variously as dispersion relations, Kramers-Kroenig relations or Hilbert transforms. A typical textbook example of this type of calculation is

$$P\int_{-\infty}^{\infty} \frac{\sin(\pi x)}{x(1-x^2)} dx = \Im P\int_{-\infty}^{\infty} \frac{\exp(i\pi x)}{x(1-x^2)} dx \tag{35}$$

the contour is indented to hop over the poles at $0,\pm 1$ on the real axis, and can be closed in the upper half plane. Thus the principal value of this integral is πi times the sum of the residues at the poles on the real axis; check that this works out to be π.

The next complication is the presence of a cut in the complex plane, introduced to keep the integrand single valued. The contour of integration cannot pass over the cut and frequently has to be deformed so that it runs along its edges, picking up the discontinuity in the integrand. Most textbook examples have a fairly simple cut in the plane, extending out to infinity. Once more a couple of examples may give some idea of what's going on. So what about:

$$\int_0^\infty \frac{x^\alpha}{1+x}dx; \quad -1<\alpha<0 \tag{36}$$

The conditions on α ensure that the integral is convergent. We take the integral $\int_C \frac{z^\alpha}{1+z}dz$ m around the contour C in the complex plane, cut from) to infinity along the positive real axis. The contour runs from "0" to R along the top of the cut, goes round a full circle of radius R until it reaches the lower edge of the cut , proceeds back along the cut and finally sneaks round the origin in a clockwise direction to get back to the starting point. We note that this contour encloses a pole at $z=-1=\exp(i\pi)$; the residue at this point will determine the value of the contour integral. On the upper edge of the cut we can write the integrand as $x^\alpha/(1+x)$ (with x real) while on the lower edge of the cut it takes the value $\exp(2\pi i\alpha)\,x^\alpha/(1+x)$. The contribution from the circle out at R vanishes as R gets progressively larger. So altogether we have

$$\left(1-\exp(2\pi i\alpha)\right)\int_0^\infty \frac{x^\alpha}{1+x}dx = 2\pi i\exp(\pi i\alpha) \tag{37}$$

which we can rearrange to give us the required result

$$\int_0^\infty \frac{x^{\alpha-1}}{1+x}dx = \frac{\pi}{\sin\pi\alpha}; \quad 0<\alpha<1. \tag{38}$$

We have already had some indication that there is significant contact between this contour integral stuff and Fourier and Laplace transforms; integrals around contours that negotiate cuts in the complex plane often crop up in the inversion of Laplace transforms. Another example in which we encounter a cut in the complex plane is the rather simple

$$\int_{-1}^1 \frac{dx}{\sqrt{1-x^2}}. \tag{39}$$

This can be evaluated by elementary methods. It also provides an interesting exercise in the properties of functions of a complex variable. We consider $1/\sqrt{1-z^2}$ in the complex plane, which must be cut to ensure that the function is single valued. The cut is inserted along the real axis from -1 to 1. On the top side of the cut the function has phase zero; on the bottom its phase is π. So to evaluate the integral we construct a contour going from " -1" to "1" across the top of the cut, then going half way round z=1 (so that the function of the real axis, with *x* greater than unity, is $\exp(i\pi/2)\big/\sqrt{x^2-1}$), scooting out to +*R* along the real axis, going round the full circle of radius *R*, coming back in along the positive real axis, negotiating *z*=1 so that one is on the underside of the cut and the function takes the value $\exp(i\pi)\big/\sqrt{1-x^2}$, proceeding to *z*=-1 then going round *z*=-1 to restore the phase on the top of the cut. The things to note here are (i) the trips back and forth along the real axis from 1 to *R* cancel out as the integrand is single valued here (ii) the circular contour out at *R* does make a contribution in this case (you can think of this as coming from 'the residue at infinity').So all told we get

$$2\int_{-1}^{1}\frac{dx}{\sqrt{1-x^2}}+\exp(i\pi).2\pi(\text{the contribution from the circle at infinity}) = \\ 0;(\text{no poles enclosed inside contour}) \tag{40}$$

from which we find, rather reassuringly, that

$$\int_{-1}^{1}\frac{dx}{\sqrt{1-x^2}}=\pi\ . \tag{41}$$

There are a couple more examples in which you have to scoot round a cut of finite extent in the exercises; they are slightly messier in detail but the same principles still apply.

Cuts in the complex plane are also needed to impose single valuedness if the logarithmic function is present in the integrand. An example of how this goes is as follows: consider the integral

$$\int_C \frac{\log(z)^2}{1+z^2}dz\,. \tag{42}$$

The complex plane is cut along the positive real axis from 0 to infinity; on the negative real axis we have $\log(z)=\log(|z|)+i\pi$. *C* comes in from -*R* along the negative real axis until it reaches the origin, sneaks up onto the top side of the cut and proceeds out to $z=R$. The contour is closed by following the semi-circle of radius *R* in the upper half plane (you should be able to convince yourself that the contribution from this fellow vanishes as *R* gets progressively larger.) This captures a pole at *z*=*i* whose residue determines the value of the contour integral. So, all told, we have

$$\int_0^\infty \frac{\log(x)^2+(\log(x)+i\pi)^2}{1+x^2}dx=2\pi i\frac{(i\pi/2)^2}{2i}=-\frac{\pi^3}{4} \tag{43}$$

On expanding out and equating real and imaginary parts we find that

$$
\begin{aligned}
&2\int_0^\infty \frac{\log(x)^2}{1+x^2}dx - \pi^2\int_0^\infty \frac{dx}{1+x^2} = -\frac{\pi^3}{4} \\
&\int_0^\infty \frac{\log(x)}{1+x^2}dx = 0
\end{aligned}
\tag{44}
$$

The first of these gives us

$$
\int_0^\infty \frac{\log(x)^2}{1+x^2}dx = \frac{\pi^3}{8} \tag{45}
$$

the second is what you would expect, even without working it out in detail (why?)

All sorts of extensions to these basic techniques can be dreamt up, particularly if you choose slightly more involved contours. However, the examples covered thus far probably suffice to illustrate the principles and help familiarise us with the behaviour of simple functions in the complex plane.

<u>Extreme values subject to constraints: Lagrange Multipliers</u>

The determination of maxima and minima of a function of a single variable is a familiar exercise in differential calculus. Basically one calculates the derivative and finds out where it vanishes. A positive (negative) second derivative identifies a minimum (maximum); a vanishing second derivative is characteristic of a point of inflection. The extrema of a function of two random variables can be analysed in a similar fashion by setting its first partial derivatives to zero, though their characterisation as maxima, minima or saddle points is a little more complicated. (Perhaps you would like to look at this as an exercise.)

Now consider the problem of determining the extreme values of a function of two variables, x, y subject to some constraint that relates x to y. We denote the function whose extreme values are required by $f(x,y)$; the constraint is represented by the equation

$$
g(x,y) = 0 \; . \tag{46}
$$

Solving this equation, we can express y as a function of x, i.e.

$$
y = y(x) \tag{47}
$$

We now look for extreme values of f, subject to (46) by solving

$$
\frac{df}{dx} = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{dy}{dx} = 0 \tag{48}
$$

The derivative dy/dx can be determined directly from (46) as

$$\delta g(x,y) = \frac{\partial g}{\partial x}\delta x + \frac{\partial g}{\partial y}\delta y = 0$$
$$\therefore \frac{dy}{dx} = -\frac{\partial g/\partial x}{\partial g/\partial y} \tag{49}$$

This leads us to the equations to be solved to determine the extreme values

$$g(x,y) = 0$$
$$\frac{\partial f}{\partial x} - \frac{\partial f}{\partial y}\frac{\partial g/\partial x}{\partial g/\partial y} = 0 \tag{50}$$

To make this discussion more concrete we consider the following: what is the shortest distance form the origin to the line

$$y = mx + c\,? \tag{51}$$

To solve this we maximise $x^2 + y^2$, subject to the constraint (51); this we do by solving

$$\frac{d}{dx}\left(x^2 + (mx+c)^2\right) = 2\left(x + m(mx+c)\right) = 0;$$
$$x_{ex} = -\frac{mc}{m^2+1}; y_{ex} = c\left(1 - \frac{m^2}{m^2+1}\right) = \frac{c}{m^2+1};$$
$$\left(x^2 + y^2\right)_{ex} = \frac{c^2}{1+m^2} \tag{52}$$

In this two-dimensional case the analysis just outlined is fairly straightforward, though it can be a bit messy in practice. For functions of more than two independent variables, subject to several constraints, this direct approach can become rather unwieldy and an equivalent, but more systematic approach is needed. This is provided by the method of Lagrange multipliers. To see how this works we approach the two dimensional problem in a slightly different way. The condition that *f* takes an extreme value can be written as

$$\delta f = \frac{\partial f}{\partial x}\delta x + \frac{\partial f}{\partial y}\delta y = 0 \tag{53}$$

In the absence of any constraints this is satisfied for arbitrary $\delta x, \delta y$ and implies that

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y} = 0 \tag{54}$$

The constraint $g(x,y) = 0$ implies that

$$\frac{\partial g}{\partial x}\delta x + \frac{\partial g}{\partial y}\delta y = 0 \tag{55}$$

This can be multiplied by a constant λ, added to (54) and re-arranged to yield

$$\left(\frac{\partial f}{\partial x}+\lambda\frac{\partial g}{\partial x}\right)\delta x+\left(\frac{\partial f}{\partial y}+\lambda\frac{\partial g}{\partial y}\right)\delta y=0 \tag{56}$$

By equating the coefficients of $\delta x, \delta y$ separately to zero we obtain two equations; by solving one of these for λ and substituting back in the other we regain our condition that identifies the constrained extreme value.

$$\begin{aligned}&\left(\frac{\partial f}{\partial x}+\lambda\frac{\partial g}{\partial x}\right)=0; \quad \left(\frac{\partial f}{\partial y}+\lambda\frac{\partial g}{\partial y}\right)\delta=0\\&\lambda=-\frac{\partial f/\partial y}{\partial g/\partial y}\\&\left(\frac{\partial f}{\partial x}-\frac{\partial f/\partial y}{\partial g/\partial y}\frac{\partial g}{\partial x}\right)=0\end{aligned} \tag{57}$$

Thus, if we write

$$K(x,y,\lambda)=f(x,y)+\lambda g(x,y) \tag{58}$$

we obtain the conditions that determine the constrained extreme values in the form

$$\frac{\partial K(x,y,\lambda)}{\partial x}=\frac{\partial K(x,y,\lambda)}{\partial y}=\frac{\partial K(x,y,\lambda)}{\partial \lambda}=0\ . \tag{59}$$

This procedure can be extended to a function $f(x_1,\cdots,x_n)$ of *n* variables, subject to *m* constraints

$$g_k(x_1,\cdots,x_n)=0, k=1,\cdots,m \tag{60}$$

(*m* is necessarily less than *n)* by constructing the function

$$K=f(x_{1,}\cdots x_n)+\sum_{k=1}^{m}\lambda_k g_k(x_{1,}\cdots x_n) \tag{61}$$

and solving the equations

$$\begin{aligned}\frac{\partial K}{\partial x_k}&=0,k=1,\cdots,n\\\frac{\partial K}{\partial \lambda_k}&=0,k=1,\cdots,m\end{aligned} \tag{62}$$

A couple of simple examples will demonstrate how this works. Let's generalise our first example to *n* dimensions i.e. find extreme values of

$$\sum_{j=1}^{n}x_j^2 \tag{63}$$

subject to the constraint

$$\sum_{j=1}^{n} a_j x_j = k \tag{64}$$

To this end we construct

$$K = \sum_{j=1}^{n} x_j^2 + \lambda\left(\sum_{j=1}^{n} a_j x_j - k\right) \tag{65}$$

We now differentiate with respect to x_j to obtain

$$2x_j + \lambda a_j = 0 \tag{66}$$

From *n* equations of this type we find that

$$\begin{aligned} &\sum_{j=1}^{n}\left(2x_j^2 + \lambda a_j x_j\right) = 0 \\ &\sum_{j=1}^{n} x_j^2 = -\frac{\lambda k}{2} \end{aligned} \tag{67}$$

We also know that

$$\begin{aligned} &x_j = -\frac{\lambda a_j}{2}, \quad \sum_{j=1}^{n} x_j^2 = \frac{\lambda^2}{4}\sum_{j=1}^{n} a_j^2 \\ &\therefore \lambda = -\frac{2k}{\sum_{j=1}^{n} a_j^2} \\ &\left(\sum_{j=1}^{n} x_j^2\right)_{ex} = \frac{k^2}{\sum_{j=1}^{n} a_j^2} \end{aligned} \tag{68}$$

which gives us our extreme value. Let us consider another example, rather reminiscent of the sort of thing one did at school: What is the largest volume of a rectangular box can take, when contained inside the ellipsoid

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1 \tag{69}$$

If one of the corners of the box is at x,y,z and all its corners lie on the ellipsoid surface then the volume of the box is given by 8*xzy*. We wish to find the extreme value this takes, subject to the condition (69). Thus we construct

$$K = 8xyz + \lambda\left(\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} - 1\right) \tag{70}$$

Evaluating the partial derivatives with respect to *x*,*y*, *z* gives us

$$
\begin{aligned}
&8yz+\frac{2\lambda x}{a^2}=8xz+\frac{2\lambda y}{b^2}=8xy+\frac{2\lambda z}{c^2}=0\\
&24xyz+2\lambda\left(\frac{x^2}{a^2}+\frac{y^2}{b^2}+\frac{z^2}{c^2}\right)=24xyz+2\lambda=0\\
&8xyz=-\frac{2\lambda}{3}
\end{aligned}
\tag{71}
$$

To determine the value of λ we write

$$y=-\frac{4xzb^2}{\lambda}\quad \text{etc.} \tag{72}$$

so that

$$xyz=-\frac{4^3(xyz)^2a^2b^2c^2}{\lambda^3} \tag{73}$$

This can be twiddled round to yield

$$
\begin{aligned}
&xyz=-\frac{\lambda^3}{4^3a^2b^2c^2}=-\frac{\lambda}{12}\\
&\lambda^2=a^2b^2c^2\frac{16}{3}
\end{aligned}
\tag{74}
$$

Bringing all this together then gives

$$(8xyz)_{ex}=\frac{8abc}{3\sqrt{3}}\,. \tag{75}$$

As a final example we consider a case where we have two constraints on a function of three variables. An ellipsoid described by (69) is intersected by a plane passing through the origin

$$lx+my+nz=0 \tag{76}$$

What are the extreme values of the distance from the origin to points where the ellipsoid cuts the plane? To determine these we introduce the two constraints (69) and (76) through two Lagrange multipliers

$$K=x^2+y^2+\lambda\left(\frac{x^2}{a^2}+\frac{y^2}{b^2}+\frac{z^2}{c^2}-1\right)+\mu(lx+my+nz) \tag{77}$$

then solve the equations

$$\frac{\partial K}{\partial x}=\frac{\partial K}{\partial y}=\frac{\partial K}{\partial z}=\frac{\partial K}{\partial \lambda}=\frac{\partial K}{\partial \mu}=0\,. \tag{78}$$

The last two of these are (69) and (76); the first three are

$$
\begin{aligned}
&2x + \frac{2\lambda x}{a^2} + \mu l = 0 \\
&2y + \frac{2\lambda y}{b^2} + m\mu = 0 \\
&2z + \frac{2\lambda z}{c^2} + n\mu = 0
\end{aligned} \tag{79}
$$

These can be combined to give us

$$
\begin{aligned}
&2\left(x^2 + y^2 + z^2\right) + 2\lambda\left(\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2}\right) + \mu(lx + my + nz) = 0 \\
&\left(x^2 + y^2 + z^2\right)_{ex} = -\lambda
\end{aligned} \tag{80}
$$

(79) can be solved for *x*, *y* and *z*, which are then substituted into (76) to give us

$$
\mu\left(\frac{l^2}{\left(1 + \lambda/a^2\right)} + \frac{m^2}{\left(1 + \lambda/b^2\right)} + \frac{n^2}{\left(1 + \lambda/c^2\right)}\right) = 0 \tag{81}
$$

As the multiplier μ cannot be equal to zero we se that this condition is equivalent to a quadratic equation in λ

$$
\lambda^2\left(\frac{l^2a^2 + m^2b^2 + n^2c^2}{a^2b^2c^2}\right) + \lambda\left(\frac{l^2 + m^2}{c^2} + \frac{l^2 + n^2}{b^2} + \frac{m^2 + n^2}{a^2}\right) + \left(l^2 + m^2 + n^2\right) = 0 \tag{82}
$$

this has two roots that can be identified with the maximum and minimum distances from the origin.

Here we have presented Lagrange multipliers as a technique for the constrained extremisation of functions of several variables; much the same idea underpins the determination of extreme values of functionals through the calculus of variations. A good reference is Chapter 2, Volume 1, Mathematics of Classical and Quantum Physics, F. W. Byron, Jr. and R. W. Fuller, Addison Wesley, New York, 1969. This covers a lot of interesting stuff, from the bitching of the Bernoulli brothers through to invariants and Noether's theorem

Exercises

Here are some examples of contour integration and the use of Lagrange multipliers; these are all about technique and not much to do with applications

1. Prove the following results; they are all based on a contour consisting of a unit circle round the origin in the complex plane

$$\int_0^{2\pi} \frac{d\theta}{1+p^2-2p\cos\theta} = \frac{2\pi}{1-p^2}$$

$$\int_0^{2\pi} \exp(\cos\theta)\cos(n\theta-\sin\theta)d\theta = \frac{2\pi}{n!}$$

$$\int_0^{2\pi} \frac{d\theta}{(a+b\cos\theta)^2} = \frac{2\pi a}{\left(a^2-b^2\right)^{3/2}}$$

$$\int_0^{2\pi} \frac{d\theta}{a^2+\cos^2\theta} = \frac{2\pi}{a\sqrt{1+a^2}}$$

$$\int_0^{2\pi} \frac{\sin^2\theta}{a+b\cos\theta}d\theta = \frac{2\pi}{b^2}\left(a-\sqrt{a^2-b^2}\right)$$

2 Prove the following, based on a contour going along the real axis then closing as a semi-circle in the upper half plane. Take care to account for poles on the real axis and, in the last fellow, a branch point at the origin. The final pair of integrals were evaluated by Cauchy, after he had discovered his theorem; he then used them, and others like them, to taunt his contemporaries something rotten.

$$\int_{-\infty}^{\infty} \frac{x^2}{\left(x^2+a^2\right)^3}dx = \frac{\pi}{8a^3}$$

$$\int_{-\infty}^{\infty} \frac{dx}{\left(a^2+x^2\right)^2\left(b^2+x^2\right)} = \frac{\pi(2a+b)}{2a^3b(a+b)^2}$$

$$\int_{-\infty}^{\infty} \frac{\cos(x)}{\left(x^2+a^2\right)\left(x^2+b^2\right)}dx = \frac{\pi}{a^2-b^2}\left(\frac{\exp(-b)}{b}-\frac{\exp(-a)}{a}\right)$$

$$\int_{-\infty}^{\infty} \frac{\cos(x)}{\left(x^2+a^2\right)^2}dx = \frac{\pi(1+a)\exp(-a)}{2a^3}$$

$$\int_{-\infty}^{\infty} \frac{a\cos x + x\sin x}{x^2+a^2}dx = 2\pi\exp(-a)$$

$$\int_0^{\infty} \frac{\sin x}{x\left(x^2+a^2\right)}dx = \frac{\pi}{2a^2}\left(1-\exp(-a)\right)$$

$$\int_0^\infty \frac{\exp(a\cos bx)\sin(a\sin bx)}{x}dx = \frac{\pi}{2}(\exp(a)-1)$$

$$\int_0^\infty x^{a-1}\sin(\pi a/2 - bx)\frac{rdx}{x^2+r^2} = \frac{\pi}{2}r^{a-1}\exp(-bx)$$

3 The following pair of integrals have integrands that must be rendered single valued by cutting the complex plane along the real axis. By following the argument that led to

$$\int_{-1}^{1}\frac{dx}{\sqrt{1-x^2}} = \pi$$

show that

$$\int_{-1}^{1}\frac{dt}{(1-t)^\alpha(1+t)^{1-\alpha}} = \frac{\pi}{\sin\pi\alpha}$$

$$\int_\alpha^\beta \left(\frac{\beta - t}{t-\alpha}\right)^{a-1}\frac{dt}{t} = \frac{\pi}{\sin\pi\alpha}\left(1-\left(\frac{\beta}{\alpha}\right)^{a-1}\right)$$

4 In the following examples the complex plane is cut along the positive real axis, out to infinity, to keep the integrand single valued. Remember that you cannot let your contour cross this cut. Show that:

$$\int_0^\infty \frac{x^{-a}dx}{1+2x\cos\theta + x^2} = \frac{\pi}{\sin\pi a}\frac{\sin a\theta}{\sin\theta}$$

$$\int_0^\infty \frac{x^z}{\left(1+x^2\right)^2}dx = \frac{\pi(1-z)}{4\cos(\pi z/2)}$$

$$\int_0^\infty \frac{x^a}{(1+x)^2}dx = \frac{\pi a}{\sin\pi a}$$

$$\int_0^\infty \frac{x^4}{1+x^8}dx = \frac{\pi}{4\sqrt{2+\sqrt{2}}}$$

The first of these fellows was derived, without the benefit of contour integration, by Euler; goodness knows how he did it.

5 A few examples with logarithms in them now. Remember that $\log(z)=\log(|z|)+i\pi$ along the negative real axis, if you cut the complex plane from 0 to +∞.

$$\int_0^\infty \frac{\log(1+x^2)}{(1+x^2)}dx=\pi\log 2$$

$$\int_0^\infty \frac{\log(x)}{1-x^2}dx=\frac{\pi^2}{4}$$

$$\int_0^\infty \frac{\log(x)}{(1+x^2)^2}dx=-\frac{\pi}{4}$$

$$\int_0^\infty \frac{\log(x)}{(x+a)^2+b^2}dx=\frac{\log\sqrt{a^2+b^2}}{b}\tan^{-1}\left(\frac{b}{a}\right)$$

In the first of these integrate $\log(z+i)/(z^2+1)$ along the real axis then round the familiar semi-circular contour in the uhp. In the second take care with poles on the real axis and principal values. The last one is definitely a bit hard; the answer just doesn't look like the usual contour integral stuff, if only because it does not have a π in it.

6 Here are a few examples of the use of Lagrange multipliers to find the extreme value of a function subject to constraints. (Ancient tomes, like Todhunter's 'Differential Calculus', Macmillan, London, 1876, devote several chapters to problems of this type. Todhunter was a celebrity of Beckham-like proportions in his day; he pops up rather unexpectedly in Finnegan's Wake as Professor Toadhaunter. If you really feel the need for extra practice, then his book is the place to look.)

Various conic sections can be represented by the equation

$$ax^2+bxy+cy^2=u$$

Using the method of Lagrange multipliers, investigate the extreme values of the distance from the origin of points on such curves, much as we did for the points on a straight line. Use your results to identify the cases where the conic section is a circle, an ellipse and a hyperbola.

Find an extreme value of $x^2y^3z^4$, subject to the constraint $2x+3y+4z=a$. Generalise this to $x^py^qz^r$, subject to $lx+my+nz=a$.

Find an extreme value of $x^4+y^4+z^4$, subject to the constraint $xyz=c^3$.

Find an extreme value of $x+y+z$, subject to the constraint $a/x+b/y+c/z=1$.

A, *B* and *C* are the angles of a triangle; for what values of *A*, *B* and *C* does $\sin^m A\sin^n B\sin^p C$ take extreme values?

A less artificial example is provided by: Consider N independent distinguishable states, the ith having an energy ε_i and an occupancy of n_i. The total energy is fixed

$$\sum_i n_i \varepsilon_i = E$$

as is the total number

$$\sum_i n_i = N$$

Given a set of populations $\{n_i\}$ we identify

$$W = \frac{N!}{\prod_i n_i!}$$

Assuming N and the n to be large enough for Stirling's approximation, in the form

$$\log n! = n \log n - n$$

find $\{\hat{n}_i\}$, the $\{n_i\}$ that maximises W subject to the constraints of fixed number and energy. This configuration dominates the determination of the entropy so that we can write

$$S = k \log \left\{ \frac{N!}{\prod_i \hat{n}_i!} \right\}$$

Identify the Lagrange multipliers that crop up here in terms of physical quantities; you might like to use the thermodynamic identity

$$\left(\frac{\partial S}{\partial E} \right)_V = \frac{1}{T}$$