Natural Sciences Tripos, Part IA

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Mathematical Methods II, Course B

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Section 2

2 FUNCTIONS OF MORE THAN ONE VARIABLE

2.1 Introduction

Functions of more than one variable are frequently encountered in scientific applications when we think about quantities that vary in more than one direction in space, or that vary in space and time.

The temperature in this room is an example of a *scalar field*. Its value is a real number (when expressed in some units such as degrees Celsius) that depends on three spatial coordinates x, y and z (and also time t).

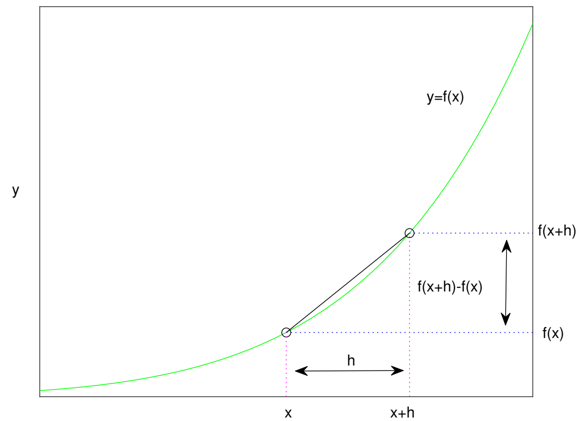
If we wanted to construct a theory of how the temperature evolves in space and time, involving processes such as thermal conduction, we would first need to understand how to do calculus in more than one variable. How do we define the temperature gradient when the temperature depends on three spatial coordinates? How do we find the points of minimum and maximum temperature?

These and related questions are answered in this section of the course.

2.2 Partial differentiation

2.2.1 Ordinary derivative

A function $f(x)$ of one variable x, where x and f are both real numbers, can be visualized as the curve $y = f(x)$ in the (x, y) plane, which is known as the *graph* of the function.



The (ordinary) *derivative* of the function is defined by

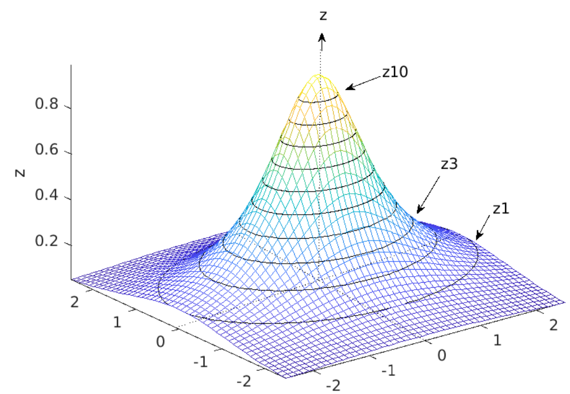
$$\frac{\mathrm{d}f}{\mathrm{d}x} = f'(x) = \lim_{h\to 0}\left[\frac{f(x+h) - f(x)}{h}\right].$$

Thus $\mathrm{d}f/\mathrm{d}x$ is the limiting value of the ratio $\delta f/\delta x$ of small increments in the function and its argument. The function is said to be *differentiable* at the point x if this limit exists.

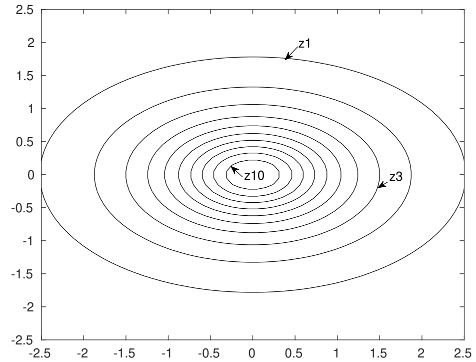
$\mathrm{d}f/\mathrm{d}x$ is the local *rate of change* of the function $f(x)$ with the variable x. Geometrically, it is the local *gradient* of the curve $y = f(x)$, i.e. the gradient of the straight line that is tangent to the curve at the point x. The derivative provides the best *linear approximation* to the function near the point considered.

2.2.2 Partial derivatives

A function $f(x, y)$ of two variables x and y, where x, y and f are all real numbers, can be visualized as the surface $z = f(x, y)$ in the (x, y, z) space, which is also known as the *graph* of the function.



Another way to visualize the function is to plot a selection of contour lines $f(x, y) = \text{constant}$ in the (x, y) plane. This is equivalent to finding the intersection of the surface $z = f(x, y)$ with a selection of horizontal planes $z = \text{constant}$. (Usually, equally spaced contour values are used.)



The *partial derivatives* of the function are defined by

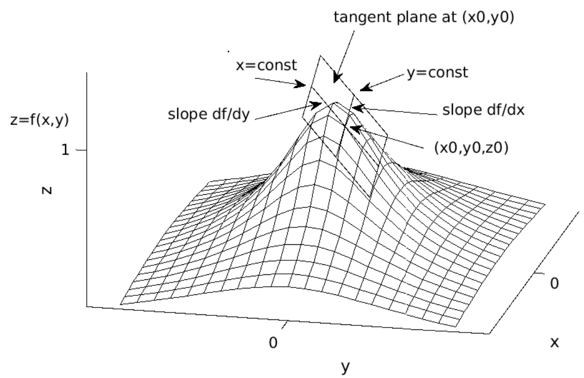
$$\frac{\partial f}{\partial x} = f_x = \lim_{h\to 0}\left[\frac{f(x+h,y)-f(x,y)}{h}\right],$$

$$\frac{\partial f}{\partial y} = f_y = \lim_{h\to 0}\left[\frac{f(x,y+h)-f(x,y)}{h}\right].$$

Therefore $\partial f/\partial x$ is the rate of change of f with x at constant y, while $\partial f/\partial y$ is the rate of change of f with y at constant x. The fact that two different derivatives exist reflects the fact that f depends on two independent variables.

Holding y at a particular constant value means that $f(x,y)$ becomes effectively a function of one variable only. The ordinary derivative of this function is exactly the same as the partial derivative $\partial f/\partial x$.

$\partial f/\partial x$ is the local gradient of the surface $z = f(x,y)$ when travelling in the x-direction, while $\partial f/\partial y$ is the gradient when travelling in the y-direction. These are the gradients of straight lines that are tangent to the surface and perpendicular to the y- and x-axes, respectively. Together, these two gradients define the orientation of the *tangent plane*, which is the best linear approximation to the surface near the point considered.



Other notations used for partial derivatives are

$$\frac{\partial f}{\partial x} = \left(\frac{\partial f}{\partial x}\right)_y = f_x = f_{,x} = \partial_x f.$$

We will use the first three. The notation

$$\left(\frac{\partial f}{\partial x}\right)_y \qquad \text{or} \qquad \left.\frac{\partial f}{\partial x}\right|_y$$

states explicitly which variable (in this case y) is held constant while carrying out the derivative. This notation is particularly useful when changing independent variables, e.g. from (x, y) to (x, v), where v

can be expressed as a function of x and y. In such cases there is a very important distinction between $\left(\frac{\partial f}{\partial x}\right)_y$ and $\left(\frac{\partial f}{\partial x}\right)_v$ (see Section 2.2.8 later).

The use of a subscript to denote differentiation, as in f_x, is compact but potentially ambiguous; we may want to use a subscript to denote a component of a vector, or for some other purpose.

∂ is sometimes pronounced 'del' rather than 'dee' to distinguish it from the ordinary differential operator d.

A vector can be formed with x and y components equal to f_x and f_y. This vector is called the *gradient* of f and may be written as

$$\operatorname{grad} f = \boldsymbol{\nabla} f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right) = \boldsymbol{i}\,\frac{\partial f}{\partial x} + \boldsymbol{j}\,\frac{\partial f}{\partial y}.$$

The symbol

$$\boldsymbol{\nabla} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right) = \boldsymbol{i}\,\frac{\partial}{\partial x} + \boldsymbol{j}\,\frac{\partial}{\partial y}$$

is the *gradient operator*, a vector differential operator. It is pronounced 'grad', 'del' or 'nabla'. Like the differential operator $\frac{\mathrm{d}}{\mathrm{d}x}$, it acts on whatever is written to the right of it.

2.2.3 Second derivatives

Second derivatives can be defined by repeated partial differentiation:

$$\frac{\partial^2 f}{\partial x^2} = f_{xx} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right),$$

$$\frac{\partial^2 f}{\partial y^2} = f_{yy} = \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial y}\right),$$

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

$$\frac{\partial^2 f}{\partial x\,\partial y} = f_{yx} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right).$$

While the first two of these just mean the second derivative of f with respect to one variable while the other is held constant, the last two mean something different and are known as *mixed partial derivatives*.

Example:

$$f(x,y) = \mathrm{e}^{-x^2-y^2}$$

$$\frac{\partial f}{\partial x} = f_x = -2x\,\mathrm{e}^{-x^2-y^2}$$

$$\frac{\partial f}{\partial y} = f_y = -2y\,\mathrm{e}^{-x^2-y^2}$$

$$\frac{\partial^2 f}{\partial x^2} = f_{xx} = \frac{\partial}{\partial x}\left(-2x\,\mathrm{e}^{-x^2-y^2}\right) = (-2+4x^2)\,\mathrm{e}^{-x^2-y^2}$$

$$\frac{\partial^2 f}{\partial y^2} = f_{yy} = \frac{\partial}{\partial y}\left(-2y\,\mathrm{e}^{-x^2-y^2}\right) = (-2+4y^2)\,\mathrm{e}^{-x^2-y^2}$$

$$\frac{\partial^2 f}{\partial y\,\partial x} = f_{xy} = \frac{\partial}{\partial y}\left(-2x\,\mathrm{e}^{-x^2-y^2}\right) = 4xy\,\mathrm{e}^{-x^2-y^2}$$

$$\frac{\partial^2 f}{\partial x\,\partial y} = f_{yx} = \frac{\partial}{\partial x}\left(-2y\,\mathrm{e}^{-x^2-y^2}\right) = 4xy\,\mathrm{e}^{-x^2-y^2}$$

Example:

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

$$\frac{\partial f}{\partial x} = f_x = -\frac{1}{(x+y^2)^2} \qquad \frac{\partial f}{\partial y} = f_y = -\frac{2y}{(x+y^2)^2}$$

$$\frac{\partial^2 f}{\partial x^2} = f_{xx} = \frac{\partial}{\partial x}\left[-\frac{1}{(x+y^2)^2}\right] = \frac{2}{(x+y^2)^3}$$

$$\frac{\partial^2 f}{\partial y^2} = f_{yy} = \frac{\partial}{\partial y}\left[-\frac{2y}{(x+y^2)^2}\right] = -\frac{2}{(x+y^2)^2} + \frac{8y^2}{(x+y^2)^3}$$

$$\frac{\partial^2 f}{\partial y\,\partial x} = f_{xy} = \frac{\partial}{\partial y}\left[-\frac{1}{(x+y^2)^2}\right] = \frac{4y}{(x+y^2)^3}$$

$$\frac{\partial^2 f}{\partial x\,\partial y} = f_{yx} = \frac{\partial}{\partial x}\left[-\frac{2y}{(x+y^2)^2}\right] = \frac{4y}{(x+y^2)^3}$$

In both examples we observe the *symmetry of mixed partial derivatives*

$$\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right) = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right).$$

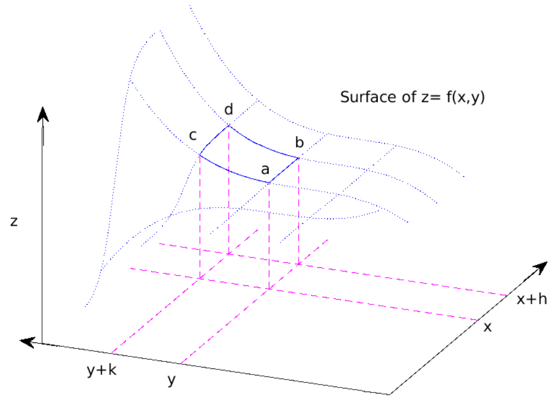
This important property holds for all functions (provided that certain smoothness properties are satisfied). We are therefore free to use any of the following notation:

$$\frac{\partial^2 f}{\partial x\,\partial y} = \frac{\partial^2 f}{\partial y\,\partial x} = f_{xy} = f_{yx}.$$

To see where this property comes from, let

$$a = f(x,y), \quad b = f(x+h,y), \quad c = f(x,y+k), \quad d = f(x+h,y+k).$$

From the definition,



$$\frac{\partial^2 f}{\partial y\,\partial x} = \lim_{k\to 0}\frac{1}{k}\left[\lim_{h\to 0}\left(\frac{d-c}{h}\right) - \lim_{h\to 0}\left(\frac{b-a}{h}\right)\right]$$

while

$$\frac{\partial^2 f}{\partial x\,\partial y} = \lim_{h\to 0}\frac{1}{h}\left[\lim_{k\to 0}\left(\frac{d-b}{k}\right) - \lim_{k\to 0}\left(\frac{c-a}{k}\right)\right].$$

In both cases, therefore, we are interested in the limit of

$$\frac{d-c-b+a}{hk}$$

as both h and k tend to zero. For sufficiently smooth functions f it can be shown that these two double limits produce the same answer.

2.2.4 Generalization

The definitions and properties of partial derivatives generalize to functions of any number of variables, such as $f(x_1, x_2, \ldots, x_n)$. Thus

$$\frac{\partial f}{\partial x_i} = \lim_{h \to 0} \left[\frac{f(x_1, x_2, \ldots, x_i + h, \ldots, x_n) - f(x_1, x_2, \ldots, x_i, \ldots, x_n)}{h} \right]$$

is a partial derivative with respect to x_i in which all of the other variables are held constant. If necessary this can be written

$$\left(\frac{\partial f}{\partial x_i} \right)_{x_1, x_2, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n} .$$

Higher partial derivatives can be calculated in any order, e.g.

$$\frac{\partial^2 f}{\partial x_i \, \partial x_j} = \frac{\partial^2 f}{\partial x_j \, \partial x_i}$$

for any i and j, while

$$\frac{\partial^3 f}{\partial x_i \, \partial x_j \, \partial x_k} = \frac{\partial^3 f}{\partial x_i \, \partial x_k \, \partial x_j} = \frac{\partial^3 f}{\partial x_j \, \partial x_i \, \partial x_k} = \cdots ,$$

etc. The partial derivative operators $\partial/\partial x_i$ and $\partial/\partial x_j$ *commute* for any i and j.

2.2.5 Integration

To undo a partial derivative with respect to x at constant y, we integrate with respect to x at constant y. For example, if $f(x, y)$ is known to satisfy

$$\frac{\partial f}{\partial x} = 2xy^2,$$

then

$$f = x^2y^2 + g(y),$$

where $g(y)$ is a function of y. This arbitrary function replaces the arbitrary constant of integration that arises when undoing an ordinary derivative. If we are also given, for example, that

$$\frac{\partial f}{\partial y} = 2x^2y + 2y,$$

then we can integrate with respect to y at constant x to find

$$f = x^2y^2 + y^2 + h(x),$$

where $h(x)$ is a function of x. Comparing the two expressions for f, we see in this case that

$$g(y) = y^2 + h(x).$$

This is possible only if $h(x) = c = \text{constant}$, in which case $g(y) = y^2 + c$. Thus $f = x^2y^2 + y^2 + c$.

2.2.6 Differentials

For a differentiable function of one variable we have a Taylor expansion

$$f(x+h) \approx f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \cdots ,$$

which gives a local approximation to the variation of f near the point x, as a polynomial in the displacement h.

(The maximum number of terms that can be included in this expansion depends on how many times the function is differentiable. If it is infinitely differentiable then we can write an infinite series that converges exactly to $f(x+h)$ within some interval $|h| < L$.)

The first-order variation, which dominates when h is sufficiently small, is described by the linear approximation

$$f(x+h) - f(x) \approx f'(x)h, \qquad \text{i.e.} \quad \delta f \approx f'(x)\,\delta x.$$

Geometrically, this corresponds to approximating the curve $y = f(x)$ by the tangent line that touches the curve at the point being considered.

Provided that $f(x)$ is indeed differentiable, this approximation is increasingly good as h tends to zero, in the sense that

$$\lim_{h\to 0} \frac{f(x+h) - f(x) - f'(x)h}{h} = 0.$$

We write the linear approximation as an exact equality of *differentials*:

$$\mathrm{d}f = f'(x)\,\mathrm{d}x.$$

For example, if $f(x) = x^3$, then $\mathrm{d}f = 3x^2\,\mathrm{d}x$. This statement is exact, whereas the statement $\delta f \approx 3x^2\,\delta x$ is an approximation.

The original (Leibniz's) interpretation of this type of statement is that it relates an *infinitesimal* change $\mathrm{d}f$ in $f(x)$ to an infinitesimal change $\mathrm{d}x$ in x. Although both quantities are vanishingly small, the absolute error in the statement is even smaller, such that the relative error in the statement is vanishingly small.

Mathematicians have since found more sophisticated ways to formalize this type of statement, but we will not investigate them here.

Now consider a function $f(x, y)$ of two variables. By analogy with the one-variable case, we expect a local linear approximation to f in the neighbourhood of any point, i.e.

$$f(x+h, y+k) \approx f(x, y) + \alpha h + \beta k,$$

for some constants α and β. Geometrically, this corresponds to approximating the surface $z = f(x, y)$ by the tangent plane that touches the surface at the point being considered.

Let the error in this approximation be

$$\epsilon(h, k) = f(x+h, y+k) - f(x, y) - \alpha h - \beta k.$$

We expect that $\epsilon(h, k)$ vanishes as h and k tend to zero. If

$$\frac{\epsilon(h, k)}{\sqrt{h^2 + k^2}} \to 0 \qquad \text{as} \quad \sqrt{h^2 + k^2} \to 0$$

then the function $f(x, y)$ is said to be differentiable at (x, y).

To find the value of α, take $k = 0$. Then

$$\frac{\epsilon(h, 0)}{h} = \frac{f(x+h, y) - f(x, y)}{h} - \alpha \to 0 \qquad \text{as} \quad h \to 0$$

and so

$$\alpha = \lim_{h \to 0} \left[\frac{f(x+h, y) - f(x, y)}{h} \right] = \frac{\partial f}{\partial x}.$$

Similarly,

$$\beta = \frac{\partial f}{\partial y}.$$

The linear approximation is therefore

$$f(x+h, y+k) - f(x,y) \approx \frac{\partial f}{\partial x} h + \frac{\partial f}{\partial y} k,$$

i.e.

$$\delta f \approx \frac{\partial f}{\partial x}\,\delta x + \frac{\partial f}{\partial y}\,\delta y.$$

This can also be written as an exact equality between infinitesimals, or differentials:

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

For example, if $f = x^2 y$, then $\mathrm{d}f = 2xy\,\mathrm{d}x + x^2\,\mathrm{d}y$.

This equation might be interpreted literally as saying that $0 = 0$. But it is valuable as a statement about how the limit is approached and implies more obviously useful results such as

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

if x and y are both functions of a parameter t. It is also useful in estimating small finite changes.

Example. The Clausius–Clapeyron equation

$$P = P_0 \exp\left[\frac{H}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right]$$

predicts the vapour pressure of a liquid at temperature T if it is known to be P_0 at temperature T_0. H is the enthalpy of vaporization and R is the ideal gas constant.

Suppose that P_0, T_0 and R are known exactly. What is the uncertainty in vapour pressure if T is known only within 5% accuracy and H is known only within 1% accuracy? We regard P as a function of T and H and calculate the small change in P associated with small changes in T and H,

$$\mathrm{d}P = \frac{\partial P}{\partial T}\,\mathrm{d}T + \frac{\partial P}{\partial H}\,\mathrm{d}H.$$

Now

$$\frac{\partial P}{\partial T} = \frac{H}{RT^2}\,P$$

$$\frac{\partial P}{\partial H} = \frac{1}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)P$$

$$\mathrm{d}P = \frac{H}{RT^2}\,P\,\mathrm{d}T + \frac{1}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)P\,\mathrm{d}H$$

$$\frac{\mathrm{d}P}{P} = \frac{H}{RT}\frac{\mathrm{d}T}{T} + \frac{H}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\frac{\mathrm{d}H}{H}.$$

This expresses the relation between the fractional errors in P, T and H when those errors are small. (**Exercise**: It can be obtained more easily by finding the partial derivatives of $\ln P$. Note that $\mathrm{d}P/P = \mathrm{d}\ln P$.) Thus the fractional error in P is approximately

$$\frac{H}{RT} \times 0.05 + \frac{H}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right) \times 0.01.$$

2.2.7 Taylor series

For a function $f(x)$ of one variable, differentiable twice for all x in an interval $[a, b]$,

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + R,$$

where the remainder term is such that

$$\frac{R}{h^2} \to 0 \qquad \text{as} \quad h \to 0.$$

The equivalent expansion for a function of two variables is

$$\begin{aligned} f(x+h, y+k) &= f(x,y) + f_x(x,y)h + f_y(x,y)k \\ &\quad + \frac{1}{2}f_{xx}(x,y)h^2 + f_{xy}(x,y)hk + \frac{1}{2}f_{yy}(x,y)k^2 + R, \end{aligned}$$

where the remainder term is such that

$$\frac{R}{h^2+k^2} \to 0 \qquad \text{as} \quad h \to 0 \quad \text{and} \quad k \to 0.$$

Another way to write this is

$$\begin{aligned}f(x,y) = f(x_0,y_0) &+ f_x(x_0,y_0)(x-x_0) + f_y(x_0,y_0)(y-y_0)\\&+ \frac{1}{2}f_{xx}(x_0,y_0)(x-x_0)^2 + f_{xy}(x_0,y_0)(x-x_0)(y-y_0)\\&+ \frac{1}{2}f_{yy}(x_0,y_0)(y-y_0)^2 + R.\end{aligned}$$

These series can be extended to higher order if the function is differentiable more than twice.

2.2.8 Chain rule

Suppose that f is a function of two variables x and y, and that, in turn, x and y are each functions of two variables u and v. This situation occurs, for example, when we change to a different system of coordinates describing location in the plane.

We could write

$$f(x, y) = f(x(u, v), y(u, v)) = g(u, v).$$

From the mathematical point of view f and g are two completely different functions. Although their values are the same, they process their arguments differently.

For example, if $f(x, y) = x + y$ is a linear function of its arguments, but $x = u^2$ and $y = v^2$, then $g(u, v) = u^2 + v^2$ is a quadratic function of its arguments. How are the partial derivatives of these two functions related?

In scientific applications we usually do *not* introduce different symbols, such as f and g, for the same quantity when expressed as a function of different arguments. One reason for this is that the choice of symbols is dictated by scientific conventions. We will call the temperature T, for example, whether it is expressed as a function of Cartesian coordinates (x, y) or polar coordinates (r, ϕ).

We will therefore write

$$f(x, y) = f(x(u, v), y(u, v)) = f(u, v)$$

although this is (like many things) a *conventional abuse of mathematical notation.* When doing this we may have to be careful to indicate (using subscripts) which variable is being held constant in a partial derivative.

Infinitesimal changes are related by

$$\mathrm{d}x = \left(\frac{\partial x}{\partial u}\right)_v \mathrm{d}u + \left(\frac{\partial x}{\partial v}\right)_u \mathrm{d}v,$$

$$\mathrm{d}y = \left(\frac{\partial y}{\partial u}\right)_v \mathrm{d}u + \left(\frac{\partial y}{\partial v}\right)_u \mathrm{d}v,$$

$$\mathrm{d}f = \left(\frac{\partial f}{\partial x}\right)_y \mathrm{d}x + \left(\frac{\partial f}{\partial y}\right)_x \mathrm{d}y.$$

Substituting the first two expressions into the third, we find

$$\begin{aligned} \mathrm{d}f = &\left[\left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial x}{\partial u}\right)_v + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial u}\right)_v\right] \mathrm{d}u \\ &+ \left[\left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial x}{\partial v}\right)_u + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial v}\right)_u\right] \mathrm{d}v. \end{aligned}$$

Since we also expect

$$\mathrm{d}f = \left(\frac{\partial f}{\partial u}\right)_v \mathrm{d}u + \left(\frac{\partial f}{\partial v}\right)_u \mathrm{d}v,$$

we deduce that

$$\left(\frac{\partial f}{\partial u}\right)_v = \left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial x}{\partial u}\right)_v + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial u}\right)_v,$$

$$\left(\frac{\partial f}{\partial v}\right)_u = \left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial x}{\partial v}\right)_u + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial v}\right)_u.$$

These are expressions of the *chain rule* of partial differentiation. To remember it, notice the pattern of the variables.

Example. Change from Cartesian coordinates (x, y) to polar coordinates (r, ϕ). By definition,

$$x = r\cos\phi, \qquad y = r\sin\phi.$$

Thus

$$\begin{aligned}\left(\frac{\partial f}{\partial r}\right)_\phi &= \left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial x}{\partial r}\right)_\phi + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial r}\right)_\phi \\ &= \cos\phi \left(\frac{\partial f}{\partial x}\right)_y + \sin\phi \left(\frac{\partial f}{\partial y}\right)_x,\end{aligned}$$

$$\begin{aligned}\left(\frac{\partial f}{\partial \phi}\right)_r &= \left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial x}{\partial \phi}\right)_r + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial \phi}\right)_r \\ &= -r\sin\phi \left(\frac{\partial f}{\partial x}\right)_y + r\cos\phi \left(\frac{\partial f}{\partial y}\right)_x .\end{aligned}$$

Note that we needed to express the old variables (x, y) in terms of the new variables (r, ϕ).

To go the other way, we can either solve these simultaneous linear equations to find (**exercise**)

$$\left(\frac{\partial f}{\partial x}\right)_y = \cos\phi \left(\frac{\partial f}{\partial r}\right)_\phi - \frac{\sin\phi}{r} \left(\frac{\partial f}{\partial \phi}\right)_r ,$$

$$\left(\frac{\partial f}{\partial y}\right)_x = \sin\phi \left(\frac{\partial f}{\partial r}\right)_\phi + \frac{\cos\phi}{r} \left(\frac{\partial f}{\partial \phi}\right)_r ,$$

or we can express

$$r = \sqrt{x^2 + y^2}, \qquad \phi = \arctan\left(\frac{y}{x}\right),$$

return to the chain rule and derive the same result (**exercise**).

A special case of the chain rule occurs when only one of the variables is changed. Suppose that $u = x$, so we are changing from (x, y) to (x, v). Then, since $(\partial x/\partial x)_v = 1$ and $(\partial x/\partial v)_x = 0$, we have

$$\left(\frac{\partial f}{\partial x}\right)_v = \left(\frac{\partial f}{\partial x}\right)_y + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial x}\right)_v ,$$

$$\left(\frac{\partial f}{\partial v}\right)_x = \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial v}\right)_x .$$

The first equation demonstrates that $(\partial f/\partial x)_v$ is, in general, not equal to $(\partial f/\partial x)_y$. (This makes sense because the constraint v = constant is different from the constraint y = constant.) The second equation corresponds to the chain rule for ordinary derivatives; here x is held constant in each derivative.

A simpler version of the chain rule occurs if both x and y are functions of a single variable t. This happens if we restrict attention to a curve in the (x, y) plane, parametrized by t. In a similar abuse of notation, we can write $f(x, y) = f(x(t), y(t)) = f(t)$. Then

$$
\begin{aligned}
\mathrm{d}x &= \frac{\mathrm{d}x}{\mathrm{d}t}\,\mathrm{d}t, \qquad \mathrm{d}y = \frac{\mathrm{d}y}{\mathrm{d}t}\,\mathrm{d}t, \\
\mathrm{d}f &= \left(\frac{\partial f}{\partial x}\right)_y \mathrm{d}x + \left(\frac{\partial f}{\partial y}\right)_x \mathrm{d}y \\
&= \left[\left(\frac{\partial f}{\partial x}\right)_y \frac{\mathrm{d}x}{\mathrm{d}t} + \left(\frac{\partial f}{\partial y}\right)_x \frac{\mathrm{d}y}{\mathrm{d}t}\right] \mathrm{d}t,
\end{aligned}
$$

and so

$$
\frac{\mathrm{d}f}{\mathrm{d}t} = \left(\frac{\partial f}{\partial x}\right)_y \frac{\mathrm{d}x}{\mathrm{d}t} + \left(\frac{\partial f}{\partial y}\right)_x \frac{\mathrm{d}y}{\mathrm{d}t}.
$$

As noted previously, this can be seen as a direct consequence of the differential relation

$$
\mathrm{d}f = \left(\frac{\partial f}{\partial x}\right)_y \mathrm{d}x + \left(\frac{\partial f}{\partial y}\right)_x \mathrm{d}y.
$$

Example. If the height of a hill is

$$h(x,y) = \frac{1}{x^2 + 2y^4 + 1}$$

and my position as a function of time t is given by $x = \sqrt{1+t}$ and $y = 1-t$, what is the rate of change of my altitude with time?
Use the chain rule in the form

$$\frac{\mathrm{d}h}{\mathrm{d}t} = \left(\frac{\partial h}{\partial x}\right)_y \frac{\mathrm{d}x}{\mathrm{d}t} + \left(\frac{\partial h}{\partial y}\right)_x \frac{\mathrm{d}y}{\mathrm{d}t}.$$

Now

$$\left(\frac{\partial h}{\partial x}\right)_y = -\frac{2x}{(x^2 + 2y^4 + 1)^2} = -\frac{2\sqrt{1+t}}{[1 + t + 2(1-t)^4 + 1]^2}$$

$$\left(\frac{\partial h}{\partial y}\right)_x = -\frac{8y^3}{(x^2 + 2y^4 + 1)^2} = -\frac{8(1-t)^3}{[1 + t + 2(1-t)^4 + 1]^2}$$

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{1}{2\sqrt{1+t}} \qquad \frac{\mathrm{d}y}{\mathrm{d}t} = -1$$

and so

$$\frac{\mathrm{d}h}{\mathrm{d}t} = \frac{-1 + 8(1-t)^3}{[2 + t + 2(1-t)^4]^2}.$$

Exercise: check that you get the same answer by substituting $x(t)$ and $y(t)$ into $h(x,y)$ to find $h(t)$ and then differentiating with respect to t.

2.2.9 Reciprocity and cyclic relations

If z is a function of two variables x and y, then equally x can be regarded as a function of y and z, or y can be regarded as a function of z and x.

(We write z rather than f here to emphasize that x, y and z are treated on an equal basis. They are three quantities sharing a functional relation, which could be written in the form $F(x, y, z) = 0$. Geometrically, this defines a surface in three-dimensional space.)

Infinitesimal changes are related by

$$\mathrm{d}x = \left(\frac{\partial x}{\partial y}\right)_z \mathrm{d}y + \left(\frac{\partial x}{\partial z}\right)_y \mathrm{d}z,$$

$$\mathrm{d}y = \left(\frac{\partial y}{\partial z}\right)_x \mathrm{d}z + \left(\frac{\partial y}{\partial x}\right)_z \mathrm{d}x,$$

$$\mathrm{d}z = \left(\frac{\partial z}{\partial x}\right)_y \mathrm{d}x + \left(\frac{\partial z}{\partial y}\right)_x \mathrm{d}y.$$

In each case we can make changes in two variables independently and deduce the change in the third.

Assuming that $(\partial y/\partial x)_z \neq 0$, we can rewrite the second equation as

$$\mathrm{d}x = \left[1 \Big/ \left(\frac{\partial y}{\partial x}\right)_z\right] \mathrm{d}y - \left[\left(\frac{\partial y}{\partial z}\right)_x \Big/ \left(\frac{\partial y}{\partial x}\right)_z\right] \mathrm{d}z$$

and compare it with the first. Since $\mathrm{d}y$ and $\mathrm{d}z$ are independent, the coefficients must agree:

$$\left(\frac{\partial x}{\partial y}\right)_z = 1 \bigg/ \left(\frac{\partial y}{\partial x}\right)_z, \tag{1}$$

$$\left(\frac{\partial x}{\partial z}\right)_y = - \left(\frac{\partial y}{\partial z}\right)_x \bigg/ \left(\frac{\partial y}{\partial x}\right)_z. \tag{2}$$

Equation (1) expresses the *reciprocity relation.* It is a straightforward generalization of the result $\frac{\mathrm{d}x}{\mathrm{d}y} = 1 \big/ \frac{\mathrm{d}y}{\mathrm{d}x}$ for ordinary derivatives. It can also be written

$$\left(\frac{\partial x}{\partial y}\right)_z \left(\frac{\partial y}{\partial x}\right)_z = 1.$$

Since x, y and z are on an equal basis, the symbols can be permuted as desired.

Equation (2) expresses the *cyclic relation.* Using the reciprocity relation, it can also be written in the more symmetrical form

$$\left(\frac{\partial x}{\partial z}\right)_y \left(\frac{\partial y}{\partial x}\right)_z \left(\frac{\partial z}{\partial y}\right)_x = -1.$$

Note the pattern of the variables and the minus sign.

Example. Given the height of a mountain $z = f(x, y)$, what is the slope of the contour lines $(\partial y/\partial x)_z$?

Using the cyclic relation,

$$\left(\frac{\partial y}{\partial x}\right)_z = - \left(\frac{\partial z}{\partial x}\right)_y \bigg/ \left(\frac{\partial z}{\partial y}\right)_x = - \left(\frac{\partial f}{\partial x}\right)_y \bigg/ \left(\frac{\partial f}{\partial y}\right)_x.$$

2.2.10 Exact differentials

The general expression

$$\omega = P(x,y)\,\mathrm{d}x + Q(x,y)\,\mathrm{d}y$$

is called a *differential form* in the variables x and y.

We say that ω is an *exact differential* if there is a function $f(x,y)$ such that

$$P(x,y)\,\mathrm{d}x + Q(x,y)\,\mathrm{d}y = \mathrm{d}f.$$

Since we know that

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

and $\mathrm{d}x$ and $\mathrm{d}y$ are independent, we must then have

$$\frac{\partial f}{\partial x} = P \qquad \text{and} \qquad \frac{\partial f}{\partial y} = Q.$$

Now the symmetry of mixed partial derivatives

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

implies

$$\frac{\partial P}{\partial y} = \frac{\partial Q}{\partial x}.$$

This is therefore a necessary condition for ω to be an exact differential. It is also (subject to certain technical restrictions) a sufficient condition. So

$$P(x,y)\,\mathrm{d}x + Q(x,y)\,\mathrm{d}y \quad \text{is an exact differential}$$

$$\text{if and only if} \quad \frac{\partial P}{\partial y} = \frac{\partial Q}{\partial x}.$$

Example. Is $y\,\mathrm{d}x - x\,\mathrm{d}y$ an exact differential, i.e. is there a function f such that $\mathrm{d}f = y\,\mathrm{d}x - x\,\mathrm{d}y$?

In this case $P = y$ and $Q = -x$, so $\partial P/\partial y = 1$ and $\partial Q/\partial x = -1$ are not equal. The answer is *no*.

Example. Is $y\,\mathrm{d}x + x\,\mathrm{d}y$ an exact differential?

In this case $P = y$ and $Q = x$, so $\partial P/\partial y = 1 = \partial Q/\partial x$. The answer is *yes*. To find f, we note that

$$\frac{\partial f}{\partial x} = y, \qquad \frac{\partial f}{\partial y} = x.$$

Integrating the first equation with respect to x and the second equation with respect to y, we find

$$f = xy + g(y), \qquad f = xy + h(x).$$

These equations are compatible only if $g(y) = h(x) =$ constant, in which case $f = xy +$ constant. We easily check that $\mathrm{d}f = y\,\mathrm{d}x + x\,\mathrm{d}y$ as required.

This idea can be applied to first-order ordinary differential equations. Another way of writing the ODE

$$\frac{\mathrm{d}y}{\mathrm{d}x} = -\frac{P(x,y)}{Q(x,y)}$$

is

$$P(x,y)\,\mathrm{d}x + Q(x,y)\,\mathrm{d}y = 0.$$

If $P\,\mathrm{d}x + Q\,\mathrm{d}y$ is an exact differential and equal to $\mathrm{d}f$ for some function $f(x,y)$, then the ODE simplifies to $\mathrm{d}f = 0$ and its solutions are given by $f(x,y) = c$, where c is an arbitrary constant.

Example. Solve the ODE $y\,\mathrm{d}x + x\,\mathrm{d}y = 0$.

We have already seen that $y\,\mathrm{d}x + x\,\mathrm{d}y = \mathrm{d}(xy)$ is an exact differential. Therefore the solutions are $xy = c$, i.e. $y = c/x$.

Compare this solution with the more conventional approach

$$\begin{aligned}
&\frac{\mathrm{d}y}{\mathrm{d}x} = -\frac{y}{x} \\
&\int \frac{\mathrm{d}y}{y} = -\int \frac{\mathrm{d}x}{x} \\
&\ln y = -\ln x + \text{constant} \\
&y = \frac{c}{x}.
\end{aligned}$$

2.2.11 Integrating factors for differential forms

The function $\mu(x,y)$ is said to be an *integrating factor* for the differential form $\omega = P(x,y)\,\mathrm{d}x + Q(x,y)\,\mathrm{d}y$ if the differential form

$$\mu(x,y)[P(x,y)\,\mathrm{d}x + Q(x,y)\,\mathrm{d}y] \qquad \text{is exact.}$$

The condition for this is

$$\frac{\partial}{\partial y}(\mu P) = \frac{\partial}{\partial x}(\mu Q).$$

Given P and Q, it is usually very difficult to solve this (linear partial differential) equation for μ.

In special cases there might be an integrating factor $\mu(x)$ that depends only on x. Then we require

$$\mu\frac{\partial P}{\partial y} = \frac{\mathrm{d}\mu}{\mathrm{d}x}Q + \mu\frac{\partial Q}{\partial x},$$

which can be rearranged to give

$$\frac{1}{\mu}\frac{\mathrm{d}\mu}{\mathrm{d}x} = \frac{1}{Q}\left(\frac{\partial P}{\partial y} - \frac{\partial Q}{\partial x}\right).$$

Given a differential form $P\,\mathrm{d}x + Q\,\mathrm{d}y$, if the right-hand side of this equation vanishes, we have an exact differential. If the right-hand side is a function of x only, then the equation is self-consistent and can be integrated to find the integrating factor $\mu(x)$. If the right-hand side depends on both x and y, then there is a contradiction and no integrating factor of the form $\mu(x)$ exists.

Similarly, an integrating factor of the form $\mu(y)$ satisfies

$$\frac{1}{\mu}\frac{\mathrm{d}\mu}{\mathrm{d}y} = -\frac{1}{P}\left(\frac{\partial P}{\partial y} - \frac{\partial Q}{\partial x}\right)$$

and exists if the right-hand side is a function of y only.

Example. $\omega = y\,\mathrm{d}x - x\,\mathrm{d}y$. Here

$$\frac{\partial P}{\partial y} - \frac{\partial Q}{\partial x} = 1 + 1 = 2,$$

so

$$\frac{1}{Q}\left(\frac{\partial P}{\partial y} - \frac{\partial Q}{\partial x}\right) = -\frac{2}{x}$$

is a function of x only. There is an integrating factor of the form $\mu(x)$, with

$$\frac{1}{\mu}\frac{\mathrm{d}\mu}{\mathrm{d}x} = -\frac{2}{x}$$

$$\ln\mu = -2\ln x + \text{constant}$$

$$\mu = \frac{c}{x^2}.$$

The simplest choice is $\mu = 1/x^2$. Indeed,

$$\mu\omega = \frac{y}{x^2}\,\mathrm{d}x - \frac{1}{x}\,\mathrm{d}y = \mathrm{d}\left(-\frac{y}{x}\right)$$

is an exact differential.

In fact

$$-\frac{1}{P}\left(\frac{\partial P}{\partial y} - \frac{\partial Q}{\partial x}\right) = -\frac{2}{y}$$

is also a function of y only, so $\mu(y) = 1/y^2$ is also an integrating factor. With this different choice,

$$\mu\omega = \frac{1}{y}\,\mathrm{d}x - \frac{x}{y^2}\,\mathrm{d}y = \mathrm{d}\left(\frac{x}{y}\right).$$

This example shows that integrating factors are not unique. However, if presented with the ODE

$$y\,\mathrm{d}x - x\,\mathrm{d}y = 0,$$

we could use either version to deduce that the general solution is $y = cx$, where c is an arbitrary constant.

2.2.12 Maxwell's relations

Partial derivatives and differentials are frequently encountered in thermodynamics, and the classic application is to gases.

A unit mass of gas has *pressure* p, *volume* V and *temperature* T.

The state of the gas is uniquely defined by any two thermodynamic variables, such as (p, V). We say that the system has two *degrees of freedom*.

The variables (p, V, T) are related by an *equation of state*. The simplest example is the ideal gas equation $pV = RT$, where R is the gas constant. This allows us to express, for example, T as a function of (p, V).

A fourth variable commonly used to describe the state of the gas is the *entropy* S. In principle, S can be expressed as a function of (p, V). In fact any two of the four variables (p, V, T, S) can be used to describe the state of the gas. The pair (p, V) are *mechanical* variables, while (T, S) are *thermal* variables.

Physical reasoning leads to the *fundamental thermodynamic relation*

$$\mathrm{d}U = T\,\mathrm{d}S - p\,\mathrm{d}V, \tag{$\star$}$$

where U is the *internal energy*. This differential relation is a statement of the first law of thermodynamics. In an infinitesimal process, the increase in internal energy is equal to the amount of heat added to the gas (by adding entropy) plus the amount of work done on it (by compressing it).

Regarding U as a function of (S, V), we have

$$\mathrm{d}U = \left(\frac{\partial U}{\partial S}\right)_V \mathrm{d}S + \left(\frac{\partial U}{\partial V}\right)_S \mathrm{d}V.$$

Therefore

$$\left(\frac{\partial U}{\partial S}\right)_V = T, \qquad \left(\frac{\partial U}{\partial V}\right)_S = -p.$$

Symmetry of the mixed partial derivatives implies

$$\frac{\partial^2 U}{\partial V\,\partial S} = \frac{\partial^2 U}{\partial S\,\partial V} \quad \Rightarrow \quad \left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial p}{\partial S}\right)_V. \tag{1}$$

This is one of *Maxwell's relations.*

We can derive similar relations by making a change of variables known as a *Legendre transformation.*

Given that

$$\mathrm{d}U = T\,\mathrm{d}S - p\,\mathrm{d}V,$$

it makes sense to consider the quantity

$$F = U - TS,$$

so that

$$\begin{aligned}
\mathrm{d}F &= \mathrm{d}U - T\,\mathrm{d}S - S\,\mathrm{d}T \\
&= -S\,\mathrm{d}T - p\,\mathrm{d}V.
\end{aligned}$$

Regarding F as a function of (T, V), we have

$$\mathrm{d}F = \left(\frac{\partial F}{\partial T}\right)_V \mathrm{d}T + \left(\frac{\partial F}{\partial V}\right)_T \mathrm{d}V.$$

Therefore

$$\left(\frac{\partial F}{\partial T}\right)_V = -S, \qquad \left(\frac{\partial F}{\partial V}\right)_T = -p,$$

and so

$$\frac{\partial^2 F}{\partial V\,\partial T} = \frac{\partial^2 F}{\partial T\,\partial V} \quad \Rightarrow \quad \left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial p}{\partial T}\right)_V. \tag{2}$$

The quantity F is called the *Helmholtz free energy* or *Helmholtz function* (some authors prefer the symbol A). Note, however, that it was just an intermediate step in this calculation. The Maxwell relation (2) is a purely mathematical consequence of the fundamental thermodynamic relation ($\star$).

Further Maxwell relations follow from the Legendre transformations $H = U + pV$ (*enthalpy*) and $G = H - TS$ (*Gibbs free energy* or *Gibbs function*), which imply

$$\mathrm{d}H = T\,\mathrm{d}S + V\,\mathrm{d}p \quad \Rightarrow \quad \left(\frac{\partial T}{\partial p}\right)_S = \left(\frac{\partial V}{\partial S}\right)_p . \tag{3}$$

$$\mathrm{d}G = -S\,\mathrm{d}T + V\,\mathrm{d}p \quad \Rightarrow \quad \left(\frac{\partial S}{\partial p}\right)_T = -\left(\frac{\partial V}{\partial T}\right)_p . \tag{4}$$

Each Maxwell relation implies the others. For example, if we assume relation (1) then we can deduce relation (2) as follows:

$$\begin{aligned}
\left(\frac{\partial S}{\partial V}\right)_T &= -\left(\frac{\partial S}{\partial T}\right)_V \left(\frac{\partial T}{\partial V}\right)_S && \text{(cyclic)}\\
&= -\left(\frac{\partial S}{\partial p}\right)_V \left(\frac{\partial p}{\partial T}\right)_V \left(\frac{\partial T}{\partial V}\right)_S && \text{(chain)}\\
&= -\left(\frac{\partial p}{\partial T}\right)_V \left(\frac{\partial T}{\partial V}\right)_S \Big/ \left(\frac{\partial p}{\partial S}\right)_V && \text{(reciprocity)}\\
&= \left(\frac{\partial p}{\partial T}\right)_V \left(\frac{\partial T}{\partial V}\right)_S \Big/ \left(\frac{\partial T}{\partial V}\right)_S && \text{(Maxwell 1)}\\
&= \left(\frac{\partial p}{\partial T}\right)_V .
\end{aligned}$$

Exercise: Choose a different pair of Maxwell relations and derive one from the other in a similar way.

A different type of relation can also be derived from equation ($\star$). By considering U as a function of the two thermal variables (T, S) we are led to write

$$
\begin{aligned}
\mathrm{d}U &= T\,\mathrm{d}S - p\,\mathrm{d}V \\
&= T\,\mathrm{d}S - p\left[\left(\frac{\partial V}{\partial T}\right)_S \mathrm{d}T + \left(\frac{\partial V}{\partial S}\right)_T \mathrm{d}S\right] \\
&= -p\left(\frac{\partial V}{\partial T}\right)_S \mathrm{d}T + \left[T - p\left(\frac{\partial V}{\partial S}\right)_T\right] \mathrm{d}S.
\end{aligned}
$$

Symmetry of the mixed partial derivatives (or, equivalently, the fact that $\mathrm{d}U$ is an exact differential) implies

$$
\left(\frac{\partial}{\partial S}\right)_T \left[-p\left(\frac{\partial V}{\partial T}\right)_S\right] = \left(\frac{\partial}{\partial T}\right)_S \left[T - p\left(\frac{\partial V}{\partial S}\right)_T\right]
$$

$$
\begin{aligned}
-\left(\frac{\partial p}{\partial S}\right)_T \left(\frac{\partial V}{\partial T}\right)_S - p\frac{\partial^2 V}{\partial S\,\partial T} \\
= 1 - \left(\frac{\partial p}{\partial T}\right)_S \left(\frac{\partial V}{\partial S}\right)_T - p\frac{\partial^2 V}{\partial T\,\partial S}
\end{aligned}
$$

$$
\left(\frac{\partial p}{\partial T}\right)_S \left(\frac{\partial V}{\partial S}\right)_T - \left(\frac{\partial p}{\partial S}\right)_T \left(\frac{\partial V}{\partial T}\right)_S = 1.
$$

2.3 Stationary points

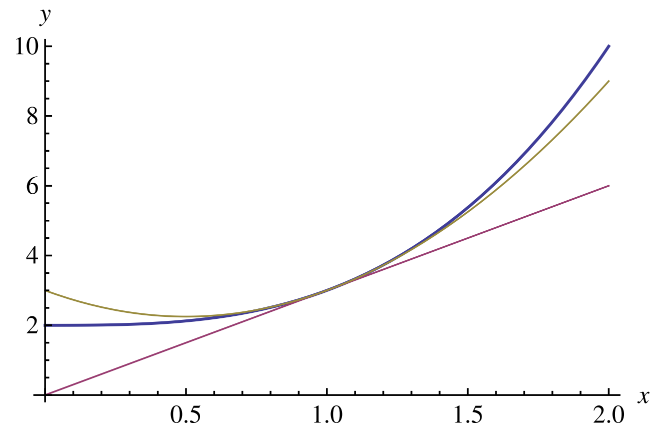
2.3.1 Functions of one variable

Consider a function $f(x)$ of one variable x, where x and f are both real numbers. Near any point $x = x_0$, we can use the Taylor expansion to approximate

$$f(x) \approx f(x_0) + f'(x_0)(x - x_0) + \tfrac{1}{2}f''(x_0)(x - x_0)^2,$$

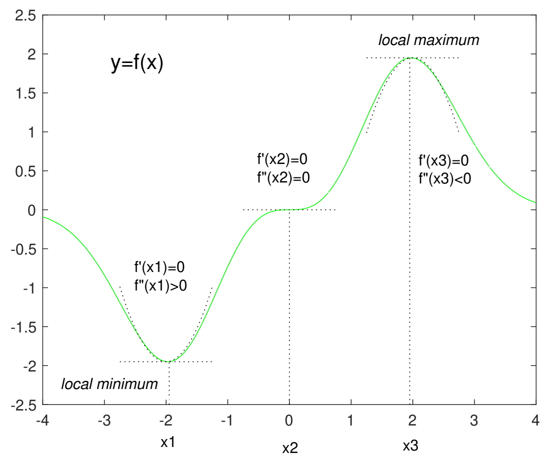
provided that the first and second derivatives exist. This approximation becomes increasing accurate as x approaches x_0.

If $f'(x_0) \neq 0$ then the variation of $f(x)$ near $x = x_0$ is dominated by the linear term, which has different signs on either side of $x = x_0$. In this case $f(x)$ has neither a local minimum nor a local maximum at $x = x_0$.



If $f'(x_0) = 0$ then $f(x)$ is said to have a *stationary point* at $x = x_0$, because then it does not vary to first order in $x - x_0$. Provided that $f''(x_0) \neq 0$, the variation of $f(x)$ near $x = x_0$ is then dominated by the quadratic term, which has the same sign on either side of $x = x_0$. In this case $f(x)$ has

- a *local minimum* at $x = x_0$ if $f''(x_0) > 0$
- a *local maximum* at $x = x_0$ if $f''(x_0) < 0$



If both $f'(x_0) = 0$ and $f''(x_0) = 0$ then we would need to inspect higher-order terms in the Taylor expansion to determine whether the function has a minimum, maximum or neither. For example, if $f'(x_0) = f''(x_0) = 0$ and $f'''(x_0) \neq 0$, then

$$f(x) \approx f(x_0) + \tfrac{1}{6} f'''(x_0)(x - x_0)^3,$$

which indicates neither a minimum nor a maximum but rather a *stationary point of inflection*.

(In general, a *point of inflection* is a point on a curve at which the curvature changes sign. The sign of the curvature of the graph $y = f(x)$ is the same as the sign of $f''(x)$. In fact the curvature is $f''(1 + f'^2)^{-3/2}$.)

2.3.2 Functions of two or more variables

Consider now a differentiable function $f(x, y)$ of two variables. Near any point (x_0, y_0) we have

$$f(x, y) \approx f(x_0, y_0) + f_x(x_0, y_0)(x - x_0) + f_y(x_0, y_0)(y - y_0).$$

The dominant variation is linear in the displacements $\delta x = x - x_0$ and $\delta y = y - y_0$.

If both $f_x(x_0, y_0) = 0$ and $f_y(x_0, y_0) = 0$ then $f(x, y)$ is said to have a *stationary point* at (x_0, y_0), because then it does not vary to first order in δx and δy.

In terms of the gradient vector

$$\boldsymbol{\nabla} f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right) = (f_x, f_y),$$

we have

$$f(\boldsymbol{x}) \approx f(\boldsymbol{x}_0) + [\boldsymbol{\nabla} f(\boldsymbol{x}_0)] \cdot \delta\boldsymbol{x},$$

where $\boldsymbol{x}_0 = (x_0, y_0)$ and $\delta\boldsymbol{x} = (\delta x, \delta y)$. The condition for a stationary point is $\boldsymbol{\nabla} f(\boldsymbol{x}_0) = \boldsymbol{0}$. This result easily generalizes to a function $f(x_1, x_2, \ldots, x_n)$ of any number of variables.

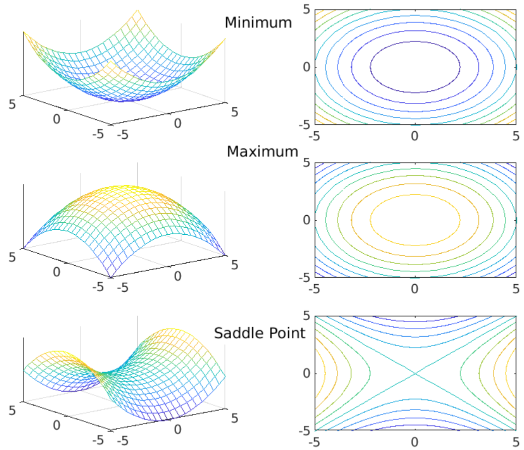
For an infinitesimal displacement $\mathrm{d}\boldsymbol{x} = (\mathrm{d}x, \mathrm{d}y)$ we can write

$$\mathrm{d}f = (\boldsymbol{\nabla} f) \cdot \mathrm{d}\boldsymbol{x}.$$

At a stationary point where $\boldsymbol{\nabla} f = \boldsymbol{0}$, $\mathrm{d}f = 0$ for all $\mathrm{d}\boldsymbol{x}$.

While a stationary point of a function of one variable is usually a minimum or a maximum (exceptions occurring only when the second derivative also vanishes), a stationary point of a function of two or more variable is usually a minimum, a maximum or a *saddle point.* Near a saddle point, the function increases in some directions and decreases in others (but to first order in the displacement it does not vary).
(The term *extremum* refers to either a minimum or a maximum, but not a saddle point.)

Pictures and contour diagrams of an idealised minimum, maximum and saddle point.



Applying a Taylor expansion (see Section 2.2.7) to a function that has a stationary point at (x_0, y_0), we obtain the approximation

$$\begin{aligned} f(x,y) \approx f(x_0,y_0) &+ \tfrac{1}{2} f_{xx}(x_0,y_0)(x-x_0)^2 \\ &+ f_{xy}(x_0,y_0)(x-x_0)(y-y_0) + \tfrac{1}{2} f_{yy}(x_0,y_0)(y-y_0)^2, \end{aligned} \tag{1}$$

which is a constant plus a homogeneous quadratic function of δx and δy.

To determine whether $f(x, y)$ has a local minimum or maximum, or neither, let us first consider the general homogeneous quadratic function of two variables

$$Q(x,y) = Ax^2 + 2Bxy + Cy^2,$$

where A, B and C are constants. Note that $Q(x, y)$ vanishes at $(0, 0)$ and has a stationary point there. Simple examples are:

- (a) $x^2 + y^2$, which has a minimum at $(0, 0)$
- (b) $-x^2 - y^2$, which has a maximum at $(0, 0)$
- (c) $x^2 - y^2$, which has a saddle point at $(0, 0)$
- (d) xy, which has a saddle point at $(0, 0)$

More generally, we can complete the square in the form

$$Q(x,y) = \frac{1}{A}\left[(Ax+By)^2 + (AC-B^2)y^2\right],$$

by noting

$$\begin{aligned} Q(x,y) =& \frac{1}{A}\left[A^2x^2 + 2ABxy + ACy^2\right] \\ =& \frac{1}{A}\left[(Ax)^2 + 2(Ax)(By) + (By)^2 - (By)^2 + ACy^2\right] \\ =& \frac{1}{A}\left[(Ax+By)^2 + (AC-B^2)y^2\right] \end{aligned}$$

which is valid provided that $A \neq 0$. Note that $(Ax+By)$ and y can be varied independently.

- If $A > 0$ and $AC > B^2$ (which requires $C > 0$) then $Q(x,y) > 0$ for all $(x,y) \neq (0,0)$ and we have a minimum.

- If $A < 0$ and $AC > B^2$ (which requires $C < 0$) then $Q(x,y) < 0$ for all $(x,y) \neq (0,0)$ and we have a maximum.

- If $AC < B^2$ then $Q(x,y)$ can be either positive or negative and we have a saddle point.

Although this analysis fails when $A = 0$, similar conclusions can be drawn from the alternative way of completing the square,

$$Q(x, y) = \frac{1}{C}\left[(Bx + Cy)^2 + (AC - B^2)x^2\right],$$

which is valid provided that $C \neq 0$. (If $A = C = 0$ then $Q = 2Bxy$, which has a saddle point, unless $B = 0$ also.) We will not discuss all the special cases that are possible if A, C or $AC - B^2$ vanishes.

Applying this analysis to the approximation (1) for f, we see that

- f has a (local) minimum if $f_{xx}f_{yy} > f_{xy}^2$ with $f_{xx} > 0$ and $f_{yy} > 0$;
- f has a (local) maximum if $f_{xx}f_{yy} > f_{xy}^2$ with $f_{xx} < 0$ and $f_{yy} < 0$;
- f has a saddle point if $f_{xx}f_{yy} < f_{xy}^2$.

In special intermediate cases, higher-order terms in the Taylor expansion are needed to determine the nature of the stationary point. We will not discuss such cases.

For later reference (this will make more sense next term), the *Hessian matrix* is defined as the matrix of second derivatives,

$$\mathsf{H} = \begin{pmatrix} f_{xx} & f_{xy} \\ f_{yx} & f_{yy} \end{pmatrix}.$$

The symmetry of mixed partial derivatives implies that the Hessian matrix is symmetric. It therefore has real eigenvalues and orthogonal eigenvectors. A stationary point is a minimum if the eigenvalues of the Hessian matrix are both positive, a maximum if they are both negative, and a saddle point if one is negative and the other positive.

- To find the *global minimum* and *global maximum* of a function of two variables may be a more difficult problem. If the function is bounded and continuous, the global extrema either correspond to local extrema or occur on the boundary of the domain.

Example. A coal bunker is to be constructed on the side of a house. Assuming that it is a cuboid of given volume V, find the shape that minimizes the external surface area A.

Let the three sides be x, y and z, with x being measured horizontally in a direction perpendicular to the side of the house. Then $V = xyz$ and $A = xy + yz + 2xz$. We can eliminate z by writing $z = V/xy$ and can then consider

$$A(x, y) = xy + \frac{V}{x} + \frac{2V}{y}.$$

To find the stationary points of A, set the partial derivatives to zero:

$$\frac{\partial A}{\partial x} = y - \frac{V}{x^2} = 0$$

$$\frac{\partial A}{\partial y} = x - \frac{2V}{y^2} = 0.$$

Eliminate y to find $x = 2x^4/V$. Since $x \neq 0$, we find $V = 2x^3$ and so

$$x = \left(\frac{V}{2}\right)^{1/3}, \qquad y = \frac{V}{x^2} = 2x, \qquad z = \frac{V}{xy} = x.$$

The optimal shape is therefore $1 : 2 : 1$. To check that A is minimized by this solution, calculate the second derivatives:

$$A_{xx} = \frac{2V}{x^3} = 4$$

$$A_{yy} = \frac{4V}{y^3} = 1$$

$$A_{xy} = 1.$$

Thus $A_{xx}A_{yy} > A_{xy}^2$ with $A_{xx} > 0$ and $A_{yy} > 0$, so A has a local minimum as expected.

(In the next section we will see an alternative method for minimizing A subject to the constraint $V =$ constant.)

Example. Find and classify the stationary points of $f(x, y) = x^3 - 4x^2 + 2xy - y^2$. Sketch the contours of f.

For stationary points,

$$f_x = 3x^2 - 8x + 2y = 0$$

$$f_y = 2x - 2y = 0.$$

Thus $y = x$ and $3x^2 - 6x = 3x(x - 2) = 0$. So the stationary points are $(0, 0)$ and $(2, 2)$.

The second derivatives are

$$f_{xx} = 6x - 8 = \begin{cases} -8 & \text{at } (0,0) \\ 4 & \text{at } (2,2) \end{cases}$$

$$f_{yy} = -2$$

$$f_{xy} = 2.$$

Therefore $(0, 0)$ is a maximum because $f_{xx} f_{yy} > f_{xy}^2$ with $f_{xx} < 0$ and $f_{yy} < 0$. But $(2, 2)$ is a saddle point because $f_{xx} f_{yy} < 0$ there.

A way to discover the orientation of the saddle point is to note that the Taylor expansion to second order near $(2, 2)$ is

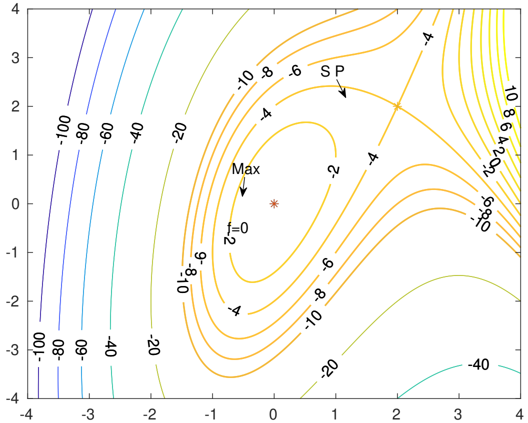
$$f \approx c + 2\,\delta x^2 + 2\,\delta x\,\delta y - \delta y^2,$$

where $c = f(2,2) = -4$, $\delta x = x - 2$ and $\delta y = y - 2$. So the contour lines that pass through the saddle point are given by $f = c$, i.e.

$$2\,\delta x^2 + 2\,\delta x\,\delta y - \delta y^2 \approx 0$$

$$-(\delta y - \delta x)^2 \approx -3\,\delta x^2$$

$$\delta y \approx (1 \pm \sqrt{3})\,\delta x.$$



2.4 Conditional stationary values

2.4.1 Two independent variables, one constraint

We have seen that the function $f(x, y)$ is stationary when $\boldsymbol{\nabla} f = \mathbf{0}$, which means that f does not change to first order when either x or y is varied. The stationary points and values found in this way are called *unconditional* or *unconstrained*.

We may be interested in a problem in which x and y cannot be varied independently, but are related by a *condition* or *constraint* of the form $g(x, y) = 0$, which means that the points (x, y) lie on a curve.

Example. Find the maximum value of $f(x, y) = xy$ on the unit circle $g(x, y) = x^2 + y^2 - 1 = 0$.

Method 1. Solve the constraint equation for y to find $y = s(1 - x^2)^{1/2}$, where $s = \pm 1$, then substitute to find $f = sx(1-x^2)^{1/2}$, which is a (double-valued) function of one variable. The derivative $\mathrm{d}f/\mathrm{d}x = s(1 - x^2)^{1/2} - sx^2(1 - x^2)^{-1/2} = s(1 - 2x^2)(1 - x^2)^{-1/2}$ vanishes at $x = \pm 1/\sqrt{2}$, where $f = \pm s/2$. Therefore the maximum of f is $1/2$ and occurs at $x = y = 1/\sqrt{2}$ and at $x = y = -1/\sqrt{2}$.

Method 2. Use a parametric representation $x = \cos\theta$, $y = \sin\theta$, $0 \leqslant \theta < 2\pi$ to satisfy the constraint. Then $f = \cos\theta \sin\theta = \frac{1}{2}\sin 2\theta$, which is a function of one variable. The derivative $\mathrm{d}f/\mathrm{d}\theta = \cos 2\theta$ vanishes at $\theta = \pi/4$, $3\pi/4$, $7\pi/4$ and $11\pi/4$. The first and third solutions give the maximum values $f = 1/2$ as above.

Either of these methods is reasonable, but they both rely on the ability to solve the constraint equation.

In more complicated cases this may not be practical, or it may lead to unwieldy algebra. A more sophisticated approach is the *method of Lagrange multipliers*.

Method 3. Suppose the maximum of f on the curve $g = 0$ is at (x_0, y_0). Consider the variation of $f(x, y)$ and $g(x, y)$ near this point. We have

$$\mathrm{d}f = f_x \,\mathrm{d}x + f_y \,\mathrm{d}y,$$

$$\mathrm{d}g = g_x \,\mathrm{d}x + g_y \,\mathrm{d}y,$$

where we recall that these differentials express the first-order variations. In order to stay on the curve $g = 0$, the displacements $\mathrm{d}x$ and $\mathrm{d}y$ are constrained by

$$g_x \,\mathrm{d}x + g_y \,\mathrm{d}y = 0.$$

This means that the vector displacement $\mathrm{d}\boldsymbol{x} = (\mathrm{d}x, \mathrm{d}y)$ is tangent to the curve $g = 0$. Solving this equation for either $\mathrm{d}x$ or $\mathrm{d}y$ and substituting into the expression for $\mathrm{d}f$, we find

$$\mathrm{d}f = (f_x g_y - f_y g_x)\frac{\mathrm{d}x}{g_y} = -(f_x g_y - f_y g_x)\frac{\mathrm{d}y}{g_x}.$$

(The first of these expressions fails when $g_y = 0$ and the second when $g_x = 0$, but in most cases at least one will work.) f is therefore stationary along the curve when

$$f_x g_y - f_y g_x = 0,$$

or, equivalently,

$$\frac{f_x}{g_x} = \frac{f_y}{g_y} = \lambda,$$

where λ is a number to be determined. This is equivalent to

$$(f_x, f_y) = \lambda(g_x, g_y), \qquad \text{i.e.} \quad \boldsymbol{\nabla} f = \lambda \boldsymbol{\nabla} g.$$

Now apply this method to the example. We have

$$f_x = y, \quad f_y = x, \quad g_x = 2x, \quad g_y = 2y,$$

so the equations $f_x = \lambda g_x$ and $f_y = \lambda g_y$ imply

$$y = 2\lambda x,$$

$$x = 2\lambda y.$$

We also have the constraint

$$x^2 + y^2 = 1,$$

which makes three equations in three unknowns (x, y, λ). The first two equations imply $x = 4\lambda^2 x$, so either $x = 0$ or $\lambda = \pm\frac{1}{2}$. $x = 0$ does not work, because then $y = 0$ and $x^2 + y^2 \neq 1$. If $\lambda = \frac{1}{2}$ then $y = x$ and we find $x = y = \pm 1/\sqrt{2}$, so $f = 1/2$. If $\lambda = -\frac{1}{2}$ then $y = -x$ and we find $x = -y = \pm 1/\sqrt{2}$, so $f = -1/2$. In this way we find all the conditional stationary points; the first two are the maxima.

2.4.2 Lagrange multipliers and Lagrangian function

To find the stationary points of $f(x, y)$ subject to the constraint $g(x, y) = 0$, solve the simultaneous equations

$$f_x = \lambda g_x, \qquad f_y = \lambda g_y, \qquad g = 0$$

for x, y and λ, where λ is a *Lagrange multiplier.*

It can be helpful to define the *Lagrangian function*

$$L(x, y, \lambda) = f(x, y) - \lambda g(x, y).$$

Then the method of Lagrange multipliers is equivalent to solving the equations

$$L_x = L_y = L_\lambda = 0,$$

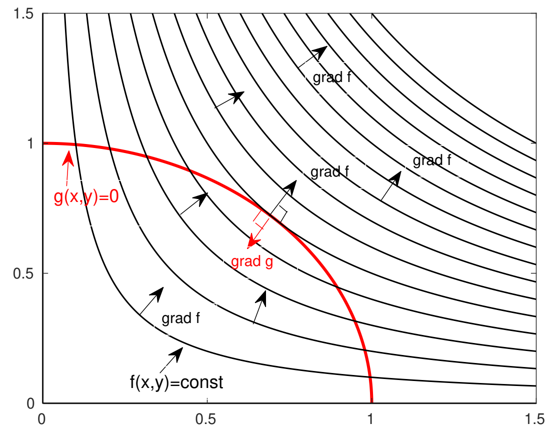
i.e. to finding the unconditional stationary values of the Lagrangian function.

Note:

- It is not really necessary to calculate the derivative L_λ because we already know the form of the constraint equation $g = 0$.
- Sometimes the Lagrangian $L = f - \lambda g$ is used to find the stationary points of f subject to the constraint $g = c$, where c is a non-zero constant. In that case we should solve the equations $L_x = L_y = 0$ and $g = c$ (not $L_\lambda = 0$).
- Sometimes $L = f + \lambda g$ is used instead of $L = f - \lambda g$. The result is the same.

2.4.3 Geometrical viewpoint

Consider a path going over a hill, but not visiting the summit. The highest point on the path is where the contour lines are parallel to the path. At the point the direction of steepest ascent is perpendicular to the path.



At each point, the vector ∇f is normal to the contour line $f =$ constant passing through that point.

This is because

$$\mathrm{d}f = (\boldsymbol{\nabla} f) \cdot \mathrm{d}\boldsymbol{x},$$

which means that the direction in which f does not change ($\mathrm{d}f = 0$) corresponds to a displacement $\mathrm{d}\boldsymbol{x}$ perpendicular to $\boldsymbol{\nabla} f$.

Similarly, the vector $\boldsymbol{\nabla} g$ is normal to the curve $g = 0$ at each point on it. When the constraint $g = 0$ is applied, displacements must be tangent to the curve and therefore satisfy $(\boldsymbol{\nabla} g) \cdot \mathrm{d}\boldsymbol{x} = 0$. For the conditional stationary point, we require that $\mathrm{d}f = (\boldsymbol{\nabla} f) \cdot \mathrm{d}\boldsymbol{x} = 0$ not for all $\mathrm{d}\boldsymbol{x}$, but only for those displacements such that $(\boldsymbol{\nabla} g) \cdot \mathrm{d}\boldsymbol{x} = 0$.

Therefore we require that $\boldsymbol{\nabla} f$ is parallel to $\boldsymbol{\nabla} g$, i.e. $\boldsymbol{\nabla} f = \lambda \boldsymbol{\nabla} g$.

2.4.4 More than two independent variables, one constraint

A similar method can be applied to functions of more than two variables, as in the following example. Note that the constraint equation $g = 0$ confines us to a surface rather than a curve.

Example. Minimize $xy + z$ subject to the constraint $x^2 + y^2 + z^2 = 1$. Let $f(x, y, z) = xy + z$ and $g(x, y, z) = x^2 + y^2 + z^2 - 1$. Form the Lagrangian function

$$L = f - \lambda g = xy + z - \lambda(x^2 + y^2 + z^2 - 1),$$

where λ is a Lagrange multiplier. Then seek unconditional stationary values of L:

$$L_x = y - 2\lambda x = 0,$$

$$L_y = x - 2\lambda y = 0,$$

$$L_z = 1 - 2\lambda z = 0,$$

$$L_\lambda = -(x^2 + y^2 + z^2 - 1) = 0.$$

As in the previous example, the first two equations imply either $x = y = 0$ or $y = \pm x$ with $\lambda = \pm\frac{1}{2}$. If $x = y = 0$ then $z = \pm 1$ (and $\lambda = \pm\frac{1}{2}$) in which case $f = \pm 1$. If $y = \pm x$ and $\lambda = \pm\frac{1}{2}$ then $z = \pm 1$ and $x^2 + y^2 = 0$, which implies $x = y = 0$. In either case we find the stationary points $(0, 0, \pm 1)$ at which $f = \pm 1$. There is therefore a minimum of -1 at $(0, 0, -1)$.

Exercise: Verify this result by parametrizing the unit sphere using spherical polar coordinates and finding the stationary points of $f(\theta, \phi)$.

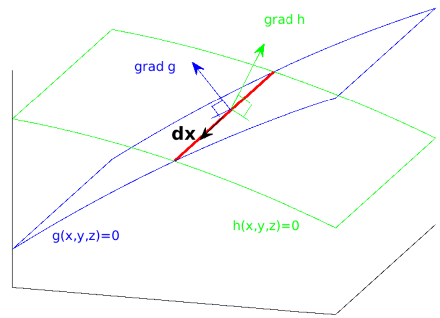
(Note that a stationary point of a function of three variables constrained to a surface could be a saddle point rather than a minimum or a maximum. It is not straightforward to determine the nature of the conditional stationary point in general using the method of Lagrange multipliers.)

2.4.5 More than one constraint

Consider the problem of two constraints in three dimensions. We seek the stationary values of $f(x, y, z)$ subject to the constraints $g(x, y, z) = 0$ and $h(x, y, z) = 0$. Each equation $g = 0$ and $h = 0$ defines a surface, so we are confined to the intersection of these surfaces, which is a curve. We have

$$
\begin{aligned}
\mathrm{d}f &= (\boldsymbol{\nabla} f) \cdot \mathrm{d}\boldsymbol{x}, \\
\mathrm{d}g &= (\boldsymbol{\nabla} g) \cdot \mathrm{d}\boldsymbol{x}, \\
\mathrm{d}h &= (\boldsymbol{\nabla} h) \cdot \mathrm{d}\boldsymbol{x}.
\end{aligned}
$$

Displacements are constrained by $\mathrm{d}g = \mathrm{d}h = 0$, which implies that $\mathrm{d}\boldsymbol{x}$ must be perpendicular to both



$\boldsymbol{\nabla} g$ and $\boldsymbol{\nabla} h$ and therefore parallel to $\boldsymbol{\nabla} g \times \boldsymbol{\nabla} h$. We require $\mathrm{d}f = 0$ for all such displacements. This is satisfied when

$$
\boldsymbol{\nabla} f = \lambda \boldsymbol{\nabla} g + \mu \boldsymbol{\nabla} h
$$

for some numbers λ and μ to be determined.

There is therefore one Lagrange multiplier for each constraint.
Equivalently, we can seek unconditional stationary values of the Lagrangian function

$$L(x, y, z, \lambda, \mu) = f(x, y, z) - \lambda g(x, y, z) - \mu h(x, y, z).$$

Example. Maximize $x + y + z$ subject to the constraints $x^2 + y^2 + z^2 = 1$ and $lx + my + nz = 0$.
Form the Lagrangian function

$$\begin{aligned} L &= f - \lambda g - \mu h \\ &= x + y + z - \lambda(x^2 + y^2 + z^2 - 1) - \mu(lx + my + nz), \end{aligned}$$

where λ and μ are Lagrange multipliers. Then seek unconditional stationary values of L:

$$\begin{aligned} L_x &= 1 - 2\lambda x - \mu l = 0, \\ L_y &= 1 - 2\lambda y - \mu m = 0, \\ L_z &= 1 - 2\lambda z - \mu n = 0, \\ L_\lambda &= -(x^2 + y^2 + z^2 - 1) = 0, \\ L_\mu &= -(lx + my + nz) = 0. \end{aligned}$$

The first three equations imply

$$(x, y, z) = \frac{1}{2\lambda}(1 - \mu l, 1 - \mu m, 1 - \mu n)$$

and so

$$f = \frac{3 - \mu(l + m + n)}{2\lambda}.$$

The fifth equation gives

$$l(1 - \mu l) + m(1 - \mu m) + n(1 - \mu n) = 0$$

$$\mu = \frac{l + m + n}{l^2 + m^2 + n^2}.$$

Finally, the fourth equation gives

$$(1 - \mu l)^2 + (1 - \mu m)^2 + (1 - \mu n)^2 = 4\lambda^2$$

$$\mu^2(l^2 + m^2 + n^2) - 2\mu(l + m + n) + 3 = 4\lambda^2.$$

Substitute for μ:

$$-\frac{(l + m + n)^2}{l^2 + m^2 + n^2} + 3 = 4\lambda^2$$

$$\lambda = \pm\frac{1}{2}\left[3 - \frac{(l + m + n)^2}{l^2 + m^2 + n^2}\right]^{1/2}.$$

Thus

$$f = \pm\left[3 - \frac{(l + m + n)^2}{l^2 + m^2 + n^2}\right]^{1/2}.$$

The maximum value is obtained by taking the + sign.

2.4.6 The Boltzmann distribution

This classic example of maximization subject to constraints comes from statistical mechanics.

Suppose we have a system consisting of a very large number of particles. Each particle occupies one of n discrete states, labelled by the index i. There is no limit on the number of particles N_i that can occupy state i. The energy of each particle in state i is E_i.

(An example of such a system is a gas in a box. The states are discrete as a result of quantum mechanics. The de Broglie wavelength of a particle has to equal one of a set of special values so that it can fit into the box in the form of a standing wave. There are many more such states available for particles of shorter wavelength, and therefore higher energy.)

The total number of particles is

$$N = \sum_{i=1}^{n} N_i.$$

The total energy of the system is

$$E = \sum_{i=1}^{n} N_i E_i.$$

The *distribution* of particles among states is described by the numbers $(N_1, N_2, \ldots, N_n)$. A given distribution $(N_1, N_2, \ldots, N_n)$ can be achieved in many different ways. The number of ways is in fact

$$W = \frac{N!}{N_1!N_2! \cdots N_n!}.$$

This is just the number of different ways of distributing N distinguishable objects between n boxes such that box i contains N_i objects. $N!$ is the number of ways of ordering all N objects, while the division by each $N_i!$ corrects for overcounting as the ordering within each box is unimportant.

W is the number of ways to distribute particles. It characterises probability of a realisation of a given state $(N_1, N_2, \ldots, N_n)$

(The assumption of distinguishable particles leads to *Maxwell–Boltzmann statistics*. The fact that particles are really indistinguishable, and fall into two categories called fermions and bosons, leads to different results, which are explored to some extent in Example Sheet 2, Question 21.)

It is argued in statistical mechanics that each permutation is equally probable, so the distribution that occurs in nature is the one with the largest value of W. This can be found by maximizing the function $W(N_1, N_2, \ldots, N_n)$ with respect to the variables $(N_1, N_2, \ldots, N_n)$. (When N is very large it turns out that the maximum is extremely sharp.)

It is easier to maximize the quantity

$$\ln W = \ln(N!) - \sum_{i=1}^{n} \ln(N_i!).$$

(The *entropy* is $S = k \ln W$, where k is Boltzmann's constant. Therefore we are finding the distribution of maximum entropy.)

If the system is isolated then we should maximize $\ln W$ subject to the constraints $N = \hat{N} =$ constant and $E = \hat{E} =$ constant, because the total number of particles and the total energy are fixed.

We therefore seek the stationary points of the Lagrangian function

$$
\begin{aligned}
L &= \ln W - \alpha(N - \hat{N}) - \beta(E - \hat{E}) \\
&= \ln(N!) - \sum_{i=1}^{n} \ln(N_i!) - \alpha\left(\sum_{i=1}^{n} N_i - \hat{N}\right) - \beta\left(\sum_{i=1}^{n} N_i E_i - \hat{E}\right),
\end{aligned}
$$

where α and β are Lagrange multipliers.

(Although $\hat{N}$ is just the fixed value of N, it is important that N is here regarded as a function of the variables $(N_1, N_2, \ldots, N_n)$ while $\hat{N}$ is a constant. Similarly for E and $\hat{E}$.)

In order to differentiate L, we make use of Stirling's approximation (see last term's lectures),

$$
x! \approx \sqrt{2\pi x}\; x^x\, \mathrm{e}^{-x},
$$

valid for $x \gg 1$. This implies

$$
\ln(x!) \approx x \ln x - x + \tfrac{1}{2}\ln(2\pi x)
$$

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}x}\ln(x!) &\approx \ln x + \frac{1}{2x} \\
&\approx \ln x \qquad \text{for} \quad x \gg 1.
\end{aligned}
$$

Applying this approximation to $N!$ and $N_i!$ for $N \gg 1$ and $N_i \gg 1$, we find

$$\frac{\partial L}{\partial N_i} = \ln N - \ln N_i - \alpha - \beta E_i,$$

where we have used $\partial N/\partial N_i = 1$ to obtain the first term. The stationary point of L therefore occurs where

$$\ln N - \ln N_i - \alpha - \beta E_i = 0$$

$$N_i = N\,\mathrm{e}^{-\alpha}\,\mathrm{e}^{-\beta E_i}.$$

This result is the *Boltzmann distribution*. Physical reasoning leads to $\beta = 1/(kT)$, where T is the temperature. Since $\beta > 0$, states of higher energy are less occupied.

The value of α (or $\mathrm{e}^{-\alpha}$) can be determined from the constraint

$$N = \sum_{i=1}^{n} N_i = N\,\mathrm{e}^{-\alpha} \sum_{i=1}^{n} \mathrm{e}^{-\beta E_i},$$

which implies

$$N_i = \frac{N\,\mathrm{e}^{-\beta E_i}}{\sum_{j=1}^{n} \mathrm{e}^{-\beta E_j}}.$$

The value of β (and therefore the temperature of the system) is determined by the second constraint, which is the total energy of the system.

Note that the Boltzmann distribution does not predict integer values of N_i. That is because we have treated the occupation numbers N_i at several stages as large real numbers rather than integers.

The Boltzmann distribution is often discussed with *degenerate states*. This situation occurs when we label the states according to their energy, but multiple states share the same energy level. The number of states sharing the energy level E_i is the *degeneracy* g_i. If N_i now denotes the combined occupation number of these degenerate states, then

$$N_i = N g_i \, \mathrm{e}^{-\alpha} \, \mathrm{e}^{-\beta E_i} = \frac{N g_i \, \mathrm{e}^{-\beta E_i}}{\sum_{j=1}^{n} g_j \, \mathrm{e}^{-\beta E_j}}.$$

This is identical to the previous result but with a different method of counting states.