Lecture-06-Partial-differentiation

Warm-up exercises

1.	$y = (2x + 6)^{1/2}$	$y' =$
2.	$y = (x^3 + 6)^{5/2}$	$y' =$
3.	$y = \dfrac{2x^2}{2 - x}$	$y' =$
4.	$y = e^x$	$y' =$
5.	$y = \sin(3x^2)$	$y' =$
6.	$\log 10$	$=$
7.	$\log A - \log A^2$	$=$
8.	$\log \dfrac{N}{2} - \log \dfrac{N}{20}$	$=$
9.	$\log_\pi \pi$	$=$
10.	$\dfrac{64 - 1}{3}$	$=$

11. Approximately what weight of Na_2CO_3 do I need to make up 100μl of a 2.5 M solution?

For you:

Answer to Week 3 challenge. The camel can travel 153.333 miles into the desert.

- Camel sets off with 100 bananas and goes 20 miles, eating 20 on way out, leaving 60 at the 20 mile post and eating 20 on the way back to base.
- She repeats this trip. Now has 120 at bananas at the 20 mile post.
- She goes there for a 3rd time and now has 200 bananas at 20 mile post. Since there are no bananas left at the starting point there is no point returning. Instead she wants to setup a cache of bananas as far into the desert as she can whilst leaving the maximum load (100) at mile 20. Hence she goes 33.333 miles, eating 33.333 on the way there and back and leaving 33.333 bananas there.
- Finally she loads up with the remaining 100 bananas at mile 20, walks another 33.3 miles, eating 33.3 bananas on the way, tops up her load to 100 bananas and then walks into the desert for another 100 miles.

Hence she has travelled 20 + 33.3 + 100 = 153.33 miles. Can you come up with a general solution for when she can carry r bananas and has n at the starting point?

Natural logarithms (cont.)

Can we differentiate $\ln x$?

$$\begin{aligned} y &= \ln x && \text{exponentiate both sides} \\ e^y &= x && \text{using the chain rule to differentiate the LHS} \\ e^y \frac{dy}{dx} &= 1 \\ \frac{dy}{dx} &= \frac{1}{e^y} \\ &= \frac{1}{x} \end{aligned}$$

In summary

$$\boxed{\frac{d}{dx}(\ln(x)) = \frac{1}{x}}$$

This is an IMPORTANT result!

Remember also that, by definition,

$$\boxed{\frac{d}{dx}(e^x) = e^x}$$

Let's put these into practice and differentiate some example functions

Example 1

$$y = x^2 e^x$$

This is a PRODUCT of two functions so we can apply the product rule to differentiate it.

$$\frac{d}{dx}(f.g) = f'g + fg'$$

Write out f and g separately and differentiate each

$$\begin{aligned} f(x) &= x^2 & f'(x) &= 2x \\ g(x) &= e^x & g'(x) &= e^x \end{aligned}$$

Now we can differentiate the function

$$
\begin{aligned}
y &= x^2 e^x \\
\frac{dy}{dx} &= 2x.e^x + x^2.e^x \\
&= xe^x(2+x)
\end{aligned}
$$

Example 2

$$y = \frac{e^x}{x}$$

This is the QUOTIENT of two functions so we can apply the quotient rule. (or, remember we can always apply the product rule as long as we correctly define both functions so they are a product).

$$\frac{d}{dx}\left(\frac{f}{g}\right) = \frac{gf' - fg'}{g^2}$$

Write out f and g separately and differentiate each

$$
\begin{aligned}
f(x) &= e^x & \qquad f'(x) &= e^x \\
g(x) &= x & \qquad g'(x) &= 1
\end{aligned}
$$

Now we can differentiate the function

$$
\begin{aligned}
y &= \frac{e^x}{x} \\
\frac{dy}{dx} &= \frac{x.e^x - e^x.1}{x^2} \\
&= \frac{e^x(x-1)}{x^2}
\end{aligned}
$$

Example 3

$$y = e^{x^2}$$

This is a function applied to a function and so we must use the CHAIN RULE. Swapping to Leibniz notation for clarity

$$\frac{d}{dx}(f(g(x)) = \frac{df}{dg} \times \frac{dg}{dx}$$

Write out f and g separately and differentiate each with respect to the correct variable as specified above

$$
\begin{aligned}
g(x) &= x^2 & \qquad \frac{dg}{dx} &= 2x \\
f(g) &= e^g & \qquad \frac{df}{dg} &= e^g
\end{aligned}
$$

Hence

$$\begin{aligned}\frac{dy}{dx} &= e^g.2x \\ &= e^{x^2}.2x \\ &= 2xe^{x^2}\end{aligned}$$

Thought:

Differentiating complex functions involving the exponential function is often easier than say, a polynomial, because by definition it is the only function that when differentiated yields itself.

Example 4

$$y = e^{ax}$$

Again we must use the CHAIN RULE.

Write out f and g separately and differentiate each with respect to the correct variable

$$g(x) = ax \qquad \frac{dg}{dx} = a$$

$$f(g) = e^v \qquad \frac{df}{dg} = e^g$$

Hence

$$\begin{aligned}\frac{dy}{dx} &= e^g.a \\ &= e^{ax}.a \\ &= ae^{ax}\end{aligned}$$

Example 5

$$y = \ln(a - x)^2$$

We can first simplify this a little using a log law (see L03) and then differentiate using the CHAIN RULE.

$$y = 2\ln(a - x)$$

As usual, write out f and g separately and differentiate each with respect to the correct variable (notice I am keeping the scalar factor 2 separate but I must remember to put it into the final expression!)

$$g(x) = a - x \qquad \frac{dg}{dx} = -1$$

$$f(g) = \ln g \qquad \frac{df}{dg} = \frac{1}{g}$$

Hence

$$\begin{aligned} \frac{dy}{dx} &= 2.\frac{1}{g}. - 1 \\ &= -\frac{2}{a - x} \end{aligned}$$

Example 6 How about this?

$$y = 2xe^{x^2}$$

We need to use the PRODUCT and the CHAIN RULEs to differentiate this!

$$y = f(x).g(j(x))$$

Apply the PRODUCT rule first..

$$\frac{d}{dx}(2xe^{x^2}) = 2e^{x^2} + 2x.\frac{d}{dx}(e^{x^2})$$

But from Example 3 above we know that

$$\frac{d}{dx}(e^{x^2}) = 2xe^{x^2}$$

Hence

$$\begin{aligned} \frac{d}{dx}(2xe^{x^2}) &= 2e^{x^2} + 2x.2xe^{x^2} \\ &= 2e^{x^2}(1 + 2x^2) \end{aligned}$$

The Binomial Theorem and the exponential function

The Binomial Theorem let's us rewrite the term in brackets below as a sum of terms in x

$$\boxed{(1 + x)^n = 1 + \frac{n}{1!}x + \frac{n(n-1)}{2!}x^2 + \frac{n(n-1)(n-2)}{3!}x^3 + \dots}$$

where the exclamation mark in e.g. 2! means 'factorial', which is easiest to show with examples.

$$
\begin{aligned}
1! &= 1 \\
2! &= 2 \times 1 = 2 \\
3! &= 3 \times 2 \times 1 = 6 \\
4! &= 4 \times 3 \times 2 \times 1 = 24
\end{aligned}
$$

The exponential function can be written using limits as

$$e^X = \lim_{n \to \infty} \left[1 + \frac{X}{n}\right]^n$$

but if we substitute $x = \frac{X}{n}$ into the Binomial theorem and use it to expand the above we get

$$e^X = \lim_{n \to \infty} \left(1 + \frac{n}{1!n} X + \frac{n(n-1)}{2!n^2} X^2 + \frac{n(n-1)(n-2)}{3!n^3} X^3 + \dots\right)$$

which when we take the limit becomes

$$e^X = 1 + X + \frac{X^2}{2!} + \frac{X^3}{3!} + \dots + \frac{X^N}{N!}$$

This is an algorithm for calculating e^x: given a value of x you can keep adding successive terms until you reach the accuracy (number of significant figures!) you need. For example, consider $x = 1$

$$
\begin{aligned}
e &= 1 + 1 + \frac{1}{2} + \frac{1}{6} + \frac{1}{24} + \frac{1}{120} + \frac{1}{720} \\
&= 2.718 \quad (3.\text{s.f})
\end{aligned}
$$

Since we have also expressed e^x as a series of polynomials and we know how to differentiate x^n, this gives us a way of 'proving' what the differential of e^x is

$$
\begin{aligned}
\frac{d}{dx}(e^x) &= 0 + 1 + \frac{2x}{2!} + \frac{3x^2}{3!} + \frac{4x^3}{4!} + \dots \\
&= 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots \\
&= e^x
\end{aligned}
$$

Partial Differentiation

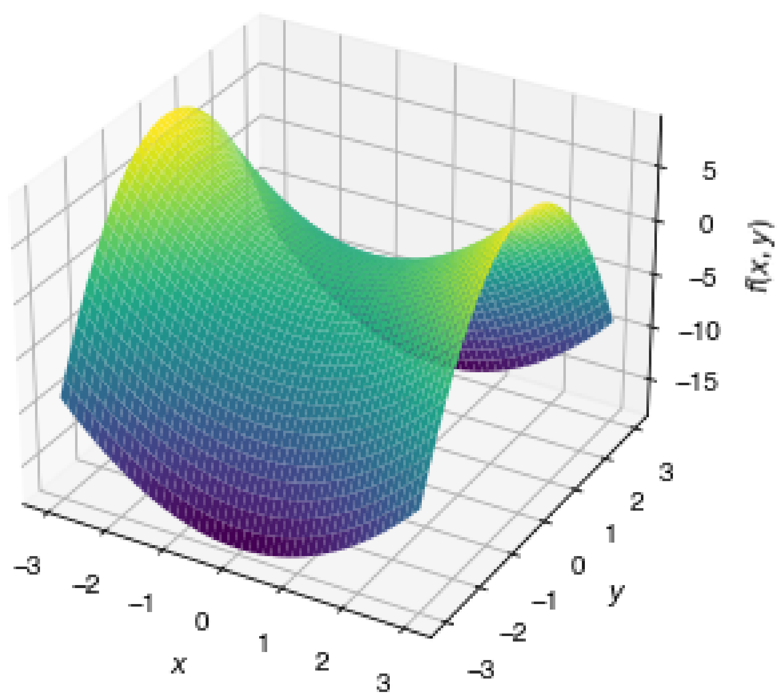
So far, we've only considered how to calculate the gradient function ($f'(x)$) of a function ($f(x)$) which has only a single variable, e.g. x.

Graphically, this is equivalent to plotting $f(x)$ against x for some function and then computing the gradient function $f'(x)$ that tells us the slope of the line at any value of x.

What about if our function has TWO (or more) variables e.g. $f(x, y)$? For example

$$f(x, y) = x^2 - 2y^2$$

This function is sketched below and forms a 'saddle'.



Asking "what is the gradient at (1,1)?" is meaningless because it is a SURFACE i.e. has more than one dimension. Instead, we have to describe the local curvature by the gradients of TWO tangents that are orthogonal (at right-angles) to one another i.e.

> What are the gradients of the two tangents to the function at (1,1) where one is parallel to the x-axis and the other is parallel to the y-axis?

Imagine yourself standing on a hill which has the above shape? How you describe the slope will depend on which way you are facing!

By analogy, we can't 'just' differentiate $f(x, y)$. We have to specify along which direction we are considering. For example, if we want to find out the gradient function of the tangents parallel to the x-axis, we have to hold y constant.

This concept of differentiating a multi-variate function w.r.t one variable whilst holding the other (or others) constant is called PARTIAL DIFFERENTIATION.

Notation

The differential of $f(x, y)$ w.r.t x whilst holding y constant is written as

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

Where the LHS is the Leibnizian form and the RHS is Newtonian. Note that on the LHS are NOT 'd's or'δ's. The subscript y outside the bracket tells you which variable (or variables) you are considering to be constant.

Since our f is a function of two independent variables, x and y, we need a second differential at right-angles to the first to describe the local curvature. Here this is

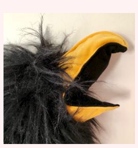
$$\left(\frac{\partial f}{\partial y}\right)_x = f_y$$

Example 1

$$\begin{aligned} f(x, y) &= x^2 - 2y^2 \\ f_x &= 2x \\ f_y &= -4y \end{aligned}$$

The trick is to remember that when you are differentiating w.r.t. x, you treat y as if it were a constant i.e. just like you would a number. Then you have to 'swap' the roles of the variables. This can easily lead to confusion!

Common misconception:



When calculating the partial differentials of a multi-variate function, don't forget which variable(s) you are holding constant and which you are differentiating with respect to! It is very easy to think we are always differentiating with respect to x but sometimes it is constant.

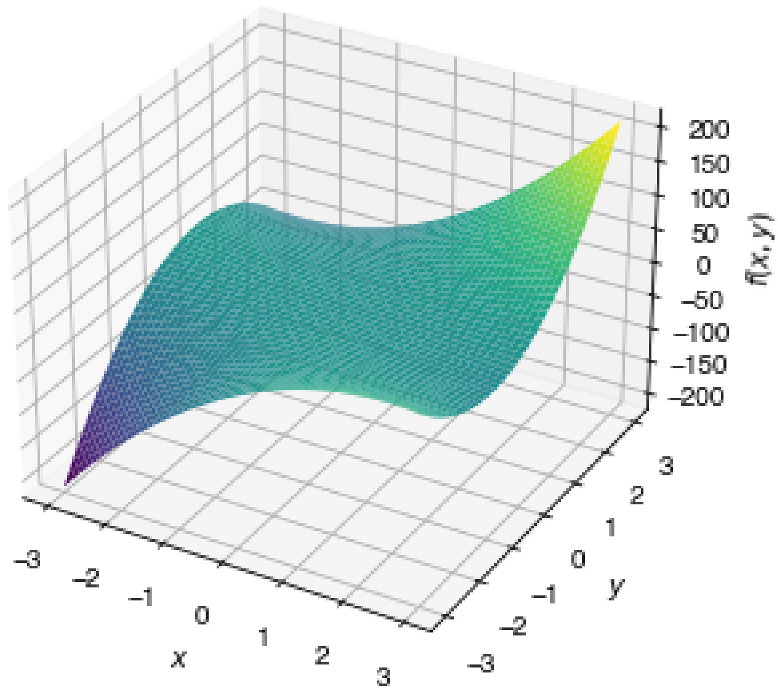
Example 2

Let's make it a bit more complex:

$$f(x, y) = 3x^2y + 5xy^2$$

Unlike the previous example where each term involved either x OR y, both terms here involve x AND y. We still follow the procedure, but the scope for confusion is greater here!

Unsurprisingly the surface is more complex as well:



$$
\begin{aligned}
f(x,y) &= 3x^2y + 5xy^2 \\
f_x &= 6xy + 5y^2 \\
f_y &= 3x^2 + 10xy
\end{aligned}
$$

Example 3

Finally we can use other functions too, such as trig functions.

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

We will approach differentiation in the same way.

$$
\begin{aligned}
f_x &= 2\sin x \cos x \cos y + \frac{1}{y^2} \\
f_y &= \sin^2 x.(-\sin y) - \frac{2x}{y^3} \\
&= -\sin^2 x \sin y - \frac{2x}{y^3}
\end{aligned}
$$

Example 4 - Ideal Gas Law

This states that

$$pV = nRT$$

where p is the pressure, V is the volume, n is the number of moles of gas, T is the temperature and R is Rydberg's gas constant (8.314 J/K/mol). Rearranging

$$p = \frac{nRT}{V}$$

Formally, p is a function of both V and T (assuming the amount of gas, n, remains constant), and hence if we want to differentiate this expression we will get two partial differentials e.g.

$$\begin{aligned}
\left(\frac{\partial p}{\partial V}\right)_T &= \frac{\partial}{\partial V}\left(\frac{nRT}{V}\right) \\
&= \frac{\partial}{\partial V}\left(nRT.V^{-1}\right) \\
&= nRT\frac{\partial}{\partial V}\left(V^{-1}\right) \\
&= nRT(-V^{-2}) \\
&= -\frac{nRT}{V^2}
\end{aligned}$$

So, the pressure of an ideal gas falls with an increase in volume when the temperature is constant as this is *always* negative.

$$\begin{aligned}
\left(\frac{\partial p}{\partial T}\right)_V &= \frac{\partial}{\partial T}\left(\frac{nRT}{V}\right) \\
&= \frac{\partial}{\partial T}\left(\frac{nR}{V}.T\right) \\
&= \frac{nR}{V}\frac{\partial}{\partial T}(T) \\
&= \frac{nR}{V}
\end{aligned}$$

This is always positive, and therefore the pressure of an ideal gas always increases if the temperature is increased.

Higher partial derivatives

Just like before, we can calculate the differential of a differential, the complexity being at each stage we can choose which variable is being held constant and with we are differentiating w.r.t!

$$f_{xx} = \frac{\partial^2 f}{\partial x^2}$$
$$f_{yy} = \frac{\partial^2 f}{\partial y^2}$$

Note that we have been lazy here and not written explicitly that in these that y is held constant in the first and x in the second as it can be assumed.

The 'cross-terms' are a different matter!

$$f_{yx} = \frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial x} f_y = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right)_x$$
$$f_{xy} = \frac{\partial^2 f}{\partial y \partial x} = \frac{\partial}{\partial y} f_x = \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right)_y$$

This makes it clear that f_{xy} means "first differentiate w.r.t x (holding y constant) and then differentiate w.r.t. y (holding x constant)".

We find that the operators $\frac{\partial}{\partial x}$ and $\frac{\partial}{\partial y}$ are COMMUTATIVE i.e.

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

Back to Example 2

Let's calculate the higher derivatives for this function. Before we had

$$f(x, y) = 3x^2 y + 5xy^2$$
$$f_x = 6xy + 5y^2$$
$$f_y = 3x^2 + 10xy$$

Now:

$$f_{xx} = 6y$$
$$f_{yy} = 10x$$
$$f_{xy} = 6x + 10y$$
$$f_{yx} = 6x + 10y$$

And $f_{xy} = f_{yx}$ as expected!

Function of a function

The CHAIN RULE for a function with 1 independent variable, x, is

$$\frac{df}{dx} = \frac{df}{du}.\frac{du}{dx}$$

where $f = f(u)$ and $u = u(x)$.

Now we can extend this to 2 (or more) variables. If $f = f(u)$ and $u = u(x, y)$, then

$$\begin{aligned} f_x &= \left(\frac{\partial f}{\partial x}\right)_y & &= \frac{df}{du}\left(\frac{\partial u}{\partial x}\right)_y \\ f_y &= \left(\frac{\partial f}{\partial y}\right)_x & &= \frac{df}{du}\left(\frac{\partial u}{\partial y}\right)_x \end{aligned}$$

Example 5

Our function is

$$f(x, y) = \frac{1}{x^2 y} \exp\left(\frac{1}{2x^2 y}\right)$$

put $u = \frac{1}{2x^2y}$ so

$$\begin{aligned} f &= 2ue^u & &\text{use product rule} \\ \frac{df}{du} &= 2e^u + 2ue^u \\ &= 2e^u(1 + u) \end{aligned}$$

So now we have $\frac{df}{du}$, but what need $\left(\frac{\partial u}{\partial x}\right)_y$ and $\left(\frac{\partial u}{\partial y}\right)_x$ so we can calculate f_x and f_y.

$$\begin{aligned} u &= \frac{1}{2x^2y} \\ \left(\frac{\partial u}{\partial x}\right)_y &= \frac{-2}{2x^3y} \\ &= \frac{-1}{x^3y} \\ \left(\frac{\partial u}{\partial y}\right)_x &= \frac{-1}{2x^2y^2} \end{aligned}$$

Hence we've got everything we need now, and just need to substitute back into our chain rule for partial differentials

$$
\begin{aligned}
f_x &= \frac{df}{du}\left(\frac{\partial u}{\partial x}\right)_y \\
&= 2e^u(1+u).\frac{-1}{x^3y} \\
&= \frac{-2}{x^3y}\left(1+\frac{1}{2x^2y}\right)\exp\left(\frac{1}{2x^2y}\right)
\end{aligned}
$$

We could combine the terms in the bracket, but I don't think it will look any simpler.

$$
\begin{aligned}
f_y &= \frac{df}{du}\left(\frac{\partial u}{\partial y}\right)_x \\
&= 2e^u(1+u).\frac{-1}{2x^2y^2} \\
&= -\frac{1}{x^2y^2}\left(1+\frac{1}{2x^2y}\right)\exp\left(\frac{1}{2x^2y}\right)
\end{aligned}
$$

Maxwell's relations

You will encounter these in Thermodynamics and they are partial differentials. If you are not familiar with the notation they are confusing!

$$
\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial P}{\partial S}\right)_V = \frac{\partial^2 U}{\partial S \partial V}
$$

where S is entropy, U is the internal energy, T is temperature, P is pressure and V volume. The LHS is the rate at which temperature changes when the volume is increased when the entropy is held constant.

Other relations are

$$
\left(\frac{\partial T}{\partial P}\right)_S = \left(\frac{\partial V}{\partial S}\right)_P = \frac{\partial^2 H}{\partial S \partial P}
$$

and

$$
\left(\frac{\partial S}{\partial P}\right)_T = \left(\frac{\partial V}{\partial T}\right)_P = \frac{\partial^2 G}{\partial T \partial P}
$$

where H is the enthalpy and G is the Gibbs free energy. Now that you can 'read' partial differentials you can hopefully translate these symbols and understand the biophysics behind them in your other courses. In other words, you'll look at them and think "oh, those are just partial differentials", rather than "what on earth does that mean?".

For you:

Week 4 challenge. Who owns the fish? According to my information, this puzzle is attributed to Albert Einstein. He claimed that 98% of the world could not work it out (if they didn't use Google!). Can you? Please send answers to philip.fowler@ndm.ox.ac.uk before the start of week 4.

There are five houses in a row in five different colours. In each house lives a person from a different country. Each person drinks a certain drink, smokes a certain cigar and keeps a certain pet. No two people drink the same drink, smoke the same cigar or keep the same pet.

- The Brit lives in the red house.

- The Swede keeps dogs.
- The Dane drinks tea.
- The green house is on the left of the white house.
- The green house owner drinks coffee.
- The person who smokes Pall Mall rears birds.
- The owner of the yellow house smokes Dunhill.
- The man living in the house right in the centre drinks milk.
- The Norwegian lives in the first house.
- The man who smokes Blends lives next to the man who keeps cats.
- The man who keeps horses lives next to the one who smokes Dunhill.
- The man who smokes Bluemaster drinks beer.
- The German smokes Prince.
- The Norwegian lives next to the blue house.
- The man who smokes Blends has a neighbour who drinks water