Lecture-08-Integration-II

Warm-up exercises

1.	$y = e^{2x}$	$y' =$
2.	$y = \ln x$	$y' =$
3.	$y = \ln 5x$	$y' =$
4.	$\int_5^{50} 2.dx$	$=$
5.	$\int_2^4 3x.dx$	$=$
6.	$\int_1^2 4x^{-3}.dx$	$=$
7.	$\int_0^{\pi/2} \cos x.dx$	$=$
8.	$\int_1^e x^{-1}.dx$	$=$
9.	$\int x^{-1}.dx$	$=$
10.	$\int \cos 2x.dx$	$=$

11. What is the H^+ concentraion of a solution with a pH of 3?
12. What would I have to do to the solution to make it have a pH of 7?

Calculus (cont.)

Integration by substitution

Protocol

If we have an integral, I, that we can write as

$$I = \int f(g(x)).dx$$

then

1. Look at the integral and see if the differential of the bracketed function is outside the brackets. If so, then substitution is an appropriate strategy.
2. Decide on the function u for substitution, find $\frac{du}{dx}$ and thus its reciprocal, $\frac{dx}{du}$.
3. Substitute u into the integral, multiply the integral by dx/du and simplify by cancelling appropriate terms.
4. If it is a definite integral, replace the limits by u(lower limit) and u(upper limit).
5. Perform the integration.
6. Substitute for u in the result to that x is again the variable.
7. If it is a definite integral, put in the appropriate limits and simplify the result.
8. If it is an indefinite integral, don't forget the constant of integration!

'Expectation' values

The *weighted average* where the weight is the probability of the result having a certain value.

e.g. the expected value, $\bar{p}$ of throwing a six-sided die is

$$\begin{aligned}\bar{p} &= \frac{1}{6}\times 1+\frac{1}{6}\times 2+\frac{1}{6}\times 3+\frac{1}{6}\times 4+\frac{1}{6}\times 5+\frac{1}{6}\times 6\\ &= \frac{1}{6}\sum_{n=1}^{n=6} n\\ &= \frac{1}{6}(1+2+3+4+5+6)\\ &= \frac{21}{6}\\ &= 3.5\end{aligned}$$

We also call this the average value.

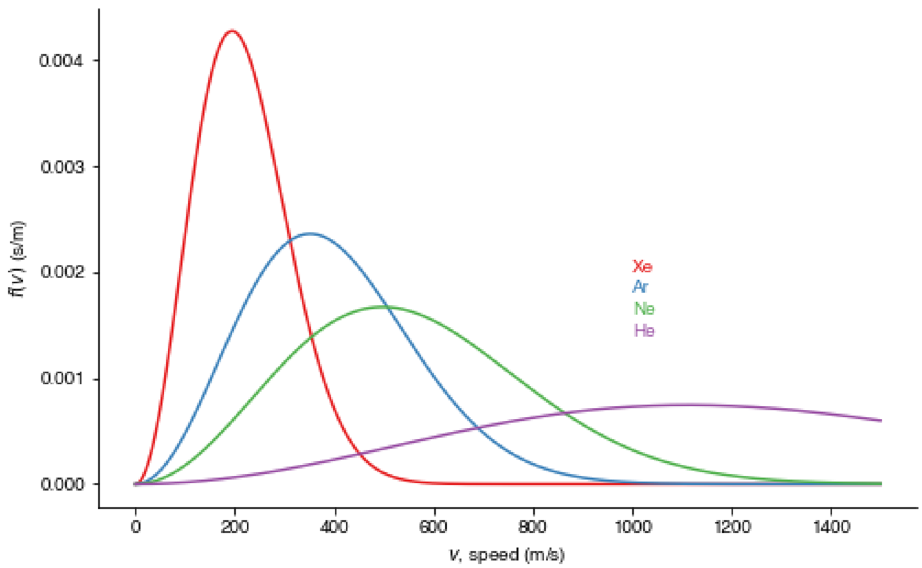
This was a *discreet* example (i.e. the numbers can only take whole values) hence the use of a *discreet* sum as signified by the $\sum$ symbol.

What is the expectation value of the speed of a molecule of gas?

The probability distribution for the speeds of molecules in an *ideal gas* is given by the Maxwell-Boltzmann distribuion

$$f(v) = 4\pi\left(\frac{m}{2\pi kT}\right)^{3/2} v^2 e^{-\frac{mv^2}{2kT}}$$

where v is the speed of the molecule, m is the mass of a molecule, T is the absolute temperature (K) and k is Boltzmann's constant (1.38×10^{-23}m^2 kg s^{-2} K^{-1}). It tells us how likely we are to find molecules with speed v, for example

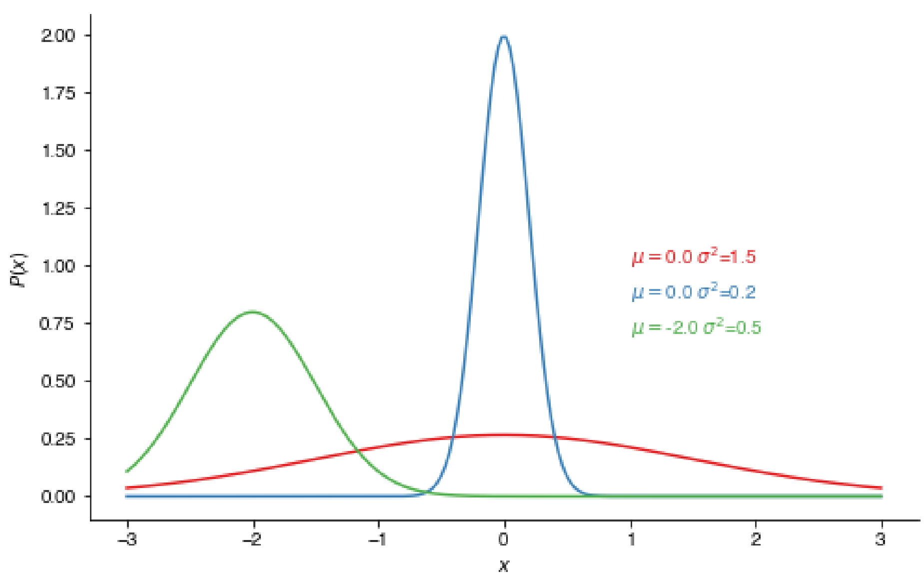


The Gaussian or 'normal' distribution

The 'exponential bit' in the Maxwell-Boltzmann equation is a Gaussian, i.e. looks like:

$$P(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2/2\sigma^2}$$

where μ is the *expectation value* of the variable x which has variance σ^2 (and hence standard deviation σ).



The expectation value, $\bar{v}$, is hence

$$\bar{v} = \int_0^\infty v.f(v).dv$$

which is going to be complex!

$$f(v) = 4\pi \left(\frac{m}{2\pi kT}\right)^{3/2} v^2 e^{-\frac{mv^2}{2kT}}$$

since the prefactor doesn't vary with x i.e. is constant once we've chosen the temperature and mass, let's call it Q.

$$Q = 4\pi \left(\frac{m}{2\pi kT}\right)^{3/2}$$

This lets us rewrite $f(v)$ as

$$f(v) = Qv^2 e^{-\frac{mv^2}{2kT}}$$

which at least looks a bit simpler. Hence the expectation value of the speed (average speed) is

$$\begin{aligned}\bar{v} &= \int_0^\infty Qv^3 e^{-\frac{mv^2}{2kT}}.dv \\ &= Q\int_0^\infty v^3 e^{-\frac{mv^2}{2kT}}.dv\end{aligned}$$

We can't do this *directly*, so because this looks like $\int f(g(v)).dv$ let's try *substituting*

$$\begin{aligned}z &= \frac{mv^2}{2kT} & v^2 &= \frac{2kTz}{m} \\ \frac{dz}{dv} &= \frac{m.2v}{2kT} \\ &= \frac{mv}{kT} \\ \frac{dv}{dz} &= \frac{kT}{mv}\end{aligned}$$

we've got what we need, let's make the substitution and see what happens

$$
\begin{aligned}
\bar{v} &= Q\int_{v=0}^{v=\infty} v^3 e^{-\frac{mv^2}{2kT}}.dv \\
&= Q\int_{z=0}^{z=\infty} v^3 \frac{kT}{mv} e^{-z}.dz \\
&= Q\int_{z=0}^{z=\infty} v^2 \frac{kT}{m} e^{-z}.dz && \text{substitute for last } v \\
&= Q\int_{z=0}^{z=\infty} \frac{2kTz}{m}\frac{kT}{m} e^{-z}.dz \\
&= 2Q\left(\frac{kT}{m}\right)^2 \int_{z=0}^{z=\infty} ze^{-z}.dz
\end{aligned}
$$

Whilst it feels like we are making progress, we STILL can't integrate the form $\int xe^{-x}.dx$. We need ANOTHER method

Integration by parts

Let's explore this new method then come back and solve our Maxwell-Boltzmann integral.

Recall the product rule for differentiation

$$
\begin{aligned}
\frac{d}{dx}(f(x)g(x)) &= f(x)\frac{dg(x)}{dx} + \frac{df(x)}{dx}g(x) \\
&= f(x)g'(x) + f'(x)g(x) && \text{integrate both sides w.r.t } x \text{ between } x=a \text{ and } x= \\
\int_a^b \frac{d}{dx}(f(x)g(x)).dx &= \int_a^b f(x)g'(x).dx + \int_a^b f'(x)g(x).dx \\
[f(x)g(x)]_a^b &= \int_a^b f(x)g'(x).dx + \int_a^b f'(x)g(x).dx && \text{rearran} \\
\int_a^b f(x)g'(x).dx &= [f(x)g(x)]_a^b - \int_a^b f'(x)g(x).dx
\end{aligned}
$$

You'll also see this written in the following forms which are all equivalent

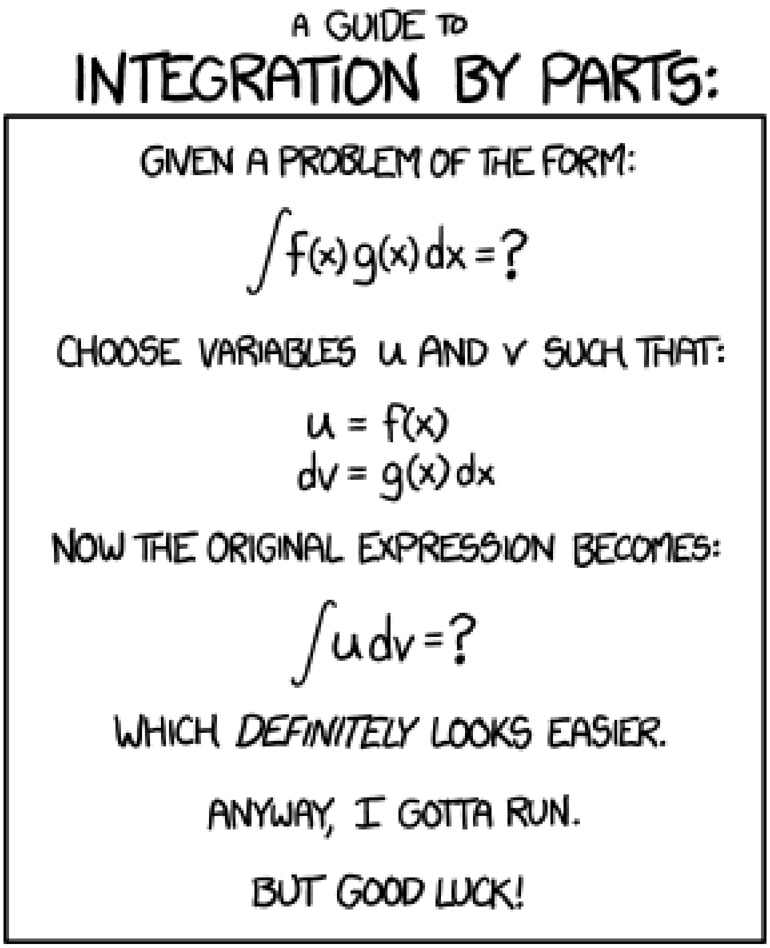
$$
\begin{aligned}
\int_a^b f.g'.dx &= [f.g]_a^b - \int_a^b f'.g.dx \\
\int_a^b u.\frac{dv}{dx}.dx &= [u.v]_a^b - \int_a^b \frac{du}{dx}.v.dx \\
\int_a^b u.v'.dx &= [u.v]_a^b - \int_a^b u'.v.dx
\end{aligned}
$$

where $f(x) \equiv f \equiv u$ and $g(x) \equiv g \equiv v$. I'll mostly use u and v. Hence our general result is

$$\boxed{\int_a^b u.v'.dx = [u.v]_a^b - \int_a^b u'.v.dx}$$

As ever, since we need to identify u and v and then calculate $\frac{du}{dx}$ and $\frac{dv}{dx}$ it really helps to make a TABLE.

So what? How does that help us? It let's us replace one integral with an evaulation and another integral? Or, as xkcd puts it:



The trick is to CHOOSE u and v such that after you've applied *integration by parts* the 'new' integral is simpler, and hopefully, doable.

The problem is that if you apply *integration by parts* where it is inappropriate, or you make the wrong choice of u and v, you will make it MORE complex not less.

Common misconception:

It is very easy to incorrectly choose u and v' when integrating by parts; if you do you will make the integral more complex rather than easier.

Example

$$\int_a^b x.\sqrt{x+1}.dx$$

Making the right choice

Choose

$$\begin{aligned} u &= x & u' &= 1 \\ v' &= \sqrt{x+1} & v &= \frac{2}{3}(x+1)^{3/2} \end{aligned}$$

Then we can apply *integration by parts*

$$\begin{aligned} \int_a^b x.\sqrt{x+1}.dx &= \left[x.\frac{2}{3}(x+1)^{3/2}\right]_a^b - \int_a^b \frac{2}{3}(x+1)^{3/2}.dx \\ &= \left[\frac{2}{3}x(x+1)^{3/2}\right]_a^b - \left[\frac{2}{3}.\frac{2}{5}(x+1)^{5/2}\right]_a^b \\ &= \left[\frac{2}{3}x(x+1)^{3/2} - \frac{4}{15}(x+1)^{5/2}\right]_a^b \end{aligned}$$

So that works! Notice how the integral on the RHS is simpler than what we started with which is what allowed us to do it.

Making the wrong choice

But what happens if we choose u and v' the 'other way round'

$$\begin{aligned} u &= \sqrt{x+1} & u' &= \frac{1}{2}(x+1)^{-1/2} \\ v' &= x & v &= \frac{1}{2}x^2 \end{aligned}$$

$$\begin{aligned}\int_a^b x.\sqrt{x+1}.dx &= \left[\sqrt{x+1}.\frac{1}{2}x^2\right]_a^b - \int_a^b \frac{1}{2}(x+1)^{-1/2}.\frac{1}{2}x^2.dx \\ &= \left[\frac{1}{2}x^2\sqrt{x+1}\right]_a^b - \frac{1}{4}\int_a^b \frac{x^2}{\sqrt{x+1}}.dx\end{aligned}$$

Our maths is correct; the LHS = RHS, but by incorrectly choosing u and v' we've swapped an integral we can't do for an integral we DEFINITELY can't do. Not helpful.

Usually the algebra does get more complicated and your lines get longer, but there comes a point where e.g. terms start to cancel or you can do an integral. If this doesn't happen and it just gets more and more complex then that is often a sign you've made a mistake. I call this 'algebra hell' and with practice you'll be able to instintively 'feel' when you've made a mistake. ("It should be getting better by now!")

What about when we have an indefinite integral?

In this case there will be no limits and we'll have to include a *constant of integration* every time we integrate.

$$\int x.\sqrt{x+1}.dx$$

Choose

$$\begin{aligned} u &= x & u' &= 1 \\ v' &= \sqrt{x+1} & v &= \frac{2}{3}(x+1)^{3/2} + c_1 \end{aligned}$$

Then we can apply *integration by parts*

$$\begin{aligned}\int_a^b x.\sqrt{x+1}.dx &= x.\left(\frac{2}{3}(x+1)^{3/2} + c_1\right) - \int_a^b \frac{2}{3}(x+1)^{3/2} + c_1.dx \\ &= \frac{2}{3}x(x+1)^{3/2} + c_1x - \left(\frac{2}{3}.\frac{2}{5}(x+1)^{5/2} + c_1x + c_2\right) \\ &= \frac{2}{3}x(x+1)^{3/2} - \frac{4}{15}(x+1)^{5/2} + c_2\end{aligned}$$

So it still works, but you need to be careful and consistent with your *constants of integration.*

For you:

Use integration by parts to integration this:

$$\int x \sin x . dx$$

$$u = \qquad\qquad u' =$$
$$v' = \qquad\qquad v =$$

$$\int_a^b u.v'.dx = [u.v]_a^b - \int_a^b u'.v.dx$$

Back to calculating the expectation value of the speed of a molecule of gas...

We want to integrate the form

$$\int_0^\infty ze^{-z}.dz$$

Apply *integration by parts*:

$$\int_a^b u.v'.dx = [u.v]_a^b - \int_a^b u'.v.dx$$

Choose u and v

$$u = z \qquad\qquad u' = 1$$
$$v' = e^{-z} \qquad\qquad v = -e^{-z}$$

$$\begin{aligned}
\int_0^\infty ze^{-z}.dz &= \left[-z.e^{-z}\right]_0^\infty - \int_0^\infty -1.e^{-z}.dz \\
&= \left[-z.e^{-z}\right]_0^\infty + \int_0^\infty e^{-z}.dz \\
&= \left[-z.e^{-z}\right]_0^\infty + \left[-e^{-z}\right]_0^\infty \\
&= \left[-z.e^{-z} - e^{-z}\right]_0^\infty \\
&= (0-0) - (0-1) \\
&= 1
\end{aligned}$$

Back to the Maxwell-Boltzmann..

$$\bar{v} = 2Q\left(\frac{kT}{m}\right)^2 \int_{z=0}^{z=\infty} ze^{-z}.dz$$

Woo. We've just shown that the integral is 1! So we can solve for the average (or expected) speed!

$$\bar{v} = 2Q\left(\frac{kT}{m}\right)^2$$

remember we grouped some constants together and called them Q, so let's substitute them back. Since $Q = 4\pi\left(\frac{m}{2\pi kT}\right)^{3/2}$

$$\bar{v} = 2 \times 4\pi\left(\frac{m}{2\pi kT}\right)^{3/2}\left(\frac{kT}{m}\right)^2$$

Let's simplify this:

$$\begin{aligned}\bar{v} &= 8\pi\left(\frac{1}{2\pi}\right)^{3/2}\left(\frac{kT}{m}\right)^{1/2} \\ &= \sqrt{\frac{8}{\pi}.\frac{kT}{m}}\end{aligned}$$

Let's check this makes sense. First, consider the *dimensions* of the constants k, T, m. We can cheat a bit since kT has units of energy so its dimensions are $[\mathrm{ML^2T^{-2}}]$ and mass has dimensions $[\mathrm{M}]$. Hence $\frac{kT}{m}$ has dimensions $[\mathrm{L^2T^{-2}}]$ but we are taking the square root, so the dimensions of the RHS (and hence the LHS) are $[\mathrm{LT^{-1}}]$, which is 'length per unit time' i.e. a speed!

Another way of checking is putting some values in and seeing if the values we get are reasonable. Let's calculate the average speed of air at room temperature. If we model air as nitrogen, then $m = 0.028$ kg/mol, or $m = 4.67 \times 10^{-26}$ kg. Boltzmann's constant $k = 1.38 \times 10^{-23}$ and $T = 298$ K. Putting all that together we estimate that the average speed is 473 m/s (3.s.f). Is that reasonable? Well we know that the speed of sound in air is 330 m/s (3 seconds gap between lightning and thunder means the storm is 1 km away) and so that is in the right range!

Tips for choosing u and v'

Look at the integrand and choose the first function in the last for u:

1. Log (e.g. $\ln x$)
2. Algebraic (e.g. x^2)
3. Trigonmetric (e.g. $\sin x$)
4. Exponetial (e.g. e^x)

We do the same for v' but this time we start at the bottom of the list and work our way UP.

An easy way of remembering this is to notice that the first letters spell out LATE.

$\boxed{\text{Hence for } u \text{ we chose the first function we encounter in LATE whilst for } v' \text{ use ETAL.}}$

The aim is to pick u and v' such that the new integral we get from applying *integration by parts* is simpler or no more complicated! If it is, we've probably made the wrong choice.

Integrating a logathrim

Consider

$$\int \ln x.dx$$

It is not obvious how we can do this! (We don't know any function that when differentiated yields $\ln x$). There is a trick, however, and that is to rewrite it as

$$\int 1.\ln x.dx$$

LATE suggests that we try $u = \ln x$ and $v' = 1$ so let's give that a go.

$$\begin{aligned} u &= \ln x & u' &= \frac{1}{x} \\ v' &= 1 & v &= x + c_1 \end{aligned}$$

$$\begin{aligned} \int 1.\ln x.dx &= (x + c_1)\ln x - \int (x + c_1).\frac{1}{x}.dx \\ &= x\ln x + c_1 \ln x - \int 1 + \frac{c_1}{x} dx \\ &= x\ln x + c_1 \ln x - x - c_1 \ln x + c_2 \\ &= x\ln x - x + c_2 \end{aligned}$$

Let's check this one by differentiating it. Notice that the first term is a product of two functions.

$$y = x\ln x + c_2$$

$$\begin{aligned} u &= x & u' &= 1 \\ v &= \ln x & v' &= \frac{1}{x} \end{aligned}$$

Hence,

$$\begin{aligned}\frac{dy}{dx} &= x.\frac{1}{x} + 1.\ln x - 1 \\ &= 1 + \ln x - 1 \\ &= \ln x\end{aligned}$$

So it it is correct. We could have considered the definite integral ($\int_a^b \ln x.dx$ which is a bit easier.

Partial fractions

How can we integrate?

$$\int \frac{1}{(2x+1)(x-5)}.dx$$

You will need to be able to integrate functions in this form in a few weeks when you consider rates.

What we need here is not another method of integrating, but a way of rewriting that expression as the sum of several terms, each of which we CAN integrate. Those terms are called PARTIAL FRACTIONS and we apply the METHOD OF UNDETERMINED COEFFICIENTS.

Since the denominator has two terms multipled together, we realise that we could rewrite the expression as the sum of two fractions

$$\frac{1}{(2x+1)(x-5)} = \frac{A}{2x+1} + \frac{B}{x-5}$$

where A and B are coefficients (constants). But how do we find A and B? The trick is to combine the two fractions on the RHS into a single fraction and then compare both sides.

$$\begin{aligned}\frac{1}{(2x+1)(x-5)} &= \frac{A}{2x+1} + \frac{B}{x-5} \\ &= \frac{A(x-5) + B(2x+1)}{(2x+1)(x-5)} \\ &= \frac{Ax - 5A + 2Bx + B}{(2x+1)(x-5)} \\ &= \frac{x(A+2B) + (B-5A)}{(2x+1)(x-5)}\end{aligned}$$

At first glance that just looks more complicated; the key is realising that on the LHS there are NO terms involving x and hence

$$A + 2B = 0$$

but since the denominator on the LHS is just unity this must also be true.

$$B - 5A = 1$$

Together these form a pair of *simultaneous equations* that we can solve to find A and B. Rearranging the first:

$$A = -2B$$

substituting into the second

$$\begin{aligned} B - (-10B) &= 1 \\ 11B &= 1 \\ B &= \frac{1}{11} \\ A &= -\frac{2}{11} \end{aligned}$$

Hence we can rewrite our complicated fraction as the sum of two simpler fractions:

$$\frac{1}{(2x+1)(x-5)} = -\frac{2}{11(2x+1)} + \frac{1}{11(x-5)}$$

That has nothing to do with integration; it is just algebra. So let's try the integration

$$\int \frac{1}{(2x+1)(x-5)}.dx = -\frac{2}{11}\int \frac{1}{2x+1}.dx + \frac{1}{11}\int \frac{1}{x-5}.dx$$

Both of the integrals on the RHS look like the function of a function (but are different!) so substitution should work on both (i.e. two substitutions at once!).

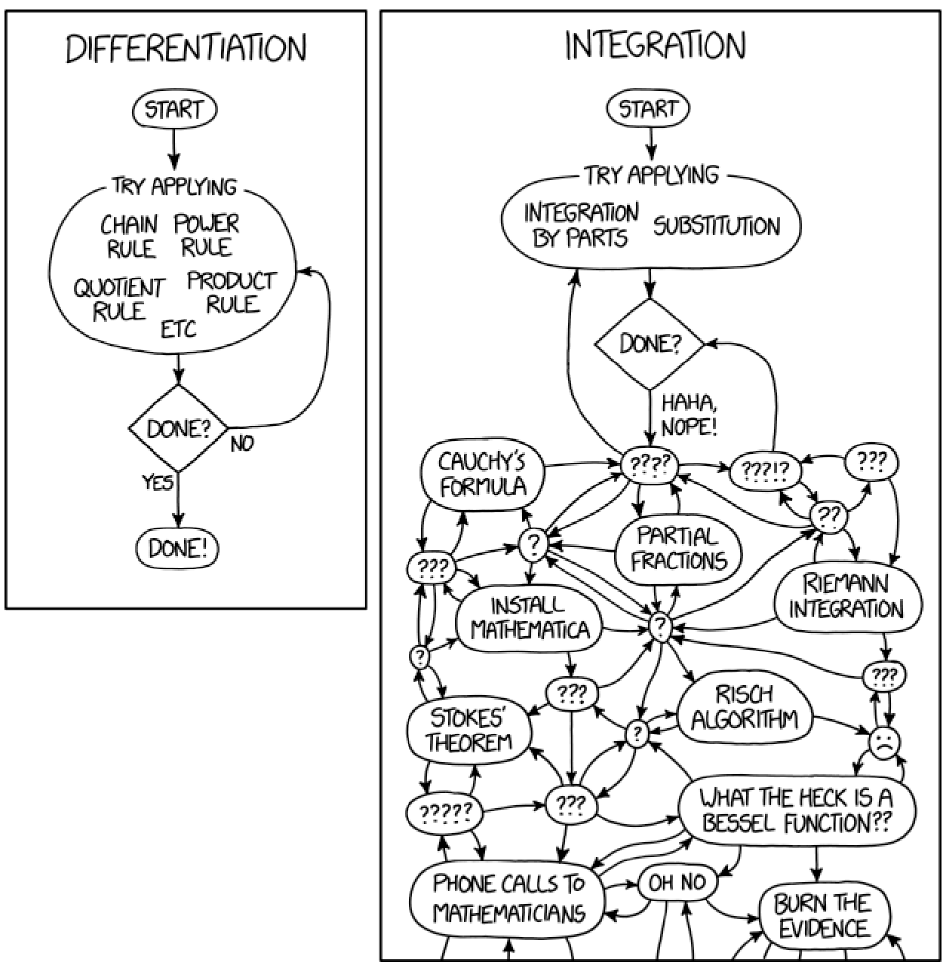
$$\begin{aligned} u &= 2x+1 \\ \frac{du}{dx} &= 2 \\ \frac{dx}{du} &= \frac{1}{2} \end{aligned} \qquad\qquad \begin{aligned} w &= x-5 \\ \frac{dw}{dx} &= 1 \\ \frac{dx}{dw} &= 1 \end{aligned}$$

$$
\begin{aligned}
\int \frac{1}{(2x+1)(x-5)}.dx &= -\frac{2}{11}\int \frac{1}{2}.\frac{1}{u}.du + \frac{1}{11}\int \frac{1}{w}.dw \\
&= -\frac{1}{11}\int \frac{1}{u}.du + \frac{1}{11}\int \frac{1}{w}.dw \\
&= -\frac{\ln|2x+1|}{11} + \frac{\ln|x-5|}{11} + k \\
&= \frac{1}{11}\ln\left(\left|\frac{x-5}{2x+1}\right|\right) + k \\
&= \frac{1}{11}\ln\left(B\left|\frac{x-5}{2x+1}\right|\right)
\end{aligned}
$$

where $k = \frac{1}{11}\ln B$.

There are more complex partial fractions whose numerator are not simply numerical, but you do not need to know these for studying reaction rates, but you may see them in textbooks.

Differentiation is usually straightforward, integration is a skill



For you:

Answer to Week 4 challenge. The German has the fish.

For you:

Week 5 challenge. A farmer has to get a grain sack, a fox and a chicken across a river in a boat. He can only carry himself and one of his burdens in one trip, but the fox will eat the chicken if he leaves them alone together, and the chicken will eat the grain given half a chance. How can he get them all across intact? Please send answers to philip.fowler@ndm.ox.ac.uk before the start of week 6.