CHEM1047 – Week 3 Lecture 1 – Deeper into derivatives

☐ *Sections 4.1-4.9 of Steiner, "The Chemistry Maths Book", 2nd edition.*

☐ *Sections 4.1-4.3 of Cockett and Doggett, "Maths for Chemists", Volume 1.*

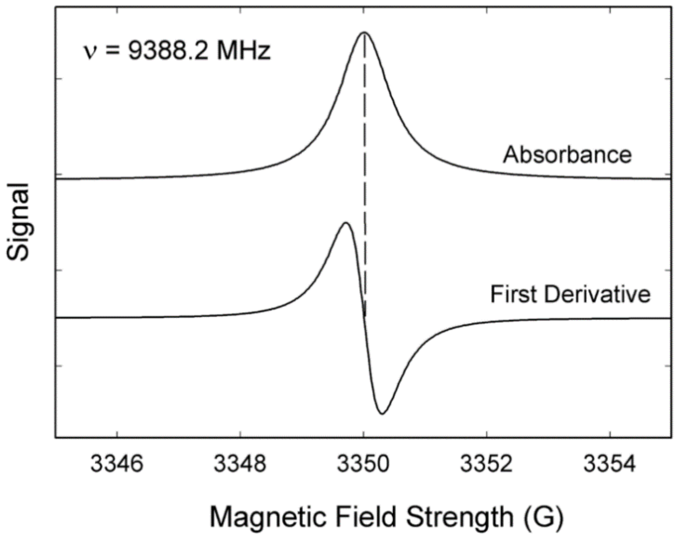
1. Formal definition of the derivative

The *derivative* $f'(x)$ of a function $f(x)$ is formally defined as the following limit:

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x} \qquad (1)$$

The process of computing derivatives is called *differentiation*. From the physical point of view, derivative may be interpreted as the rate of change of the function. For example, the derivative of coordinate with respect to time is velocity. The derivative of ground height with respect to distance is the slope of that ground.

An example from chemical sciences is given in the figure on the right. It shows a radio wave absorbance spectrum of an organic radical as a function of the applied magnetic field. The absorbance signal is a simple bell-shaped curve. Its derivative indicates the rate of change in the value of that function. When the function is increasing, the derivative is positive. When the function is decreasing, the derivative is negative.



2. Differentiation using limits

Technically, all derivatives may be computed using the definition in Equation (1), for example:

$$f(t) = 5t^2 - 2t + 8, \qquad f'(t) = \lim_{\Delta t \to 0} \frac{\left[5(t+\Delta t)^2 - 2(t+\Delta t) + 8\right] - \left[5t^2 - 2t + 8\right]}{\Delta t} = [\ldots] = 10t - 2$$

However, the intermediate expressions are bulky even for simple functions:

$$f(x) = 2 - \sqrt{x+1}, \qquad f'(x) = \lim_{\Delta x \to 0} \frac{\left[2 - \sqrt{x+\Delta x+1}\right] - \left[2 - \sqrt{x+1}\right]}{\Delta x} =$$

$$= \lim_{\Delta x \to 0} \frac{\sqrt{x+1} - \sqrt{x+\Delta x+1}}{\Delta x} = \lim_{\Delta x \to 0} \left[\frac{\sqrt{x+1} - \sqrt{x+\Delta x+1}}{\Delta x} \frac{\sqrt{x+1} + \sqrt{x+\Delta x+1}}{\sqrt{x+1} + \sqrt{x+\Delta x+1}}\right] =$$

$$= \lim_{\Delta x \to 0} \left[\frac{x+1-x-\Delta x-1}{\Delta x\left(\sqrt{x+1} + \sqrt{x+\Delta x+1}\right)}\right] = \lim_{\Delta x \to 0} \left[-\frac{\Delta x}{\Delta x\left(\sqrt{x+1} + \sqrt{x+\Delta x+1}\right)}\right] =$$

$$= \lim_{\Delta x \to 0} \left[-\frac{1}{\sqrt{x+1} + \sqrt{x+\Delta x+1}}\right] = -\frac{1}{2\sqrt{x+1}}$$

It is therefore common practice to simply memorise a set of differentiation rules, and to use those rules for calculating derivatives. We will now derive these rules from Equation (1).

3. Derivatives of sums and multiples

The rules for sums and multiples are simple. The derivative of a sum is a sum of derivatives:

$$\begin{aligned}\left[f(x)+g(x)\right]' &= \lim_{\Delta x\to 0}\frac{\left[f(x+\Delta x)+g(x+\Delta x)\right]-\left[f(x)+g(x)\right]}{\Delta x}= \\ &=\lim_{\Delta x\to 0}\frac{f(x+\Delta x)-f(x)}{\Delta x}+\lim_{\Delta x\to 0}\frac{g(x+\Delta x)-g(x)}{\Delta x}=f'(x)+g'(x)\end{aligned} \tag{2}$$

Constant multipliers can be taken out of the differentiation operation:

$$\left[\alpha f(x)\right]'=\lim_{\Delta x\to 0}\frac{\alpha f(x+\Delta x)-\alpha f(x)}{\Delta x}=\alpha\lim_{\Delta x\to 0}\frac{f(x+\Delta x)-f(x)}{\Delta x}=\alpha\left[f(x)\right]' \tag{3}$$

This applies equally to real and complex numbers.

4. Formal derivation of product, quotient and chain rules

To derive the differentiation rule for a product of functions, we need to make a few preliminary observations. The limit definition of the derivative:

$$f'(x)=\lim_{\Delta x\to 0}\frac{f(x+\Delta x)-f(x)}{\Delta x} \tag{4}$$

holds strictly for infinitely small values of Δx. For finite values of Δx we would have:

$$f'(x)=\frac{f(x+\Delta x)-f(x)}{\Delta x}+\varphi(x,\Delta x) \tag{5}$$

where the unknown function $\varphi(x,\Delta x)$ goes to zero when Δx goes to zero. After rearranging this formula to make $f(x+\Delta x)$ the subject, we obtain:

$$f(x+\Delta x)=f(x)+f'(x)\Delta x-\varphi(x,\Delta x)\Delta x \tag{6}$$

If we take some other function $g(x)$ and perform a similar treatment, we would obtain:

$$g(x+\Delta x)=g(x)+g'(x)\Delta x-\psi(x,\Delta x)\Delta x \tag{7}$$

with some other unknown function $\psi(x,\Delta x)$ which also goes to zero when Δx goes to zero. Now, for the derivative of the product of $f(x)$ and $g(x)$:

$$\begin{aligned}\left[f(x)g(x)\right]' &= \lim_{\Delta x\to 0}\frac{f(x+\Delta x)g(x+\Delta x)-f(x)g(x)}{\Delta x}= \\ &=\lim_{\Delta x\to 0}\frac{\left[f(x)+f'(x)\Delta x-\varphi(x,\Delta x)\Delta x\right]\left[g(x)+g'(x)\Delta x-\psi(x,\Delta x)\Delta x\right]-f(x)g(x)}{\Delta x}= \\ &=\lim_{\Delta x\to 0}\frac{f'(x)g(x)\Delta x+f(x)g'(x)\Delta x+[\ldots]}{\Delta x}=f'(x)g(x)+f(x)g'(x)\end{aligned} \tag{8}$$

where all terms in square brackets $[\ldots]$ have a zero limit when Δx goes to zero (inspect them as an exercise). Therefore, the *product rule* is:

$$\left[f(x)g(x)\right]'=f'(x)g(x)+f(x)g'(x) \tag{9}$$

A similar procedure (Appendix A) for a ratio of two functions produces the *quotient rule*:

$$\left[\frac{f(x)}{g(x)}\right]' = \frac{f'(x)g(x) - f(x)g'(x)}{g(x)^2} \tag{10}$$

A page of mathematics (Appendix B) along similar lines results in the *chain rule*:

$$\frac{d}{dx} f\left[g(x)\right] = f'\left[g(x)\right]g'(x) \tag{11}$$

You are expected to memorize Equations (9)-(11) and to understand their derivation.

5. Derivatives of common functions

This section contains a boring enumeration of common function derivatives. The simplest case is the derivative of a constant:

$$\left[\alpha\right]' = \lim_{\Delta x \to 0} \frac{\alpha - \alpha}{\Delta x} = 0 \tag{12}$$

The next most popular function is the linear function:

$$f(x) = ax + b \tag{13}$$

We can already handle sums and constants, and so the question is about the derivative of x:

$$\left[x\right]' = \lim_{\Delta x \to 0} \frac{x + \Delta x - x}{\Delta x} = \lim_{\Delta x \to 0} \frac{\Delta x}{\Delta x} = 1 \tag{14}$$

The next step on the difficulty ladder is a polynomial, or rather its individual terms that contain powers of x. We can use the product rule here:

$$\left[x^n\right]' = \left[xx^{n-1}\right]' = \left[x\right]' x^{n-1} + x\left[x^{n-1}\right]' = x^{n-1} + x\left[x^{n-1}\right]' \tag{15}$$

This is a recursively defined sequence. We know from Equation (14) that $\left[x\right]' = 1$, therefore:

$$\begin{aligned}
&\left[x\right]' = 1 \\
&\left[x^2\right]' = x + x\left[x\right]' = 2x \\
&\left[x^3\right]' = x^2 + x\left[x^2\right]' = x^2 + x\left[2x\right] = 3x^2 \\
&\left[x^4\right]' = x^3 + x\left[x^3\right]' = x^3 + x\left[3x^2\right] = 4x^3
\end{aligned} \tag{16}$$

and so on. It is easy to see by direct inspection that $\left[x^n\right]' = nx^{n-1}$. This formula is also valid for negative and fractional powers (prove this as an exercise).

The limit definition of the derivative may be applied to all elementary functions. The result is a table that you are expected to memorize:

Function	**Derivative**
c (constant)	0
x^n	nx^{n-1}
e^x	e^x
a^x	$a^x \ln a$

$\sin x$	$\cos x$
$\cos x$	$-\sin x$
$\ln x$	$1/x$
$\log_b x$	$1/(x\ln b)$

Together with Equations (9)-(11), this table makes it possible to differentiate most functions in chemistry and physics, for example:

$$\left[\frac{\cos(x)\ln(x)}{x^2}\right]' = \frac{\left[\cos(x)\ln(x)\right]' x^2 - \cos(x)\ln(x)\left[x^2\right]'}{x^4} =$$

$$= \frac{\left(\left[\cos(x)\right]'\ln(x) + \cos(x)\left[\ln(x)\right]'\right)x^2 - 2x\cos(x)\ln(x)}{x^4} =$$

$$= \frac{\left(-\sin(x)\ln(x) + \dfrac{\cos(x)}{x}\right)x^2 - 2x\cos(x)\ln(x)}{x^4} = \frac{\left(1-2\ln(x)\right)\cos(x)}{x^3} - \frac{\sin(x)\ln(x)}{x^2}$$

A lot of practice is required before such calculations become easy and natural.

6. Alternative notations for the derivative

The definition of the derivative involves the increment of the function divided by the increment of the argument. This suggests an alternative notation for the derivative that will be useful later because it can actually be interpreted as a fraction:

$$g'(x) \equiv \frac{dg(x)}{dx} \equiv \frac{d}{dx}g(x) \tag{17}$$

The d/dx prefix is called *differentiation operator*. It is an instruction to calculate the derivative of whatever occurs in front, in the same sense as the prime symbol is an instruction to compute the derivative of whatever comes before it. In this notation, the problem we have just solved above would be

$$\frac{d}{dx}\left[\frac{\cos(x)\ln(x)}{x^2}\right]$$

We will see more of this notation when we consider integrals and differential equations. A less common notation used in physics for derivatives with respect to time is $\dot{g}(t) \equiv g'(t) \equiv dg(t)/dt$.

One particular task that is simplified by the use of df/dx notation is computing derivatives for inverse functions. If the derivative of some complicated function $y = f(x)$ is

$$\frac{dy}{dx} = f'(x) \tag{18}$$

then the derivative of the corresponding inverse function $x = f^{-1}(y)$ is

$$\frac{dx}{dy} = \frac{1}{f'(x)} = \frac{1}{f'\left(f^{-1}(y)\right)} \tag{19}$$

Appendix A – Derivation of the quotient rule

The problem of differentiating the ratio of two functions may be simplified by using the product rule:

$$\left[\frac{f(x)}{g(x)}\right]' = \left[f(x)\frac{1}{g(x)}\right]' = f'(x)\frac{1}{g(x)} + f(x)\left[\frac{1}{g(x)}\right]' \tag{20}$$

Now the question is reduced to finding out what the derivative of $1/g(x)$ is. That is quite easy:

$$\begin{gathered}\left[\frac{1}{g(x)}\right]' = \lim_{\Delta x\to 0}\left[\frac{1}{\Delta x}\left(\frac{1}{g(x+\Delta x)} - \frac{1}{g(x)}\right)\right] = \lim_{\Delta x\to 0}\left[\frac{1}{\Delta x}\left(\frac{g(x)-g(x+\Delta x)}{g(x+\Delta x)g(x)}\right)\right] = \\ = -\lim_{\Delta x\to 0}\left[\frac{g(x+\Delta x)-g(x)}{\Delta x}\frac{1}{g(x+\Delta x)g(x)}\right] = -\frac{g'(x)}{g(x)^2}\end{gathered} \tag{21}$$

We can now continue the simplification of Equation (20):

$$\left[\frac{f(x)}{g(x)}\right]' = f'(x)\frac{1}{g(x)} - f(x)\frac{g'(x)}{g(x)^2} = \frac{f'(x)g(x) - f(x)g'(x)}{g(x)^2} \tag{22}$$

Therefore, the rule for differentiation of fractions is:

$$\left[\frac{f(x)}{g(x)}\right]' = \frac{f'(x)g(x) - f(x)g'(x)}{g(x)^2} \tag{23}$$

Appendix B – Derivation of the chain rule

In the case of nested functions:

$$\frac{d}{dx} f\left[g\left(x\right)\right] = \lim_{\Delta x \to 0} \frac{f\left[g\left(x+\Delta x\right)\right] - f\left[g\left(x\right)\right]}{\Delta x} \tag{24}$$

To make progress with this expression, we will take advantage of the finite Δx expressions that we have already used above. For the functions $f\left(x\right)$ and $g\left(x\right)$ separately:

$$\begin{aligned} f'\left(x\right) &= \lim_{\Delta x \to 0} \frac{f\left(x+\Delta x\right) - f\left(x\right)}{\Delta x} \quad \Rightarrow \quad f'\left(x\right) = \frac{f\left(x+\Delta x\right) - f\left(x\right)}{\Delta x} + \varphi\left(x, \Delta x\right) \\ g'\left(x\right) &= \lim_{\Delta x \to 0} \frac{g\left(x+\Delta x\right) - g\left(x\right)}{\Delta x} \quad \Rightarrow \quad g'\left(x\right) = \frac{g\left(x+\Delta x\right) - g\left(x\right)}{\Delta x} + \psi\left(x, \Delta x\right) \end{aligned} \tag{25}$$

where the unknown functions $\varphi\left(x, \Delta x\right)$ and $\psi\left(x, \Delta x\right)$ go to zero when Δx goes to zero. After rearranging these expressions to expose $f\left(x+\Delta x\right)$ and $g\left(x+\Delta x\right)$, we obtain:

$$\begin{aligned} f\left(x+\Delta x\right) &= f\left(x\right) + f'\left(x\right)\Delta x - \varphi\left(x, \Delta x\right)\Delta x \\ g\left(x+\Delta x\right) &= g\left(x\right) + g'\left(x\right)\Delta x - \psi\left(x, \Delta x\right)\Delta x \end{aligned} \tag{26}$$

The second equation allows us to make progress with $g\left(x+\Delta x\right)$ term that appears in Equation (24):

$$\begin{aligned} \frac{d}{dx} f\left[g\left(x\right)\right] &= \lim_{\Delta x \to 0} \frac{f\left[g\left(x+\Delta x\right)\right] - f\left[g\left(x\right)\right]}{\Delta x} = \\ &= \lim_{\Delta x \to 0} \frac{f\left[g\left(x\right) + g'\left(x\right)\Delta x - \psi\left(x, \Delta x\right)\Delta x\right] - f\left[g\left(x\right)\right]}{\Delta x} \end{aligned} \tag{27}$$

In this new expression, the argument of $f\left(x\right)$ has a primary part and an increment:

$$f\left[g\left(x\right) + g'\left(x\right)\Delta x - \psi\left(x, \Delta x\right)\Delta x\right] = f\left(g + \Delta g\right) \tag{28}$$

where $\Delta g = g'\left(x\right)\Delta x - \psi\left(x, \Delta x\right)\Delta x$ also goes to zero when Δx goes to zero. Equation (28) is similar to the first part of Equation (26), and we can therefore make further progress with Equation (27):

$$\begin{aligned} \frac{d}{dx} f\left[g\left(x\right)\right] &= \lim_{\Delta x \to 0} \frac{f\left(g\right) + f'\left(g\right)\Delta g - \varphi\left(x, \Delta g\right)\Delta g - f\left(g\right)}{\Delta x} = \\ &= \lim_{\Delta x \to 0} \frac{f'\left(g\right)\Delta g - \varphi\left(x, \Delta g\right)\Delta g}{\Delta x} = \lim_{\Delta x \to 0} \frac{f'\left(g\right)\Delta g}{\Delta x} = f'\left(g\right) \lim_{\Delta x \to 0} \frac{\Delta g}{\Delta x} \end{aligned} \tag{29}$$

Finally, the remaining limit is:

$$\lim_{\Delta x \to 0} \frac{\Delta g}{\Delta x} = \lim_{\Delta x \to 0} \frac{g'\left(x\right)\Delta x - \psi\left(x, \Delta x\right)\Delta x}{\Delta x} = g'\left(x\right) \tag{30}$$

After putting the last two equations together, we conclude that:

$$\frac{d}{dx} f\left[g\left(x\right)\right] = f'\left[g\left(x\right)\right] g'\left(x\right) \tag{31}$$