CHEM1033 - Week 5 Lecture - Derivatives and differentiation III

Section 4.6 of Steiner, "The Chemistry Maths Book", 2nd edition.
Chapters 19 and 20 of Monk and Munro, "Maths for Chemistry", 2nd edition.

1. Nested function rule

The last remaining case that we must consider before our differentiation toolkit is complete is the case of nested functions:

$$\frac{d}{dx} f\left(g\left(x\right)\right) = \lim_{\Delta x \to 0} \frac{f\left(g\left(x+\Delta x\right)\right) - f\left(g\left(x\right)\right)}{\Delta x} \tag{1}$$

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

$$\begin{aligned} f'\left(x\right) = \lim_{\Delta x \to 0} \frac{f\left(x+\Delta x\right) - f\left(x\right)}{\Delta x} \quad &\Rightarrow \quad f'\left(x\right) = \frac{f\left(x+\Delta x\right) - f\left(x\right)}{\Delta x} + \varphi\left(x, \Delta x\right) \\ g'\left(x\right) = \lim_{\Delta x \to 0} \frac{g\left(x+\Delta x\right) - g\left(x\right)}{\Delta x} \quad &\Rightarrow \quad g'\left(x\right) = \frac{g\left(x+\Delta x\right) - g\left(x\right)}{\Delta x} + \psi\left(x, \Delta x\right) \end{aligned} \tag{2}$$

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:

$$\begin{aligned} f\left(x+\Delta x\right) &= f\left(x\right) + f'\left(x\right)\Delta x - \varphi\left(x, \Delta x\right)\Delta x \\ g\left(x+\Delta x\right) &= g\left(x\right) + g'\left(x\right)\Delta x - \psi\left(x, \Delta x\right)\Delta x \end{aligned} \tag{3}$$

The second equation allows us to make progress with the $g\left(x+\Delta x\right)$ term that appears in Equation (1):

$$\begin{aligned} \frac{d}{dx} f\left(g\left(x\right)\right) &= \lim_{\Delta x \to 0} \frac{f\left(g\left(x+\Delta x\right)\right) - f\left(g\left(x\right)\right)}{\Delta x} = \\ &= \lim_{\Delta x \to 0} \frac{f\left(g\left(x\right) + g'\left(x\right)\Delta x - \psi\left(x, \Delta x\right)\Delta x\right) - f\left(g\left(x\right)\right)}{\Delta x} \end{aligned} \tag{4}$$

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

$$f\left(g\left(x\right) + g'\left(x\right)\Delta x - \psi\left(x, \Delta x\right)\Delta x\right) = f\left(g + \Delta g\right) \tag{5}$$

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 (5) is similar to the first part of Equation (3), and we can therefore make further progress with Equation (4):

$$\begin{aligned} \frac{d}{dx} f\left(g\left(x\right)\right) &= \lim_{\Delta x \to 0} \frac{f\left(g\right) + f'\left(g\right)\Delta g - \varphi\left(x, \Delta g\right)\Delta g - f\left(g\right)}{\Delta x} = \\ &= \lim_{\Delta x \to 0} \frac{f'\left(g\right)\Delta g - \varphi\left(x, \Delta g\right)\Delta g}{\Delta x} = \lim_{\Delta x \to 0} \frac{f'\left(g\right)\Delta g}{\Delta x} = f'\left(g\right) \lim_{\Delta x \to 0} \frac{\Delta g}{\Delta x} \end{aligned} \tag{6}$$

Finally, the remaining limit is:

$$\lim_{\Delta x \to 0} \frac{\Delta g}{\Delta x} = \lim_{\Delta x \to 0} \frac{g'\left(x\right)\Delta x - \psi\left(x, \Delta x\right)\Delta x}{\Delta x} = g'\left(x\right) \tag{7}$$

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

$$\frac{d}{dx} f\left(g\left(x\right)\right) = f'\left(g\left(x\right)\right) g'\left(x\right) \tag{8}$$

That is, the derivative of a nested function is the derivative of the outer function, with its argument unchanged, multiplied by the derivative of the argument. For example:

$$\left[\sin\left(x^2\right)\right]' = \left\{ \begin{matrix} f(x)=\sin(x), & f'(x)=\cos(x) \\ g(x)=x^2, & g'(x)=2x \end{matrix} \right\} = \cos\left(x^2\right)\cdot 2x = 2x\cos\left(x^2\right) \tag{9}$$

2. Higher order derivatives

Many problems in physical sciences require the calculation of the rate of change for another rate of change (*e.g.* acceleration is a rate of change in the velocity, which is itself the rate of change in the coordinate). In those cases a repeated evaluation of the derivative is needed. The corresponding second and higher derivatives are denoted with either multiple dashes, or multiple dots, or with powers of d and dt in the Leibnitz notation:

$$a(t) = x''(t) \equiv \ddot{x}(t) \equiv \frac{d^2 x(t)}{dt^2} \equiv \frac{d^2}{dt^2} x(t) \tag{10}$$

Higher derivatives are computed by applying the same differentiation rules repeatedly, for example:

$$\left[\sin\left(x^2\right)\right]'' = \left[2x\cos\left(x^2\right)\right]' = 2\cos\left(x^2\right) + 2x\left[-2x\sin\left(x^2\right)\right] = 2\cos\left(x^2\right) - 4x^2\sin\left(x^2\right) \tag{11}$$

Many functions that occur in physical sciences have an infinite number of non-zero derivatives.

3. Differentials

The differential is a generalization of the notion of a small increment. In the discussion so far, we were either dealing with finite increments (*e.g.* Δf and Δx) or with limit expressions in which those increments vanished after the limit was taken. Differential expressions combine those methods: dx stands for an increment of x that is infinitely small. This eliminates the need to account for the correction factors of the kind that we had in Equations (3):

$$\begin{gathered} f(x+\Delta x) = f(x) + f'(x)\Delta x - \varphi(x,\Delta x)\Delta x \\ \Downarrow \\ f(x+\Delta x) - f(x) = f'(x)\Delta x - \varphi(x,\Delta x)\Delta x \\ \Downarrow \\ \Delta f = f'(x)\Delta x - \varphi(x,\Delta x)\Delta x \\ \Downarrow \\ df = f'(x)\,dx \end{gathered} \tag{12}$$

It is clear that differential expressions are smaller and more convenient than the expressions involving limits of finite increments. Equation (12) also clarifies the origin of the Leibnitz notation for the derivative:

$$df = f'(x)\,dx \quad \Rightarrow \quad \frac{df}{dx} = f'(x) \tag{13}$$

The properties of differentials follow directly from the corresponding derivative properties. For linear combinations of functions we have:

$$d[f+g] = df + dg, \qquad d[\alpha f] = \alpha df \tag{14}$$

where α is a constant. For products and fractions, likewise:

$$d\left[fg\right]=fdg+gdf,\qquad d\left[\frac{f}{g}\right]=\frac{fdg-gdf}{g^2} \tag{15}$$

where d is not a variable or function, but a differential operator – an instruction to carry out the differentiation of whatever appears in front. This notation is the reason why you never see letter d used for anything else in mathematics, it is firmly reserved for differentials. Interestingly, the chain rule may now be derived in just one line:

$$d\left[f(g)\right]=f'(g)dg,\quad dg(x)=g'(x)dx\quad\Rightarrow\quad d\left[f(g(x))\right]=f'(g(x))g'(x)dx \tag{16}$$

The simplicity (to a trained eye) of such transformations is the primary reason why differentials are so widely used in physical sciences – quantum theory in particular is full of such things. Example:

$$d\left[\exp\left(-x^2/2\right)\right]=\left[\exp\left(-x^2/2\right)\right]'dx=-x\exp\left(-x^2/2\right)dx$$

Expressions for higher order differentials may be obtained using the product rule in Equation (15):

$$\begin{aligned}d^2f&=d\left[df\right]=d\left[f'(x)dx\right]=d\left[f'(x)\right]dx+f'(x)d\left[dx\right]=\\&=\left[f''(x)dx\right]dx+f'(x)d^2x=f''(x)dx^2+f'(x)d^2x\end{aligned} \tag{17}$$

Note that dx^2 in this equation is the square of the first differential of x, whereas $d^2x=ddx$ is the second differential of x.

4. Inverse function rule

One particular task that is simplified significantly by the use of differentials is that of computing derivatives for inverse functions. It is easy to see that, 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

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

and so, instead of laboriously solving $y=f(x)$ for x and then taking the derivative of the result with respect to y, we can simply put $f'(x)$ in the denominator and be done with it. Example:

$$y=a\sin(x)\quad\Rightarrow\quad\frac{dy}{dx}=a\cos(x)\quad\Rightarrow\quad\frac{dx}{dy}=\frac{1}{a\cos(x)}$$

$$\frac{dx}{dy}=\frac{1}{a\sqrt{1-\sin^2(x)}}=\frac{1}{a\sqrt{1-y^2/a^2}}=\frac{1}{\sqrt{a^2-y^2}}$$

Week 6 workshop exercises

Monk and Munro, 2nd edition: self-tests 19.1, 19.2, 20.1-20.3; problems 19.1-19.10.

Steiner, 2nd edition: Section 4.13 (29-32, 37-44).

Extra difficulty exercises for the brave

Steiner, 2nd edition: Section 4.13 (33-36, 45-64).