CHEM1034 - Week 23 Lecture - Multivariate functions: differentiation

Sections 4.12, 9.1-9.3, 9.5-9.7 of Steiner, "The Chemistry Maths Book", 2nd edition.

Chapter 22 of Monk and Munro, "Maths for Chemistry", 2nd edition.

Partial derivatives

A partial derivative of a function is a derivative with respect to just one of its arguments. The same differentiation rules apply, all other arguments should be treated as constants. Examples:

$$\frac{\partial}{\partial y}(xyz) = xz \qquad \frac{\partial}{\partial x}\left(\frac{1-x}{\sin y}\right) = \frac{-1}{\sin y}$$

Higher derivatives, such as $\partial^2 f/\partial x^2$, and mixed derivatives, such as $\partial^2 f/\partial x \partial y$ are obtained by sequential partial differentiation. For well-behaved functions (the derivatives in question should be continuous), the value of mixed derivatives does not depend on the order of partial differentiation.

Partial derivatives have the same limit definition as the derivatives of univariate functions:

$$\frac{\partial f(x,y,z,\ldots)}{\partial x} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x, y, z, \ldots) - f(x,y,z,\ldots)}{\Delta x} \tag{1}$$

and therefore, for finite increments of the argument, the same approximate expressions apply:

$$\begin{aligned} f(x+\Delta x) &= f(x) + \frac{df}{dx}\Delta x + O\left[\Delta x^2\right] \\ f(x+\Delta x, y, z, \ldots) &= f(x,y,z,\ldots) + \frac{\partial f}{\partial x}\Delta x + O\left[\Delta x^2\right] \end{aligned} \tag{2}$$

In the case of increments of multiple variables, these expressions are generalized further:

$$\Delta f = \frac{\partial f}{\partial x}\Delta x + \frac{\partial f}{\partial y}\Delta y + \ldots + O\left[\Delta x^2\right] + O\left[\Delta y^2\right] + \ldots \tag{3}$$

Writing every argument of a function out explicitly tends to be voluminous. The arguments are therefore often collected into a vector, for example:

$$f(x,y,z) = f(\vec{r}), \qquad \vec{r} = \begin{bmatrix} x & y & z \end{bmatrix} \tag{4}$$

Partial derivatives can also be collected into arrays. In particular, the vector of first partial derivatives

$$\vec{\nabla} f = \begin{bmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} & \frac{\partial f}{\partial z} & \cdots \end{bmatrix} \tag{5}$$

is called the *gradient* of the function. Gradient indicates the direction of steepest growth and has many uses in physical sciences – for example, force may be defined *via* the gradient of the potential energy.

Chain rules for differentiation of multivariate functions

In situations when a function depends on multiple arguments that are themselves functions of other arguments, the chain rule for differentiation must be extended appropriately. Several situations exist:

1. A function of one variable that depends on multiple other variables:

$$\frac{\partial}{\partial x} f\left(g(x,y,z,\ldots)\right) \tag{6}$$

We can use Equations (2) and (3) to write out Δf when the argument x is incremented by Δx and then take the limit:

$$\Delta f = \frac{df}{dg}\Delta g + O\left[\Delta g^2\right] = \frac{df}{dg}\left(\frac{\partial g}{\partial x}\Delta x + O\left[\Delta x^2\right]\right) + O\left[\Delta g^2\right]$$
$$\frac{\partial f}{\partial x} = \lim_{\Delta x \to 0}\frac{\Delta f}{\Delta x} = \frac{df}{dg}\frac{\partial g}{\partial x} \tag{7}$$

We therefore arrive at the following chain rule:

$$\frac{\partial}{\partial x} f\left(g\left(x, y, z, \ldots\right)\right) = \frac{df}{dg}\frac{\partial g}{\partial x} \tag{8}$$

2. A function of multiple variables that depend on the same variable:

$$\frac{d}{dt} f\left(x(t), y(t), \ldots\right) \tag{9}$$

This is a full derivative because the function ultimately only depends on one argument. Using Equation (3) followed by the univariate case of Equation (2) we obtain:

$$\Delta f = \frac{\partial f}{\partial x}\Delta x + \frac{\partial f}{\partial y}\Delta y + \ldots + O\left[\Delta x^2\right] + O\left[\Delta y^2\right] + \ldots =$$
$$= \frac{\partial f}{\partial x}\frac{dx}{dt}\Delta t + \frac{\partial f}{\partial y}\frac{dy}{dt}\Delta t + \ldots + O\left[\Delta x^2\right] + O\left[\Delta y^2\right] \tag{10}$$

After using the limit definition of the derivative with respect to t, we can conclude that:

$$\frac{d}{dt} f\left(x(t), y(t), \ldots\right) = \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\partial f}{\partial y}\frac{dy}{dt} + \ldots \tag{11}$$

3. A function of multiple variables that each depend on multiple other variables. This is a combination of the two situations above and the corresponding rule may be derived in a similar fashion:

$$\frac{\partial}{\partial \alpha} f\left(x(\alpha, \beta, \ldots), y(\alpha, \beta, \ldots), \ldots\right) = \frac{\partial f}{\partial x}\frac{\partial x}{\partial \alpha} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial \alpha} + \ldots \tag{12}$$

<u>Example 1</u>:

$$z = \sin(x), \quad x = u^2 v^2$$
$$\frac{\partial z}{\partial u} = \frac{dz}{dx}\frac{\partial x}{\partial u} = \left[\cos(x)\right]\left[2uv^2\right] = 2uv^2\cos\left(u^2v^2\right)$$

<u>Example 2</u>:

$$z = x^2 y - y^2, \quad x = t^2, \quad y = 2t$$
$$\frac{dz}{dt} = \frac{\partial z}{\partial x}\frac{dx}{dt} + \frac{\partial z}{\partial y}\frac{dy}{dt} = \left[2xy\right]\left[2t\right] + \left[x^2 - 2y\right]\left[2\right] = \ldots = 10t^4 - 8t$$

<u>Example 3</u>:

$$z = e^{x^2 y}, \quad x(u,v) = \sqrt{uv}, \quad y(u,v) = 1/v$$
$$\frac{\partial z}{\partial u} = \frac{\partial z}{\partial x}\frac{\partial x}{\partial u} + \frac{\partial z}{\partial y}\frac{\partial y}{\partial u} = \left[2xye^{x^2 y}\right]\left[\frac{\sqrt{v}}{2\sqrt{u}}\right] + \left[x^2 e^{x^2 y}\right]\left[0\right] = \ldots = e^u$$

Differentials

The differential df of a function $f(x)$ is a function that relates an infinitesimal increment of the argument and the corresponding infinitesimal increment of the function. It is defined in the following way:

$$df = f'(x)dx \tag{13}$$

This definition makes the fraction notation for the derivatives particularly transparent and useful:

$$df = \frac{df}{dx}dx \tag{14}$$

The physical meaning of the differential becomes clear if we replace the infinitesimal increments dy and dx with finite increments Δy and Δx:

$$\Delta y \approx y'(x)\Delta x \tag{15}$$

The differential approximates the rate of change in the function: Δy is the approximate amount by which the function changes when the argument is changed by Δx.

Multivariate functions change value if any of their arguments changes. The expression for the differential of a multivariate function is:

$$df(x,y,z,...) = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy + \frac{\partial f}{\partial z}dz + ... \tag{16}$$

<u>Example 1</u>: calculate the differential of $f(x,y) = x\sin y$.

$$df = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy = \frac{\partial}{\partial x}(x\sin y)dx + \frac{\partial}{\partial y}(x\sin y)dy =$$
$$= \sin(y)dx + x\cos(y)dy$$

Differentials are particularly useful for variable substitution in expressions involving derivatives and integrals – the differentials that occur in those expressions simply need to be evaluated.

<u>Example 2</u>: $df/dx = \cos x,\ x = t^3$ – derive the expression for df/dt.

$$dx = 3t^2dt \quad \Rightarrow \quad \frac{df}{3t^2dt} = \cos(t^3) \quad \Rightarrow \quad \frac{df}{dt} = 3t^2\cos(t^3)$$

<u>Example 3</u>: perform the variable substitution $t = 1/x$ in the following integral

$$\int_1^2 x\ln(x)dx$$

In this example three things need to be transformed: the limits, the expression under the integral and the differential.

$$t(1) = 1, \quad t(2) = 1/2; \qquad x\ln x = \frac{1}{t}\ln\frac{1}{t} = -\frac{\ln t}{t}; \qquad dx = -\frac{1}{t^2}dt$$

The resulting integral is:

$$\int_1^{1/2}\frac{\ln t}{t^3}dt = -\int_{1/2}^{1}\frac{\ln t}{t^3}dt$$

Multivariate Taylor series

The generalisation of the Taylor series to functions of multiple arguments is:

$$f(x_1,\ldots,x_m) = f(a_1,\ldots,a_m) + \sum_{j=1}^{m} \frac{\partial f(a_1,\ldots,a_m)}{\partial x_j}(x_j - a_j) + \\ + \frac{1}{2!}\sum_{j=1}^{m}\sum_{k=1}^{m} \frac{\partial^2 f(a_1,\ldots,a_m)}{\partial x_j \partial x_k}(x_j - a_j)(x_k - a_k) + \\ + \frac{1}{3!}\sum_{j=1}^{m}\sum_{k=1}^{m}\sum_{l=1}^{m} \frac{\partial^3 f(a_1,\ldots,a_m)}{\partial x_j \partial x_k \partial x_l}(x_j - a_j)(x_k - a_k)(x_l - a_l) + \ldots \tag{17}$$

The best practical way of generating such a series is to use *Mathematica*'s `Series` command.

Week 24 workshop exercises

Monk and Munro, 2nd edition: problems 22.1-22.4.

Steiner, 2nd edition: Section 4.13, problems 89-92; Section 9.12, problems 3-14, 31-35.

Extra difficulty exercises for the brave

Steiner, 2nd edition: section 9.12, problems 15-19.