Chemistry 231_Math_Toolbox

Ordinary Derivatives of Functions with One Independent Variable

The **ordinary derivative of $f(x)$** is defined as $\dfrac{\mathrm{d}f(x)}{\mathrm{d}x} = \lim_{\Delta x \to 0} \dfrac{f(x+\Delta x) - f(x)}{\Delta x}$ which gives:

$$\frac{\mathrm{d}x}{\mathrm{d}x} = 1 \qquad \frac{\mathrm{d}x^2}{\mathrm{d}x} = 2x \qquad \frac{\mathrm{d}x^3}{\mathrm{d}x} = 3x^2$$

$$\frac{\mathrm{d}\left(\frac{1}{x}\right)}{\mathrm{d}x} = -\frac{1}{x^2} \qquad \frac{\mathrm{d}e^x}{\mathrm{d}x} = e^x \qquad \frac{\mathrm{d}\ln x}{\mathrm{d}x} = \frac{1}{x} \qquad \textit{etc.}$$

Useful rules for ordinary derivatives (a is a constant):

$$\frac{\mathrm{d}}{\mathrm{d}x} af(x) = a\frac{\mathrm{d}f}{\mathrm{d}x} \qquad \frac{\mathrm{d}}{\mathrm{d}x} x^a = ax^{a-1} \qquad \frac{\mathrm{d}}{\mathrm{d}x} f(u(x)) = \frac{\mathrm{d}f}{\mathrm{d}x}\frac{\mathrm{d}u}{\mathrm{d}x} \quad \text{(chain rule)}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\frac{f(x)}{u(x)} = \frac{u\dfrac{\mathrm{d}f}{\mathrm{d}x} - f\dfrac{\mathrm{d}u}{\mathrm{d}x}}{u^2} \qquad \frac{\mathrm{d}}{\mathrm{d}x} f(x)u(x) = f\frac{\mathrm{d}u}{\mathrm{d}x} + u\frac{\mathrm{d}f}{\mathrm{d}x} \quad \text{(product rule)}$$

Examples:

$$\frac{\mathrm{d}}{\mathrm{d}x}(2 + 4x - 7x^3) = 4 - 21x^2$$

$$\frac{\mathrm{d}}{\mathrm{d}x} 10e^{-2x} = -20e^{-2x}$$

$$\frac{\mathrm{d}}{\mathrm{d}x} 15xe^{-ax} = 15(1 - ax)e^{-ax}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}(10 + 3x^3 - 5\ln x) = 9x^2 - \frac{5}{x}$$

Useful Integrals (*a* is a constant)

$$\int_{x_1}^{x_2} \mathrm{d}x = x_2 - x_1$$

$$\int_{x_1}^{x_2} \frac{1}{x}\mathrm{d}x = \ln x_2 - \ln x_1 = \ln\frac{x_2}{x_1}$$

$$\int_{x_1}^{x_2} x\mathrm{d}x = \frac{1}{2}x_2^2 - \frac{1}{2}x_1^2$$

$$\int_{x_1}^{x_2} \mathrm{e}^{ax}\mathrm{d}x = \frac{1}{a}\mathrm{e}^{ax_2} - \frac{1}{a}\mathrm{e}^{ax_1}$$

$$\int_{x_1}^{x_2} x^2\mathrm{d}x = \frac{1}{3}x_2^3 - \frac{1}{3}x_1^3$$

$$\int_{x_1}^{x_2} \ln x\,\mathrm{d}x = x_2 \ln x_2 - x_2 - x_1 \ln x_1 + x_1$$

$$\int_{x_1}^{x_2} x^a\mathrm{d}x = \frac{1}{a+1}x_2^{a+1} - \frac{1}{a+1}x_1^{a+1}$$

$$\int_{x_1}^{x_2} af(x)\mathrm{d}x = a\int_{x_1}^{x_2} f(x)\mathrm{d}x$$

Other Useful Expressions

$$\ln(\mathrm{e}^{ax}) = ax$$

$$\ln a + \ln b = \ln(ab)$$

$$\ln a - \ln b = \ln(a/b)$$

$$\mathrm{e}^a + \mathrm{e}^b = \mathrm{e}^{a+b}$$

$$\ln a = (\ln 10)\log_{10} a$$

$$\mathrm{e}^x = 1 + x + \frac{1}{2!}x^2 + \frac{1}{3!}x^3 + \cdots$$

$$f(x+\Delta x) = f(x) + \frac{\mathrm{d}f}{\mathrm{d}x}\Delta x + \frac{1}{2!}\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}(\Delta x)^2 + \frac{1}{3!}\frac{\mathrm{d}^3 f}{\mathrm{d}x3}(\Delta x)^3 + \cdots$$

Partial Derivatives of Functions with Two Independent Variables

The **partial *x* derivative of *f(x,y)*** holding *y* constant is defined as

$$\left(\frac{\partial f}{\partial x}\right)_y = \lim_{\Delta x \to 0} \frac{f(x+\Delta x, y) - f(x,y)}{\Delta x}$$

Similarly, the **partial *y* derivative of *f(x,y)*** holding *x* constant is defined as

$$\left(\frac{\partial f}{\partial y}\right)_x = \lim_{\Delta y \to 0} \frac{f(x, y+\Delta y) - f(x,y)}{\Delta y}$$

If you can do ordinary differentiation, then you can do partial differentiation! Just keep track of the variable being held constant.

Example $f(x,y) = 37xy^3$

holding *y* constant: $\left(\frac{\partial f}{\partial x}\right)_y = \left[\frac{\partial}{\partial x}(37xy^3)\right]_y = 37y^3\left[\frac{\partial}{\partial x}(x)\right] = 37y^3\,[1] = 37y^3$

holding *x* constant: $\left(\frac{\partial f}{\partial y}\right)_x = \left[\frac{\partial}{\partial y}(37xy^3)\right]_x = 37x\left[\frac{\partial}{\partial x}(y^3)\right] = 37x\left[3y^2\right] = 111xy^2$

Example $V_{\text{m}}(p,T) = RT/p$ for the molar volume of an ideal gas (note that R is a constant)

holding *T* constant: $\left(\frac{\partial V_{\text{m}}}{\partial p}\right)_T = \left[\frac{\partial}{\partial x}\left(\frac{RT}{p}\right)\right]_T = RT\left[\frac{\partial}{\partial p}\left(\frac{1}{p}\right)\right] = RT\left[-\frac{1}{p^2}\right] = -\frac{RT}{p^2} = -\frac{V_{\text{m}}}{p}$

holding *p* constant: $\left(\frac{\partial V_{\text{m}}}{\partial T}\right)_p = \left[\frac{\partial}{\partial T}\left(\frac{RT}{p}\right)\right]_p = \frac{R}{p}\left[\frac{\partial}{\partial T}(T)\right] = \frac{R}{p}[1] = \frac{R}{p} = \frac{V_{\text{m}}}{T}$

Useful Rules for the Partial Derivatives of the Function *f*(*x*,*y*)

Differential of *f*(*x*,*y*)

$$df = \left(\frac{\partial f}{\partial x}\right)_y dx + \left(\frac{\partial f}{\partial y}\right)_x dy$$

Inverse Rule

$$\left(\frac{\partial f}{\partial x}\right)_y = \frac{1}{\left(\frac{\partial x}{\partial f}\right)_y} \quad \text{and} \quad \left(\frac{\partial f}{\partial y}\right)_x = \frac{1}{\left(\frac{\partial y}{\partial f}\right)_x}$$

Cyclic Rule

$$\left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial x}{\partial y}\right)_f \left(\frac{\partial y}{\partial f}\right)_x = -1 \quad \text{and} \quad \left(\frac{\partial f}{\partial x}\right)_y = -\left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial x}\right)_f$$

Mixed Second Derivatives

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

Test for the Existence of the Function *u*(*x*,*y*)

Given $du = g(x,y)dx + h(x,y)dy$

the function *u*(*x*,*y*) exists if

$$\left(\frac{\partial g}{\partial y}\right)_x = \left(\frac{\partial h}{\partial x}\right)_y$$