Univariate Calculus, Integration and Series: Introduction to Thermodynamics

1 Introduction to Integrals

Why do we care about integrals?

Derivatives in natural science are widely used as they help understanding some phenomena. Some of the most common case uses of integrals are:

- Quantum chemistry.
- Spectroscopy, the intensity of absorption or emission is related to the transition dipole moment, which is calculated using an integral:
- Thermodynamics, integrals are used to calculate work done on or by a system and the heat exchanged in processes such as expansion or compression:

2 Deffinition

Integrals are sums.

Integrals were developed to compute the area under the curve (function). One of the most used numerical integration methods is the sum of “bins”. Geometrically this sum represents the represents the sum of the areas of each rectangle, Fig. 1. This approach is know as *Riemann sum.* As we can observe, there is a limitation, depending on the topology of the function we may require more or less “rectangles” to correctly compute the area under the curve for a given function. In the infinite limit of number of “bins”, $(x_i - x_j) \approx 0$, we can defined this sum as a limiting process,

$$\lim_{h\to 0} \sum_{i}^{N} f(\varepsilon_i)h = \int_a^b f(x)dx. \tag{1}$$

Eq. 1 is also known as *Riemann integral.* $f(x)$ is known as the **integrand**.

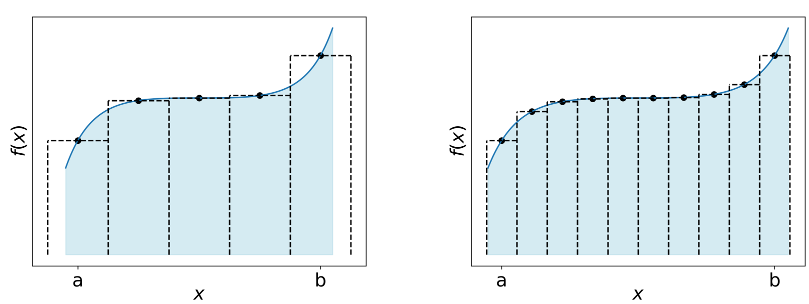

Figure 1: An illustration of integrals.

There are two different types of integrals,

1. definite integrals

$$\int_a^b f(x)dx \tag{2}$$

2. indefinite integrals

$$\int f(x)dx = \int_{-\infty}^{\infty} f(x)dx \tag{3}$$

3 Properties of integrals

Similar to derivatives, integrals have some nice properties that we can use to our advantage.

1. Integrals are linear operations

$$\int_a^b (f(x) + g(x))dx = \int_a^b f(x)dx + \int_a^b g(x)dx \tag{4}$$

2. Constants do not affect integrals

$$\int af(x)dx = a \int f(x)dx \tag{5}$$

3.

$$\int dx = x + c \tag{6}$$

4. Polynomials, $n \neq -1$

$$\int x^n dx = \frac{x^{n+1}}{n+1} + C \tag{7}$$

5. Polynomials, $n = -1$

$$\int \frac{1}{x} dx = lnx + C \tag{8}$$

6. Polynomials, $n = -1$

$$\int e^x dx = e^x + C \tag{9}$$

7. Trigonometric functions

$$\int \cos(x)dx = \sin(x) + C \tag{10}$$

$$\int \sin(x)dx = -\cos(x) + C \tag{11}$$

Exercise: Compute the integral of $f(x) = c$ within the interval a and b.

$$\int_a^b cdx = c \int_a^b dx = cx|_a^b = c(b-a) \tag{12}$$

3.1 Change of variable

Some times it is convenient to use a chain of variable to make the integral easier. This is similar to the chain rule in derivatives.
Exercise: Compute the integral of $f(x) = e^{ax}$ if we define $u = ax$, the total differential of u is

$$du = \left(\frac{\partial u}{\partial x}\right) dx = a dx, \tag{13}$$

meaning $dx = \frac{1}{a} du$.

$$\int e^{ax} dx = \frac{1}{a} \int e^u du = \frac{1}{a} e^u + c = \frac{e^{ax}}{a} + c \tag{14}$$

4 Integration by parts

: Integration by parts is one of the most used methods for computing the integral of complex functions. Integration by parts is defined as,

$$\int u dv = uv - \int v du, \tag{15}$$

where u and v are both functions of x; $u = u(x)$. In Spanish, there is a good mnemonic to memorize integration by parts.

un **d**ia **v**i **u**na **v**aca **v**estida **d**e **u**niforme.

Exercise: Evaluate the following integral

$$\begin{aligned} \int f(x) dx &= \int 10 + \left(\frac{x}{10}\right)^3 e^{\left(\frac{x}{10}\right)^2} dx & (16) \\ &= 10 \int dx + \int \left(\frac{x}{10}\right)^3 e^{\left(\frac{x}{10}\right)^2} dx & (17) \end{aligned}$$

Let's focus on the second integral and use a change of variable, $u = \left(\frac{x}{10}\right)^2$,

$$\begin{aligned} \int \left(\frac{x}{10}\right)^3 e^{\left(\frac{x}{10}\right)^2} dx &= \int \left(\frac{x}{10}\right)^3 \frac{50}{x} e^u du = \int \left(\frac{x}{10}\right)^3 \frac{50}{x} e^u du & (18) \\ &= 5 \int u e^u du & (19) \end{aligned}$$

For this integral it is convenient to use the following definitions for u and v,

$$\begin{aligned} u = u \quad &\text{and} \quad du = du & (20) \\ dv = e^u du \quad &\text{and} \quad v = \int dv = \int e^u du = e^u & (21) \end{aligned}$$

Plugging these equations into Eq. 4, we get,

$$\int u e^u du = u e^u - \int e^u du = u e^u - e^u. \tag{22}$$

Let's bring back the definitions based on x,

$$\int \left(\frac{x}{10}\right)^3 e^{\left(\frac{x}{10}\right)^2} dx = 5 \int u e^u du = 5 e^{\left(\frac{x}{10}\right)^2} \left(\left(\frac{x}{10}\right)^2 - 1\right) \tag{23}$$

The full integral of $f(x)$ is,

$$\int 10 + \left(\frac{x}{10}\right)^3 e^{\left(\frac{x}{10}\right)^2} dx = 10x + \frac{1}{20} e^{\left(\frac{x}{10}\right)^2} \left(x^2 - 100\right) + c \tag{24}$$