Section: Double Integrals and the Meshing Principle

1 Double Integrals: Meshing and Integration by Slicing

In theoretical chemistry and physics (e.g., computing electron densities in a plane, calculating work on a $P-V$ surface, or evaluating the probability of finding a particle $\iint |\Psi|^2\, dxdy$), it is necessary to integrate functions of two variables $f(x,y)$.

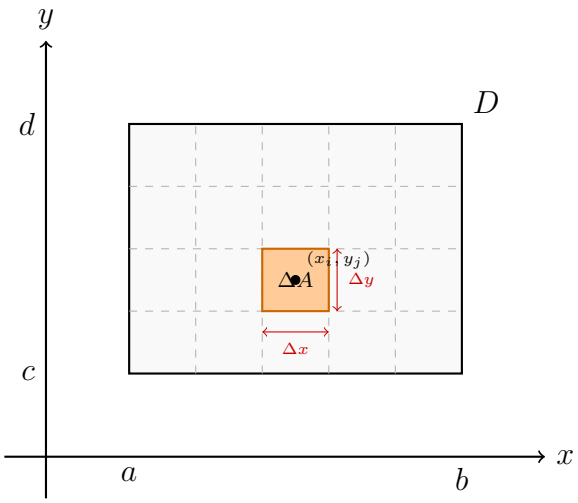
1.1 The Grid Mesh: From Discrete to Continuous

Let $D = [a,b] \times [c,d]$ be a rectangular domain in the plane. To compute the double integral of $f(x,y)$ over D, we begin by partitioning (meshing) this domain:

- The interval $[a,b]$ along the x-axis is divided into n subintervals of width $\Delta x = \frac{b-a}{n}$.
- The interval $[c,d]$ along the y-axis is divided into m subintervals of height $\Delta y = \frac{d-c}{m}$.

This partitioning forms a grid mesh composed of $n \times m$ small rectangular subregions with elementary area:

$$\Delta A = \Delta x \cdot \Delta y$$



Each cell in the grid contributes to the total volume under the surface $z = f(x,y)$ by an elementary volume $\Delta V_{i,j} = f(x_i, y_j)\, \Delta x \Delta y$.

Taking the continuous limit ($\Delta x \to 0$ and $\Delta y \to 0$, i.e., $n, m \to \infty$), the discrete sum becomes the double integral:

$$\iint_D f(x,y)\, dxdy = \lim_{\substack{\Delta x \to 0 \\ \Delta y \to 0}} \sum_{i=1}^{n} \sum_{j=1}^{m} f(x_i, y_j)\, \Delta x\, \Delta y$$

where $dA = dx\, dy$ is the differential surface element.

1.2 Principle of Partial Integration (Fubini's Theorem)

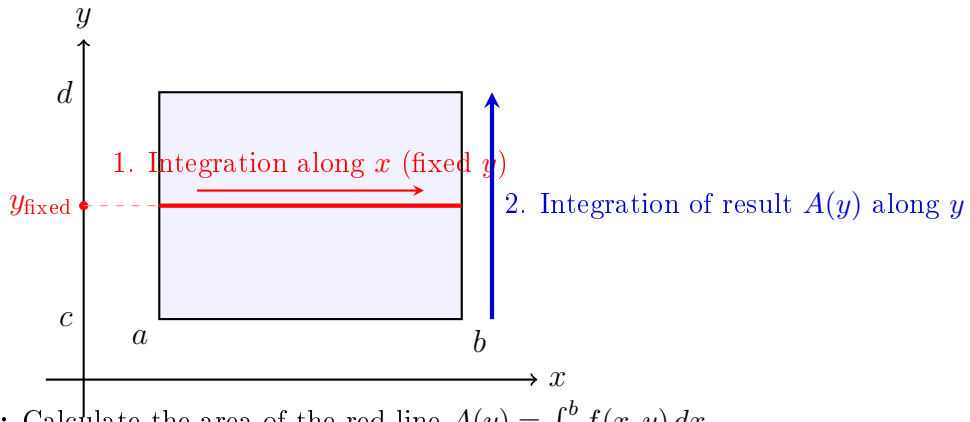
To compute a double integral analytically, we use Fubini's Theorem, which converts the double integral into two successive single-variable integrals (iterated integrals).

Method:

1. Temporarily fix the variable y at a constant value.
2. Integrate the function solely with respect to x from a to b. During this calculation, y is treated exactly as a constant number. This yields an intermediate area function $A(y)$:
$$A(y) = \int_a^b f(x, y)\, dx$$
3. Then integrate this area function $A(y)$ with respect to y from c to d:
$$I = \int_c^d A(y)\, dy = \int_c^d \left(\int_a^b f(x, y)\, dx \right) dy$$

1.3 Schematic Representation: The Method of Slices

Schematically, integrating with respect to x for a fixed y is equivalent to making a "cross-section" or "slice" through the volume under the surface $z = f(x, y)$.



Step 1: Calculate the area of the red line $A(y) = \int_a^b f(x, y)\, dx$.

Step 2: Sum all lines from $y = c$ to $y = d$.

1.4 Detailed Analytical Example

Let us evaluate the following double integral over the domain $D = [0, 2] \times [1, 3]$:

$$I = \iint_D (x^2 y + 3y^2)\, dx\, dy$$

Step 1: Inner integration with respect to x (y is kept FIXED) Isolate the inner integral:

$$A(y) = \int_0^2 (x^2 y + 3y^2)\, dx$$

Since y is treated as a constant:

- An antiderivative of x^2y with respect to x is $\frac{x^3}{3}y$.
- An antiderivative of the constant $3y^2$ with respect to x is $3y^2x$.

Evaluating from $x = 0$ to $x = 2$:

$$A(y) = \left[\frac{x^3}{3}y + 3y^2x\right]_{x=0}^{x=2} = \left(\frac{8}{3}y + 6y^2\right) - (0) = \frac{8}{3}y + 6y^2$$

Step 2: Outer integration with respect to y Now we evaluate a simple single-variable integral with respect to y from $y = 1$ to $y = 3$:

$$I = \int_1^3 A(y)\,dy = \int_1^3 \left(\frac{8}{3}y + 6y^2\right) dy$$

Calculating the antiderivatives with respect to y:

$$I = \left[\frac{8}{3} \cdot \frac{y^2}{2} + 6 \cdot \frac{y^3}{3}\right]_1^3 = \left[\frac{4}{3}y^2 + 2y^3\right]_1^3$$

Evaluating at the boundaries:

$$\begin{aligned} I &= \left(\frac{4}{3}(3)^2 + 2(3)^3\right) - \left(\frac{4}{3}(1)^2 + 2(1)^3\right) \\ &= \left(\frac{4}{3}(9) + 2(27)\right) - \left(\frac{4}{3} + 2\right) \\ &= (12 + 54) - \left(\frac{4}{3} + \frac{6}{3}\right) \\ &= 66 - \frac{10}{3} = \frac{198 - 10}{3} = \boxed{\mathbf{\frac{188}{3}}} \approx \mathbf{62.67} \end{aligned}$$