Multiple Integrals, Numerical Integration and Monte Carlo Methods

I-exercises

Exercise I1: Double integral

Calculate:

$$I = \int_0^1 \int_0^1 (x + y) dy dx.$$

Explain the physical meaning of the result.

Exercise I2: Triple integral

Calculate the volume:

$$V = \int_0^2 \int_0^1 \int_0^1 1 \, dz \, dy \, dx.$$

Explain why this is a triple integral.

Exercise I3: Numerical integration with the *Trapezoidal Rule*

A function:

$$f(x) = x^2$$

is integrated over:

$$0 \leq x \leq 1.$$

Use:

$$N = 10$$

intervals. Compare the numerical result with the exact value:

$$\frac{1}{3}.$$

Exercise I4: Curse of dimensionality

A grid uses:

$$N = 50$$

points per dimension.
Calculate the number of points for:

$$d = 1, 2, 3, 6.$$

Explain why this becomes impossible.

Exercise I5: Monte Carlo estimate

Random samples give:

$$f(x_1), f(x_2), \ldots, f(x_N).$$

Explain how:

$$\frac{1}{N}\sum_i f(x_i)$$

can approximate an integral.

Exercise I6: Chemical application

A molecule contains:

$$N = 500$$

atoms. Calculate the number of spatial degrees of freedom:

$$d = 3N.$$

Explain why grid integration is impossible and why Monte Carlo methods are appropriate.

Final Conclusion

The main message of this course is:

High-dimensional scientific problems require intelligent sampling.

The progression is:

calculus
↓
multiple integrals
↓
numerical methods
↓
Monte Carlo
↓
modern computational chemistry

Monte Carlo integration provides a bridge between mathematics, computation and chemistry.

Extra exercises

Exercise I7

Approximate $\int_0^1 x^2\,dx$ using the trapezoidal rule with $\Delta x = 1$. What is the numerical error? Compare this error with the prediction:

$$\text{error} \approx -\frac{(b-a)}{12}(\Delta x)^2\,\overline{f''}.$$

Comment on your result. Make a sketch of the approximation alongside the graph of $y = x^2$.

Exercise I8

Calculate $\int_0^\pi \sin(x)\,dx$ using both the midpoint rule (rectangular rule) and the trapezoidal rule using 3 subintervals. How accurate are both approximations? Make a sketch of the approximation alongside the graph of $y = \sin(x)$.

The Trapezoidal Rule in Two Dimensions

Consider the domain $\Omega = [a, b] \times [c, d]$ in two dimensions, as shown in Figure **??**. The two-dimensional version of the trapezoidal rule for the double integral $\int_c^d \int_a^b f(x, y)\,dx\,dy$ is obtained by applying the one-dimensional rule sequentially in both spatial directions:

$$\int_c^d \int_a^b f(x, y)\,dx\,dy \approx \tag{1}$$

$$\begin{aligned}
&\int_c^d \left\{ \frac{\Delta x}{2} \left[f(x_0, y) + 2f(x_1, y) + 2f(x_2, y) + \cdots + 2f(x_{n-1}, y) + f(x_n, y) \right] \right\} dy \\
&= \frac{\Delta x}{2} \left[\int_c^d f(x_0, y)\,dy + 2\int_c^d f(x_1, y)\,dy + \cdots + 2\int_c^d f(x_{n-1}, y)\,dy + \int_c^d f(x_n, y)\,dy \right] \\
&\approx \frac{\Delta x}{2} \left[\frac{\Delta y}{2} \left\{ f(x_0, y_0) + 2f(x_0, y_1) + \cdots + 2f(x_0, y_{m-1}) + f(x_0, y_m) \right\} \right. \\
&\quad + \frac{\Delta y}{2} \cdot 2 \left\{ f(x_1, y_0) + 2f(x_1, y_1) + \cdots + 2f(x_1, y_{m-1}) + f(x_1, y_m) \right\} + \ldots \\
&\quad + \frac{\Delta y}{2} \cdot 2 \left\{ f(x_{n-1}, y_0) + 2f(x_{n-1}, y_1) + \cdots + 2f(x_{n-1}, y_{m-1}) + f(x_{n-1}, y_m) \right\} \\
&\quad \left. + \frac{\Delta y}{2} \left\{ f(x_n, y_0) + 2f(x_n, y_1) + \cdots + 2f(x_n, y_{m-1}) + f(x_n, y_m) \right\} \right] \\
&= \frac{\Delta x \Delta y}{4} \{ \ldots \}.
\end{aligned}$$

Exercise I9

Calculate $\int_0^1 \int_0^1 xy\,dx\,dy$ with $\Delta x = \Delta y = 1$ using the two-dimensional trapezoidal rule. Determine the exact value of the integral as well. What is the resulting numerical error?

Exercise I10

Derive the midpoint rule (rectangular rule) for a double integral $\int_c^d \int_a^b f(x, y)\,dx\,dy$. Next, apply your derived formula to evaluate:

$$\int_{-2}^{2} \int_0^4 (x^2 - 3y^2 + xy^3)\,dx\,dy$$

using $\Delta x = \Delta y = 1$. What is the numerical error? (Calculate the exact value of this integral as well for comparison.)

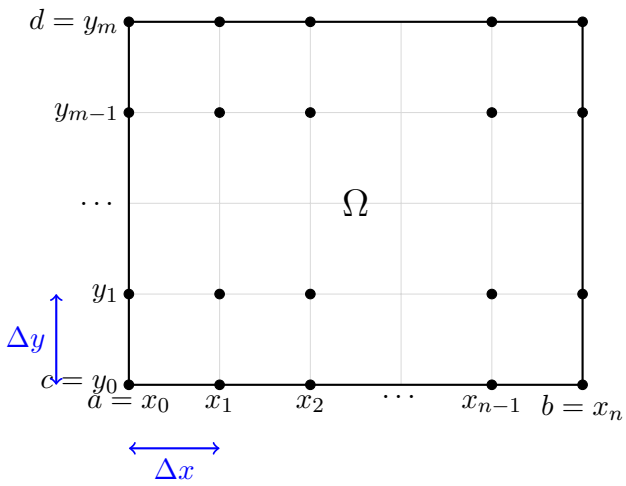


Figure 1: A rectangular domain $\Omega = [a, b] \times [c, d]$ with its associated numerical grid on which the double integral from (**??**) is approximated.