Multiple Integrals, Numerical Integration and Monte Carlo Methods

Solutions: I1–I6

Exercise I1: Double integral

Problem. Calculate

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

and explain the physical meaning of the result.

Solution

We integrate first with respect to y. Since x is constant during this integration,

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

The first term is

$$\int_0^1 x\, dy = x[y]_0^1 = x,$$

and the second term is

$$\int_0^1 y\, dy = \left[\frac{y^2}{2}\right]_0^1 = \frac{1}{2}.$$

Therefore

$$\int_0^1 (x + y)\, dy = x + \frac{1}{2}.$$

We now integrate with respect to x:

$$I = \int_0^1 \left(x + \frac{1}{2}\right) dx.$$

Thus

$$I = \left[\frac{x^2}{2} + \frac{x}{2}\right]_0^1 = \frac{1}{2} + \frac{1}{2} = 1.$$

Hence

$$\boxed{I = 1}.$$

Physical interpretation. The integral adds up the quantity represented by the density or field $x + y$ over the unit square

$$0 \le x \le 1, \qquad 0 \le y \le 1.$$

For example, if $x + y$ represents a surface density (mass per unit area), then I is the total mass of the square. Thus the result

$$\boxed{1}$$

is the total accumulated quantity over the two-dimensional region.

Exercise I2: Triple integral

Problem. Calculate the volume

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

and explain why this is a triple integral.

Solution

The integrand is simply 1. We first integrate with respect to z:

$$\int_0^1 1 \, dz = [z]_0^1 = 1.$$

Therefore

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

Next,

$$\int_0^1 1 \, dy = 1,$$

so

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

Finally,

$$V = [x]_0^2 = 2.$$

Hence

$$\boxed{V = 2}.$$

Geometrical interpretation. The integration region is

$$0 \le x \le 2, \qquad 0 \le y \le 1, \qquad 0 \le z \le 1.$$

This is a rectangular box with side lengths

$$2, \quad 1, \quad 1.$$

Its volume is therefore

$$2 \cdot 1 \cdot 1 = 2,$$

in agreement with the triple integral.

Why is this a triple integral? There are three independent spatial coordinates, x, y, and z. The volume element is

$$dV = dx \, dy \, dz.$$

Consequently, a volume calculation in three-dimensional space is naturally written as a three-dimensional, or triple, integral:

$$\boxed{\iiint_\Omega 1 \, dV}.$$

Exercise I3: Numerical integration

Problem. For

$$f(x) = x^2, \qquad 0 \le x \le 1,$$

use $N = 10$ intervals to obtain a numerical integral and compare it with the exact value $1/3$.

Solution

The interval length is

$$\Delta x = \frac{1-0}{10} = 0.1.$$

Using the composite trapezoidal rule,

$$T_N = \Delta x \left[\frac{1}{2} f(x_0) + \sum_{i=1}^{N-1} f(x_i) + \frac{1}{2} f(x_N) \right],$$

where

$$x_i = i\Delta x = 0.1i.$$

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

$$f(x_0) = 0, \qquad f(x_{10}) = 1.$$

The interior points give

$$\sum_{i=1}^{9} f(x_i) = \sum_{i=1}^{9} (0.1i)^2 = 0.01 \sum_{i=1}^{9} i^2.$$

Using

$$\sum_{i=1}^{9} i^2 = \frac{9(10)(19)}{6} = 285,$$

we obtain

$$\sum_{i=1}^{9} f(x_i) = 2.85.$$

Therefore

$$T_{10} = 0.1 \left(0 + 2.85 + \frac{1}{2} \right) = 0.1(3.35) = 0.335.$$

Thus the numerical result is

$$\boxed{T_{10} = 0.335}.$$

The exact integral is

$$\int_0^1 x^2 \, dx = \left[\frac{x^3}{3} \right]_0^1 = \boxed{\frac{1}{3} \approx 0.333333}.$$

The absolute error is

$$|T_{10} - 1/3| = 0.335 - 0.333333\ldots \approx 0.001667.$$

Hence the numerical result is already quite close to the exact answer.

Remark. The original exercise only specifies $N = 10$ intervals, not a particular quadrature rule. Here the composite trapezoidal rule has been used explicitly. Different numerical rules, such as the midpoint or Simpson rule, give different approximations.

Exercise I4: Curse of dimensionality

Problem. A grid uses $N = 50$ points per dimension. Calculate the number of points for

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

and explain why this becomes impossible.

Solution

If there are $N = 50$ points in each dimension and there are d dimensions, then the total number of grid points is

$$N_{\text{total}} = N^d = 50^d.$$

For $d = 1$,

$$50^1 = 50.$$

For $d = 2$,

$$50^2 = 2500.$$

For $d = 3$,

$$50^3 = 125000.$$

For $d = 6$,

$$50^6 = 15\,625\,000\,000.$$

Therefore,

d	50^d
1	50
2	2 500
3	125 000
6	15 625 000 000

Why is this a problem? The crucial point is that the number of grid points grows exponentially with the dimension:

$$\boxed{N_{\text{total}} = N^d}.$$

This is called the *curse of dimensionality*.
Going from three to six dimensions does not merely double the number of grid points. Instead,

$$50^6$$

is more than fifteen billion points.
If each point requires function evaluations, memory, and computational work, the cost rapidly becomes prohibitive. This is why methods based on a full tensor-product grid become unsuitable for many high-dimensional problems.

Exercise I5: Monte Carlo estimate

Problem. 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.

Solution

Suppose first that we want to calculate

$$I = \int_a^b f(x)\,dx.$$

The interval has length

$$L = b - a.$$

Choose independent random points

$$x_1, \ldots, x_N$$

uniformly from $[a, b]$.
For a uniformly distributed random variable X on $[a, b]$,

$$\mathbb{E}[f(X)] = \frac{1}{b-a}\int_a^b f(x)\,dx.$$

Therefore,

$$\int_a^b f(x)\,dx = (b-a)\mathbb{E}[f(X)].$$

The Monte Carlo approximation replaces the expectation by the sample average:

$$\mathbb{E}[f(X)] \approx \frac{1}{N}\sum_{i=1}^{N} f(x_i).$$

Consequently,

$$\boxed{I \approx \frac{b-a}{N}\sum_{i=1}^{N} f(x_i).}$$

If the integration region has volume V_Ω in d dimensions, the corresponding formula is

$$\boxed{\int_\Omega f(\mathbf{x})\,d\mathbf{x} \approx V_\Omega \frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}_i).}$$

Why does this work? The law of large numbers states that, for independent samples,

$$\frac{1}{N}\sum_{i=1}^{N} f(x_i) \longrightarrow \mathbb{E}[f(X)] \qquad \text{as } N \to \infty.$$

Therefore the Monte Carlo estimate converges to the desired integral.
For independent samples with finite variance, the statistical error typically scales as

$$\boxed{\text{error} \sim N^{-1/2}}.$$

Important point for high dimensions. Monte Carlo does not require a full tensor-product grid. The number of samples can therefore be increased without multiplying the sampling points by a factor of N in every dimension. This is the main reason Monte Carlo methods become attractive for high-dimensional integrals.

Exercise I6: Chemical application

Problem. 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.

Solution

Each atom has three spatial coordinates:

$$(x_i, y_i, z_i).$$

Therefore, for N atoms, the number of spatial coordinates is

$$d = 3N.$$

With

$$N = 500,$$

we obtain

$$d = 3(500) = 1500.$$

Hence

$$\boxed{d = 1500}.$$

Why is a grid impossible? Suppose, only as an illustration, that we used 50 grid points in every coordinate direction. A full tensor-product grid would then contain

$$50^{1500}$$

points.
This number is astronomically large. For comparison, its decimal order of magnitude is

$$50^{1500} = 10^{1500\log_{10}(50)} \approx 10^{2548.5}.$$

Thus a direct grid representation is completely impractical.
The problem is precisely the curse of dimensionality:

$$\boxed{N_{\text{grid}} = N_{\text{points}}^{d}}.$$

Even a moderate number of points per coordinate becomes impossible when d is large.

Why is Monte Carlo appropriate? Monte Carlo methods do not construct the complete tensor-product grid. Instead, they generate a collection of sample configurations

$$\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_M$$

in the high-dimensional configuration space.
An integral can then be estimated from an average such as

$$\int_\Omega f(\mathbf{x})\, d\mathbf{x} \approx V_\Omega \frac{1}{M} \sum_{j=1}^{M} f(\mathbf{x}_j).$$

The number of samples M does not have to scale as

$$50^{1500}.$$

This makes stochastic sampling feasible even when the configuration space has hundreds or thousands of dimensions.

Chemical interpretation. For a molecule with 500 atoms, the configuration is described by 1500 spatial coordinates before accounting for possible constraints such as translation, rotation, or molecular bonds. Many quantities in molecular simulation involve integrals or averages over this high-dimensional configuration space. Monte Carlo sampling provides a practical way to explore that space without constructing an impossible full grid.

Final Conclusion

The six exercises illustrate a natural progression:

calculus $\longrightarrow$ multiple integrals $\longrightarrow$ numerical methods $\longrightarrow$ Monte Carlo $\longrightarrow$ high-dimensional scientific applic

The central computational difficulty is that tensor-product grids scale exponentially with dimension:

$$N_{\text{grid}} = N^d.$$

Monte Carlo methods avoid this particular exponential grid construction by replacing systematic coverage of the entire domain with statistical sampling.
Thus the main message is

High-dimensional scientific problems require intelligent sampling.

Monte Carlo integration provides an important bridge between mathematics, computation, and applications such as computational chemistry.