Multiple Integrals, Numerical Quadrature, and Monte Carlo Methods

Extra file for Lecture 6

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Abstract

These lecture notes provide a systematic transition from classical multivariate calculus to modern high-dimensional computational algorithms. Starting with double and triple integrals, we introduce deterministic quadrature rules and examine their fundamental limitation: the curse of dimensionality. To bypass this computational bottleneck, we develop the theory of Monte Carlo integration based on probability theory, the Law of Large Numbers, and the Central Limit Theorem. Finally, we discuss high-dimensional applications in physical and computational chemistry, such as molecular phase-space integration with hundreds of degrees of freedom.

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1 Multivariate Calculus: Double and Triple Integrals

In single-variable calculus, the definite integral $\int_a^b f(x)\,dx$ represents the net signed area under a curve $f(x)$ over a one-dimensional interval $[a, b]$. When extending integration to functions of multiple variables, the domain of integration expands from intervals to higher-dimensional regions in $\mathbb{R}^n$.

1.1 Double Integrals over Planar Regions

Consider a continuous function $f(x, y)$ defined over a bounded closed region $R \subset \mathbb{R}^2$.

Definition 1.1 (Double Integral)**.** *The double integral of $f(x, y)$ over R is defined as the limit of a 2D Riemann sum:*

$$\iint_R f(x, y)\,dA = \lim_{\Delta x, \Delta y \to 0} \sum_i \sum_j f(x_i^*, y_j^*)\,\Delta x \Delta y,$$

where $dA = dx\,dy$ denotes the differential area element.

1.1.1 Physical Interpretations of the Double Integral

- **Volume under a Surface:** If $f(x, y) \geq 0$, then $I = \iint_R f(x, y)\,dA$ computes the three-dimensional volume bounded above by $z = f(x, y)$ and below by the planar region R.
- **Total Mass / Charge:** If $f(x, y) = \rho(x, y)$ represents a surface mass or charge density, the integral gives the total accumulated mass or total electric charge over R.
- **Average Value / Expectation:** The spatial average of $f(x, y)$ over R is given by:

$$\bar{f} = \frac{1}{\text{Area}(R)} \iint_R f(x, y)\,dA.$$

Theorem 1.1 (Fubini's Theorem)**.** *If $f(x, y)$ is continuous on a rectangular region $R = [a, b] \times [c, d]$, the double integral can be evaluated as an iterated integral in any order:*

$$\iint_R f(x, y)\,dA = \int_a^b \left(\int_c^d f(x, y)\,dy \right) dx = \int_c^d \left(\int_a^b f(x, y)\,dx \right) dy.$$

Example 1.1 (Evaluation of a Double Integral)**.** *Evaluate $I = \int_0^1 \int_0^1 (x + y)\,dy\,dx$ and interpret its meaning.*

Solution: *We evaluate the inner integral with respect to y first, treating x as a constant:*

$$\int_0^1 (x + y)\,dy = \left[xy + \frac{1}{2}y^2 \right]_{y=0}^{y=1} = x(1) + \frac{1}{2}(1)^2 - 0 = x + \frac{1}{2}.$$

Next, we integrate this intermediate result with respect to x:

$$I = \int_0^1 \left(x + \frac{1}{2} \right) dx = \left[\frac{1}{2}x^2 + \frac{1}{2}x \right]_0^1 = \frac{1}{2}(1)^2 + \frac{1}{2}(1) = 1.$$

Physical Meaning: *Since the area of the domain $R = [0, 1] \times [0, 1]$ is 1, $I = 1$ represents both the 3D volume under $z = x + y$ and the spatial average value $\bar{f} = 1/1 = 1$.*

1.2 Triple Integrals and Volumes in 3D Space

Extending the integral to three-dimensional domains $V \subset \mathbb{R}^3$ yields the triple integral:

$$\iiint_V f(x,y,z)\,dV = \lim_{\Delta x,\Delta y,\Delta z\to 0} \sum_i \sum_j \sum_k f(x_i^*, y_j^*, z_k^*)\,\Delta x \Delta y \Delta z,$$

where $dV = dz\,dy\,dx$ is the differential volume element.

When $f(x,y,z) = 1$ everywhere, the integral computes the exact geometric volume of the domain:

$$\text{Volume}(V) = \iiint_V 1\,dz\,dy\,dx.$$

Example 1.2 (Volume of a Rectangular Box)**.** *Calculate* $V = \int_0^2 \int_0^1 \int_0^1 1\,dz\,dy\,dx$.

Solution: *Integrating layer by layer:*

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

This computes the volume of a $2\times 1\times 1$ *cuboid.*

2 Deterministic Numerical Integration (Quadrature)

In real-world applications, closed-form analytical integration is rarely possible. We must approximate integrals numerically using a finite set of N function evaluations.

2.1 1D Quadrature Rules

To approximate $I = \int_a^b f(x)\,dx$, we divide $[a,b]$ into N equal subintervals of width $h = \frac{b-a}{N}$, with grid points $x_i = a + ih$.

1. **Left/Right Riemann Sums:**

$$I_{\text{Left}} = h\sum_{i=0}^{N-1} f(x_i), \quad \text{Error: } \mathcal{O}(h) = \mathcal{O}(N^{-1}).$$

2. **Midpoint Rule:**

$$I_{\text{Mid}} = h\sum_{i=0}^{N-1} f\left(x_i + \frac{h}{2}\right), \quad \text{Error: } \mathcal{O}(h^2) = \mathcal{O}(N^{-2}).$$

3. **Trapezoidal Rule:**

$$I_{\text{Trap}} = h\left(\frac{f(x_0)}{2} + \sum_{i=1}^{N-1} f(x_i) + \frac{f(x_N)}{2}\right), \quad \text{Error: } \mathcal{O}(h^2) = \mathcal{O}(N^{-2}).$$

Example 2.1 (Numerical Convergence)**.** *Consider integrating* $f(x) = x^2$ *over* $[0,1]$ *(*$I_{exact} = 1/3 \approx 0.33333$*). For* $N = 10$*,* $h = 0.1$*:*

$$x_i = 0.1\cdot i \implies I_{Mid} = 0.1\sum_{i=0}^{9}(0.1i + 0.05)^2 = 0.3325.$$

The error is $|0.33333 - 0.3325| = 0.000833$*, which decays quadratically as* N *increases.*

3 The Curse of Dimensionality

When extending deterministic grid-based numerical integration to d-dimensional hypercubes $[0,1]^d$:

$$I = \int_{[0,1]^d} f(x_1, x_2, \ldots, x_d)\, dx_1\, dx_2 \cdots dx_d,$$

we place N_1 grid points along each coordinate axis.

3.1 Exponential Growth of Computational Cost

The total number of evaluation points M required to cover the d-dimensional grid is:

$$M = (N_1)^d.$$

Table 1: Grid points $M = 50^d$ required for $N_1 = 50$ points per dimension.

Dimension (d)	**Total Points (M)**	**Feasibility**
1	$50^1 = 50$	Instantaneous (< 1 ms)
2	$50^2 = 2{,}500$	Instantaneous (< 1 ms)
3	$50^3 = 125{,}000$	Fast (< 0.1 s)
6	$50^6 = 1.5625 \times 10^{10}$	Seconds to Minutes
10	$50^{10} \approx 9.77 \times 10^{16}$	Terabytes/Days
100	$50^{100} \approx 7.88 \times 10^{169}$	Physically Impossible ($>$ atoms in universe)

3.2 Error Scaling in High Dimensions

If a 1D quadrature rule has error $\mathcal{O}(N_1^{-r})$, expressing the error in terms of total function evaluations $M = N_1^d$ gives:

$$\text{Error} = \mathcal{O}\left(M^{-r/d}\right).$$

As dimension $d \to \infty$, the rate of convergence $r/d \to 0$. Grid methods completely fail in high dimensions.

4 Monte Carlo Integration

Monte Carlo integration overcomes the curse of dimensionality by replacing deterministic grid points with N independent uniformly distributed random samples $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N \sim \text{Uniform}(\Omega)$.

4.1 Mathematical Foundation

Let $\Omega \subset \mathbb{R}^d$ be a domain with volume $V = \int_\Omega d\mathbf{x}$. The integral of $f(\mathbf{x})$ can be reinterpreted as an expectation value:

$$I = \int_\Omega f(\mathbf{x})\, d\mathbf{x} = V \cdot \mathbb{E}[f(\mathbf{X})], \quad \text{where } \mathbf{X} \sim \text{Uniform}(\Omega).$$

The Monte Carlo estimator $\hat{I}_N$ is defined as the sample mean:

$$\hat{I}_N = \frac{V}{N} \sum_{i=1}^{N} f(\mathbf{x}_i).$$

4.2 Statistical Properties

1. **Unbiasedness:**
$$\mathbb{E}[\hat{I}_N] = \frac{V}{N}\sum_{i=1}^{N}\mathbb{E}[f(\mathbf{x}_i)] = \frac{V}{N}\cdot N\cdot\frac{I}{V} = I.$$

2. **Variance and Standard Error:** Let $\sigma^2 = \mathrm{Var}[f(\mathbf{X})]$. The variance of the estimator is:
$$\mathrm{Var}[\hat{I}_N] = \frac{V^2}{N^2}\sum_{i=1}^{N}\mathrm{Var}[f(\mathbf{x}_i)] = \frac{V^2\sigma^2}{N}.$$
The standard error σ_N is:
$$\sigma_N = \sqrt{\mathrm{Var}[\hat{I}_N]} = \frac{V\sigma}{\sqrt{N}} = \mathcal{O}\left(\frac{1}{\sqrt{N}}\right).$$

Theorem 4.1 (Dimension Independence of Monte Carlo)**.** *The statistical error of Monte Carlo integration decays as $\mathcal{O}(N^{-1/2})$,* ***regardless of the spatial dimension*** *d.*

5 Applications in Computational Chemistry

In molecular modeling, computational chemistry, and statistical mechanics, physical observables are computed as ensemble averages over molecular microstates.

5.1 Phase-Space Integration

Consider a macro-molecule (e.g., a protein or polymer) composed of N_{atom} atoms.

- Each atom i has 3 spatial coordinates (x_i, y_i, z_i).
- The total spatial dimension of the configuration space is:
$$d = 3N_{\text{atom}}.$$

For $N_{\text{atom}} = 500$, the dimension is $d = 3\times 500 = 1500$.

The thermodynamic expectation value of a physical property $A(\mathbf{q})$ (such as potential energy or binding affinity) is given by the high-dimensional Boltzmann integral:
$$\langle A\rangle = \frac{\int_{\mathbb{R}^{3N}} A(\mathbf{q})\, e^{-\frac{U(\mathbf{q})}{k_BT}}\, d\mathbf{q}}{\int_{\mathbb{R}^{3N}} e^{-\frac{U(\mathbf{q})}{k_BT}}\, d\mathbf{q}}.$$

5.2 Why Grid Methods Fail and Monte Carlo Succeeds

1. **Impossibility of Grid Integration:** Even using a ultra-coarse grid of $N_1 = 2$ points per coordinate, evaluating $d = 1500$ dimensions requires $2^{1500} \approx 3.5\times 10^{451}$ function evaluations!

2. **Efficiency of Stochastic Sampling:** Markov Chain Monte Carlo (MCMC) methods (such as the Metropolis-Hastings algorithm) sample configurations $\mathbf{q}_i$ directly from the probability density $P(\mathbf{q}) \propto e^{-U(\mathbf{q})/k_BT}$, concentrating compute power strictly in low-energy, physically relevant regions.

6 Summary & Conceptual Hierarchy

Modern computational modelling relies on a clear progression from classical calculus to stochastics:

Calculus
(Single-variable integration)
↓
Multiple Integrals
(Area, volume, multi-variable density)
↓
Numerical Quadrature
(Riemann, Trapezoidal, Grid methods)
↓
Curse of Dimensionality
(Exponential grid explosion $M = N_1^d$)
↓
Monte Carlo Methods
(Stochastic sampling, $\mathcal{O}(1/\sqrt{N})$ convergence)
↓
Computational Chemistry & Physics
(High-dimensional molecular state integration)