Quadrature Rules and the Curse of Dimensionality

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Overview

1. Ubiquitous high dimensional integrals in physics
2. Numerical quadratures for high dimensional integrals
3. Breaking the curse of dimensionality
4. Some open issues concerning applications in physics

Ubiquitous high dimensional integrals in physics

In statistical, condensed matter and high energy physics high dimensional integrals are ubiquitous.

- Classical Monte Carlo (statistical physics)

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{O}(X)\, e^{-\beta V(X)}\, dX, \quad dX := dx_1 dx_2 \ldots dx_n, \; \beta = \frac{1}{k_B T}$$

- Path integral Monte Carlo (quantum physics)

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{O}(X) \rho(X, X, \beta)\, dX$$

heat kernel

$$\rho(X, \tilde{X}, \beta) = \sum_{\alpha} \bar{\Psi}_{\alpha}(\tilde{X}) \Psi_{\alpha}(X) e^{-\beta E_{\alpha}}$$

- Feynman Kac (diffusion MC)

$$|\Psi_0\rangle \sim \lim_{\tau \to \infty} e^{-\tau(H - E_0)} |\Phi_0\rangle$$

Ubiquitous high dimensional integrals in physics

- Feynman diagrams (configuration space)

$$F(a_1,\dots,a_m) = \int \Gamma_n(a_1,\dots,a_m,x_1,\dots,x_n)\,dx_1\cdots dx_n$$

$$\Gamma_n(a_1,\dots,a_m,x_1,\dots,x_n) = \prod_{i<j} u(x_i,x_j)^{n_{ij}}$$

n_{ij}: number of propagators between the vertices i and j.

- Lattice gauge theory

$$\langle \mathcal{O} \rangle = \frac{\int \prod_{p,\nu,B} dA_\nu^B(p)\mathcal{O}(A_\nu^B)\big(\det\Delta\big)^{N_f} e^{-S_{\text{measure}}-S_g}}{\int \prod_{p,\nu,B} dA_\nu^B(p)\big(\det\Delta\big)^{N_f} e^{-S_{\text{measure}}-S_g}}$$

Numerical quadratures for high dimensional integrals

Problem: approximate the integral

$$I(f) := \int_{\Omega} f(x)\rho(x)dx$$

with $\Omega \subset \mathbb{R}^d$, $f : \Omega \to \mathbb{R}$, by a quadrature rule

$$Q_N(f) = \sum_{i=1}^{N} w_i f(x_i)$$

where $x_i \in \Omega$ and w_i, $i = 1, \ldots, N$ denote quadrature points and weights, respectively.

Product quadrature rules

Uni-variate quadrature rules, e.g., Gaussian quadratures which provide polynomial exactness, can be tensorized in order to get quadrature rules in higher dimensions

$$
\begin{aligned}
Q^{\text{prod}}_{N_{l_1}\dots N_{l_d}}(f) &:= Q_{l_1} \otimes \cdots \otimes Q_{l_d}(f) \\
&= \sum_{i_1=1}^{N_{l_1}} \cdots \sum_{i_d=1}^{N_{l_d}} w_{i_1} \cdots w_{i_d} f(x_{i_1}, \cdots, x_{i_d})
\end{aligned}
$$

- Number of quadrature points: $\prod_{i=1}^{d} N_{l_i}$
- Convergence rate: $|I(f) - Q^{\text{prod}}_{N\dots N}(f)| \lesssim N^{-s/d}$
- Simply tensorising one-dimensional quadrature rules leads to the curse of dimensionality.

Monte Carlo methods

Let $x_1, \ldots, x_N$ be independend and identically distributed samples

$$Q_N^{\mathrm{MC}}(f) := \frac{1}{N} \sum_{i=1}^{N} f(x_i)$$

- Mean square error

$$\mathbb{E}\left[|I(f) - Q_N^{\mathrm{MC}}(f)|^2 \right] \leq \frac{1}{N} \mathrm{Var}(f)$$

- Slow but dimension independent convergence $\sim N^{-\frac{1}{2}}$
- Variance reduction techniques.
- Requires rather weak assumptions on the integrand.

Some input from functional analysis

Function spaces and their properties

- Standard Sobolev spaces ($|\alpha|_1 := \alpha_1 + \cdots \alpha_d$)

$$H^s(\Omega) := \{f : \Omega \to \mathbb{R},\ \partial^\alpha f \in L_2(\Omega) \text{ for all } |\alpha|_1 \leq s\}$$

- Sobolev spaces of mixed regularity ($|\alpha|_\infty := max\{\alpha_1, \ldots, \alpha_d\}$)

$$H^s_{\text{mix}}(\Omega) := \{f : \Omega \to \mathbb{R},\ \partial^\alpha f \in L_2(\Omega) \text{ for all } |\alpha|_\infty \leq s\}$$

- Best possible convergence rates for quadrature rules
  - $H^s([0,1]^d)$: $N^{-s/d}$
  - $H^s_{\text{mix}}([0,1]^d)$: $N^{-s}\log(N)^{(d-1)/2}$
- Mathematical complexity theory usually refers to a large class of functions, e.g. Sobolev spaces, in constrast to this solutions of physical models are often in rather narrow classes.

Quasi Monte Carlo methods

Deterministic quadrature points with good descrepancy

$$D^*(x^{(1)}, \dots, x^{(N)}) := \sup_{y \in [0,1)^d} \left| \frac{|\{x^{(i)} \in [0,y]\}|}{N} - \mathrm{vol}([0,y]) \right|$$

QMC convergence rate for star-descrepancy

$$\left| \frac{1}{N} \sum_{i=1}^{N} f(x^{(i)}) - \int_{[0,1]^d} f(x)dx \right| \lesssim D^*(x^{(1)}, \dots, x^{(N)}) \|f\|_{H^1_{\mathrm{mix}}}$$

Low-descrepancy sequences (Halton, Hammersley or Sobol points) satisfy

$$D^*(x^{(1)}, \dots, x^{(N)}) \lesssim N^{-1} \log(N)^{d-1}$$

$$D^*(x^{(1)}, \dots, x^{(N)}) \lesssim N^{-1} \log(N)^{d}$$

Sparse grid quadratures

Construction of a sparse grid quadrature rule

- Sequences of one-dimensional quadrature rules with nested sets of quadrature points $\Gamma_k \subset \Gamma_{k+1}$
- difference operators (1d) using the quadrature points $\Lambda_k := \Gamma_k \setminus \Gamma_{k-1}$:

$$\begin{aligned} \Delta_k(f) &= Q_k(f) - Q_{k-1}(f), \text{ for } k \geq 1 \\ \Delta_0(f) &= Q_0(f) \end{aligned}$$

- Sparse grid quadrature $|\mathbf{k}|_1 := k_1 + \cdots k_d$

$$Q_\ell^{\text{sg}}(f) = \sum_{|\mathbf{k}|_1 \leq \ell + d - 1} \Delta_{k_1} \otimes \cdots \otimes \Delta_{k_d}(f)$$

- For comparison: product quadrature $|\mathbf{k}|_\infty := max\{k_1, \ldots, k_d\}$

$$Q_\ell^{\text{prod}}(f) = \sum_{|\mathbf{k}|_\infty \leq \ell + d - 1} \Delta_{k_1} \otimes \cdots \otimes \Delta_{k_d}(f)$$

Sparse grid quadratures

- Sparse grid quadrature points

$$\Gamma_\ell^{\mathrm{sg}} = \bigcup_{|\mathbf{k}|_1 \le \ell + d - 1} \Lambda_{k_1}^{(1)} \otimes \cdots \otimes \Lambda_{k_d}^{(d)}$$

- Number of grid points

$$N := |\Gamma_\ell^{\mathrm{sg}}| = \mathcal{O}\left(2^\ell \ell^{d-1}\right) \text{ for } |\Gamma_k| = \mathcal{O}(2^k)$$

- Convergence rate for $f \in H^s_{\mathrm{mix}}(\Omega)$

$$|I(f) - Q_\ell^{\mathrm{sg}}(f)| \lesssim N^{-s} \log(N)^{\frac{(d-1)(s*1)}{2}}$$

- For comparison: product quadrature

$$|I(f) - Q_{N\ldots N}^{\mathrm{prod}}(f)| \lesssim N^{-s/d}$$

Some open issues concerning applications in physics

- **Feynman diagrams in configuration space**
  - Propagators are singular along their diagonals.
  - Complicated singularities (intersecting hyperplanes).
  - Does Fulton-MacPhearson compactification of configuration space or so called *wonderful models* of subspace arrangements help?

    R. Fulton and R. MacPherson, *Ann. of Math.* **139**, 183-225 (1994).
    C. De Concini and C. Procesi, *Selecta Mathematica (N.S)*, **1**, 459-494 (1995).
    C. Bergbauer, R. Brunetti, D. Kreimer, arXiv:0908.0633 [hep-th].

- **Path integrals for lattice gauge theories**
  - Does it make sense to speak of the regularity of the integrand?
  - Taking the continuum limit has to be accompanied by a renormalization of the coupling constant.
  - How to approximate in this context the Callan-Symanzik equation?
  - What are good parameters for the sparse grid combination technique?