Tractability of Multivariate Integration in Hermite Spaces

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Multivariate integration over $\mathbb{R}^s$ – linear algorithms

We study the numerical approximation of integrals

$$I_s(f) = \int_{\mathbb{R}^s} f(\mathbf{x}) \varphi_s(\mathbf{x}) \, \mathrm{d}\mathbf{x},$$

where

- φ_s is the density of the s-dimensional standard Gaussian measure, and
- $f \in \mathcal{H}(K)$ (RKHS) with norm $\|\cdot\|_K$.

We use **linear algorithms**

$$A_{n,s}(f) = \sum_{k=1}^{n} \alpha_k f(\mathbf{t}_k)$$

for $\alpha_k \in \mathbb{R}$ and $\mathbf{t}_k \in \mathbb{R}^s$.
Linear algorithms are optimal (Smolyak 1965, Bakhvalov 1971)

Multivariate integration over $\mathbb{R}^s$ – worst-case setting

- **Worst-case error**:

$$e(A_{n,s}, K) = \sup_{\substack{f \in \mathcal{H}(K) \\ \|f\|_K \le 1}} |I_s(f) - A_{n,s}(f)|.$$

- n**th minimal worst-case error**:

$$e(n, s) = \inf_{A_{n,s}} e(A_{n,s}, K).$$

- **Initial error**: For $n = 0$, we approximate $I_s(f)$ by zero, and

$$e(0, s) = \|I_s\| \quad \text{for all} \quad s \in \mathbb{N}.$$

- **Information complexity**: For $\varepsilon \in (0, 1)$,

$$n(\varepsilon, s) = \min\{n \ : \ e(n, s) \le \varepsilon \, e(0, s)\}.$$

Smoothness of the problems

We study problems with **infinite** smoothness.

- It is natural to demand more
  - of the nth minimal errors $e(n, s)$ and
  - of the information complexity $n(\varepsilon, s)$

  than for those cases where we only have finite smoothness.
- For problems with unbounded smoothness we are interested in obtaining (uniform) exponential convergence of the minimal errors.

Well studied: **Korobov spaces** of periodic functions over $[0, 1]^s$ with infinite smoothness (Dick, Kritzer, Larcher, Woźniakowski)

Exponential convergence

Definition

Exponential convergence (EXP) if $\exists\, q \in (0,1)$ and functions $p, C, C_1 : \mathbb{N} \to (0, \infty)$ such that

$$e(n,s) \le C(s)\, q^{\,(n/C_1(s))^{\,p(s)}} \quad \text{for all} \quad s, n \in \mathbb{N}.$$

The largest possible rate of EXP is

$$p^*(s) = \sup\left\{ p > 0 : \exists\, C, C_1 > 0 \text{ s.t. } \forall n \in \mathbb{N} : e(n,s) \le C q^{(n/C_1)^p} \right\}.$$

Uniform exponential convergence

Definition

Uniform exponential convergence (UEXP) if $\exists\, q \in (0,1),\ \exists\, p > 0$ and functions $C, C_1 : \mathbb{N} \to (0,\infty)$ such that

$$e(n,s) \le C(s)\, q^{\,(n/C_1(s))^{\,p}} \quad \text{for all} \quad s, n \in \mathbb{N}.$$

The largest rate of UEXP is

$$p^* \;=\; \sup\Big\{p > 0 : \exists C, C_1 : \mathbb{N} \to (0,\infty) \text{ s.t. } \forall n, s \in \mathbb{N} : e(n,s) \le C(s) q^{(n/C_1(s))^p}\Big\}.$$

Exponential convergence

UEXP implies

$$n(\varepsilon, s) \leq \left\lceil C_1(s) \left(\frac{\log C(s) + \log \varepsilon^{-1}}{\log q^{-1}} \right)^{1/p} \right\rceil \quad \text{for all} \quad s \in \mathbb{N},\ \varepsilon \in (0,1).$$

With respect to $\varepsilon \to 0$, we need $O\left(\left[\log \varepsilon^{-1}\right]^{1/p}\right)$ function values to reduce the initial error by a factor of ε.

EC-tractability

(a) **Exponential Convergence-Weak Tractability (EC-WT)** if

$$\lim_{s+\varepsilon^{-1}\to\infty} \frac{\log\ n(\varepsilon, s)}{s + \log\ \varepsilon^{-1}} = 0.$$

(b) **Exponential Convergence-Polynomial Tractability (EC-PT)** if $\exists\, c, \tau_1, \tau_2 > 0$ such that

$$n(\varepsilon, s) \le c\, s^{\tau_1} (1 + \log\ \varepsilon^{-1})^{\tau_2} \quad \text{for all} \quad s \in \mathbb{N},\ \varepsilon \in (0, 1).$$

(c) **Exponential Convergence-Strong Polynomial Tractability (EC-SPT)** if $\exists\, c, \tau > 0$ such that

$$n(\varepsilon, s) \le c\, (1 + \log\ \varepsilon^{-1})^{\tau} \quad \text{for all} \quad s \in \mathbb{N},\ \varepsilon \in (0, 1).$$

The exponent τ^* of EC-SPT is the infimum of τ for which EC-SPT holds, i.e.,

$$\tau^* = \inf\{\tau \ge 0 : \exists c > 0 \text{ s.t. } n(\varepsilon, s) \le c(1 + \log \varepsilon^{-1})^{\tau}\ \forall s, \varepsilon\}.$$

EC-tractability

Proposition

1. EC-SPT $\Rightarrow$ EC-PT $\Rightarrow$ UEXP
2. EC-WT $\Rightarrow \lim_{n\to\infty} n^{\alpha} e(n,s) = 0$ for all $\alpha > 0$
3. If we have UEXP ($e(n,s) \le C(s)\, q^{(n/C_1(s))^p}$), then:
   - $C(s) = \exp(\exp(o(s)))$ and $C_1(s) = \exp(o(s))$ $\Rightarrow$ EC-WT
   - $C(s) = \exp(O(s^{\tau}))$ and $C_1(s) = O(s^{\eta})$ $\Rightarrow$ EC-PT
   - $C(s) = O(1)$ and $C_1(s) = O(1)$ $\Rightarrow$ EC-SPT

Hermite polynomials

- Univariate Hermite polynomials

$$H_k(x) = \frac{(-1)^k}{\sqrt{k!}} \mathrm{e}^{\frac{x^2}{2}} \frac{\mathrm{d}^k}{\mathrm{d}x^k} \mathrm{e}^{-\frac{x^2}{2}} \quad \text{for} \quad k \in \mathbb{N}_0, \; x \in \mathbb{R}$$

E.g. $H_0(x) = 1$, $H_1(x) = x$, $H_2(x) = \frac{x^2}{\sqrt{2}} - \frac{1}{\sqrt{2}}$, $H_3(x) = \frac{x^3}{\sqrt{3}} - \sqrt{\frac{3}{2}}x$

- Multivariate Hermite polynomials

$$H_{\mathbf{k}}(\mathbf{x}) = \prod_{j=1}^{s} H_{k_j}(x_j) \quad \text{for} \quad \mathbf{k} \in \mathbb{N}_0^s, \; \mathbf{x} \in \mathbb{R}^s$$

- $(H_{\mathbf{k}})_{\mathbf{k} \in \mathbb{N}_0^s}$ is an ONB of $L_2(\mathbb{R}^s, \varphi_s)$
- Hermite expansion of $f \in L_2(\mathbb{R}^s, \varphi_s)$:

$$f(\mathbf{x}) \sim \sum_{\mathbf{k} \in \mathbb{N}_0^s} \widehat{f}(\mathbf{k}) H_{\mathbf{k}}(\mathbf{x})$$

with $\mathbf{k}$th Hermite coefficient $\widehat{f}(\mathbf{k}) = \int_{\mathbb{R}^s} f(\mathbf{x}) H_{\mathbf{k}}(\mathbf{x}) \varphi_s(\mathbf{x}) \, \mathrm{d}\mathbf{x}$

Hermite spaces

- Let $r : \mathbb{N}_0^s \to \mathbb{R}^+$ be a summable function.
- Define a kernel

$$K_r(\mathbf{x}, \mathbf{y}) = \sum_{\mathbf{k} \in \mathbb{N}_0^s} r(\mathbf{k}) H_{\mathbf{k}}(\mathbf{x}) H_{\mathbf{k}}(\mathbf{y}) \quad \text{for } \mathbf{x}, \mathbf{y} \in \mathbb{R}^s,$$

- and a inner product

$$\langle f, g \rangle_{K_r} := \sum_{\mathbf{k} \in \mathbb{N}_0^s} \frac{1}{r(\mathbf{k})} \widehat{f}(\mathbf{k}) \widehat{g}(\mathbf{k}).$$

  Let $\|f\|_{K_r}^2 = \langle f, f \rangle_{K_r}$.

- We call the RKHS $\mathcal{H}(K_r)$ a **Hermite space**.

The Hermite space $\mathcal{H}(K_{s,\mathbf{a},\mathbf{b},\omega})$

Let $\mathbf{a} = \{a_j\}_{j\geq 1}$ and $\mathbf{b} = \{b_j\}_{j\geq 1}$, where we assume that

$$1 \leq a_1 \leq a_2 \leq a_3 \leq \ldots \quad \text{and} \quad 1 \leq b_1 \leq b_2 \leq b_3 \leq \ldots .$$

Fix $\omega \in (0,1)$. For a vector $\mathbf{k} = (k_1, \ldots, k_s) \in \mathbb{N}_0^s$, consider

$$r(\mathbf{k}) = \omega^{\sum_{j=1}^s a_j k_j^{b_j}}.$$

We modify the notation for the kernel function to

$$K_{s,\mathbf{a},\mathbf{b},\omega}(\mathbf{x},\mathbf{y}) := \sum_{\mathbf{k}\in\mathbb{N}_0^s} \omega^{\sum_{j=1}^s a_j k_j^{b_j}} H_{\mathbf{k}}(\mathbf{x}) H_{\mathbf{k}}(\mathbf{y}).$$

Proposition

- $f \in \mathcal{H}(K_{s,\mathbf{a},\mathbf{b},\omega}) \;\Rightarrow\; f$ is analytic
- $\mathbb{R}[\mathbf{x}] \subset \mathcal{H}(K_{s,\mathbf{a},\mathbf{b},\omega})$
- $f(\mathbf{x}) = \exp(\boldsymbol{\lambda} \cdot \mathbf{x})$ belongs to $\mathcal{H}(K_{s,\mathbf{a},\mathbf{b},\omega})$ for suitable $\mathbf{a}, \mathbf{b}$
- $e(0,s) = 1$

The main result

Main Theorem

1. EXP holds for all **a** and **b** and

$$p^*(s) = 1/B(s) \quad \text{with} \quad B(s) := \sum_{j=1}^{s} b_j^{-1}.$$

2. Let $B := \sum_{j=1}^{\infty} b_j^{-1}$. Then

$$B < \infty \Leftrightarrow \text{UEXP} \Leftrightarrow \text{EC-PT} \Leftrightarrow \text{EC-SPT}$$

   and $p^* = 1/B$ and the exponent τ^* of EC-SPT is B.

3. EC-WT $\Rightarrow$ $\lim_{j\to\infty} a_j 2^{b_j} = \infty$
4. $\lim_{j\to\infty} a_j = \infty$ $\Rightarrow$ EC-WT

Remarks on the theorem

- We always have EXP, independent of **a** and **b**.
- The best rate $p^*(s)$ is $1/B(s)$, which decreases for growing s.
- A necessary and sufficient condition for UEXP, EC-PT and EC-SPT is that
$$B = \sum_{j=1}^{\infty} b_j^{-1} < \infty$$
with **no** extra conditions on **a** and ω.
- The best rate p^* is $1/B < 1$. Small B implies a large p^*.
- **a** and ω have no influence on UEXP, EC-PT and EC-SPT.
- There is a gap between the necessary and sufficient condition for EC-WT.
- The results for EXP, UEXP, EC-PT and EC-SPT are constructive.

Gauss-Hermite rules – one-dimensional case

A **Gauss-Hermite rule of order** n is a linear integration rule A_n of the form

$$A_n(f) = \sum_{i=1}^{n} \alpha_i f(x_i)$$

that is exact for all $p \in \mathbb{R}[x]$ with $\deg(p) < 2n$, i.e.

$$\int_{\mathbb{R}} p(x)\varphi(x)\,\mathrm{d}x = A_n(p) \quad \forall p \in \mathbb{R}[x] \ \text{ with } \ \deg(p) < 2n.$$

The nodes $x_1, \ldots, x_n \in \mathbb{R}$ are exactly the zeros of the nth Hermite polynomial H_n and the weights are given by

$$\alpha_i = \frac{1}{n H_{n-1}^2(x_i)}.$$

Gauss-Hermite rules – multivariate case

For $j = 1, 2, \ldots, s$ let

$$A_{m_j}^{(j)}(f) = \sum_{i=1}^{m_j} \alpha_i^{(j)} f(x_i^{(j)})$$

Let $n = m_1 m_2 \cdots m_s$ and set

$$A_{n,s} = A_{m_1}^{(1)} \otimes \cdots \otimes A_{m_s}^{(s)},$$

i.e., for $f \in \mathcal{H}(K_{s,\mathbf{a},\mathbf{b},\omega})$

$$A_{n,s}(f) = \sum_{i_1=1}^{m_1} \ldots \sum_{i_s=1}^{m_s} \alpha_{i_1}^{(1)} \cdots \alpha_{i_s}^{(s)} f(x_{i_1}^{(1)}, \ldots, x_{i_s}^{(s)}).$$

Proposition

$$e^2(A_{n,s}, K_{s,\mathbf{a},\mathbf{b},\omega}) \leq -1 + \prod_{j=1}^{s} \left(1 + \omega^{a_j (2m_j)^{b_j}} \frac{\sqrt{8\pi}}{1 - \omega^2}\right).$$

Gauss-Hermite rules – multivariate case

Theorem

For $s \in \mathbb{N}$, let $B(s) := \sum_{j=1}^{s} b_j^{-1}$. For $\varepsilon \in (0,1)$, let

$$m = \max_{j=1,2,\ldots,s} \left\lceil \left(\frac{1}{a_j} \frac{\log\left(\frac{\sqrt{8\pi}}{1-\omega^2} \frac{s}{\log(1+\varepsilon^2)}\right)}{\log \omega^{-1}} \right)^{B(s)} \right\rceil .$$

and define

$$m_j := \lfloor m^{1/(B(s)\cdot b_j)} \rfloor .$$

Then

$$e(A_{n,s}, K_{s,\mathbf{a},\mathbf{b},\omega}) \le \varepsilon \quad \text{and} \quad n(\varepsilon, s) \ll_s \log^{B(s)}\left(1 + \frac{1}{\varepsilon}\right).$$

This implies EXP.

Gauss-Hermite rules – multivariate case

Theorem

Assume that $B = \sum_{j=1}^{\infty} b_j^{-1} < \infty$. For $\varepsilon \in (0,1)$ define

$$m_j = \left\lceil \left(\frac{\log\left(\frac{\sqrt{8\pi}}{1-\omega^2}\ \frac{\pi^2}{6}\ \frac{j^2}{\log(1+\varepsilon^2)}\right)}{a_j 2^{b_j}\ \log \omega^{-1}} \right)^{1/b_j} \right\rceil .$$

Then

$$e(A_{n,s}, K_{s,\mathbf{a},\mathbf{b},\omega}) \leq \varepsilon \quad \text{and} \quad n(\varepsilon, s) \ll_\delta \log^{B+\delta}\left(1 + \frac{1}{\varepsilon}\right).$$

This implies EC-SPT with τ^* at most B and also UEXP.

Finite smoothness

For $k \in \mathbb{N}_0$ define $\beta_0(k) = 1$ and for $\tau \in \mathbb{N}$ define

$$\beta_\tau(k) = \begin{cases} 0 & \text{if } 0 \le k < \tau, \\ \frac{k!}{(k-\tau)!} & \text{if } k \ge \tau. \end{cases}$$

For $\alpha \in \mathbb{N}$ we define

$$r_\alpha(k) = \left(\sum_{\tau=0}^{\alpha} \beta_\tau(k) \right)^{-1} \asymp_\alpha \frac{1}{k^\alpha}.$$

For $\mathbf{k} = (k_1, \ldots, k_s) \in \mathbb{N}_0^s$ let

$$r(\mathbf{k}) = r_\alpha(\mathbf{k}) = \prod_{j=1}^{s} r_\alpha(k_j).$$

Finite smoothness

For $s \in \mathbb{N}$ define the kernel function

$$K_{s,\alpha}(\mathbf{x},\mathbf{y}) = \sum_{\mathbf{k}\in\mathbb{N}_0^s} r_\alpha(\mathbf{k}) H_{\mathbf{k}}(\mathbf{x}) H_{\mathbf{k}}(\mathbf{y}) \quad \text{for} \quad \mathbf{x},\mathbf{y} \in \mathbb{R}^s$$

and inner product

$$\langle f, g\rangle_{K_{s,\alpha}} = \sum_{\mathbf{k}\in\mathbb{N}_0^s} \frac{1}{r_\alpha(\mathbf{k})} \widehat{f}(\mathbf{k}) \widehat{g}(\mathbf{k}).$$

The inner product can also be written as

$$\langle f, g\rangle_{K_{s,\alpha}} = \sum_{\boldsymbol{\tau}\in\{0,\ldots,\alpha\}^s} \int_{\mathbb{R}^s} \frac{\partial^{\boldsymbol{\tau}} f}{\partial \mathbf{x}^{\boldsymbol{\tau}}}(\mathbf{x}) \frac{\partial^{\boldsymbol{\tau}} g}{\partial \mathbf{x}^{\boldsymbol{\tau}}}(\mathbf{x})\, \varphi_s(\mathbf{x}) \,\mathrm{d}\mathbf{x}.$$

We call $\mathcal{H}(K_{s,\alpha})$ the **Hermite space of smoothness** α.

Integration in $\mathcal{H}(K_{s,\alpha})$

Theorem (Irrgeher and Leobacher 2014)

There exist QMC rules $Q_{n,s}(f) = \frac{1}{n}\sum_{i=1}^{n} f(\mathbf{x}_i)$ such that

$$e(Q_{n,s}, K_{s,\alpha}) \ll_s \frac{1}{\sqrt{n}}.$$

A Smolyak algorithm based on Gauss-Hermite rules

For $i \in \mathbb{N}_0$ let $A_{2^i}(f)$ be one-dimensional Gauss-Hermite rules of order 2^i. Define

$$\Delta_i = \begin{cases} A_1 & \text{if } i = 0, \\ A_{2^i} - A_{2^{i-1}} & \text{if } i \in \mathbb{N}. \end{cases}$$

The **Smolyak algorithm** based on Gauss-Hermite rules is defined as

$$\mathcal{A}_{q,s} = \sum_{\substack{i_1,\ldots,i_s=0 \\ i_1+\cdots+i_s \le q}}^{\infty} \bigotimes_{j=1}^{s} \Delta_{i_j}.$$

$\mathcal{A}_{q,s}$ is linear and requires

$$n = \sum_{t=q-s+1}^{q} 2^t \binom{t+s-1}{s-1}$$

function evaluations. Hence $q \asymp_s \log n$.

A Smolyak algorithm based on Gauss-Hermite rules

Theorem

$$e(\mathcal{A}_{q,s}, K_{s,\alpha}) \ll_{s,\alpha} \frac{(\log n)^{s-1}}{n^{(\alpha-1)/2}}$$

For $\alpha > 2$ this improves the existence result for QMC rules.
For $1 \leq \alpha \leq 2$ the QMC result is better.

Theorem (Dick, 2014)

For any linear quadrature rule $A_{n,s}$ we have

$$e(A_{n,s}, K_{s,1}) \gg_s \frac{1}{n}.$$

Summary

- For **infinite** smoothness:
  - exponential convergence holds always
  - *if and only if* condition for UEXP, EC-PT and EC-SPT
  - gap between the sufficient and necessary condition for EC-WT
- For **finite** smoothness α:
  - convergence of order $O\left(\frac{1}{\sqrt{n}}\right)$ for QMC, and $O\left(\frac{(\log n)^{s-1}}{n^{(\alpha-1)/2}}\right)$ for Smolyak rules based on Gauss-Hermite

Open question

What is the exact convergence order for $e(n,s)$ in $\mathcal{H}(K_{s,\alpha})$ and what are the optimal algorithms?

  - tractability not yet studied

Announcement

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