# On higher-order integration algorithms in (weighted) Hermite spaces

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# Integration problem

Consider the following integration problem:

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

where

$$\varphi_s(\boldsymbol{x}) = \frac{1}{(2\pi)^{s/2}} \exp\left(-\frac{\boldsymbol{x}\cdot\boldsymbol{x}}{2}\right)$$

and where $f$ belongs to a Hermite space with smoothness $\alpha$.

# Hermite spaces (1)

- Hermite polynomials $\{H_{\boldsymbol{k}}\}_{\boldsymbol{k}\in\mathbb{N}_0^s}$ form an ONB of $L^2(\mathbb{R}^s,\varphi_s)$
- Hermite coefficient: $\widehat{f}(\boldsymbol{k}) = \int_{\mathbb{R}^s} f(\boldsymbol{x})H_{\boldsymbol{k}}(\boldsymbol{x})\varphi_s(\boldsymbol{x})\mathrm{d}\boldsymbol{x}$ for $f\in L^2(\mathbb{R}^s,\varphi_s)$
- For $\boldsymbol{k}\in\mathbb{N}_0^s$ define
  $\sigma_{\boldsymbol{k}} := \sup_{\boldsymbol{x}\in\mathbb{R}^s}|H_{\boldsymbol{k}}(\boldsymbol{x})|\varphi_s(\boldsymbol{x})^{1/2} = \prod_{j=1}^s \sup_{x\in\mathbb{R}}|H_{k_j}(x)|\phi(x)^{1/2}$
- For $r:\mathbb{N}_0^s\to(0,\infty)$ with $\sum_{\boldsymbol{k}\in\mathbb{N}_0^s}\sigma(\boldsymbol{k})^2 r(\boldsymbol{k})<\infty$ and continuous $f:\mathbb{R}^s\to\mathbb{R}$ define $\|f\|_r^2 := \sum_{\boldsymbol{k}\in\mathbb{N}_0^s}\widehat{f}(\boldsymbol{k})^2 r_{\boldsymbol{k}}^{-1}$ and let
  $$\mathscr{H}_r := \{f:\mathbb{R}^s\to\mathbb{R}\colon f \text{ continuous and } \|f\|_r<\infty\}$$
- $\mathscr{H}_r$ is a reproducing kernel Hilbert space with reproducing kernel
  $$K_r(\boldsymbol{x},\boldsymbol{y}) = \sum_{\boldsymbol{k}\in\mathbb{N}_0} r_{\boldsymbol{k}}H_{\boldsymbol{k}}(\boldsymbol{x})H_{\boldsymbol{k}}(\boldsymbol{y})\,,\quad (\boldsymbol{x},\boldsymbol{y}\in\mathbb{R}^s)$$

# Hermite spaces (2)

- Irrgeher & L.(2015): integration is tractable for certain weighted Hermite spaces with polynomially or exponentially decreasing functions
- Dick, Irrgeher, L., Pillichshammer (2015): exponential convergence tractability for certain weighted Hermite spaces with exponentially decreasing functions

# Hermite spaces with finite smoothness (1)

- Let $\alpha \in \mathbb{N} \setminus \{0\}$
- Define $r_{s,\alpha} : \mathbb{N}_0^s \to \mathbb{R}_+$ by $r_{s,\alpha}(\boldsymbol{k}) = \prod_{j=1}^s r_\alpha(k_j)$, where

$$r_\alpha(k) = \begin{cases} 1 & \text{if } k = 0 \\ \left(\sum_{\tau=0}^{\alpha} \beta_\tau(k)\right)^{-1} & \text{if } k \geq 1 \end{cases}$$

  and for integers $\tau \geq 1$,

$$\beta_\tau(k) = \begin{cases} \frac{k!}{(k-\tau)!} & \text{if } k \geq \tau, \\ 0 & \text{otherwise} \end{cases}$$

- Note $r_\alpha(k) \asymp_\alpha \frac{1}{k^\alpha}$
- $\mathscr{H}_{s,\alpha} := \mathscr{H}_{r_{s,\alpha}}$
- Space of Gaussian square-integrable functions with polynomially decaying Hermite coefficients (degree $\alpha$)

# Hermite spaces with finite smoothness (2)

$\mathscr{H}_{s,\alpha}$ is a Sobolev-type space of functions on $\mathbb{R}^s$ with smoothness $\alpha$:

**Proposition**

*$\mathscr{H}_{s,\alpha}$ is isometrically isomorphic to the completion of*

$$\operatorname{span}\{f_1 \otimes \cdots \otimes f_s \colon f_k \in C_c^\alpha(\mathbb{R}),\ k = 1, \ldots, s\}$$

*with respect to the inner product*

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

# Numerical Integration

Consider approximation of $I_s$ by linear algorithms:

$$A_{N,s}(f) = \sum_{i=1}^{N} w_i f(\boldsymbol{x}_i) \qquad \text{for} \qquad f \in \mathscr{H}_{s,\alpha}$$

with integration nodes $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \in \mathbb{R}^s$ and weights $w_1, \ldots, w_N \in \mathbb{R}$.

# Worst-case error

- **Integration error** for $f \in \mathscr{H}_{s,\alpha}$:

$$\mathrm{err}(f) := I_s(f) - A_{N,s}(f).$$

- **Worst-case error** of the algorithm $A_{N,s}$:

$$e(A_{N,s}, \mathscr{H}_{s,\alpha}) = \sup_{\substack{f \in \mathscr{H}_{s,\alpha} \\ \|f\|_{s,\alpha} \leq 1}} \left|\mathrm{err}(f)\right|.$$

- $N$**-th minimal worst-case error**:

$$e(N, \mathscr{H}_{s,\alpha}) = \inf_{A_{N,s}} e(A_{N,s}, \mathscr{H}_{s,\alpha})$$

# Lower bound on the worst-case error (1)

**Theorem (Lower bound – Dick, Irrgeher, L., Pillichshammer (2018))**

*Let $s, \alpha \in \mathbb{N}$. Then for all $N \in \mathbb{N}$ the $N$-th minimal worst-case error for integration in the Hermite space $\mathscr{H}_{s,\alpha}$ is bounded from below by*

$$e(N, \mathscr{H}_{s,\alpha}) \gtrsim_{s,\alpha} N^{-\alpha}(\log N)^{(s-1)/2}$$

# Lower bound on the worst-case error (2)

Idea of proof:

- Consider point set $\mathscr{P} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)$ in $\mathbb{R}^s$
- Construct function $0 \neq h \in \mathscr{H}_{s,\alpha}$ with support contained in $[0,1]^s$, such that $h(\boldsymbol{x}_n) = 0$ for all $n \in \{1, \ldots, N\}$

  Basic building block: $x \mapsto 1_{[0,1]}(x) x^\alpha (1-x)^\alpha$
- Show that $\int_{\mathbb{R}^s} h(\boldsymbol{x}) \phi_s(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} \gtrsim_{s,\alpha} \log(N)^{s-1}$

  makes use – among others – of $x \in [0,1]^s \Rightarrow \varphi_s(x) \geq \varphi(1)^s$
- Show that $\|h\|_{s,\alpha}^2 \lesssim_{s,\alpha} \log(N)^{s-1} N^{2\alpha}$
  - use $\|\varphi_s\|_\infty \leq 1$ such that $\|h\|_{s,\alpha}^2 \leq \sum_{\boldsymbol{\tau} \in \{0,\ldots,\alpha\}^s} \int_{[0,1]^s} \left(\partial^{\boldsymbol{\tau}} h(\boldsymbol{x})\right)^2 \mathrm{d}\boldsymbol{x}$,
  - use equivalence of unanchored and anchored Sobolov norm for functions on $[0,1]^s$

# Main questions

- Is $\mathscr{O}_{s,\alpha}(N^{-\alpha})$ the optimal order (up to log-terms) for the integration problem?
- If so, can we construct a quadrature rule with convergence rate (up to log-terms) of $\mathscr{O}_{s,\alpha}(N^{-\alpha})$?
- If so, can we get rid of exponential dependence on the dimension by introducing weights?

# First try: Higher order QMC+inverse CDF

- **Idea**:
  - Choose a higher order digital net $\mathscr{P} = \{\boldsymbol{z}_1, \ldots, \boldsymbol{z}_N\} \subset [0,1)^s$
  - Map $\mathscr{P}$ from $[0,1)^s$ to $\mathbb{R}^s$ using the inverse CDF $\Phi^{-1}$ coordinate-wise, where

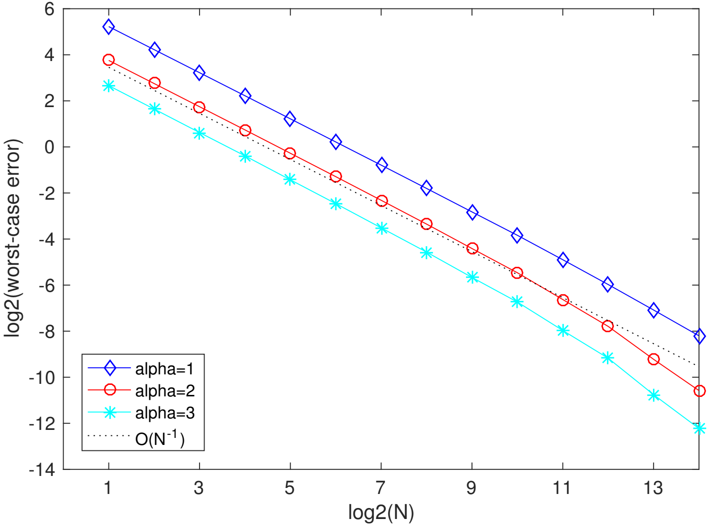
$$\Phi(x) = \int_{(-\infty,x]} \varphi(u)\mathrm{d}u$$

- Quadrature rule:

$$A_{N,s}(f) = \frac{1}{N}\sum_{i=1}^{N} f(\Phi_s^{-1}(\boldsymbol{z}_i))$$

$\Phi_s(x_1, \ldots, x_s) = (\Phi(x_1), \ldots, \Phi(x_s))$

# Worst-case error of higher order QMC+inverse CDF



# Another try: Smolyak's quadrature rule

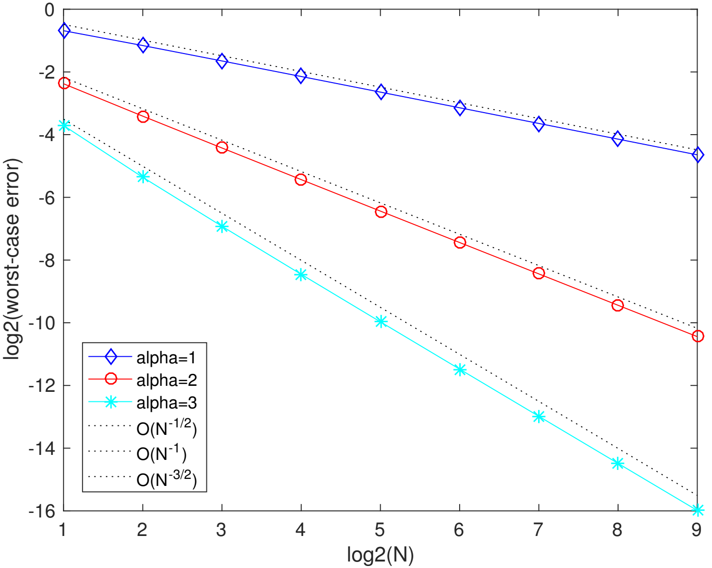
- **Idea**:
  - Choose a suitable one-dimensonal quadrature rule: Gauss-Hermite rule
  - Build an $s$-dimensional algorithm by a sparse tensor product construction
- $1$-dimensional quadrature rule: Gauss-Hermite rule of order $N$

$$A_{N,s}(f) = \sum_{i=1}^{N} w_i f(x_i)$$

where

- $x_1, \ldots, x_N$ are the roots of the $N$th Hermite polynomial and
- $w_i = \frac{1}{NH_{N-1}(x_i)}$ for $i = 1, \ldots, N$.

# Worst-case error of Gauss-Hermite rules



# Final concept

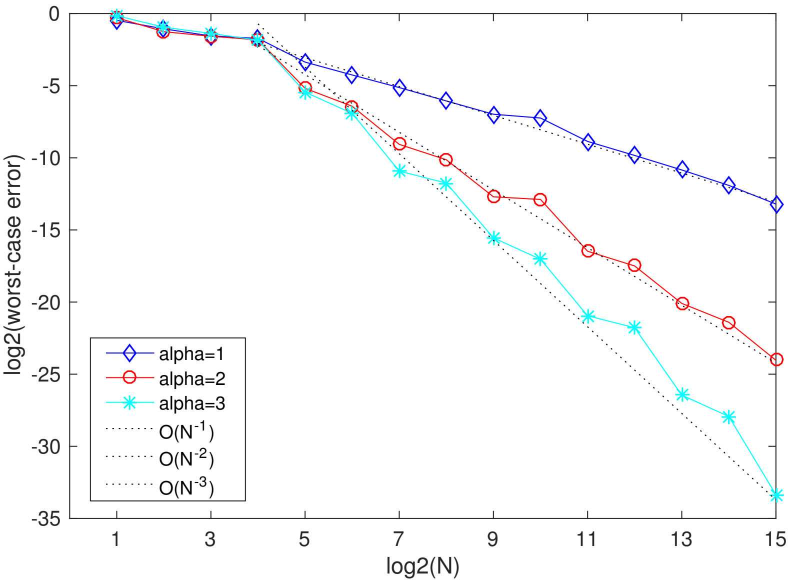
- **Idea**:
  - Choose a suitable QMC rule $Q_{N,s}$ with point set $\mathscr{P} = \{\boldsymbol{z}_1, \ldots, \boldsymbol{z}_N\} \subset [0,1)^s$
  - Map the point set $\mathscr{P}$ to an appropriate chosen box $[-\boldsymbol{b}, \boldsymbol{b}] \subset \mathbb{R}^s$ with $\boldsymbol{b} = (b, \ldots, b)$
  - Choose integration weights according to the Gaussian measure
  - Ignore what happens outside of the box $[-\boldsymbol{b}, \boldsymbol{b}]$
- Quadrature rule:

$$A_{N,s}(f) = \frac{(2b)^s}{N} \sum_{i=1}^{N} f(\mathscr{B}_b(\boldsymbol{z}_i))\varphi_s(\mathscr{B}_b(\boldsymbol{z}_i))$$

with $b = 2\sqrt{\alpha \log N}$ and $\mathscr{B}_b : [0,1)^s \to [-\boldsymbol{b}, \boldsymbol{b}]$ given by

$$\mathscr{B}_b(\boldsymbol{z}) = 2\boldsymbol{b}\boldsymbol{z} - \boldsymbol{b}$$

# Worst-case error of the presented algorithm



# Estimate of the integration error

- Triangle inequality:

$$
\begin{aligned}
|\mathrm{err}(f)| \le & \underbrace{\left| \int_{\mathbb{R}^s \setminus [-\boldsymbol{b}, \boldsymbol{b}]} f(\boldsymbol{x}) \varphi_s(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} \right|}_{=:\mathrm{err}_1(f)} \\
& + \underbrace{\left| \int_{[-\boldsymbol{b}, \boldsymbol{b}]} f(\boldsymbol{x}) \varphi_s(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} - \frac{(2b)^s}{N} \sum_{i=1}^{N} f(\boldsymbol{x}_i) \varphi_s(\boldsymbol{x}_i) \right|}_{=:\mathrm{err}_2(f)}
\end{aligned}
$$

# Estimate of $\mathrm{err}_1$

- Key observations:
  - For $f \in \mathscr{H}_{s,\alpha}$,

$$|f(\boldsymbol{x})\sqrt{\varphi_s(\boldsymbol{x})}| \lesssim_{s,\alpha} \|f\|_{s,\alpha} \quad \text{for all } \boldsymbol{x} \in \mathbb{R}^s$$

  - For $\boldsymbol{b} = (b, \ldots, b)$ with $b = 2\sqrt{\alpha \log N}$,

$$\int_{\mathbb{R}^s \setminus [-\boldsymbol{b}, \boldsymbol{b}]} \sqrt{\varphi_s(\boldsymbol{x})} \mathrm{d}\boldsymbol{x} \lesssim_s N^{-\alpha}$$

- Upper bound on $\mathrm{err}_1$:

$$|\mathrm{err}_1(f)| \lesssim_{s,\alpha} \|f\|_{s,\alpha} N^{-\alpha}$$

# Estimate of $\mathrm{err}_2$

- Transformation to the unit cube

$$\left|\int_{[-\boldsymbol{b},\boldsymbol{b}]} f(\boldsymbol{x})\varphi_s(\boldsymbol{x})\mathrm{d}\boldsymbol{x} - \frac{(2b)^s}{N}\sum_{i=1}^{N} f(\boldsymbol{x}_i)\varphi_s(\boldsymbol{x}_i)\right|$$

$$= (2b)^s \left|\int_{[0,1]^s} f(\mathscr{B}_b(\boldsymbol{z}))\varphi_s(\mathscr{B}_b(\boldsymbol{z}))\mathrm{d}\boldsymbol{z} - \frac{1}{N}\sum_{i=1}^{N} f(\mathscr{B}_b(\boldsymbol{z}_i))\varphi_s(\mathscr{B}_b(\boldsymbol{z}_i))\right|$$

# Estimate of $\mathrm{err}_2$

- Analysis of $g = (f \cdot \varphi_s) \circ \mathscr{B}_b$:
  - $g$ belongs to the ANOVA space (or unanchored Sobolev space) $\mathscr{H}^{\mathrm{sob}}_{s,\alpha}$ of smoothness $\alpha$ defined over $[0,1)^s$ with norm $\|\cdot\|_{\mathrm{sob},s,\alpha}$
  - Norm relation to the Hermite space:

$$\|g\|_{\mathrm{sob},s,\alpha} \lesssim_{s,\alpha} b^{s(\alpha-1/2)} \|f\|_{s,\alpha}$$

  - Integration in the ANOVA space:

$$\left| \int_{[0,1)^s} g(\boldsymbol{z}) \mathrm{d}\boldsymbol{z} - \frac{1}{N} \sum_{i=1}^{N} g(\boldsymbol{z}_i) \right| \leq \|g\|_{\mathrm{sob},s,\alpha} e(Q_{N,s}, \mathscr{H}^{\mathrm{sob}}_{s,\alpha})$$

- Upper bound on $\mathrm{err}_2$:

$$|\mathrm{err}_2(f)| \lesssim_{s,\alpha} \|f\|_{s,\alpha} (\log N)^{s\frac{2\alpha+1}{4}} e(Q_{N,s}, \mathscr{H}^{\mathrm{sob}}_{s,\alpha})$$

# Relation to integration in the ANOVA space

**Theorem (Dick, Irrgeher, L., Pillichshammer)**

*Let $\alpha \in \mathbb{N}$ and $A_{N,s}$ be the quadrature rule defined as before. Then for the worst-case error of $A_{N,s}$ in the Hermite space $\mathscr{H}_{s,\alpha}$ we have*

$$e(A_{N,s}, \mathscr{H}_{s,\alpha}) \lesssim_{s,\alpha} (\log N)^{s\frac{2\alpha+1}{4}} e(Q_{N,s}, \mathscr{H}_{s,\alpha}^{\mathrm{sob}}) + \frac{1}{N^\alpha}.$$

# Optimal order of integration in the ANOVA space

- Higher order nets (Dick '07)
  - Generalization of digital nets
  - Optimal for integration in the ANOVA space of smoothness $\alpha$
  - Achieve convergence rates of order $N^{-\alpha}$
- Construction of higher order nets
  - Interlacing method using digital nets (e.g. Sobol', Faure, Niederreiter)
- Upper bound on the worst-case error of QMC integration with order $(2\alpha+1)$ nets (Goda, Suzuki and Yoshiki '16):

$$e(Q_{N,s}, \mathscr{H}^{\mathrm{sob}}_{s,\alpha}) \lesssim_{s,\alpha} (\log N)^{(s-1)/2} N^{-\alpha}$$

# Upper bound on the worst-case error

**Theorem (Dick, Irrgeher, L., Pillichshammer)**

*Let $\alpha \in \mathbb{N}$ and $A_{N,s}$ be the quadrature rule defined as before based on a higher order net of order $(2\alpha + 1)$ over the finite field $\mathbb{F}_q$ with $N = q^m$ elements. Then for the worst-case error of $A_{N,s}$ in the Hermite space $\mathscr{H}_{s,\alpha}$ we have*

$$e(A_{N,s}, \mathscr{H}_{s,\alpha}) \lesssim_{s,\alpha} \frac{(\log N)^{s\frac{2\alpha+3}{4}-\frac{1}{2}}}{N^\alpha} \quad \textit{where } N = q^m.$$

# Weighted case

- So far no result beyond tractability with order $N^{-\frac{1}{2}}$ (for functions with polynomially decaying Hermite coefficients)
- Try to integrate over $\prod_{j=1}^{s}[-b_j, b_j]$
- Cannot balance truncation error with integration error (so far)

# Thank you!


- J. Dick, C. Irrgeher, G. Leobacher and F. Pillichshammer. *On the optimal order of integration in Hermite spaces with finite smoothness*, SIAM J. Numer. Anal. 56(2), pp. 684-707, 2018.
- C. Irrgeher and G. Leobacher. *High-dimensional integration on $\mathbb{R}^d$, weighted Hermite spaces, and orthogonal transforms*, Journal of Complexity, 31(2):174–205, 2015.
- C. Irrgeher, P. Kritzer, G. Leobacher, and F. Pillichshammer. *Integration in Hermite spaces of analytic functions*, Journal of Complexity, 31(3):380 – 404, 2015.