

Infinite-Dimensional Integration (and Function Recovery): Randomized Algorithms and Their Analysis

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June 30, 2023

Infinite-Variate Integration Problem

Given: $D \neq \emptyset$ domain, μ probability measure on D , class F of input functions $f : D^{\mathbb{N}} \rightarrow \mathbb{R}$, and $\mu^{\mathbb{N}} := \bigotimes_{j=1}^{\infty} \mu$ probability measure on $D^{\mathbb{N}}$.

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Some Motivation:

- **Theory:** Multivariate integration problems are of interest – infinite-variate integration is limit case when number of variables tends to infinity.
- **Application:** Stochastic models are often based on sequences of i.i.d. r.v., implying that expectations can be represented as infinite-variate integrals.

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To answer these questions, we have to...

- impose some **structure** on the (class of) integrands,
- **specify the setting** (class of admissible algorithms/cost/error criterion).

Outline

- Infinite-variate Integration
 - ① Structure of function spaces
 - ② Specification of the setting
 - ③ Optimal results in a class of function spaces
 - ④ Extension of optimal results to more general class of function spaces
 - ⑤ Further extension of optimal results to different class of function spaces
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Requirement satisfied *iff* H **reproducing kernel Hilbert space (RKHS)**, i.e., if there exists **reproducing kernel (RK)** $K : X \times X \rightarrow \mathbb{R}$ such that

- 1 $K(\cdot, x) \in H$ for all $x \in X$,
- 2 $f(x) = \langle f, K(\cdot, x) \rangle_H$ for all $f \in H$, $x \in X$.

Convention: For RK K denote its RKHS by $H(K)$ and norm in $H(K)$ by $\|\cdot\|_K$.

Structure II: Weighted RKHSs, ...

Fix RK $k : D \times D \rightarrow \mathbb{R}$ with $\int_D k(x, x) d\mu(x) < \infty$ and $1 \notin H(k)$. Then

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Observation: If $\|f\|_{1+\gamma_j k} \leq 1$, then $\|g\|_k \leq \sqrt{\gamma_j}$.

Structure III: ... Tensor Products, and Function Decomposition

For $u \subset_f \mathbb{N}$ (read as “ u is a finite subset of \mathbb{N} ”) put

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Then

$$H(K_\gamma) = \bigotimes_{j \in \mathbb{N}} H(1 + \gamma_j k) = \bigoplus_{u \subset_f \mathbb{N}} H(k_u),$$

resulting in orthogonal function decomposition of $f \in H(K_\gamma)$

$$f(\mathbf{x}) = \sum_{u \subset_f \mathbb{N}} f_u(\mathbf{x}_u), \quad f_u \in H(k_u), \quad \text{with} \quad \|f\|_{K_\gamma}^2 = \sum_{u \subset_f \mathbb{N}} \gamma_u^{-1} \|f_u\|_{k_u}^2.$$

Example of FSD: Anchored Decomposition (aka Cut-HDMR)

If there is **anchor** $a \in D$ such that $k(a, a) = 0$ (“anchor condition”), then decomposition $f = \sum_{u \subset_f \mathbb{N}} f_u$ on $H(K_\gamma)$ is the **anchored decomposition** which can be **calculated directly** as

$$f_u(\mathbf{x}) := \sum_{v \subseteq u} (-1)^{|u \setminus v|} f(\mathbf{x}_v, \mathbf{a}_{\mathbb{N} \setminus v}),$$

see [Kuo, Sloan, Wasilkowski, Woźniakowski '10b].

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Example: Wiener kernel $k : [0, 1] \times [0, 1] \rightarrow \mathbb{R}$, $k(x, y) := \min(x, y)$.

with anchor $a = 0$.

$H(1 + k) = \{f : f, f' \in L^2([0, 1])\}$ Sobolev space of order 1

with anchored norm $\|f\|_{1+k}^2 = |f(0)|^2 + \|f'\|_{L^2[0,1]}^2$.

Specifying the Setting I: Admissible Algorithms & Cost Models

Integration functional:

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Deterministic Setting:

Admissible deterministic quadrature formulas:

$$Q_n(f) = \sum_{i=1}^n w_i f(\mathbf{x}^{(i)}), \quad \text{where } w_i \in \mathbb{R}, \mathbf{x}^{(i)} \in D^{\mathbb{N}}.$$

Cost: Fix default value $a \in D$.

Unrestricted Subspace Sampling [Kuo, Sloan, Wasilkowski, Woźniakowski'10a]

$$\text{cost}(Q_n) := \sum_{i=1}^n |\{j \in \mathbb{N} : x_j^{(i)} \neq a\}|$$

Specifying the Setting I: Admissible Algorithms & Cost Model

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Specifying the Setting II: Error Criterion

Error criterion: (worst case) randomized error of quadrature Q

$$e(Q; K_{\gamma})^2 := \sup_{\|f\|_{K_{\gamma}} \leq 1} E((S(f) - Q(f))^2)$$

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“(Polynomial) Convergence rate” of decreasing null sequence $\mathbf{s} := (s_n)_{n \in \mathbb{N}}$:

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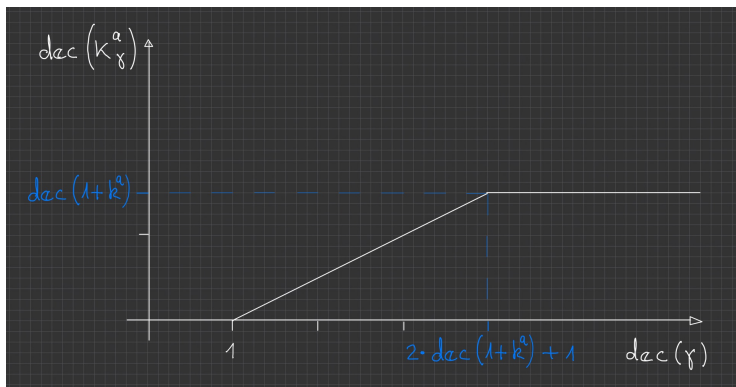
$$\text{dec}(K_\gamma) := \text{dec}((e(n, K_\gamma))_{n \in \mathbb{N}})$$

Result 1: Weighted RKHS Based on Anchored Kernel k^a

Theorem 1. Let $k = k^a$ be RK *anchored in* $a \in D$ and $K_\gamma = K_\gamma^a$ corresponding weighted RK. Then

$$\text{dec}(K_\gamma^a) = \min \left(\text{dec}(1 + k^a), \frac{\text{dec}(\gamma) - 1}{2} \right),$$

where $\text{dec}(1 + k^a)$ denotes convergence rate of n th minimal errors of univariate integration on $H(1 + k^a)$.



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$$k_u(\mathbf{x}_u, \mathbf{y}_u) := \prod_{j \in u} k(x_j, y_j), \quad \mathbf{x}_u = (x_j)_{j \in u}, \mathbf{y}_u = (y_j)_{j \in u} \in D^u.$$

Then $H(k_u) = \otimes_{j \in u} H(k)$. Put $\gamma_u := \prod_{j \in u} \gamma_j$ (“product weight”).

“Weighted RK”:

$$K_\gamma(\mathbf{x}, \mathbf{y}) := \prod_{j \in \mathbb{N}} (1 + \gamma_j k(x_j, y_j)) = \sum_{u \subset_f \mathbb{N}} \gamma_u k_u(\mathbf{x}_u, \mathbf{y}_u), \quad \mathbf{x}, \mathbf{y} \in D^{\mathbb{N}}.$$

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Then

$$H(K_\gamma) = \bigotimes_{j \in \mathbb{N}} H(1 + \gamma_j k) = \bigoplus_{u \subset_f \mathbb{N}} H(k_u),$$

resulting in orthogonal function decomposition of $f \in H(K_\gamma)$

$$f(\mathbf{x}) = \sum_{u \subset_f \mathbb{N}} f_u(\mathbf{x}_u), \quad f_u \in H(k_u), \quad \text{with} \quad \|f\|_{K_\gamma}^2 = \sum_{u \subset_f \mathbb{N}} \gamma_u^{-1} \|f_u\|_{k_u}^2.$$

Example of FSD: Anchored Decomposition (aka Cut-HDMR)

If there is **anchor** $a \in D$ such that $k(a, a) = 0$ (“anchor condition”), then decomposition $f = \sum_{u \subset_f \mathbb{N}} f_u$ on $H(K_\gamma)$ is the **anchored decomposition** which can be **calculated directly** as

$$f_u(\mathbf{x}) := \sum_{v \subseteq u} (-1)^{|u \setminus v|} f(\mathbf{x}_v, \mathbf{a}_{\mathbb{N} \setminus v}),$$

see [Kuo, Sloan, Wasilkowski, Woźniakowski '10b].

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Example: Wiener kernel $k : [0, 1] \times [0, 1] \rightarrow \mathbb{R}$, $k(x, y) := \min(x, y)$.

with anchor $a = 0$.

$H(1 + k) = \{f : f, f' \in L^2([0, 1])\}$ Sobolev space of order 1

with anchored norm $\|f\|_{1+k}^2 = |f(0)|^2 + \|f'\|_{L^2[0,1]}^2$.

Specifying the Setting I: Admissible Algorithms & Cost Models

Integration functional:

$$S(f) = \int_{D^{\mathbb{N}}} f(\mathbf{x}) \, d\mu^{\mathbb{N}}(\mathbf{x})$$

Deterministic Setting:

Admissible deterministic quadrature formulas:

$$Q_n(f) = \sum_{i=1}^n w_i f(\mathbf{x}^{(i)}), \quad \text{where } w_i \in \mathbb{R}, \mathbf{x}^{(i)} \in D^{\mathbb{N}}.$$

Cost: Fix default value $a \in D$.

Unrestricted Subspace Sampling [Kuo, Sloan, Wasilkowski, Woźniakowski'10a]

$$\text{cost}(Q_n) := \sum_{i=1}^n |\{j \in \mathbb{N} : x_j^{(i)} \neq a\}|$$

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Error criterion: (worst case) randomized error of quadrature Q

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“(Polynomial) Convergence rate” of decreasing null sequence $\mathbf{s} := (s_n)_{n \in \mathbb{N}}$:

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“(Polynomial) Convergence rate” of $e(n, K_\gamma)$:

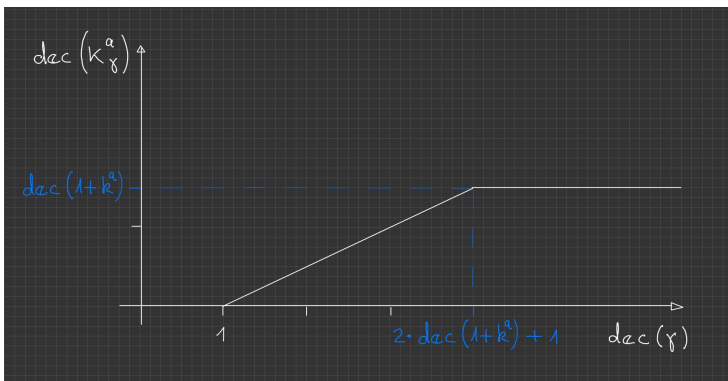
$$\text{dec}(K_\gamma) := \text{dec}((e(n, K_\gamma))_{n \in \mathbb{N}})$$

Result 1: Weighted RKHS Based on Anchored Kernel k^a

Theorem 1. Let $k = k^a$ be RK *anchored in* $a \in D$ and $K_\gamma = K_\gamma^a$ corresponding weighted RK. Then

$$\text{dec}(K_\gamma^a) = \min \left(\text{dec}(1 + k^a), \frac{\text{dec}(\gamma) - 1}{2} \right),$$

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Contributions to proof of Theorem 1:

- Lower error bounds: Kuo, Sloan, Wasilkowski & Woźniakowski'10a (deterministic case); G.'13 (randomized case)
- Upper error bounds: Plaskota & Wasilkowski'11 (via multivariate decomposition method (MDM))

Earlier partial results in deterministic case: Kuo, Sloan, Wasilkowski & Woźniakowski'10a (via MDM); Niu, Hickernell, Müller-Gronbach & Ritter'11; G.'12 (both via multilevel algorithms)

Multivariate Decomposition Method

Recall: k^a RK anchored in $a \in D$ and K_γ^a corresponding weighted RK.

Anchored decomposition for $f \in H(K_\gamma^a)$: $f = \sum_{u \subset_f \mathbb{N}} f_u$, $f_u \in H(k_u)$.

Observation: S continuous on $H(K_\gamma^a)$, hence

$$S(f) = \int_{D^{\mathbb{N}}} f(\mathbf{x}) \, \mathrm{d}\mu(\mathbf{x}) = \sum_{u \subset_f \mathbb{N}} \int_{D^u} f_u(\mathbf{x}_u) \, \mathrm{d}\mu^u(\mathbf{x}_u).$$

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Multivariate decomposition method (MDM):

- ① Choose finite set \mathcal{A} ("set of active variables") of most important groups of variables.
- ② Choose for each $u \in \mathcal{A}$ quadrature Q_{u,n_u} using n_u samples to approximate $\int_{D^u} f_u(\mathbf{x}_u) \, d\mu^u(\mathbf{x}_u)$.

Final algorithm Q^{MDM} is of form

$$Q^{\text{MDM}}(f) = \sum_{u \in \mathcal{A}} Q_{u,n_u}(f_u)$$

Multivariate Decomposition Method

MDM *aka* **changing dimension algorithm** for ∞ -variate setting introduced in

- Kuo, Sloan, Wasilkowski & Woźniakowski'10; Plaskota & Wasilkowski'11 (∞ -variate integration)
- Wasilkowski & Woźniakowski'11a, '11b (∞ -variate approximation).

Further papers on MDM include: Wasilkowski'12; G.'13; Dick & G.'14a, 14b; Plaskota & Wasilkowski'14; Wasilkowski'14; Gilbert & Wasilkowski'17; G., Hefter, Hinrichs & Ritter'17; G., Hefter, Hinrichs, Ritter & Wasilkowski'17; Kuo, Nuyens, Plaskota, Sloan, Wasilkowski'17; Gilbert, Kuo, Nuyens & Wasilkowski'18; G., Hefter, Hinrichs, Ritter & Wasilkowski'19; G. & Wnuk'20; G., Hinrichs, Ritter & Rüßmann'23+

Similar idea used for **multivariate integration** in Griebel & Holtz'10 (**dimension-wise quadrature methods**).

How to choose building blocks Q_{u,n_u} for MDM?

- 1 Choose sequence $(Q_k)_{k \in \mathbb{N}}$ of quadratures for **univariate integration** on $H(1 + k^a)$.
- 2 Employ **Smolyak's method** to obtain Q_{u,n_u} : For $f_u \in H(k_u^a)$

$$Q_{u,n_u} f_u = \left(\sum_{L-|u|+1 \leq |\ell|_1 \leq L} (-1)^{L-|\ell|_1} \binom{|u|-1}{L-|\ell|_1} \otimes_{j \in u} Q_{\ell_j} \right) f_u.$$

Smolyak's method (*aka* **sparse grid method**, etc.) is “universal method” for approximation of **tensor product problems**, see, e.g.,

- **Deterministic Case**: [Smolyak'63; Temlyakov'87; Baszenski & Delvos'93; Wasilkowski & Woźniakowski'95; Novak & Ritter'96; Gerstner, Griebel'98;...
Surveys: [Bungartz, Griebel'04; Novak & Woźniakowski'08; Düng, Temlyakov & T. Ullrich'16; Tempone & Wolfers'18;...]
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Examples of Non-Anchored RKHSs

The following RKHSs are not based on an anchored kernel $k = k^a$:

Spaces defined via ...

... derivatives:

- Sobolev spaces with classical norms,
- unanchored Sobolev spaces,
- ...

... Fourier coefficients w.r.t. orthonormal basis of L^2 (including 1):

- Korobov spaces,
- Walsh spaces,
- Haar wavelet spaces,
- Hermite spaces,
- cosine spaces,
- ...

Result 2: Weighted RKHS Based on General RK k

Theorem 2 [G., Hefter, Hinrichs & Ritter'17; G. & Wnuk'20]¹. Let k be *general RK* and K_γ corresponding weighted RK. Then

$$\text{dec}(K_\gamma) = \min \left(\text{dec}(1 + k), \frac{\text{dec}(\gamma) - 1}{2} \right),$$

where $\text{dec}(1 + k)$ denotes convergence rate of N th minimal errors of univariate integration on $H(1 + k)$.

¹Results for ANOVA kernels in randomized setting were proved earlier in [Hickernell, Müller-Gronbach, Niu & Ritter'10], [Baldeaux & G. 14], [Dick & G.'14b].

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How to prove the more general Theorem 2?

Simple observation: For Banach spaces $X \subseteq Y$ of integrable functions:

$$X \hookrightarrow Y$$

with embedding constant C implies

$$e(Q, X) \leq Ce(Q, Y) \quad \text{for all quadratures } Q,$$

resulting in

$$e(n, X) \leq Ce(n, Y) \quad \text{and} \quad \text{dec}(X) \geq \text{dec}(Y).$$

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“Universality of Anchored Spaces”

Construction of associated anchored RKHS of $H(1 + k)$

Subspace $\{f \in H(1 + k) \mid f(a) = 0\}$ of RKHS $H(1 + k)$ has RK

$$k^a : D \times D \rightarrow \mathbb{R} \quad \text{with} \quad k^a(a, a) = 0$$

and $H(1 + k^a) = H(1 + k)$ as vector spaces with equivalent norms,
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With associated anchored kernel k^a of k again construct **weighted space** of ∞ -variate functions $H(K_\gamma^a)$:

$$K_\gamma^a(\mathbf{x}, \mathbf{y}) = \prod_{j \in \mathbb{N}} (1 + \gamma_j k^a(x_j, y_j)), \quad \mathbf{x}, \mathbf{y} \in D^{\mathbb{N}}.$$

“Embedding Triple”

In general, $H(K_\gamma) \not\subseteq H(K_\gamma^a)$ and $H(K_\gamma^a) \not\subseteq H(K_\gamma)$ [Heffer & Ritter ‘14].

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Remedy: Manipulate the Weights!

For $c > 0$ let $c\gamma := (c\gamma_j)_{j \in \mathbb{N}}$. Note that $\text{dec}(c\gamma) = \text{dec}(\gamma)$.

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Proposition [G., Hefer, Hinrichs & Ritter’17]. *There exists $0 < c_0 < 1$ such that*

$$H(K_{c_0\gamma}^a) \hookrightarrow H(K_\gamma) \hookrightarrow H(K_{c_0^{-1}\gamma}^a).$$

In general, $H(K_{c_0\gamma}^a) \subsetneq H(K_\gamma) \subsetneq H(K_{c_0^{-1}\gamma}^a)$.

Structure IV: Spaces of Increasing Smoothness

Let $(e_\nu)_{\nu \in \mathbb{N}_0}$ ONB of $L^2(D, \mu)$ with $e_0 = 1$.

Consider “Fourier weights” $\alpha_{\nu,j} \geq 1$, $\nu, j \in \mathbb{N}$, with

(A 1) $\alpha_{\nu,j} \leq \alpha_{\nu+1,j}$ and $\alpha_{\nu,j} \leq \alpha_{\nu,j+1}$ for all $\nu, j \in \mathbb{N}$,

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For each variable $j \in \mathbb{N}$ define RK

$$k_j(x, y) = \sum_{\nu \in \mathbb{N}} \alpha_{\nu,j}^{-1} \cdot e_\nu(x) \cdot e_\nu(y), \quad x, y \in \mathbb{R};$$

Then

$$H(1 + k_j) = \left\{ f \in L^2(D, \mu) : \sum_{\nu \in \mathbb{N}} \alpha_{\nu,j} \langle f, e_\nu \rangle_{L^2}^2 < \infty \right\}.$$

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Examples: Korobov spaces, Walsh spaces, Haar spaces, Hermite spaces,....

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Build “increasing smoothness RK”

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Result 3: Spaces of Increasing Smoothness

Define weights

$$\gamma_j := \sup_{\nu \in \mathbb{N}} \frac{\alpha_{\nu,1}}{\alpha_{\nu,j}}, \quad j \in \mathbb{N}.$$

Interpretation of weights: $\sqrt{\gamma_j}$ norm of embedding $H(k_j) \hookrightarrow H(k_1)$.

Sequence $\gamma = (\gamma_j)_{j \in \mathbb{N}}$ monotone decreasing. Assume $\sum_{j \in \mathbb{N}} \gamma_j < \infty$.

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Theorem 3 [G., Hefter, Hinrichs, Ritter & Wasilkowski'19;
G., Hinrichs, Ritter & Rüßmann'23+].

$$\begin{aligned} \min \left(\text{dec}(1 + k_1), \frac{\text{dec}(\gamma) - 1}{2} \right) &\leq \text{dec}(K) \\ &\leq \min \left(\text{dec}(1 + k_1), \frac{\text{dec}((\alpha_{1,j}^{-1})_{j \in \mathbb{N}}) - 1}{2} \right) \end{aligned}$$

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Examples: Let $1 < r_1 \leq r_2 \leq r_3 \leq \dots$

Fourier weights of ...

- ... polynomial growth (PG): $\alpha_{\nu,j} := (\nu + 1)^{r_j}$,
- ... exponential growth (EG): $\alpha_{\nu,j} := 2^{r_j \cdot \nu}$.

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Fourier weights of ...

- ... polynomial growth (PG): $\alpha_{\nu,j} := (\nu + 1)^{r_j}$,
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For both cases (PG) & (EG): $\alpha_{1,j}^{-1} = 2^{-r_j}$ and $\gamma_j = 2^{r_1 - r_j}$, hence

$$\text{dec}(\gamma) = \text{dec}((\alpha_{1,j}^{-1})_{j \in \mathbb{N}}) = \liminf_{j \rightarrow \infty} \left(\frac{\ln(2)}{\ln(j)} r_j \right),$$

resulting in matching bounds in Theorem 3.

L^2 -Approximation

Solution Operator: **Embedding operator** $S : H(K) \rightarrow L^2(D^{\mathbb{N}}, \mu^{\mathbb{N}}), f \mapsto f$.

Algorithms: **Linear algorithms** $A : H(K) \rightarrow \mathbb{R}$ of form

$$A(f) := \sum_{i=1}^m w_i \cdot f(\mathbf{x}^{(i)}) \quad (3)$$

where $m \in \mathbb{N}$, $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)} \in D^{\mathbb{N}}$, and $w_1, \dots, w_m \in L^2(D^{\mathbb{N}}, \mu^{\mathbb{N}})$.

Cost: We only account for function evaluations, fix nominal value $a \in \mathbb{R}$, ...

Error Criterion: Worst case randomized/deterministic error of algorithm A ...

Results: Theorem 1, 2, and 3 hold verbatim²! Again, upper error bounds are established via MDM based on Smolyak algorithms.

²But the univariate convergence rates of n -th minimal errors of integration and L^2 -approximation may differ.

Summary

- Infinite-variate Integration:

- ① On spaces of integrands we first imposed structure (reproducing kernels, tensor product structure, weights, anchored function decomposition).
- ② Afterwards we fixed the setting (admissible algorithms, costs, and error criterion). In that setting...
- ③ ... MDM achieved optimal results on anchored weighted RKHSs by exploiting the anchored function decomposition.
- ④ ... an Embedding framework was used to prove that MDM achieve also optimal results on general weighted RKHSs.
- ⑤ ... another embedding strategy was used to prove that MDM achieve also optimal results on RKHSs of increasing smoothness.

- Infinite-variate L^2 -Approximation:

Same holds for L^2 -approximation (main results Theorem 1, 2 & 3 for integration hold verbatim for L^2 -approximation).

- **Concluding Remark:** Our embedding techniques allow to transfer error bounds for linear algorithms for multi- or ∞ -variate linear problems on one RKHS of weighted type or of increasing smoothness to different ones.

Sketch of Proof of Theorem 3

Consider *new* weighted RKs

$$k_j^{\text{up}}(x, y) := \gamma_j k_1(x, y), \quad \text{and} \quad k_j^{\text{low}}(x, y) := \alpha_{1,j}^{-1} e_1(x) e_1(y),$$

and put

$$K_{\gamma}^{\text{up}}(\mathbf{x}, \mathbf{y}) := \prod_{j=1}^{\infty} (1 + k_j^{\text{up}}(x_j, y_j)), \quad \text{and} \quad K_{\alpha_{1,j}}^{\text{low}}(\mathbf{x}, \mathbf{y}) := \prod_{j=1}^{\infty} (1 + k_j^{\text{low}}(x_j, y_j)).$$

Then

$$H(K_{\alpha_{1,j}}^{\text{low}}) \hookrightarrow H(K) \hookrightarrow H(K_{\gamma}^{\text{up}}).$$

Since $\text{dec}(1 + k_1^{\text{up}}) = \text{dec}(1 + k_1)$ and $\text{dec}(1 + k_1) \geq \text{dec}(K)$, we obtain

$$\begin{aligned} \min \left(\text{dec}(1 + k_1), \frac{\text{dec}(\gamma) - 1}{2} \right) &\leq \text{dec}(K) \\ &\leq \min \left(\text{dec}(1 + k_1), \frac{\text{dec}((\alpha_{1,j}^{-1})_{j \in \mathbb{N}}) - 1}{2} \right) \end{aligned}$$

Observation: $\dim(H(1 + k_j^{\text{low}})) = 2$, while $\dim(H(1 + k_j)) = \infty$ and typically $H(1 + k_{j+1}) \hookrightarrow H(1 + k_j)$ compactly, while $H(1 + k_{j+1}^{\text{up}}) = H(1 + k_j^{\text{up}})$ with equivalent norms.

An Alternative Cost Model

Randomized Quadrature: $Q_n(f) = \sum_{i=1}^n w_i f(\mathbf{x}^{(i)})$, where $w_i \in \mathbb{R}$, $\mathbf{x}^{(i)} \in D^{v_i}$.

Unrestricted Subspace Sampling [Kuo, Sloan, Wasilkowski, Woźniakowski'10a]

$$\text{cost}_{\text{unr}}(Q_n) := E \left[\sum_{i=1}^n |\{j \in \mathbb{N} : x_j^{(i)} \neq a\}| \right]$$

Nested Subspace Sampling [Creutzig, Dereich, Müller-Gronbach, Ritter'09]

$$\text{cost}_{\text{nest}}(Q_n) := E \left[\sum_{i=1}^n \max \{j \in \mathbb{N} : x_j^{(i)} \neq a\} \right]$$

"Rule of Thumb": For USS use multivariate decomposition method (MDM), but for NSS use multilevel algorithms!

General references for multilevel algorithms: Heinrich '98, '01 (integral equations/parametric integration); Giles '08a, '08b; Giles, Higham & Mao (SDEs); Giles & Waterhouse '09 (QMC-ML); ... now better look at http://people.maths.ox.ac.uk/gilesm/mlmc_community.html

Multilevel for ∞ -dimensional integration problem: Hickernell, Müller-Gronbach, Niu & Ritter '10; Niu, Hickernell, Müller-Gronbach & Ritter '11; G. '12; Baldeaux '12; G.'13; Baldeaux & G. '14; Dick & G. '14a; Hefter '14; G., Hefter, Hinrichs & Ritter '17.

Comparison: Multilevel Algorithms and MDM

QMC-Multilevel Algorithm: $Q_L^{\text{ML}}(f) := \sum_{\ell=1}^L Q_{\ell}(f)$, where

$$Q_{\ell}(f) := \frac{1}{n_{\ell}} \sum_{i=1}^{n_{\ell}} \left(f(x_1^{(\ell,i)}, \dots, x_{2^{\ell}}^{(\ell,i)}, a, a, \dots) - f(x_1^{(\ell,i)}, \dots, x_{2^{\ell-1}}^{(\ell,i)}, a, a, \dots) \right)$$

Let $f \in H(K_{\gamma}^a)$ with anchored function decomposition $f = \sum_{u \subset_f \mathbb{N}} f_u$.

Solution operator:

$$S(f) = \int_{D^{\mathbb{N}}} f(\mathbf{x}) \, d\mu^{\mathbb{N}}(\mathbf{x}) = \sum_{u \subset_f \mathbb{N}} \int_{D^u} f_u(\mathbf{x}_u) \, d\mu^u(\mathbf{x}_u)$$

Multivariate decomposition method:

$$Q^{\text{MDM}}(f) = \sum_{u \subset_f \mathbb{N}} Q_{u, n_u}(f_u)$$

Multilevel algorithm:

$$Q^{\text{ML}}(f) = \sum_{\ell=1}^L \left(\sum_{\substack{u \subseteq \{1, 2, \dots, 2^{\ell}\} \\ u \not\subseteq \{1, 2, \dots, 2^{\ell-1}\}}} Q_{\ell}(f_u) \right)$$

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Cost:
$$\text{cost}_{\text{nest}}(Q_L^{\text{ML}}) = \text{cost}_{\text{unr}}(Q_L^{\text{ML}}) \leq \sum_{\ell=1}^L 2 n_{\ell} 2^{\ell}$$

Multivariate decomposition method: Q^{MDM} :

$$Q^{\text{MDM}}(f) = \sum_{u \in \mathcal{A}_{\varepsilon}} Q_{u, n_u}(f_u)$$

$$f_u(\mathbf{x}) = \sum_{v \subseteq u} (-1)^{|u \setminus v|} f(\mathbf{x}_v)$$

Cost:
$$\text{cost}_{\text{unr}}(Q_L^{\text{MDM}}) = O\left(\sum_{u \in \mathcal{A}_{\varepsilon}} n_u 2^{|u|} |u|\right)$$

(Recall: $f_u(\mathbf{x}) = \sum_{v \subseteq u} (-1)^{|u \setminus v|} f(\mathbf{x}_v)$.)

Cost for evaluating f_u in unrestricted model: $O(2^{|u|} |u|)$.

“Typically”: $u \in \mathcal{A}_{\varepsilon} \implies |u| = o(\ln(1/\varepsilon)).$

Example of Non-Anchored Decomposition: ANOVA Decomp.

ANOVA condition $\int_D k(x, y) d\mu(y) = 0 \quad \forall x \in D$ implies that function decomp. $f = \sum_{u \subset_f \mathbb{N}} f_u$ in $H(K_\gamma)$ is **ANOVA decomp.** (in $L^2(D^{\mathbb{N}}, \mu^{\mathbb{N}})$):

$$f_\emptyset(\mathbf{x}) := \int_{D^{\mathbb{N}}} f(\mathbf{y}) d\mu^{\mathbb{N}}(\mathbf{y}),$$

$$f_u(\mathbf{x}) := \int_{D^{\mathbb{N} \setminus u}} f(\mathbf{x}_u, \mathbf{y}_{\mathbb{N} \setminus u}) d\mu^{\mathbb{N} \setminus u}(\mathbf{y}_{\mathbb{N} \setminus u}) - \sum_{v \subsetneq u} f_v(\mathbf{x}),$$

where $\mathbf{x}_u := (x_j)_{j \in u}$, $\mathbf{y}_{\mathbb{N} \setminus u} := (y_j)_{j \in \mathbb{N} \setminus u}$.

This implies

$$\|f\|_{L^2(D^{\mathbb{N}}, \mu^{\mathbb{N}})}^2 = \sum_{u \subset_f \mathbb{N}} \|f_u\|_{L^2(D^u, \mu^u)}^2 \quad \text{and} \quad \text{Var}(f) = \sum_{u \subset_f \mathbb{N}} \text{Var}(f_u).$$

(∞ -variate ANOVA decomposition was studied in:

Hickernell, Müller-Gronbach, Niu, Ritter '10; G., Baldeaux '14; Dick, G. '14b; Griebel, Kuo, Sloan '16;...)

Some Motivation

Given: $X = (X_t)_{t \in [0,1]}$ stochastic process with series expansion

$$X_t = \sum_{j=1}^{\infty} \xi_j e_j(t),$$

e_1, e_2, \dots deterministic functions on $[0, 1]$, ξ_1, ξ_2, \dots i.i.d. r.v. with distribution μ on D and $E[\xi_i] = 0$.

Examples: Consider $D = \mathbb{R}$ and $\mu = N(0, 1)$.

- Karhunen-Loève expansion of zero-mean Gaussian process X ; then $(e_j)_{j \in \mathbb{N}}$ orthogonal system in $L^2([0, 1])$ with $\sum_{j=1}^{\infty} \|e_j\|_{L^2([0,1])}^2 < \infty$.
- Lévy-Ciesielski or Brownian Bridge construction of Brownian motion X ; then e_1, e_2, \dots Schauder functions.

Task: For given functional φ on path space of X evaluate $E[\varphi(X)]$.

Observation:

$$E[\varphi(X)] = \int_{D^{\mathbb{N}}} f(\mathbf{x}) \, d\mu^{\mathbb{N}}(\mathbf{x}), \quad \text{where} \quad f(\mathbf{x}) = \varphi\left(\sum_{j=1}^{\infty} x_j e_j\right).$$

Computational Approach

Step 1: “Truncation”:

$$\sum_{j=1}^{\infty} \xi_j e_j \approx \sum_{j=1}^d \xi_j e_j \quad \text{and} \quad E[\varphi(X)] \approx E \left[\varphi \left(\sum_{j=1}^d \xi_j e_j \right) \right]$$

Step 2: Approximate

$$\begin{aligned} E \left[\varphi \left(\sum_{j=1}^d \xi_j e_j \right) \right] &= \int_{D^{\mathbb{N}}} f(x_1, \dots, x_d, 0, 0, \dots) \, d\mu^{\mathbb{N}}(\mathbf{x}) \\ &= \int_{D^d} f(x_1, \dots, x_d, 0, 0, \dots) \, d\mu^d(x_1, \dots, x_d) \end{aligned}$$

with algorithms for multivariate integration (recall $f(\mathbf{x}) = \varphi(\sum_{j=1}^{\infty} x_j e_j)$).

Result 1: Weighted RKHS Based on Anchored Kernel k^a

Theorem 1. Let $k = k^a$ be RK *anchored in* $a \in D$ and $K_\gamma = K_\gamma^a$ corresponding weighted RK. Then

$$\text{dec}(K_\gamma^a) = \min \left(\text{dec}(1 + k^a), \frac{\text{dec}(\gamma) - 1}{2} \right),$$

where $\text{dec}(1 + k^a)$ denotes convergence rate of n th minimal errors of univariate integration on $H(1 + k^a)$.

Contributions to proof of Theorem 1:

- Lower error bounds: Kuo, Sloan, Wasilkowski & Woźniakowski'10a (deterministic case); G.'13 (randomized case)
- Upper error bounds: Plaskota & Wasilkowski'11 (via multivariate decomposition method (MDM))

Earlier partial results in deterministic case: Kuo, Sloan, Wasilkowski & Woźniakowski'10a (via MDM); Niu, Hickernell, Müller-Gronbach & Ritter'11; G.'12 (both via multilevel algorithms)

Multivariate Decomposition Method

Recall: k^a RK anchored in $a \in D$ and K_γ^a corresponding weighted RK.

Anchored decomposition for $f \in H(K_\gamma^a)$: $f = \sum_{u \subset_f \mathbb{N}} f_u$, $f_u \in H(k_u)$.

Observation: S continuous on $H(K_\gamma^a)$, hence

$$S(f) = \int_{D^{\mathbb{N}}} f(\mathbf{x}) \, \mathrm{d}\mu(\mathbf{x}) = \sum_{u \subset_f \mathbb{N}} \int_{D^u} f_u(\mathbf{x}_u) \, \mathrm{d}\mu^u(\mathbf{x}_u).$$

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Multivariate decomposition method (MDM):

- ① Choose finite set \mathcal{A} ("set of active variables") of most important groups of variables.
- ② Choose for each $u \in \mathcal{A}$ quadrature Q_{u,n_u} using n_u samples to approximate $\int_{D^u} f_u(\mathbf{x}_u) \, d\mu^u(\mathbf{x}_u)$.

Final algorithm Q^{MDM} is of form

$$Q^{\text{MDM}}(f) = \sum_{u \in \mathcal{A}} Q_{u,n_u}(f_u)$$

Multivariate Decomposition Method

MDM *aka* **changing dimension algorithm** for ∞ -variate setting introduced in

- Kuo, Sloan, Wasilkowski & Woźniakowski'10; Plaskota & Wasilkowski'11 (∞ -variate integration)
- Wasilkowski & Woźniakowski'11a, '11b (∞ -variate approximation).

Further papers on MDM include: Wasilkowski'12; G.'13; Dick & G.'14a, 14b; Plaskota & Wasilkowski'14; Wasilkowski'14; Gilbert & Wasilkowski'17; G., Hefter, Hinrichs & Ritter'17; G., Hefter, Hinrichs, Ritter & Wasilkowski'17; Kuo, Nuyens, Plaskota, Sloan, Wasilkowski'17; Gilbert, Kuo, Nuyens & Wasilkowski'18; G., Hefter, Hinrichs, Ritter & Wasilkowski'19; G. & Wnuk'20; G., Hinrichs, Ritter & Rüßmann'23+

Similar idea used for **multivariate integration** in Griebel & Holtz'10 (**dimension-wise quadrature methods**).

How to choose building blocks Q_{u,n_u} for MDM?

- 1 Choose sequence $(Q_k)_{k \in \mathbb{N}}$ of quadratures for **univariate integration** on $H(1 + k^a)$.
- 2 Employ **Smolyak's method** to obtain Q_{u,n_u} : For $f_u \in H(k_u^a)$

$$Q_{u,n_u} f_u = \left(\sum_{L-|u|+1 \leq |\ell|_1 \leq L} (-1)^{L-|\ell|_1} \binom{|u|-1}{L-|\ell|_1} \otimes_{j \in u} Q_{\ell_j} \right) f_u.$$

Smolyak's method (*aka* **sparse grid method**, etc.) is “universal method” for approximation of **tensor product problems**, see, e.g.,

- **Deterministic Case**: [Smolyak'63; Temlyakov'87; Baszenski & Delvos'93; Wasilkowski & Woźniakowski'95; Novak & Ritter'96; Gerstner, Griebel'98;...
Surveys: [Bungartz, Griebel'04; Novak & Woźniakowski'08; Düng, Temlyakov & T. Ullrich'16; Tempone & Wolfers'18;...]
- **Randomized Case**: [Dick, Leobacher & Pillichshammer'07; Heinrich & Milla'11; G. & Wnuk'20; Wnuk & G.'21].

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Examples of Non-Anchored RKHSs

The following RKHSs are not based on an anchored kernel $k = k^a$:

Spaces defined via ...

... derivatives:

- Sobolev spaces with classical norms,
- unanchored Sobolev spaces,
- ...

... Fourier coefficients w.r.t. orthonormal basis of L^2 (including 1):

- Korobov spaces,
- Walsh spaces,
- Haar wavelet spaces,
- Hermite spaces,
- cosine spaces,
- ...

Result 2: Weighted RKHS Based on General RK k

Theorem 2 [G., Hefter, Hinrichs & Ritter'17; G. & Wnuk'20]. Let k be *general RK* and K_γ corresponding weighted RK. Then

$$\text{dec}(K_\gamma) = \min \left(\text{dec}(1 + k), \frac{\text{dec}(\gamma) - 1}{2} \right),$$

where $\text{dec}(1 + k)$ denotes convergence rate of N th minimal errors of univariate integration on $H(1 + k)$.

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where $\text{dec}(1+k)$ denotes convergence rate of N th minimal errors of univariate integration on $H(1+k)$.

How to prove the more general Theorem 2?

Simple observation: For Banach spaces $X \subseteq Y$ of integrable functions:

$$X \hookrightarrow Y$$

with embedding constant C implies

$$e(Q, X) \leq Ce(Q, Y) \quad \text{for all quadratures } Q,$$

resulting in

$$e(n, X) \leq Ce(n, Y) \quad \text{and} \quad \text{dec}(X) \geq \text{dec}(Y).$$

“Universality of Anchored Spaces”

Construction of associated anchored RKHS of $H(1 + k)$

Subspace $\{f \in H(1 + k) \mid f(a) = 0\}$ of RKHS $H(1 + k)$ has RK

$$k^a : D \times D \rightarrow \mathbb{R} \quad \text{with} \quad k^a(a, a) = 0$$

and $H(1 + k^a) = H(1 + k)$ as vector spaces with equivalent norms,
hence $\text{dec}(1 + k^a) = \text{dec}(1 + k)$.

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hence $\text{dec}(1 + k^a) = \text{dec}(1 + k)$.

With associated anchored kernel k^a of k again construct **weighted space** of ∞ -variate functions $H(K_\gamma^a)$:

$$K_\gamma^a(\mathbf{x}, \mathbf{y}) = \prod_{j \in \mathbb{N}} (1 + \gamma_j k^a(x_j, y_j)), \quad \mathbf{x}, \mathbf{y} \in D^{\mathbb{N}}.$$

“Embedding Triple”

In general, $H(K_\gamma) \not\subseteq H(K_\gamma^a)$ and $H(K_\gamma^a) \not\subseteq H(K_\gamma)$ [Heftner & Ritter '14].

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Remedy: Manipulate the Weights!

For $c > 0$ let $c\gamma := (c\gamma_j)_{j \in \mathbb{N}}$. Note that $\text{dec}(c\gamma) = \text{dec}(\gamma)$.

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Proposition [G., Hefter, Hinrichs & Ritter’17]. *There exists $0 < c_0 < 1$ such that*

$$H(K_{c_0\gamma}^a) \hookrightarrow H(K_\gamma) \hookrightarrow H(K_{c_0^{-1}\gamma}^a).$$

In general, $H(K_{c_0\gamma}^a) \subsetneq H(K_\gamma) \subsetneq H(K_{c_0^{-1}\gamma}^a)$.

Structure IV: Spaces of Increasing Smoothness

Let $(e_\nu)_{\nu \in \mathbb{N}_0}$ ONB of $L^2(D, \mu)$ with $e_0 = 1$.

Consider “Fourier weights” $\alpha_{\nu,j} \geq 1$, $\nu, j \in \mathbb{N}$, with

(A 1) $\alpha_{\nu,j} \leq \alpha_{\nu+1,j}$ and $\alpha_{\nu,j} \leq \alpha_{\nu,j+1}$ for all $\nu, j \in \mathbb{N}$,

(A 2) $\sum_{j \in \mathbb{N}} \sum_{\nu \in \mathbb{N}} \alpha_{\nu,j}^{-1} < \infty$.

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For each variable $j \in \mathbb{N}$ define RK

$$k_j(x, y) = \sum_{\nu \in \mathbb{N}} \alpha_{\nu,j}^{-1} \cdot e_\nu(x) \cdot e_\nu(y), \quad x, y \in \mathbb{R};$$

Then

$$H(1 + k_j) = \left\{ f \in L^2(D, \mu) : \sum_{\nu \in \mathbb{N}} \alpha_{\nu,j} \langle f, e_\nu \rangle_{L^2}^2 < \infty \right\}.$$

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Examples: Korobov spaces, Walsh spaces, Haar spaces, Hermite spaces,....

Structure IV: Spaces of Increasing Smoothness

Let $(e_\nu)_{\nu \in \mathbb{N}_0}$ ONB of $L^2(D, \mu)$ with $e_0 = 1$.

Consider “Fourier weights” $\alpha_{\nu,j} \geq 1$, $\nu, j \in \mathbb{N}$, with

(A 1) $\alpha_{\nu,j} \leq \alpha_{\nu+1,j}$ and $\alpha_{\nu,j} \leq \alpha_{\nu,j+1}$ for all $\nu, j \in \mathbb{N}$,

(A 2) $\sum_{j \in \mathbb{N}} \sum_{\nu \in \mathbb{N}} \alpha_{\nu,j}^{-1} < \infty$.

For each variable $j \in \mathbb{N}$ define RK

$$k_j(x, y) = \sum_{\nu \in \mathbb{N}} \alpha_{\nu,j}^{-1} \cdot e_\nu(x) \cdot e_\nu(y), \quad x, y \in \mathbb{R};$$

Then

$$H(1 + k_j) = \left\{ f \in L^2(D, \mu) : \sum_{\nu \in \mathbb{N}} \alpha_{\nu,j} \langle f, e_\nu \rangle_{L^2}^2 < \infty \right\}.$$

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Build “increasing smoothness RK”

$$K(\mathbf{x}, \mathbf{y}) := \prod_{j \in \mathbb{N}} (1 + k_j(x_j, y_j)), \quad \mathbf{x}, \mathbf{y} \in D^{\mathbb{N}}.$$

Result 3: Spaces of Increasing Smoothness

Define weights

$$\gamma_j := \sup_{\nu \in \mathbb{N}} \frac{\alpha_{\nu,1}}{\alpha_{\nu,j}}, \quad j \in \mathbb{N}.$$

Interpretation of weights: $\sqrt{\gamma_j}$ norm of embedding $H(k_j) \hookrightarrow H(k_1)$.

Sequence $\gamma = (\gamma_j)_{j \in \mathbb{N}}$ monotone decreasing. Assume $\sum_{j \in \mathbb{N}} \gamma_j < \infty$.

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Theorem 3 [G., Hefter, Hinrichs, Ritter & Wasilkowski'19;
G., Hinrichs, Ritter & Rüßmann'23+].

$$\begin{aligned} \min \left(\text{dec}(1 + k_1), \frac{\text{dec}(\gamma) - 1}{2} \right) &\leq \text{dec}(K) \\ &\leq \min \left(\text{dec}(1 + k_1), \frac{\text{dec}((\alpha_{1,j}^{-1})_{j \in \mathbb{N}}) - 1}{2} \right) \end{aligned}$$

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Examples: Let $1 < r_1 \leq r_2 \leq r_3 \leq \dots$

Fourier weights of ...

- ... polynomial growth (PG): $\alpha_{\nu,j} := (\nu + 1)^{r_j}$,
- ... exponential growth (EG): $\alpha_{\nu,j} := 2^{r_j \cdot \nu}$.

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For both cases (PG) & (EG): $\alpha_{1,j}^{-1} = 2^{-r_j}$ and $\gamma_j = 2^{r_1 - r_j}$, hence

$$\text{dec}(\gamma) = \text{dec}((\alpha_{1,j}^{-1})_{j \in \mathbb{N}}) = \liminf_{j \rightarrow \infty} \left(\frac{\ln(2)}{\ln(j)} r_j \right),$$

resulting in matching bounds in Theorem 3.

L^2 -Approximation

Solution Operator: **Embedding operator** $S : H(K) \rightarrow L^2(D^{\mathbb{N}}, \mu^{\mathbb{N}}), f \mapsto f$.

Algorithms: **Linear algorithms** $A : H(K) \rightarrow \mathbb{R}$ of form

$$A(f) := \sum_{i=1}^m w_i \cdot f(\mathbf{x}^{(i)}) \quad (3)$$

where $m \in \mathbb{N}$, $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)} \in D^{\mathbb{N}}$, and $w_1, \dots, w_m \in L^2(D^{\mathbb{N}}, \mu^{\mathbb{N}})$.

Cost: We only account for function evaluations, fix nominal value $a \in \mathbb{R}$, ...

Error Criterion: Worst case randomized/deterministic error of algorithm A ...

Results: Theorem 1, 2, and 3 hold verbatim¹! Again, upper error bounds are established via MDM based on Smolyak algorithms.

¹But the univariate convergence rates of n -th minimal errors of integration and L^2 -approximation may differ.

Summary

- Infinite-variate Integration:

- ① On spaces of integrands we first imposed structure (reproducing kernels, tensor product structure, weights, anchored function decomposition).
- ② Afterwards we fixed the setting (admissible algorithms, costs, and error criterion). In that setting...
- ③ ... MDM achieved optimal results on anchored weighted RKHSs by exploiting the anchored function decomposition.
- ④ ... an Embedding framework was used to prove that MDM achieve also optimal results on general weighted RKHSs.
- ⑤ ... another embedding strategy was used to prove that MDM achieve also optimal results on RKHSs of increasing smoothness.

- Infinite-variate L^2 -Approximation:

Same holds for L^2 -approximation (main results Theorem 1, 2 & 3 for integration hold verbatim for L^2 -approximation).

- **Concluding Remark:** Our embedding techniques allow to transfer error bounds for linear algorithms for multi- or ∞ -variate linear problems on one RKHS of weighted type or of increasing smoothness to different ones.

Sketch of Proof of Theorem 3

Consider *new* weighted RKs

$$k_j^{\text{up}}(x, y) := \gamma_j k_1(x, y), \quad \text{and} \quad k_j^{\text{low}}(x, y) := \alpha_{1,j}^{-1} e_1(x) e_1(y),$$

and put

$$K_{\gamma}^{\text{up}}(\mathbf{x}, \mathbf{y}) := \prod_{j=1}^{\infty} (1 + k_j^{\text{up}}(x_j, y_j)), \quad \text{and} \quad K_{\alpha_{1,j}}^{\text{low}}(\mathbf{x}, \mathbf{y}) := \prod_{j=1}^{\infty} (1 + k_j^{\text{low}}(x_j, y_j)).$$

Then

$$H(K_{\alpha_{1,j}}^{\text{low}}) \hookrightarrow H(K) \hookrightarrow H(K_{\gamma}^{\text{up}}).$$

Since $\text{dec}(1 + k_1^{\text{up}}) = \text{dec}(1 + k_1)$ and $\text{dec}(1 + k_1) \geq \text{dec}(K)$, we obtain

$$\begin{aligned} \min \left(\text{dec}(1 + k_1), \frac{\text{dec}(\gamma) - 1}{2} \right) &\leq \text{dec}(K) \\ &\leq \min \left(\text{dec}(1 + k_1), \frac{\text{dec}((\alpha_{1,j}^{-1})_{j \in \mathbb{N}}) - 1}{2} \right) \end{aligned}$$

Observation: $\dim(H(1 + k_j^{\text{low}})) = 2$, while $\dim(H(1 + k_j)) = \infty$ and typically $H(1 + k_{j+1}) \hookrightarrow H(1 + k_j)$ compactly, while $H(1 + k_{j+1}^{\text{up}}) = H(1 + k_j^{\text{up}})$ with equivalent norms.

An Alternative Cost Model

Randomized Quadrature: $Q_n(f) = \sum_{i=1}^n w_i f(\mathbf{x}^{(i)})$, where $w_i \in \mathbb{R}$, $\mathbf{x}^{(i)} \in D^{v_i}$.

Unrestricted Subspace Sampling [Kuo, Sloan, Wasilkowski, Woźniakowski'10a]

$$\text{cost}_{\text{unr}}(Q_n) := E \left[\sum_{i=1}^n |\{j \in \mathbb{N} : x_j^{(i)} \neq a\}| \right]$$

Nested Subspace Sampling [Creutzig, Dereich, Müller-Gronbach, Ritter'09]

$$\text{cost}_{\text{nest}}(Q_n) := E \left[\sum_{i=1}^n \max \{j \in \mathbb{N} : x_j^{(i)} \neq a\} \right]$$

"Rule of Thumb": For USS use multivariate decomposition method (MDM),
but for NSS use multilevel algorithms!

General references for multilevel algorithms: Heinrich '98, '01 (integral equations/parametric integration); Giles '08a, '08b; Giles, Higham & Mao (SDEs); Giles & Waterhouse '09 (QMC-ML); ... now better look at http://people.maths.ox.ac.uk/gilesm/mlmc_community.html

Multilevel for ∞ -dimensional integration problem: Hickernell, Müller-Gronbach, Niu & Ritter '10; Niu, Hickernell, Müller-Gronbach & Ritter '11; G. '12; Baldeaux '12; G.'13; Baldeaux & G. '14; Dick & G. '14a; Hefter '14; G., Hefter, Hinrichs & Ritter '17.

Comparison: Multilevel Algorithms and MDM

QMC-Multilevel Algorithm: $Q_L^{\text{ML}}(f) := \sum_{\ell=1}^L Q_{\ell}(f)$, where

$$Q_{\ell}(f) := \frac{1}{n_{\ell}} \sum_{i=1}^{n_{\ell}} \left(f(x_1^{(\ell,i)}, \dots, x_{2^{\ell}}^{(\ell,i)}, a, a, \dots) - f(x_1^{(\ell,i)}, \dots, x_{2^{\ell-1}}^{(\ell,i)}, a, a, \dots) \right)$$

Let $f \in H(K_{\gamma}^a)$ with anchored function decomposition $f = \sum_{u \subset_f \mathbb{N}} f_u$.

Solution operator:

$$S(f) = \int_{D^{\mathbb{N}}} f(\mathbf{x}) \, d\mu^{\mathbb{N}}(\mathbf{x}) = \sum_{u \subset_f \mathbb{N}} \int_{D^u} f_u(\mathbf{x}_u) \, d\mu^u(\mathbf{x}_u)$$

Multivariate decomposition method:

$$Q^{\text{MDM}}(f) = \sum_{u \subset_f \mathbb{N}} Q_{u, n_u}(f_u)$$

Multilevel algorithm:

$$Q^{\text{ML}}(f) = \sum_{\ell=1}^L \left(\sum_{\substack{u \subseteq \{1, 2, \dots, 2^{\ell}\} \\ u \not\subseteq \{1, 2, \dots, 2^{\ell-1}\}}} Q_{\ell}(f_u) \right)$$

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Cost:
$$\text{cost}_{\text{nest}}(Q_L^{\text{ML}}) = \text{cost}_{\text{unr}}(Q_L^{\text{ML}}) \leq \sum_{\ell=1}^L 2 n_{\ell} 2^{\ell}$$

Multivariate decomposition method: Q^{MDM} :

$$Q^{\text{MDM}}(f) = \sum_{u \in \mathcal{A}_{\varepsilon}} Q_{u, n_u}(f_u)$$

$$f_u(\mathbf{x}) = \sum_{v \subseteq u} (-1)^{|u \setminus v|} f(\mathbf{x}_v)$$

Cost:
$$\text{cost}_{\text{unr}}(Q_L^{\text{MDM}}) = O\left(\sum_{u \in \mathcal{A}_{\varepsilon}} n_u 2^{|u|} |u|\right)$$

(Recall: $f_u(\mathbf{x}) = \sum_{v \subseteq u} (-1)^{|u \setminus v|} f(\mathbf{x}_v)$.)

Cost for evaluating f_u in unrestricted model: $O(2^{|u|} |u|)$.

“Typically”: $u \in \mathcal{A}_{\varepsilon} \implies |u| = o(\ln(1/\varepsilon)).$

Example of Non-Anchored Decomposition: ANOVA Decomp.

ANOVA condition $\int_D k(x, y) d\mu(y) = 0 \quad \forall x \in D$ implies that function decomp. $f = \sum_{u \subset_f \mathbb{N}} f_u$ in $H(K_\gamma)$ is **ANOVA decomp.** (in $L^2(D^{\mathbb{N}}, \mu^{\mathbb{N}})$):

$$f_\emptyset(\mathbf{x}) := \int_{D^{\mathbb{N}}} f(\mathbf{y}) d\mu^{\mathbb{N}}(\mathbf{y}),$$

$$f_u(\mathbf{x}) := \int_{D^{\mathbb{N} \setminus u}} f(\mathbf{x}_u, \mathbf{y}_{\mathbb{N} \setminus u}) d\mu^{\mathbb{N} \setminus u}(\mathbf{y}_{\mathbb{N} \setminus u}) - \sum_{v \subsetneq u} f_v(\mathbf{x}),$$

where $\mathbf{x}_u := (x_j)_{j \in u}$, $\mathbf{y}_{\mathbb{N} \setminus u} := (y_j)_{j \in \mathbb{N} \setminus u}$.

This implies

$$\|f\|_{L^2(D^{\mathbb{N}}, \mu^{\mathbb{N}})}^2 = \sum_{u \subset_f \mathbb{N}} \|f_u\|_{L^2(D^u, \mu^u)}^2 \quad \text{and} \quad \text{Var}(f) = \sum_{u \subset_f \mathbb{N}} \text{Var}(f_u).$$

(∞ -variate ANOVA decomposition was studied in:

Hickernell, Müller-Gronbach, Niu, Ritter '10; G., Baldeaux '14; Dick, G. '14b; Griebel, Kuo, Sloan '16;...)

Some Motivation

Given: $X = (X_t)_{t \in [0,1]}$ stochastic process with series expansion

$$X_t = \sum_{j=1}^{\infty} \xi_j e_j(t),$$

e_1, e_2, \dots deterministic functions on $[0, 1]$, ξ_1, ξ_2, \dots i.i.d. r.v. with distribution μ on D and $E[\xi_i] = 0$.

Examples: Consider $D = \mathbb{R}$ and $\mu = N(0, 1)$.

- Karhunen-Loève expansion of zero-mean Gaussian process X ; then $(e_j)_{j \in \mathbb{N}}$ orthogonal system in $L^2([0, 1])$ with $\sum_{j=1}^{\infty} \|e_j\|_{L^2([0,1])}^2 < \infty$.
- Lévy-Ciesielski or Brownian Bridge construction of Brownian motion X ; then e_1, e_2, \dots Schauder functions.

Task: For given functional φ on path space of X evaluate $E[\varphi(X)]$.

Observation:

$$E[\varphi(X)] = \int_{D^{\mathbb{N}}} f(\mathbf{x}) \, d\mu^{\mathbb{N}}(\mathbf{x}), \quad \text{where} \quad f(\mathbf{x}) = \varphi\left(\sum_{j=1}^{\infty} x_j e_j\right).$$

Computational Approach

Step 1: “Truncation”:

$$\sum_{j=1}^{\infty} \xi_j e_j \approx \sum_{j=1}^d \xi_j e_j \quad \text{and} \quad E[\varphi(X)] \approx E \left[\varphi \left(\sum_{j=1}^d \xi_j e_j \right) \right]$$

Step 2: Approximate

$$\begin{aligned} E \left[\varphi \left(\sum_{j=1}^d \xi_j e_j \right) \right] &= \int_{D^{\mathbb{N}}} f(x_1, \dots, x_d, 0, 0, \dots) \, d\mu^{\mathbb{N}}(\mathbf{x}) \\ &= \int_{D^d} f(x_1, \dots, x_d, 0, 0, \dots) \, d\mu^d(x_1, \dots, x_d) \end{aligned}$$

with algorithms for multivariate integration (recall $f(\mathbf{x}) = \varphi(\sum_{j=1}^{\infty} x_j e_j)$).