# Adapting quasi-Monte Carlo methods to simulation problems in weighted Korobov spaces

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joint work with G. Leobacher

RICAM Special Semester – Workshop 1
"Uniform distribution and quasi-Monte Carlo methods"
October 2013, Linz

- Efficient computation of $\mathbb{E}(g(B))$
  - $B \ldots$ standard Brownian motion with index set $[0, T]$
  - $g \ \ldots$ suitable function

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- Examples in finance, biology, physics,. . .
- e.g.: Financial derivative pricing
  - Gaussian financial market models
  - European-style options

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- Error of QMC algorithm $Q_{d,N}$

$$\text{err} := |\mathbb{E}(g(B)) - Q_{d,N}(f_d)|$$

- First estimate:

$$\text{err} \leq \underbrace{\left|\mathbb{E}(g(B)) - I(f_d)\right|}_{\textit{discretization error}} + \underbrace{\left|I(f_d) - Q_{d,N}(f_d)\right|}_{\textit{integration error}}$$

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- Analysis of both errors
  - emphasis on integration error
  - but discretization error not negligible

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  with convergence rate $p > 0$ and constant $c_1 > 0$
- Convergence rate depends on
  - discretization method
  - function $g$

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- $\{H_{\boldsymbol{k}}\}_{\boldsymbol{k}}$ is an ONB of $L^2(\mathbb{R}^d, \varphi)$

- Hermite expansion of $f \in L^2(\mathbb{R}^d, \varphi)$

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{k} \in \mathbb{N}_0^d} \hat{f}(\boldsymbol{k}) H_{\boldsymbol{k}}(\boldsymbol{x}) \qquad \text{in } L^2$$

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**Theorem**

*Let $f \in L^2(\mathbb{R}^d, \varphi) \cap C(\mathbb{R}^d)$ and $\sum_{\boldsymbol{k} \in \mathbb{N}_0^d} \hat{f}(\boldsymbol{k}) < \infty$. Then*

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{k} \in \mathbb{N}_0^d} \hat{f}(\boldsymbol{k}) H_{\boldsymbol{k}}(\boldsymbol{x})$$

*for all $\boldsymbol{x} \in \mathbb{R}^d$.*

- Let $\alpha > 1$, $\gamma > 0$. Define for $k \in \mathbb{N}_0$:

$$r(\alpha, \gamma, k) := \begin{cases} 1 & \text{if } k = 0 \\ \gamma k^{-\alpha} & \text{if } k \neq 0 \end{cases}$$

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$$\langle f, g \rangle_{\alpha,\gamma} := \sum_{k=0}^{\infty} r(\alpha, \gamma, k)^{-1} \hat{f}(k) \hat{g}(k)$$

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- Function space:

$$\mathcal{H}_{\alpha,\gamma}(\mathbb{R},\varphi) := \{ f \in L^2(\mathbb{R},\varphi) \cap C(\mathbb{R}) : \|f\|_{\alpha,\gamma} < \infty \}$$

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- Reproducing kernel function $K_{\alpha,\gamma}:\mathbb{R}\times\mathbb{R}\longrightarrow\mathbb{R}$
  - $K_{\alpha,\gamma}(\cdot,y)\in\mathcal{H}_{\alpha,\gamma}(\mathbb{R},\varphi) \quad \forall y\in\mathbb{R}$
  - $\langle f,K_{\alpha,\gamma}(\cdot,y)\rangle_{\alpha,\boldsymbol{\gamma}} = f(y) \quad \forall y\in\mathbb{R}\,\forall f\in\mathcal{H}_{\alpha,\gamma}(\mathbb{R},\varphi)$

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  - $\langle f, K_{\alpha,\gamma}(\cdot, y)\rangle_{\alpha,\boldsymbol{\gamma}} = f(y) \quad \forall y \in \mathbb{R}\ \forall f \in \mathcal{H}_{\alpha,\gamma}(\mathbb{R},\varphi)$
- Series representation of the reproducing kernel

$$K_{\alpha,\gamma}(x,y) = 1 + \gamma \sum_{k=1}^{\infty} k^{-\alpha} H_k(x) H_k(y)$$

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**Theorem (I. & Leobacher)**

*Let $\beta > 2$ be an integer and $f : \mathbb{R} \longrightarrow \mathbb{R}$ be a $\beta$ times differentiable function such that*

(i) $D_x^j f(x)\varphi(x)^{\frac{1}{2}} \in L^1(\mathbb{R})$ *for each* $j \in \{1, \ldots, \beta\}$ *and*

(ii) $D_x^j f(x) = \mathcal{O}\left(e^{x^2/(2c)}\right)$ *as* $|x| \to \infty$ *for each* $j \in \{0, \ldots, \beta - 1\}$ *and some* $c > 1$.

*Then* $f \in \mathcal{H}_{\alpha,\gamma}(\mathbb{R}, \varphi)$ *with* $1 < \alpha < \beta - 1$.

- For non-increasing weights $\boldsymbol{\gamma} = (\gamma_1, \dots, \gamma_d)$

$$\mathcal{H}_{\alpha,\boldsymbol{\gamma}}(\mathbb{R}^d, \varphi) := \mathcal{H}_{\alpha,\gamma_1}(\mathbb{R}, \varphi) \otimes \ldots \otimes \mathcal{H}_{\alpha,\gamma_d}(\mathbb{R}, \varphi)$$

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- Inner product: $\langle f, g \rangle_{\alpha,\boldsymbol{\gamma}} = \sum_{\boldsymbol{k} \in \mathbb{N}_0^d} \boldsymbol{r}(\alpha, \boldsymbol{\gamma}, \boldsymbol{k})^{-1} \hat{f}(\boldsymbol{k}) \hat{g}(\boldsymbol{k})$ with $\boldsymbol{r}(\alpha, \boldsymbol{\gamma}, \boldsymbol{k}) = \prod_{j=1}^{d} r(\alpha, \gamma_j, k_j)$

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- $\mathcal{H}_{\alpha,\boldsymbol{\gamma}}(\mathbb{R}^d, \varphi)$ is a weighted reproducing kernel Hilbert space
  - Reproducing kernel $K_{\alpha,\boldsymbol{\gamma}}(\boldsymbol{x}, \boldsymbol{y}) = \prod_{j=1}^d K_{\alpha,\gamma_j}(x_j, y_j)$
  - Influence of variables is given by the choice of weights $\boldsymbol{\gamma}$

- Let $f_d \in \mathcal{H}_{\alpha,\boldsymbol{\gamma}}(\mathbb{R}^d, \varphi)$.
  - $I(f_d) = \int_{\mathbb{R}^d} f_d(\boldsymbol{x})\varphi(\boldsymbol{x})d\boldsymbol{x} = \int_{\mathbb{R}^d} \langle f_d, K_{\alpha,\boldsymbol{\gamma}}(\cdot,\boldsymbol{x})\rangle_{\alpha,\boldsymbol{\gamma}}\varphi(\boldsymbol{x})d\boldsymbol{x}$
    $= \langle f_d, \int_{\mathbb{R}^d} K_{\alpha,\boldsymbol{\gamma}}(\cdot,\boldsymbol{x})\varphi(\boldsymbol{x})d\boldsymbol{x}\rangle_{\alpha,\boldsymbol{\gamma}}$
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  - $Q_{d,N}(f_d) = \langle f_d, \frac{1}{N}\sum_{n=1}^N K_{\alpha,\boldsymbol{\gamma}}(\cdot,\boldsymbol{x}_n)\rangle_{\alpha,\boldsymbol{\gamma}}$
- Integration error

$$\begin{aligned}\mathrm{err}_{\mathrm{QMC}} &= |I(f_d) - Q_{d,N}(f_d)| \\ &\le \|f_d\|_{\alpha,\boldsymbol{\gamma}} \underbrace{\left\| \int_{\mathbb{R}^d} K_{\alpha,\boldsymbol{\gamma}}(\cdot,\boldsymbol{x})\varphi(\boldsymbol{x})d\boldsymbol{x} - \frac{1}{N}\sum_{n=1}^N K_{\alpha,\boldsymbol{\gamma}}(\cdot,\boldsymbol{x}_n)\right\|_{\alpha,\boldsymbol{\gamma}}}_{=:e_{d,N}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N)}\end{aligned}$$

- Considering the Gaussian-weighted root-mean-square error for QMC integration:

$$\bar{e}_{d,N} := \left( \int_{\mathbb{R}^{dN}} e_{d,N}^2(\boldsymbol{x}_1, \dots, \boldsymbol{x}_N) \varphi(\boldsymbol{x}_1) \dots \varphi(\boldsymbol{x}_N) d(\boldsymbol{x}_1, \dots, \boldsymbol{x}_N) \right)^{\frac{1}{2}}$$

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## Theorem (I. & Leobacher)

*The Gaussian-weighted root-mean-square error for QMC integration in the Korobov space $\mathcal{H}_{\alpha,\gamma}(\mathbb{R}^d, \varphi)$ is*

$$\bar{e}_{d,N} = \frac{1}{\sqrt{N}} \left( \prod_{j=1}^{d} (1 + \gamma_j \zeta(\alpha)) - 1 \right)^{\frac{1}{2}}.$$

- There exists a point set $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ such that

$$e_{d,N} \leq \frac{1}{\sqrt{N}} \exp\left(\frac{\zeta(\alpha)}{2} \sum_{j=1}^{d} \gamma_j\right)$$

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- $\mathrm{err} \leq c_1 d^{-p} + \|f_d\|_{\alpha,\boldsymbol{\gamma}} c_2 N^{-1/2} d^q$
- $\|f_d\|_{\alpha,\boldsymbol{\gamma}}$ can grow in $d$

- For any orthogonal transform $U$ on $\mathbb{R}^d$:

$$\int_{\mathbb{R}^d} f_d(\boldsymbol{x})\varphi(\boldsymbol{x})d\boldsymbol{x} = \int_{\mathbb{R}^d} f_d(U\boldsymbol{x})\varphi(\boldsymbol{x})d\boldsymbol{x}$$

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- Equivalence principle (Wang & Sloan 2011)
  - Roughly spoken: every construction that is good for one function is bad for another

- Bound of the integration error:

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- Bound of the integration error:

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- In general, $\|f_d\|_{\alpha,\gamma} \neq \|f_d \circ U\|_{\alpha,\gamma}$
- Goal: Find $U$ such that $\|f_d \circ U\|_{\alpha,\gamma}$ grows slower in $d$ than $\|f_d\|_{\alpha,\gamma}$ or is even bounded.
  - LT-method (Imai & Tan 2007)
  - Regression algorithm (I. & Leobacher 2012)

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- $\|f_d\|_{\alpha,\boldsymbol{\gamma}}^2 = \sum_{\boldsymbol{k}\in\mathbb{N}_0^d} r(\alpha,\boldsymbol{\gamma},\boldsymbol{k})^{-1} \widehat{f_d}(\boldsymbol{k})^2 \approx \exp(1 + \frac{1}{d} \sum_{j=1}^{d} \gamma_j^{-1})$

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- If $\gamma_j = j^{-2}$,
  - $e_{d,N}$ is bounded by $cN^{-1/2}$ with constant $c > 0$,
  - But $\|f_d\|_{\alpha,\boldsymbol{\gamma}} = \mathcal{O}(e^d)$

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- Norm is independent of $d$

$$\|f_d \circ U\|^2_{\alpha,\boldsymbol{\gamma}} = \sum_{\boldsymbol{k} \in \mathbb{N}_0^d} r(\alpha, \boldsymbol{\gamma}, \boldsymbol{k}) \widehat{f_d \circ U}(\boldsymbol{k})^2 = e + \sum_{k=1}^{\infty} \gamma_1^{-1} k_1^{\alpha} \frac{e}{k_1!}$$
$$= e + \gamma_1^{-1} e^2 c(\alpha)$$

- Define:
  - $\mathcal{A}_U : L^2(\mathbb{R}^d, \varphi) \longrightarrow L^2(\mathbb{R}^d, \varphi)$ by $\mathcal{A}_U f = f \circ U$
  - $\mathcal{H}_m := \mathrm{span}\{H_{\boldsymbol{k}}(x) : |\boldsymbol{k}| = m\}$
  - $\mathcal{A}_{U,m} := \mathcal{A}_U\big|_{\mathcal{H}_m}$

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  - $\mathcal{A}_U : L^2(\mathbb{R}^d, \varphi) \longrightarrow L^2(\mathbb{R}^d, \varphi)$ by $\mathcal{A}_U f = f \circ U$
  - $\mathcal{H}_m := \mathrm{span}\{H_{\boldsymbol{k}}(x) : |\boldsymbol{k}| = m\}$
  - $\mathcal{A}_{U,m} := \mathcal{A}_U\big|_{\mathcal{H}_m}$
- Then:
  - $\mathcal{A}_U$ is a Hilbert space automorphism of $L^2(\mathbb{R}^d, \varphi)$
  - $\mathcal{A}_{U,m}$ is a Hilbert space automorphism of $\mathcal{H}_m$
  - $L^2(\mathbb{R}^d, \varphi) = \bigoplus_{m \geq 0} \mathcal{H}_m$
  - $\mathcal{A}_U = \bigoplus_{m \geq 0} \mathcal{A}_{U,m}$

- $H_{\boldsymbol{k}}(\boldsymbol{x}) = \frac{\partial^{|\boldsymbol{k}|}}{\partial \boldsymbol{t}^{\boldsymbol{k}}} G(\boldsymbol{x}, \boldsymbol{t})\Big|_{\boldsymbol{t}=0}$ with exponential generating function $G$

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- For any $(\beta_1, \ldots, \beta_m) \in \{1, \ldots, d\}^m$:

$$\frac{\partial}{\partial t_{\beta_m}} \cdots \frac{\partial}{\partial t_{\beta_1}} G(U\boldsymbol{x}, \boldsymbol{t})\Big|_{\boldsymbol{t}=0} = \\ = \sum_{\xi_1, \ldots, \xi_m = 1}^{d} U_{\beta_m \xi_m} \cdots U_{\beta_1 \xi_1} \left( \frac{\partial}{\partial t_{\xi_m}} \cdots \frac{\partial}{\partial t_{\xi_1}} G(\boldsymbol{x}, \boldsymbol{t})\Big|_{\boldsymbol{t}=0} \right)$$

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- Many $(\beta_1, \ldots, \beta_m)$ correspond to the same multi-index $\boldsymbol{k}$

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$$
\begin{array}{ccc}
\mathcal{H}_m & \xrightarrow{\mathcal{A}_{U,m}} & \mathcal{H}_m \\
J_m \big\downarrow & & \big\uparrow J_m^\top \\
\mathcal{K}_m & \xrightarrow[U^{\otimes m}]{} & \mathcal{K}_m
\end{array}
$$

$$\begin{array}{ccc} L^2(\mathbb{R}^d,\varphi) & \xrightarrow{\ \mathcal{A}_U\ } & L^2(\mathbb{R}^d,\varphi) \\ J\big\downarrow & & \big\uparrow J^\top \\ \mathcal{K} & \xrightarrow[\bigoplus_{m\geq 0} U^{\otimes m}]{} & \mathcal{K} \end{array}$$

with

$$\mathcal{K} = \bigoplus_{m\geq 0} \mathcal{K}_m, \qquad J = \bigoplus_{m\geq 0} J_m, \qquad J^\top = \bigoplus_{m\geq 0} J_m^\top.$$

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- Thus $\mathcal{A} = J^\top \left( \bigoplus_{m \geq 0} U^{\otimes m} \right) J$

- Is $\mathcal{A}_U$ well defined on the Korobov space?
- Other weight structures (choice of weights)
- Sobolev space setting (RKHS, tractability)
- Concrete point sets (worst case error analysis, tractability)

# Thank you for your attention