The Multivariate Decomposition Method

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On joint work with
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specifically: using the anchored decomposition:

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Method: approximate $I_{\mathfrak{u}}$ on sets of important dimensions $\mathfrak{u} \in \mathcal{U}_\epsilon$ by cubature formulae $Q_{\mathfrak{u},n_{\mathfrak{u}}}$ using function values.

Baldeaux, Gilbert, Gnewuch, Hefter, Hickernell, Hinrichs, Kuo, Müller-Gronbach, N., Plaskota, Ritter, Sloan, Wasilkowski, Woźniakowski, ...

Anchored decomposition and point evaluations

Prototype infinite variate function as depending on a series decomposition, e.g.,

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$$f(\boldsymbol{y}_{\mathfrak{u}};0) = g\left(\sum_{j\in\mathfrak{u}} y_j\, c_j\right),$$

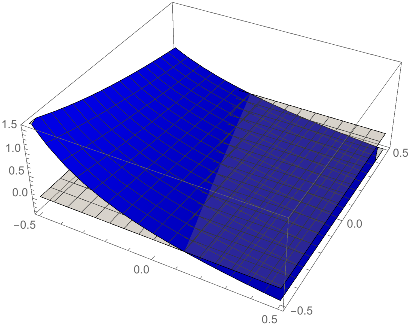
and the cost of evaluating $f_{\mathfrak{u}}$, denoted later by $\pounds(\mathfrak{u})$,

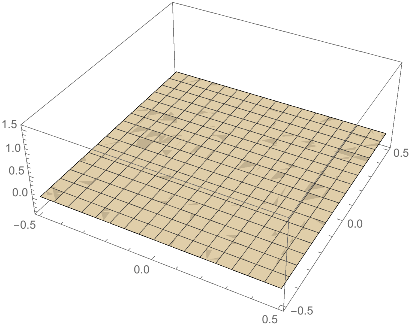
$$f_{\mathfrak{u}}(\boldsymbol{y}_{\mathfrak{u}}) = \sum_{\mathfrak{v}\subseteq\mathfrak{u}} (-1)^{|\mathfrak{u}|-|\mathfrak{v}|}\, f(\boldsymbol{y}_{\mathfrak{v}};0),$$

can be bounded as $\pounds(\mathfrak{u}) \leq 2^{|\mathfrak{u}|}\$(\mathfrak{u})$ (with here $\$(\mathfrak{u}) \sim |\mathfrak{u}|$).

Example of anchored decomposition (on $[-1/2, 1/2]^{\mathbb{N}}$)

$$f(\boldsymbol{y}) = \left(1 + \sum_{j\geq 1} j^{-2}\, y_j\right)^{-1} - 1 \qquad f_\emptyset$$





$$f_\emptyset = f(0, 0, \ldots)$$

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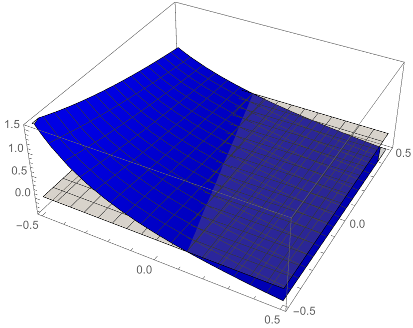

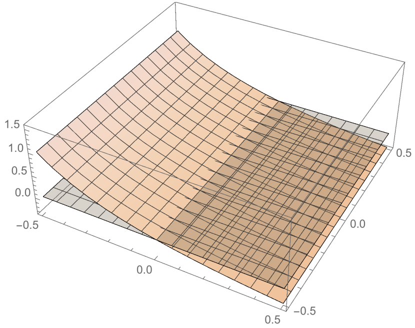

$$f_{\{1\}}(y_1) = f(y_1, 0, 0, \ldots) - f(0, 0, \ldots)$$

Example of anchored decomposition (on $[-1/2, 1/2]^{\mathbb{N}}$)

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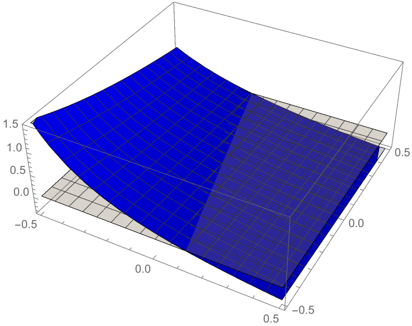

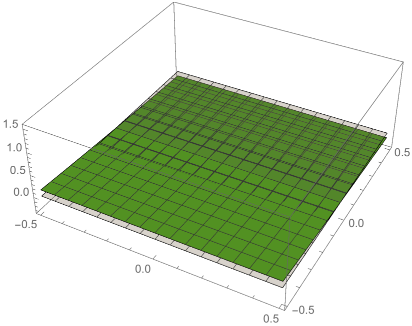

$$f_{\{2\}}(y_2) = f(0, y_2, 0, \ldots) - f(0, 0, \ldots)$$

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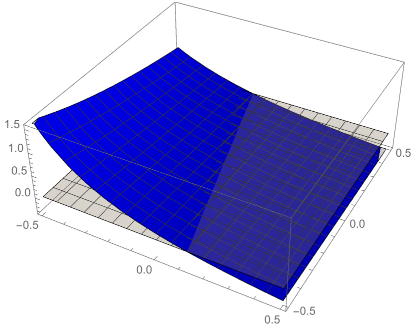

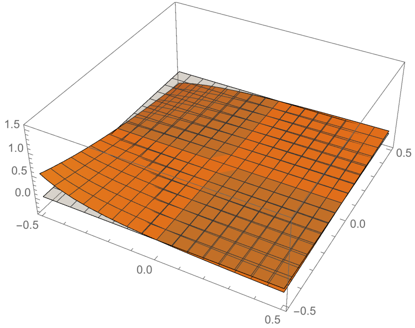

$$f_{\{1,2\}}(y_1, y_2) = f(y_1, y_2, 0, \ldots) - f(y_1, 0, \ldots) - f(0, y_2, 0, \ldots) + f(0, 0, \ldots)$$

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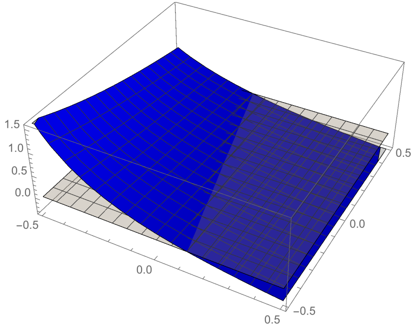

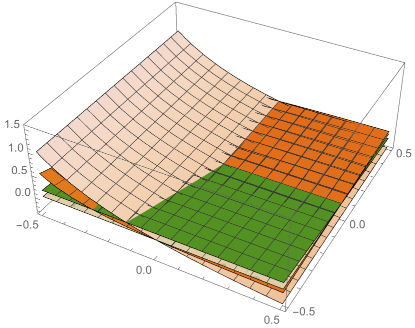

$$f(y_1, y_2, 0, 0, \ldots) = f_{\emptyset} + f_{\{1\}}(y_1) + f_{\{2\}}(y_2) + f_{\{1,2\}}(y_1, y_2)$$

Standard problem

Consider the following elliptic PDE

$$-\nabla \cdot \big(a(\boldsymbol{x}, \boldsymbol{y}) \nabla u(\boldsymbol{x}, \boldsymbol{y})\big) = w(\boldsymbol{x}), \qquad \text{for } \boldsymbol{x} \in D, \text{ a.s. } \boldsymbol{y} \in [-1/2, 1/2]^{\mathbb{N}},$$

and $u(\boldsymbol{x}, \boldsymbol{y}) = 0$ for $\boldsymbol{x} \in \delta D$, where

- $D \subset \mathbb{R}^d$ is a "nice" bounded physical domain, $d = 1, 2, 3$,
- $\boldsymbol{y}$ is parameter/parametrization of random field,
- $a(\boldsymbol{x}, \boldsymbol{y})$ is a scalar random field, e.g.,

$$a(\boldsymbol{x}, \boldsymbol{y}) = a_0(\boldsymbol{x}) + \sum_{j \ge 1} y_j \, \varphi_j(\boldsymbol{x}), \qquad y_j \sim U[-1/2, 1/2],$$

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- and $\sum_{j\ge1} \|\varphi_j\|_{L_\infty}^p < \infty$ for some $0 < p < 1$.

Lots of references: Adcock, Babuska, Brugiapaglia, Chkifa, Cohen, Dahmen, DeVore, Dexter, Ghanem, Gittelson, Graham, Griebel, Hoang, Karniadakis, Nobile, Scheichl, Schwab, Spanos, Tempone, Todor, Webster, Xiu, Zhang, EVERYBODY, ...

Calculate expected value (could also approximate function)

For a continuous linear functional G we wish to approximate

$$\mathbb{E}[G(u)] = I_\infty(G(u)) = \int_{[-1/2,1/2]^{\mathbb{N}}} G(u(\boldsymbol{x}, \boldsymbol{y}))\, \mathrm{d}\boldsymbol{y}.$$

From cubature point of view (MC, QMC or sparse grid, but QMC biased) there are 3 options with corresponding (dimension independent) error analysis (= truncation error + FEM error + cubature error) for parametrized PDE:

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NB: both first order and higher order convergence with QMC.

The general MDM setting (no PDE for now)

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with error

$$|I_\infty(f) - Q_\epsilon(G)| \leq \underbrace{\sum_{\mathfrak{u}\notin\mathcal{U}_\epsilon} |I_{\mathfrak{u}}(f_{\mathfrak{u}})|}_{\lesssim \epsilon/2} +$$

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$$|I_\infty(f) - Q_\epsilon(G)| \le \underbrace{\sum_{\mathfrak{u}\notin\mathcal{U}_\epsilon} |I_{\mathfrak{u}}(f_{\mathfrak{u}})|}_{\lesssim\epsilon/2} + \underbrace{\sum_{\mathfrak{u}\notin\mathcal{U}_\epsilon} |I_{\mathfrak{u}}(f_{\mathfrak{u}}) - Q_{\mathfrak{u},n_{\mathfrak{u}}}(f_{\mathfrak{u}})|}_{\lesssim\epsilon/2} \lesssim \epsilon.$$

$\Rightarrow$ Need properties on $f_{\mathfrak{u}} \in F_{\mathfrak{u}}$ to use optimal algorithms.

$\Rightarrow$ error = truncation error + cubature errors.

Truncation error

From application:
Assume that $f_{\mathfrak{u}} \in F_{\mathfrak{u}}$ with $\|f_{\mathfrak{u}}\|_{F_{\mathfrak{u}}} \le B_{\mathfrak{u}}$ and $\|I_{\mathfrak{u}}\| \le C_{\mathfrak{u}}$.

Construct the active set $\mathcal{U}_\epsilon$ such that

$$\sum_{\mathfrak{u} \notin \mathcal{U}_\epsilon} |I_{\mathfrak{u}}(f_{\mathfrak{u}})| \le \sum_{\mathfrak{u} \notin \mathcal{U}_\epsilon} \|I_{\mathfrak{u}}\| \|f_{\mathfrak{u}}\|_{F_{\mathfrak{u}}} \le \sum_{\mathfrak{u} \notin \mathcal{U}_\epsilon} C_{\mathfrak{u}} B_{\mathfrak{u}} \le \frac{\epsilon}{2}.$$

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Moreover there is a decay with respect to increasing $|\mathfrak{u}|$:

$$\alpha_0 := \sup \left\{ \alpha : \sum_{|\mathfrak{u}| < \infty} (C_{\mathfrak{u}} B_{\mathfrak{u}})^{1/\alpha} < \infty \right\} > 1.$$

Compare this with ℓ_p summability with $0 < p < 1$ where $p = 1/\alpha$.

Constructing the active set $\mathcal{U}_\epsilon$ to control truncation error

Remember $|I_{\mathfrak{u}}(f_{\mathfrak{u}})| \le C_{\mathfrak{u}} B_{\mathfrak{u}}$, then for any $\alpha \in (1, \alpha_0)$ we may define

$$\mathcal{U}_\epsilon = \mathcal{U}_\epsilon(\alpha) := \left\{ \mathfrak{u} \subset \mathbb{N} : (C_{\mathfrak{u}} B_{\mathfrak{u}})^{1-1/\alpha} > \frac{\epsilon/2}{\sum_{|\mathfrak{v}|<\infty} (C_{\mathfrak{v}} B_{\mathfrak{v}})^{1/\alpha}} \right\}.$$

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We have

$$|\mathcal{U}_\epsilon(\alpha)| < \left(\frac{2}{\epsilon}\right)^{\frac{1}{\alpha-1}} \left[\sum_{|\mathfrak{u}|<\infty} (C_{\mathfrak{u}} B_{\mathfrak{u}})^{\frac{1}{\alpha}} \right]^{\frac{\alpha}{\alpha-1}}.$$

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In implementation we assume product and order dependent (POD)

$$C_{\mathfrak{u}} B_{\mathfrak{u}} = (|\mathfrak{u}|!)^{b_1} \mu \prod_{j \in \mathfrak{u}} (\kappa j^{-b_2}), \quad \text{with } b_2 > \max(b_1, 0), \mu > 0, \kappa > 0,$$

then for $\epsilon \to 0$

$$d(\epsilon) := \max_{\mathfrak{u} \in \mathcal{U}_\epsilon} |\mathfrak{u}| = O(\ln(1/\epsilon) \,/\, \ln(\ln(1/\epsilon))).$$

Cubature errors: worst case error

Assume we have cubature rules $Q_{\mathfrak{u},n_\mathfrak{u}}$ which for all $f_\mathfrak{u} \in F_\mathfrak{u}$:

$$|Q_{\mathfrak{u},n_\mathfrak{u}}(f_\mathfrak{u}) - I_\mathfrak{u}(f_\mathfrak{u})| \le \frac{G_{\mathfrak{u},q} \|f_\mathfrak{u}\|_{F_\mathfrak{u}}}{(n_\mathfrak{u}+1)^q}, \qquad n_\mathfrak{u} = 0, 1, 2, \ldots,$$

e.g., QMC or sparse grid rules, where $\|I_\mathfrak{u}\|_{F_\mathfrak{u}} \le C_\mathfrak{u} \le G_{\mathfrak{u},q}$ such that this also holds for the zero algorithm $Q_{\mathfrak{u},0} = 0$.
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Then, again with $\|f_\mathfrak{u}\|_{F_\mathfrak{u}} \le B_\mathfrak{u}$, we need

$$\sum_{\mathfrak{u} \in \mathcal{U}_\epsilon} |I_\mathfrak{u}(f_\mathfrak{u}) - Q_{\mathfrak{u},n_\mathfrak{u}}(f_\mathfrak{u})| \le \sum_{\mathfrak{u} \in \mathcal{U}_\epsilon} \frac{G_{\mathfrak{u},q} B_\mathfrak{u}}{(n_\mathfrak{u}+1)^q} \le \frac{\epsilon}{2}.$$

The number of cubature samples $n_\mathfrak{u}$ now follows from a Lagrange multiplier argument minimizing the cost to reach error ϵ.

Synopsis

Main result, e.g., Kuo, N., Plaskota, Sloan, Wasilkowski (2017),

$$Q_\epsilon(f) = \sum_{\mathfrak{u}\in\mathcal{U}_\epsilon} Q_{\mathfrak{u},n_\mathfrak{u}}(f_\mathfrak{u}) = \sum_{\mathfrak{v}\in\mathcal{U}_\epsilon^{\mathrm{ext}}} \sum_{\substack{\mathfrak{u}\in\mathcal{U}_\epsilon \\ \text{s.t. } \mathfrak{v}\subseteq\mathfrak{u}}} (-1)^{|\mathfrak{u}|-|\mathfrak{v}|} Q_{\mathfrak{u},n_\mathfrak{u}}(f(\cdot_\mathfrak{v};0)).$$

$$\begin{aligned}\mathrm{cost}(Q_\epsilon) &\le \sum_{\mathfrak{u}\in\mathcal{U}_\epsilon(\alpha)} n_\mathfrak{u}\,\pounds(\mathfrak{u}) \le \sum_{\mathfrak{u}\in\mathcal{U}_\epsilon(\alpha)} n_\mathfrak{u}\, 2^{|\mathfrak{u}|}\$(\mathfrak{u}) \\ &\le \left(\frac{2}{\epsilon}\right)^{1/q} \left(\sum_{\mathfrak{u}\in\mathcal{U}_\epsilon} (G_{\mathfrak{u},q} B_\mathfrak{u})^{1/(q+1)}\right)^{1+1/q} \max_{\mathfrak{u}\in\mathcal{U}_\epsilon} 2^{|\mathfrak{u}|}\$(\mathfrak{u}).\end{aligned}$$

Then for all f with $\|f_\mathfrak{u}\|_{F_\mathfrak{u}} \le B_\mathfrak{u}$:

$$e(Q_\epsilon;\mathcal{F}) := \sup_{f\in\mathcal{F}} |I_\infty(f) - Q_\epsilon(f)| \le \epsilon.$$

Error = truncation error + FEM error + cubature error

Back to the PDE example, the total error then is

$$I_\infty(G(u)) - \sum_{\mathfrak{u} \in \mathcal{U}_\epsilon} Q_{\mathfrak{u},n_\mathfrak{u}}(G(u^{h_\mathfrak{u}}(\boldsymbol{x}, (\boldsymbol{y}_\mathfrak{u}; 0))))$$

$$=$$

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$$= \left(I_\infty(G(u)) - \sum_{\mathfrak{u}\in\mathcal{U}_\epsilon} I_\mathfrak{u}(G(u(\boldsymbol{x},(\boldsymbol{y}_\mathfrak{u};0)))) \right)$$

$$+$$

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$$+ \left(\sum_{\mathfrak{u}\in\mathcal{U}_\epsilon} I_\mathfrak{u}(G(u(\boldsymbol{x},(\boldsymbol{y}_\mathfrak{u};0)))) - I_\mathfrak{u}(G(u^{h_\mathfrak{u}}(\boldsymbol{x},(\boldsymbol{y}_\mathfrak{u};0)))) \right)$$

$$+$$

Error = truncation error + FEM error + cubature error

Back to the PDE example, the total error then is

$$
\begin{aligned}
I_\infty(G(u)) - \sum_{\mathfrak{u}\in\mathcal{U}_\epsilon} Q_{\mathfrak{u},n_\mathfrak{u}}(G(u^{h_\mathfrak{u}}(\boldsymbol{x},(\boldsymbol{y}_\mathfrak{u};0))))
&= \left(I_\infty(G(u)) - \sum_{\mathfrak{u}\in\mathcal{U}_\epsilon} I_\mathfrak{u}(G(u(\boldsymbol{x},(\boldsymbol{y}_\mathfrak{u};0))))\right) \\
&\quad + \left(\sum_{\mathfrak{u}\in\mathcal{U}_\epsilon} I_\mathfrak{u}(G(u(\boldsymbol{x},(\boldsymbol{y}_\mathfrak{u};0)))) - I_\mathfrak{u}(G(u^{h_\mathfrak{u}}(\boldsymbol{x},(\boldsymbol{y}_\mathfrak{u};0))))\right) \\
&\quad + \left(\sum_{\mathfrak{u}\in\mathcal{U}_\epsilon} I_\mathfrak{u}(G(u^{h_\mathfrak{u}}(\boldsymbol{x},(\boldsymbol{y}_\mathfrak{u};0)))) - Q_{\mathfrak{u},n_\mathfrak{u}}(G(u^{h_\mathfrak{u}}(\boldsymbol{x},(\boldsymbol{y}_\mathfrak{u};0))))\right).
\end{aligned}
$$

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$$I_\infty(G(u)) - \sum_{\mathfrak{u}\in\mathcal{U}_\epsilon} Q_{\mathfrak{u},n_\mathfrak{u}}(G(u^{h_\mathfrak{u}}(\boldsymbol{x},(\boldsymbol{y}_\mathfrak{u};0))))$$

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$$+ \left(\sum_{\mathfrak{u}\in\mathcal{U}_\epsilon} I_\mathfrak{u}(G(u^{h_\mathfrak{u}}(\boldsymbol{x},(\boldsymbol{y}_\mathfrak{u};0)))) - Q_{\mathfrak{u},n_\mathfrak{u}}(G(u^{h_\mathfrak{u}}(\boldsymbol{x},(\boldsymbol{y}_\mathfrak{u};0))))\right).$$

$\Rightarrow$ Balance errors such that total error is ϵ.

Function spaces

Now we need to choose the function spaces.
The details are a story for another day... but

Use [Cohen, De Vore, Schwab (2010)]:

$$\|\partial^{\boldsymbol{\nu}} u(\cdot,\boldsymbol{y})\|_V \le |\boldsymbol{\nu}|!\, \boldsymbol{b}^{\boldsymbol{\nu}} \, \frac{\|w\|_{V^*}}{a_{\min}} \qquad \text{with } b_j := \frac{\|\varphi_j\|_{L_\infty}}{a_{\min}},$$

and combine, e.g., with the (first order convergence) norm

$$\|f_{\mathfrak{u}}\|_{F_{\mathfrak{u}}}^2 = \int_{[-1/2,1/2]^{|\mathfrak{u}|}} \left|\partial_{\boldsymbol{y}_{\mathfrak{u}}}^{|\mathfrak{u}|} f_{\mathfrak{u}}(\boldsymbol{y}_{\mathfrak{u}})\right|^2 \mathrm{d}\boldsymbol{y}_{\mathfrak{u}} = \int_{[-1/2,1/2]^{|\mathfrak{u}|}} \left|\partial_{\boldsymbol{y}_{\mathfrak{u}}}^{|\mathfrak{u}|} f(\boldsymbol{y}_{\mathfrak{u}};0)\right|^2 \mathrm{d}\boldsymbol{y}_{\mathfrak{u}},$$

for $f(\boldsymbol{y}_{\mathfrak{u}};0) = G(u^{h_{\mathfrak{u}}}(\boldsymbol{x},(\boldsymbol{y}_{\mathfrak{u}};0)))$.

Test function

Consider $f : [-1/2, 1/2]^{\mathbb{N}} \to \mathbb{R}$ given by

$$f(\boldsymbol{y}) = \frac{1}{1 + \sum_{j \geq 1} j^{-\beta}\, y_j},$$

for $\beta > 1$.
Note: β is the decay (i.e., ℓ_p summability with $p > 1/\beta$).

We use

- (Randomly shifted) lattice rule with tent-transform,
- Sparse grid based on trapezoidal rule (starting with 1-point),

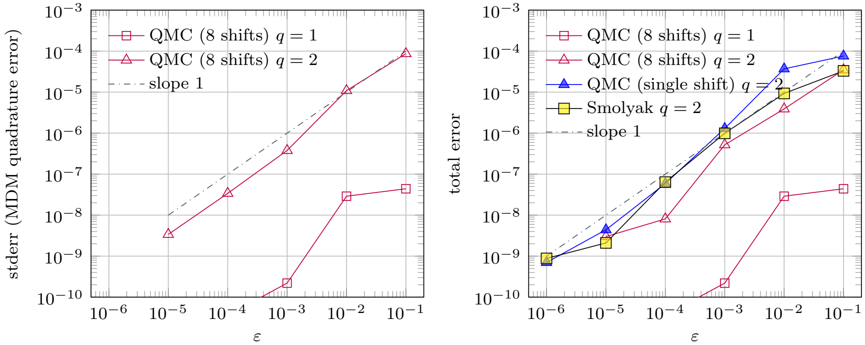
both have order 2 (deterministic).

(We took great care in implementing this efficiently in reusing computations $\to$ see Gilbert, Kuo, N., Wasilkowski (201x).)

Active set constructions for different β and ϵ

	$\beta = 4$			$\beta = 3$			$\beta = 2.5$	
ϵ	1e-1	1e-2	1e-3	1e-1	1e-2	1e-3	1e-1	1e-2
T	1.4e-4	2.8e-6	6.4e-8	4.0e-6	3.6e-8	3.8e-10	1.5e-8	4.9e-11
max $\lvert\mathfrak{u}\rvert$	3	4	5	5	6	7	8	10
$\max_{\mathfrak{u}} \mathfrak{u}$	10	28	72	86	418	1907	2528	24724
size 1	9	26	68	76	370	1686	2019	19750
2	12	48	159	195	1285	7327	10077	126882
3	5	28	132	202	1828	13117	21996	354377
4	0	4	36	80	1234	11907	26258	559155
5	0	0	1	10	361	5578	17874	536133
6	0	0	0	0	32	1145	6513	313623
7	0	0	0	0	0	69	1088	106877
8	0	0	0	0	0	0	47	18582
9	0	0	0	0	0	0	0	1210
10	0	0	0	0	0	0	0	8

Convergence orders $\beta = 3$



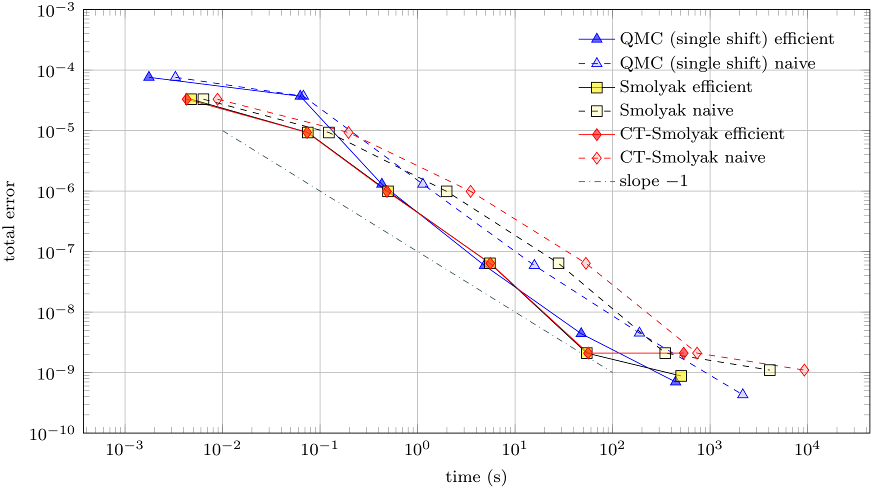
Error request against estimated standard error (lft) and total error (rgt).

Efficient implementations vs naive implementations

$\beta = 3$, reference value = 1.1011984577041

ε	method	efficient total error	efficient time (s)	naive total error	naive time (s)	speedup
1e-01	QMC	7.57e-05	0.0017576	7.57e-05	0.0032837	1.9
$t_1 = 0.000768$	Smolyak	3.26e-05	0.0047466	3.26e-05	0.0063622	1.3
$t_2 = 0.00339$	CT-Smolyak	3.26e-05	0.0042816	3.26e-05	0.0088774	2.1
1e-02	QMC	3.66e-05	0.062643	3.66e-05	0.067456	1.1
$t_1 = 0.00899$	Smolyak	9.34e-06	0.074826	9.34e-06	0.12321	1.6
$t_1 = 0.00899$	Smolyak	9.34e-06	0.074826	9.34e-06	0.12321	1.6
$t_2 = 0.049$	CT-Smolyak	9.34e-06	0.073692	9.34e-06	0.19568	2.7
1e-03	QMC	1.26e-06	0.4301	1.26e-06	1.1336	2.6
$t_1 = 0.0401$	Smolyak	9.92e-07	0.49712	9.92e-07	1.9859	4.0
$t_2 = 0.339$	CT-Smolyak	9.92e-07	0.48502	9.92e-07	3.4984	7.2
1e-04	QMC	5.90e-08	4.8547	5.90e-08	15.766	3.2
$t_1 = 0.34$	Smolyak	6.39e-08	5.5186	6.39e-08	27.89	5.1
$t_2 = 4.08$	CT-Smolyak	6.39e-08	5.5692	6.39e-08	53.191	9.6
1e-05	QMC	4.41e-09	47.64	4.51e-09	188.61	4.0
$t_1 = 2.79$	Smolyak	2.13e-09	54.331	2.12e-09	346.79	6.4
$t_2 = 41.7$	CT-Smolyak	2.11e-09	56.083	2.12e-09	734.87	13.1
1e-06	QMC	7.01e-10	442.8	4.31e-10	2163.1	4.9
$t_1 = 20.2$	Smolyak	8.76e-10	504.78	1.14e-09	4093.9	8.1
$t_2 = 435$	CT-Smolyak	2.08e-09	535.74	1.14e-09	9255.4	17.3

Total error against time



Thank you for your attention

- Implementation of the MDM for infinite dimensional integration.
- Overview papers for QMC and PDE: Kuo & N. (2016, 2018).
- Also function reconstruction using QMC point sets.
- And higher order convergence.

The Magic Point Shop!

QMC4PDE

See https://www.cs.kuleuven.be/~dirkn/qmc4pde/ and https://www.cs.kuleuven.be/~dirkn/qmc-generators/.