Introduction to the (sparse grid) stochastic collocation

Simona Domesová

November 22, 2019

Outline

Bibliography

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- Nobile, F., R. Tempone, and C. G. Webster. "A Sparse Grid Stochastic Collocation Method for Partial Differential Equations with Random Input Data." SIAM Journal on Numerical Analysis 46, no. 5 (January 2008): 2309–45. https://doi.org/10.1137/060663660.

Problem setting

Problem setting

Stochastic boundary value problem

Find a random function $u : \Omega \times \overline{D} \to \mathbb{R}$:

$$\mathcal{L}(a)(u) = f \quad \text{in } D$$
$$+ \text{ boundary conditions}$$

holds P-almost everywhere in Ω (i.e. almost surely).

$$\left.\begin{aligned} a &= a(\omega, x) \\ f &= f(\omega, x) \\ u &= u(\omega, x) \end{aligned}\right\} \omega \in \Omega, x \in D$$

- $a(\omega, x) \geq a_{min}(\omega) > 0$ almost surely and almost everywhere in D
- $f(\omega, \cdot)$ is square integrable w.r.t. P, i.e. $\int_D E\left(f^2\right) dx < \infty$

Problem setting - example

Stochastic linear elliptic boundary value problem

Find a function $u : \Omega \times \overline{D} \to \mathbb{R}$:

$$\begin{aligned} -\text{div}\left(a\left(\omega,x\right)\nabla u\left(\omega,x\right)\right) &= f\left(\omega,x\right) \ \ \forall x \in D \\ u\left(\omega,x\right) &= 0 \ \ \forall x \in \partial D \end{aligned}$$

holds P-almost everywhere in Ω (i.e. almost surely).

$$\left.\begin{aligned} a &= a\left(\omega,x\right) \\ f &= f\left(\omega,x\right) \\ u &= u\left(\omega,x\right) \end{aligned}\right\} \omega \in \Omega, x \in \overline{D}$$

- $a\left(\omega,x\right) \geq a_{min}\left(\omega\right) > 0$ almost surely and almost everywhere in D
- $f\left(\omega,\cdot\right)$ is square integrable w.r.t. P, i.e. $\int_D E\left(f^2\right) dx < \infty$

Assumption: finite dimension of uncertainty

$$\left.\begin{array}{l} a = a(\omega, x) = a(Y_1(\omega), \dots, Y_N(\omega), x) \\ f = f(\omega, x) = f(Y_1(\omega), \dots, Y_N(\omega), x) \\ u = u(\omega, x) = u(Y_1(\omega), \dots, Y_N(\omega), x) \end{array}\right\} \omega \in \Omega, x \in \overline{D}$$

- $Y_n : \Omega \to \Gamma_n \subset \mathbb{R}$, $n \in \{1, \dots, N\}$ ... real valued random variables (not necessarily independent)
- $\Gamma = \prod_{n=1}^{N} \Gamma_n$ ... set of outcomes
- $\rho : \Gamma \to \mathbb{R}_+$, $\rho \in L^\infty(\Gamma)$ ... joint probability density function of $(Y_1, \dots, Y_n)$
  $\longrightarrow$ probability space $\left(\Gamma, \mathcal{B}^N, \rho dy\right)$

Assumption: finite dimension of uncertainty

Stochastic boundary value problem

Find a random function $u : \Gamma \times \overline{D} \to \mathbb{R}$:

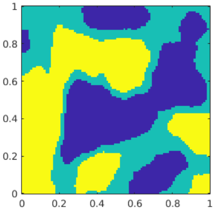
$$\mathcal{L}(a)(u) = f \quad \text{in } D$$
$$+ \text{ boundary conditions}$$

holds almost surely.

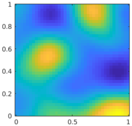
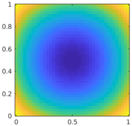
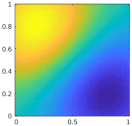
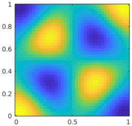
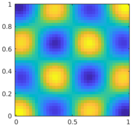
- assume a unique solution $u \in L^2_\rho(\Gamma; W(D))$

$\longrightarrow$ Instead of $u(\omega, x)$ on $\Omega \times \overline{D}$, we consider $u(y, x)$ on $\Gamma \times \overline{D}$.
The aim is to find an approximation of u (for any $y \in \Gamma$ and $x \in \overline{D}$) in a suitable finite dimensional subspace.

- example 1 (exact representation)



- example 2 (suitable truncation)

 ∈span( ,  ,...,  ,..., )

Finite element operator

- $W_h(D) \subset W(D)$ ... standard finite element space; triangulation $\mathcal{T}_h$
- consider a finite element operator $FEM_h : W(D) \to W_h(D)$ with the optimality condition

$$\|\varphi - FEM_h\varphi\|_{W(D)} \leq c \min_{v \in W_h(D)} \|\varphi - v\|_{W(D)} \quad \forall \varphi \in W(D)$$

  (c is independent of h)
- denote:

$$FEM_h u = u_h : \Gamma \to W_h(D),$$

  i.e.

$$FEM_h u(y) = u_h(y) \in W_h(D)$$

Stochastic collocation

Stochastic collocation

= a method that produces an approximation $u_{h,p} \in C^0(\Gamma; W_h(D))$ of a function $u \in L^2_\rho(\Gamma; W(D))$ constructed by a linear combination of point values $u_h(y_k) \in W_h(D)$, where $y_k \in \Gamma$, $k \in \{1, \ldots, N_p\}$, i.e.

$$u_{h,p}(y, x) = \sum_{k=1}^{N_p} u_h(y_k, x)\, l_k(y)$$

Stochastic collocation provides:

- approximation of u
- estimation of statistical moments of the solution u (mean value, variance, covariance, ...)

$$E(u) \approx E(u_{h,p}) = \sum_{k=1}^{N_p} u_h(y_k, x)\, E(l_k(y))$$

- statistics of quantities of interest $\psi(u)$

Discretization of the probability space

- $\mathcal{P}_{\mathbf{p}}(\Gamma) \subset L^2_\rho(\Gamma)$ ... span of tensor product polynomials with degrees at most $\mathbf{p} = (p_1, \dots, p_N)$

$$\mathcal{P}_{\mathbf{p}}(\Gamma) = \bigotimes_{n=1}^{N} \mathcal{P}_{p_n}(\Gamma_n)$$

- $\mathcal{P}_{p_n}(\Gamma_n)$ ... all univariate polynomials with degree at most p_n
- dimension of $\mathcal{P}_{\mathbf{p}}(\Gamma)$ is $\prod_{n=1}^{N}(p_n + 1)$
- Lagrange basis of $\mathcal{P}_{p_n}(\Gamma_n)$:

$$\{l_{n,j}\}_{j=1}^{p_n+1}, \ l_{n,j}(y_{n,k}) = \delta_{jk}, \ j,k \in \{1, \dots, p_n + 1\},$$

where $y_{n,1}, \dots, y_{n,p_{n+1}} \in \Gamma_n$
$\longrightarrow$ one-dimensional interpolation operator

$$\mathscr{U}(u)(y) = \sum_{j=1}^{p_n+1} u(y_{n,j})\, l_{n,j}(y)$$

Full tensor stochastic collocation

full tensor product interpolation operator

$\mathcal{I}^N : C^0(\Gamma; W(D)) \to \mathcal{P}_{\mathbf{p}}(\Gamma) \otimes W(D)$:

$$\begin{aligned}\mathcal{I}^N(u)(y) &= \left(\mathscr{U}^{(1)} \otimes \cdots \otimes \mathscr{U}^{(N)}\right)(u)(y) = \\ &= \sum_{j_1=1}^{p_1+1} \cdots \sum_{j_N=1}^{p_N+1} u\left(y_{1,j_1}, \ldots, y_{N,j_N}\right)\left(l_{1,j_1}(y) \otimes \cdots \otimes l_{N,j_N}(y)\right)\end{aligned}$$

The aim was to approximate $u \in L^2_\rho(\Gamma; W(D))$ by $u_{h,p}$ of the form

$$u_{h,p}(y,x) = \sum_{k=1}^{N_p} u_h(y_k, x)\, l_k(y),$$

where $y_k \in \Gamma$. Using $\mathcal{I}^N$, we can simply write $u_{h,p} = \mathcal{I}^N(u_h)$,
i.e. $N_p = \prod_{n=1}^N (p_n + 1)$, $l_k = \prod_{n=1}^N l_{n,k_n}$.

Choice of $y_{n,j}$

$$\mathcal{I}^N(u)(y) = \sum_{j_1=1}^{p_1+1} \cdots \sum_{j_N=1}^{p_N+1} u\left(y_{1,j_1}, \ldots, y_{N,j_N}\right)\left(l_{1,j_1}(y) \otimes \cdots \otimes l_{N,j_N}(y)\right)$$

auxiliary probability density $\widehat{\rho} : \Gamma \to \mathbb{R}^+$:

$$\widehat{\rho}(y) = \prod_{n=1}^{N} \widehat{\rho}_n(y_n), \ \forall y \in \Gamma, \quad \text{and} \quad \left\| \frac{\rho}{\widehat{\rho}} \right\|_{L^\infty(\Gamma)} < \infty$$

- $y_{n,1}, \ldots, y_{n,p_n+1} \in \Gamma_n$ are roots of the polynomial Q of degree $p_n + 1$ orthogonal with respect to $\widehat{\rho}_n$, i.e.

$$\int_{\Gamma_n} Q(y)\, r(y)\, \widehat{\rho}_n(y)\, dy = 0 \ \ \forall r \in \mathcal{P}_{p_n}(\Gamma_n)$$

Relation to Gaussian quadrature

$$\int p(x)\, \rho dx = \sum_{i=1}^{n} w_i p(x_i)$$

- choice of w_i, x_i ... $2n$ degrees of freedom $\rightarrow$ exact integration of polynomials up to degree $2n-1$

Back to 1d interpolation operator $\mathscr{U}(u)(y) = \sum_{j=1}^{p_n+1} u(y_{n,j})\, l_{n,j}(y)$,
where $y_{n,1}, \ldots, y_{n,p_n+1}$ are roots of polynomial Q of degree $p_n + 1$:
$\int_{\Gamma_n} Qr\widehat{\rho}_n dy = 0 \;\; \forall r \in \mathcal{P}_{p_n}$

$$\int u(y)\, \widehat{\rho} dy \overset{u \in \mathcal{P}_{2p_n+1}}{=} \int \mathscr{U}(u)(y)\, \widehat{\rho} dy = \sum_{j=1}^{p_n+1} u(y_{n,j}) \overbrace{\int l_{n,j}(y)\, \widehat{\rho} dy}^{=w_j}$$

Integrated polynomial $u(y)$ can be written as $\underset{\in}{\overset{\mathcal{P}_{2p_n+1}}{u}}(y) = \underset{\in}{\overset{\mathcal{P}_{p_n}}{s}}(y) \underset{\in}{\overset{\mathcal{P}_{p_n+1}}{Q}}(y) + \underset{\in}{\overset{\mathcal{P}_{p_n}}{r}}(y)$

$$\int u(x)\, \widehat{\rho} dx = \sum_{j=1}^{p_n+1} w_j s(y_{n,j}) \overbrace{Q(y_{n,j})}^{=0} + \sum_{j=1}^{p_n+1} w_j r(y_{n,j})$$

$$\forall i \in \{1, \ldots, p_n + 1\} : \int l_{n,i} \widehat{\rho} dy = \sum_{j=1}^{p_n+1} w_j l_{n,i}(y_{n,j}) = w_i \overbrace{l_{n,i}(y_{n,i})}^{=1}$$

Example: $N = 3$, degree $= 3$

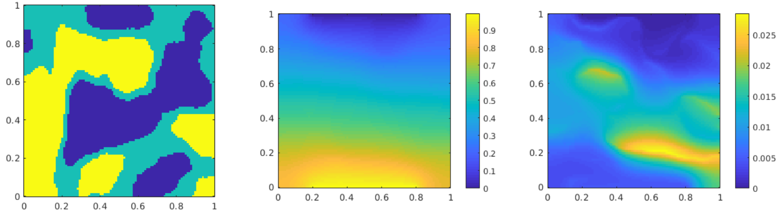
Stochastic linear elliptic boundary value problem

Find a function $u : \Omega \times \overline{D} \to \mathbb{R}$:

$$-\mathrm{div}\left(a\left(Y_1(\omega), Y_2(\omega), Y_3(\omega), x\right)\nabla u(\omega, x)\right) = 0 \;\; \forall x \in D$$
$$+ \text{ boundary conditions}$$

holds almost surely.

$$Y_n \sim \mathcal{N}(5; 1)$$



$a(\cdot, x)$ ... 3 parameters; approx. of $E(u)$; approx. of $Var(u)$

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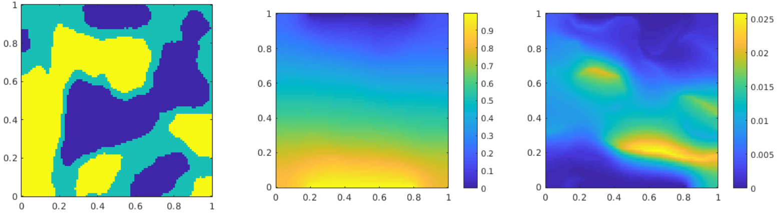

$a\left(\cdot, x\right)$ ... 3 parameters; approx. of $E\left(u\right)$; approx. of $Var\left(u\right)$

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Find a function $u : \Omega \times \overline{D} \to \mathbb{R}$:

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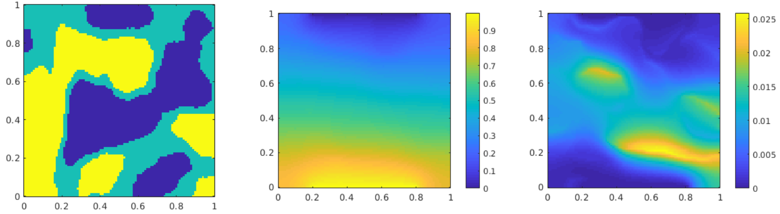
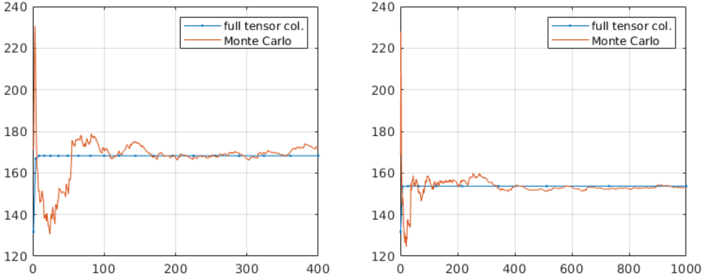


$a\left(\cdot, x\right)$ ... 3 parameters; approx. of $E\left(u\right)$; approx. of $Var\left(u\right)$

Quantity of interest $\psi(u)$: flow through outflow boundary part

$$Y_n \sim \mathcal{N}(5;1)$$



Convergence of $E(\psi(u))$ for $N = 2$ (left) and $N = 3$ (right) with increasing number of collocation points

Consider again:

Stochastic linear elliptic boundary value problem

Find a function $u : \Gamma \times \overline{D} \to \mathbb{R}$:

$$\begin{aligned} -\text{div}\left(a\left(y,x\right)\nabla u\left(y,x\right)\right) &= f\left(y,x\right) \;\; \forall x \in D \\ u\left(y,x\right) &= 0 \;\; \forall x \in \partial D \end{aligned}$$

holds almost surely.

Stochastic Galerkin

Find $u_{h,p}^G \in \mathcal{P}_p(\Gamma) \otimes W_h(D)$:

$$\int_\Gamma \int_D a \nabla u \nabla v \, dx \, \rho dy = \int_\Gamma \int_D fv \, dx \, \rho dy \quad \forall \in P_p(\Gamma) \otimes W_h(D)$$

$\longrightarrow$ fully coupled linear system of dimension $N_p \times N_h$

replace integrals over Γ by quadrature formula $E_{\widehat{\rho}}^p(g) = \sum_{k=1}^{N_p} \omega_k g(y_k)$
& choose test functions $v(y,x) = l_k(y) \phi(x)$ $(\phi(x) \in W_h(x))$

Stochastic collocation

Find $u_{h,p} \in \mathcal{P}_p(\Gamma) \otimes W_h(D)$: $\quad \forall \in P_p(\Gamma) \otimes W_h(D)$

$$\sum_{k=1}^{N_p} \omega_k \frac{\rho(y_k)}{\widehat{\rho}(y_k)} \int_D a(y_k) \nabla u_{h,p}(y_k) \nabla v(y_k) \, dx = \sum_{k=1}^{N_p} \omega_k \frac{\rho(y_k)}{\widehat{\rho}(y_k)} \int_D f(y_k) v(y_k) \, dx$$

$\longrightarrow$ sequence of N_p uncoupled linear system of dimension N_h

Relation to Stochastic Galerkin method

Stochastic collocation

- replaces the integration of $\int_D a\nabla u \nabla v\, dx$ over Γ by a quadrature formula $\Rightarrow$ if $\int_D a\nabla u \nabla v\, dx$ (function of y) is a polynomial at most of degree $2p_n + 1$, the integration is exact
- decouples the linear system (also when a and f are non-linear functions of Y_n)
- treats efficiently the case of non-independent random variables Y_n (using $\widehat{\rho}$)

1d interpolation operator (direction n omitted) $\mathscr{U}(u) = \sum_{j=1}^{m_i} u(y_j)\, l_j$

- consider a sequence of 1d interpolation operators $\mathscr{U}^i(u)$ given by
  - m_i
  - points y_j^i; $j \in \{1, \ldots, m_i\}$
  - functions l_j^i; $j \in \{1, \ldots, m_i\}$
- multivariate "building block" for multiindex $\mathbf{i} = (i_1, \ldots, i_N)$

$$\left(\mathscr{U}^{i_1} \otimes \cdots \otimes \mathscr{U}^{i_N}\right)(u) = \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_N=1}^{m_{i_N}} u\left(y_{j_1}^{i_1}, \ldots, y_{j_N}^{i_N}\right)\left(l_{j_1}^{i_1} \otimes \cdots \otimes l_{j_N}^{i_N}\right)$$

Smolyak sparse grids - notation

Isotropic Smolyak formula for level w and dimension N:

$$\mathscr{A}(w,N) = \sum_{\mathbf{i}\in Y(w,N)} (-1)^{w+N-|\mathbf{i}|} \begin{pmatrix} N-1 \\ w+N-|\mathbf{i}| \end{pmatrix} \cdot \left(\mathscr{U}^{i_1} \otimes \cdots \otimes \mathscr{U}^{i_N}\right),$$

where $Y(w,N) = \left\{\mathbf{i} \in \mathbb{N}_+^N, \mathbf{i} \geq \mathbf{1} : w+1 \leq |\mathbf{i}| \leq w+N\right\}$

How to choose the sequence of 1d interpolation operators $\mathscr{U}^i(u)$?

- $m_1 = 1,\ m_i = 2^{i-1}+1$ for $i > 1$
- Clenshaw-Curtis abscissas
  - nested, i.e. $\left\{y_1^i, \ldots, y_{m_1}^i\right\} \subset \left\{y_1^{i+1}, \ldots, y_{m_{1+1}}^{i+1}\right\}$
  - points y_j^i are extremes of Chebyshev polynomials $\in \langle -1, 1\rangle$
- Gaussian abscissas
  - in general not nested
  - points y_j^i are zeros of orthogonal polynomials w.r.t. a positive weight

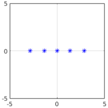
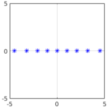
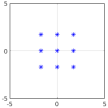
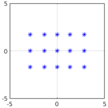
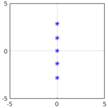
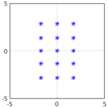
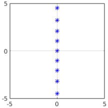
Example - sequence $\mathscr{U}^i(u)$ and set $Y(w,N)$

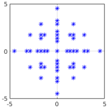
Setting: $m_i = 2^{i-1}+1$ for $i>1$; Gaussian abscissas; points y_j^i are zeros of Hermite polynomials H_j; $w=3$; $N=2$

- $\mathscr{U}^1(u)$: $m_1 = 1$, roots of $H_1 \in \mathcal{P}_1$
- $\mathscr{U}^2(u)$: $m_2 = 3$, roots of $H_3 \in \mathcal{P}_3$
- $\mathscr{U}^3(u)$: $m_3 = 5$, roots of $H_5 \in \mathcal{P}_5$
- $\mathscr{U}^4(u)$: $m_4 = 9$, roots of $H_9 \in \mathcal{P}_9$

$$
\begin{aligned}
Y(w,N) &= \left\{\mathbf{i} \in \mathbb{N}_+^2, \mathbf{i} \geq \mathbf{1} : 4 \leq |\mathbf{i}| \leq 5\right\} = \\
&= \{\underset{1\cdot 9}{\underset{\downarrow}{(1,4)}}, \underset{1\cdot 5}{\underset{\downarrow}{(1,3)}}, \underset{3\cdot 5}{\underset{\downarrow}{(2,3)}}, \underset{3\cdot 3}{\underset{\downarrow}{(2,2)}}, \underset{5\cdot 3}{\underset{\downarrow}{(3,2)}}, \underset{5\cdot 1}{\underset{\downarrow}{(3,1)}}, \underset{9\cdot 1}{\underset{\downarrow}{(4,1)}}\}
\end{aligned}
$$

Example: $Y(\omega = 3, N = 2) = \{\mathbf{i} \in \mathbb{N}^N : \mathbf{i} \geq \mathbf{1} \wedge 4 \leq |\mathbf{i}| \leq 5\}$

	$i_2 = 1$	$i_2 = 2$	$i_2 = 3$	$i_2 = 4$
$i_1 = 1$	$\lvert\mathbf{i}\rvert = 2$	$\lvert\mathbf{i}\rvert = 3$		
$i_1 = 2$	$\lvert\mathbf{i}\rvert = 3$			$\lvert\mathbf{i}\rvert = 6$
$i_1 = 3$			$\lvert\mathbf{i}\rvert = 6$	$\lvert\mathbf{i}\rvert = 7$
$i_1 = 4$		$\lvert\mathbf{i}\rvert = 6$	$\lvert\mathbf{i}\rvert = 7$	$\lvert\mathbf{i}\rvert = 8$

$\rightarrow$ 

Convergence properties

Stochastic boundary value problem

Find a random function $u : \Omega \times \overline{D} \to \mathbb{R}$:

$$\mathcal{L}(a)(u) = f \quad \text{in } D$$
$$+ \text{ boundary conditions}$$

holds P-almost everywhere in Ω (i.e. almost surely).

- the solution has realizations in $W(D)$, i.e. $u(\cdot, \omega) \in W(D)$ almost surely
- $\exists c \; \forall \omega \in \Omega$: $\|u(\cdot, \omega)\|_{W(D)} \leq c \|f(\cdot, \omega)\|_{W^*(D)}$
- forcing term $f \in L_P^2(\Omega; W^*(D))$ is such that the solution u is unique and bounded in $L_P^2(\Omega; W(D))$

For functions $u \in C^0(\Gamma; W(D))$ which admit an analytic extension in $\{z \in \mathbb{C} : \operatorname{dist}(z,\Gamma) < \tau\}$ for some $\tau > 0$ the isotropic Smolyak formula based on Gaussian abscissas satisfies

$$\|u - \mathscr{A}(\omega, N)(u)\|_{L^2_\rho(\Gamma;W(D))} \leq$$

$$\leq \sqrt{\left\|\frac{\rho}{\widehat{\rho}}\right\|_{L^\infty(\Gamma)}} e^{\sigma e \log(2)} C(\sigma) \frac{\max\{1, C(\sigma)\}^N}{|1 - C(\sigma)|} \eta^{-D},$$

- η is the number of collocation points,
- $D = \frac{\sigma e \log(2)}{\zeta + \log(N)}$,
- $\zeta \approx 2.1$, $C(\sigma)$ incorporates the interpolation error with Lagrange polynomials, $\sigma = \sigma(\tau, \Gamma)$.

[3, Theorem 3.17]

For functions $u \in C^0(\Gamma; W(D))$ which admit an analytic extension in $\{z \in \mathbb{C} : \operatorname{dist}(z, \Gamma) < \tau\}$ for some $\tau > 0$

- isotropic Smolyak formula based on Gaussian abscissas satisfies

$$\|u - \mathscr{A}(\omega, N)(u)\|_{L^2_\rho(\Gamma; W(D))} \leq C_1(\sigma, N)\, \eta^{-\frac{\sigma e \log(2)}{\zeta + \log(N)}}$$

- full tensor product interpolation satisfies

$$\|u - \mathscr{A}(\omega, N)(u)\|_{L^2_\rho(\Gamma; W(D))} \leq C_2(\sigma, N)\, \eta^{-\frac{\sigma}{N}}$$

[3, Theorem 3.17], [1, Theorem 1]

For comparison:

- crude Monte Carlo convergence rate is

$$\mathcal{O}\left(\eta^{-\frac{1}{2}}\right)$$

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