Polytope Division Method: Greedy Sampling in High Dimensions

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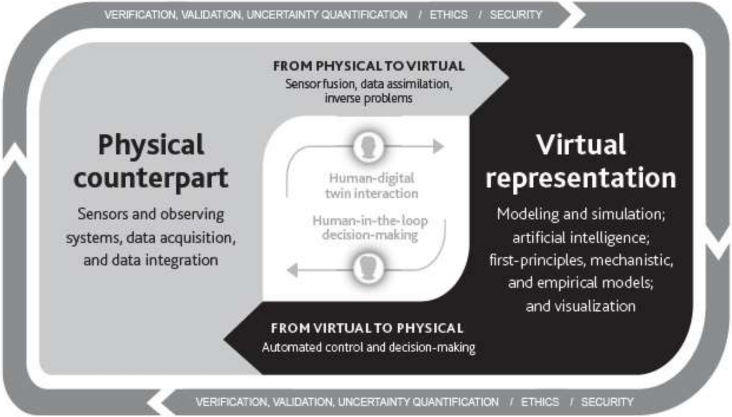
Image by Bart van Overbeeke Photography



Credit: National Academies of Science, Engineering and Medicine

Outline

$$a(u(p), v; p) = f(v; p), \qquad \forall v \in \mathbb{V},$$

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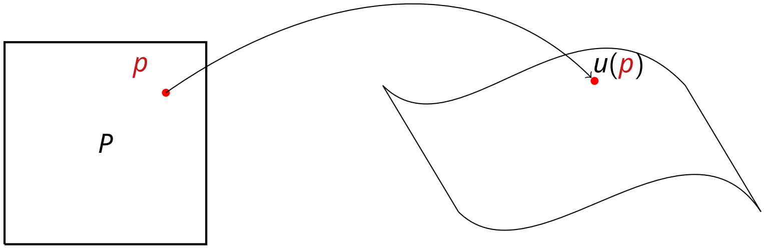

Parameter space

Solution manifold

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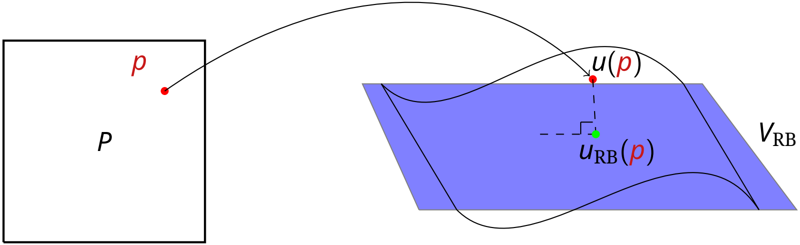

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Reduced Basis Method

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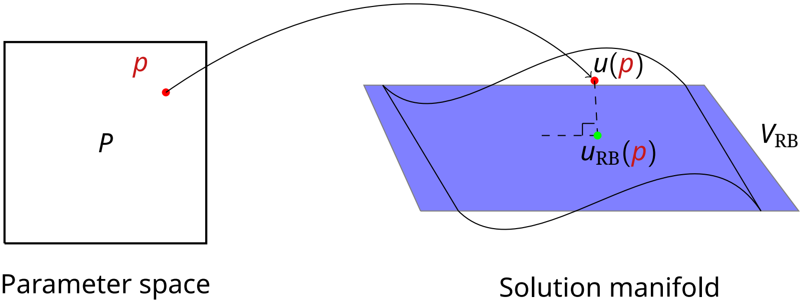

Goal: Construct an approximation space
$V_{\mathrm{RB}} := \mathrm{span}\{u(p_1), \ldots, u(p_n)\}.$

Reduced basis Method

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- In reduced basis methods, the loss function is given by

$$\mathcal{L}(\gamma) = \max_{q \in P} \left\| u(q) - P_{V_{\mathrm{RB}}(\gamma)} u(q) \right\|^2 . \tag{1}$$

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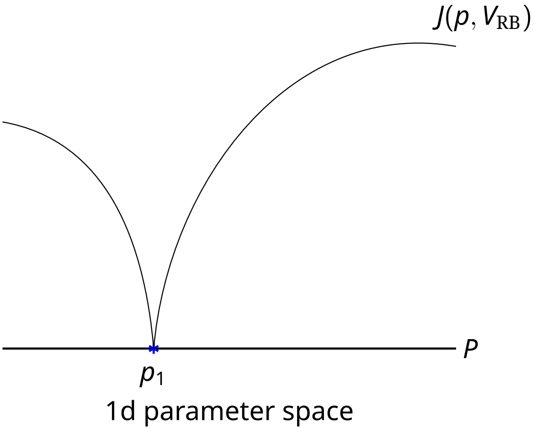
- We use an error estimate $J(p, V_{\mathrm{RB}})$ to approximate the norm $\|u(q) - P_{V_{\mathrm{RB}}} u(q)\|^2$.

- We sample p_1 randomly and set $V_{\text{RB}} = \text{span}\{u(p_1)\}$



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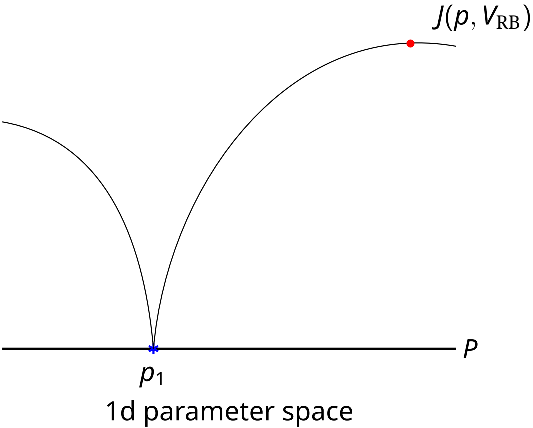

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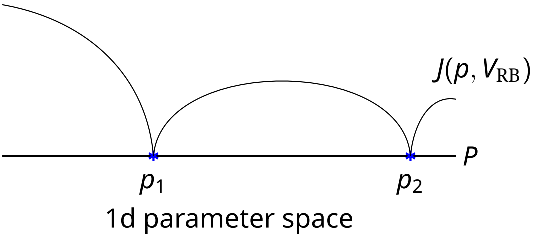

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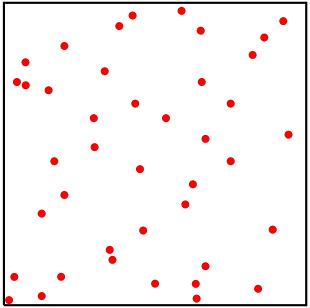

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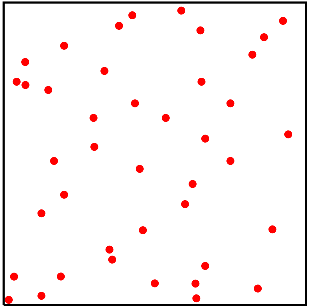

Compute

$\xrightarrow{J(p, V_{\mathrm{RB}})}$

TU/e

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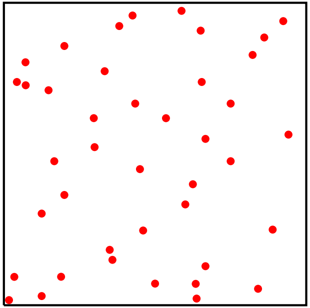

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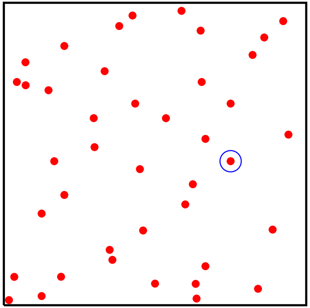

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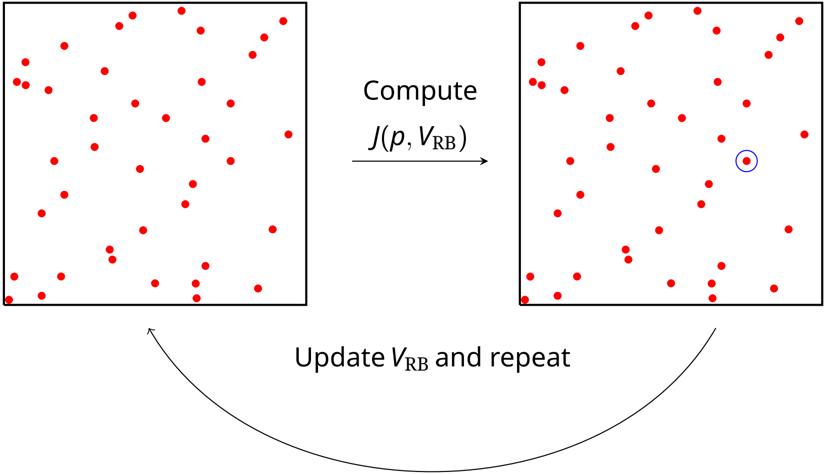

High-dimensionality

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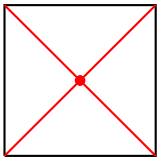
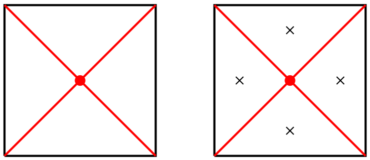
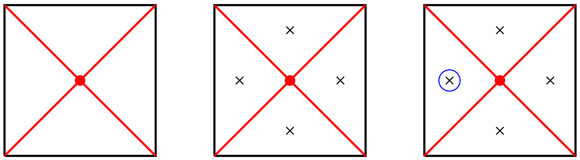
- In high-dimensionality cases, the sampling becomes problematic.
- In each update step, we have to compute the error estimate for each sample.
- Can we do something else?

Polytope Division Method







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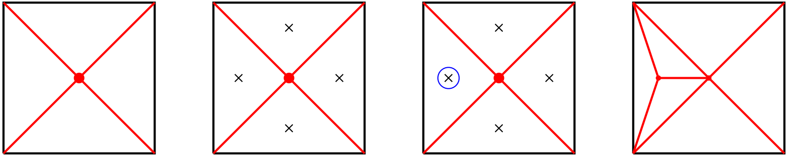

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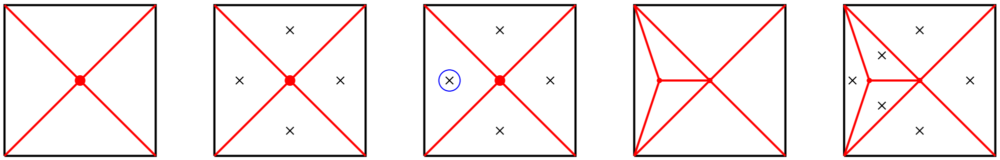

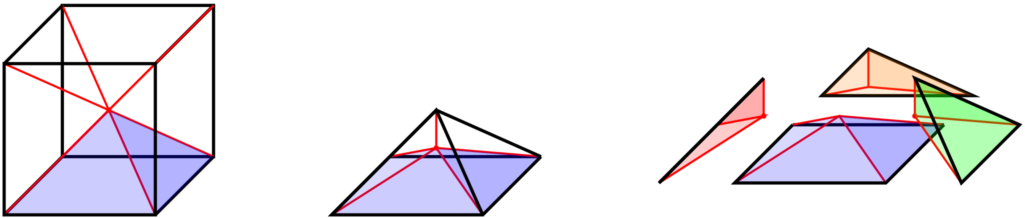

Higher-dimensional

- Can we still find the facets in the higher-dimensional case?
- Do we keep the satisfactory scaling properties?

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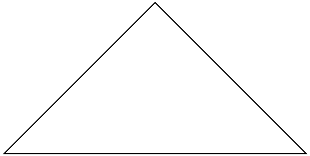
Yes!



2d simplex

Simplices, subfacets and P-boundary polytopes

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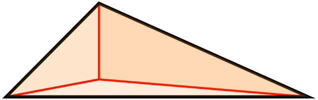
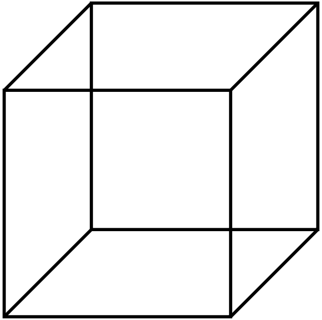
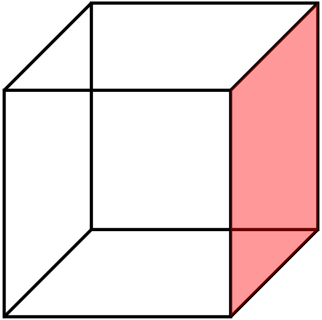


3d simplex

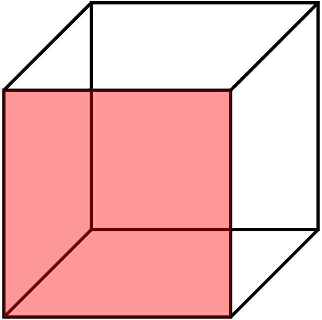
Simplices, subfacets and P-boundary polytopes

TU/e





Example of a facet



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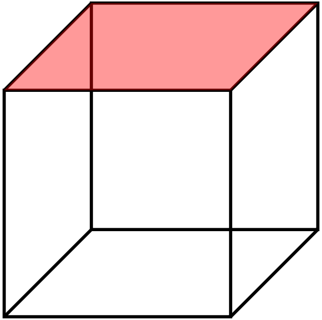

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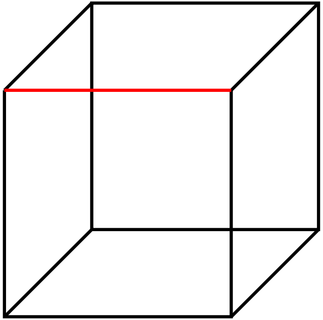
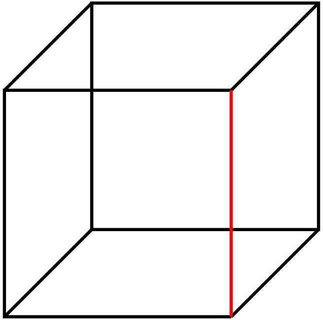


Example of a 2-subfacet



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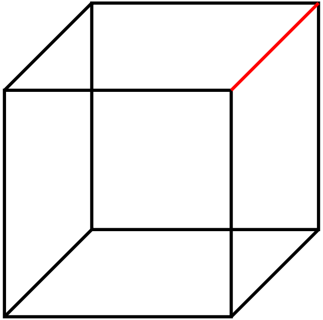

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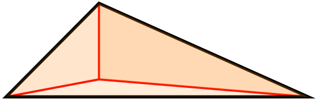

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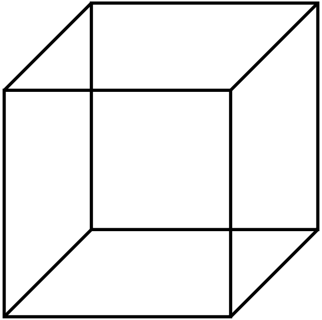

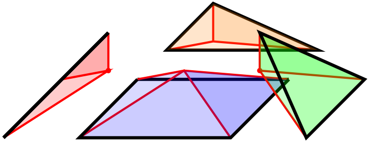

$\square = \mathrm{Conv}(\{x_1, \ldots, x_n\} \cup F)$

Theorem

Let P be a d-dimensional hyperrectangle and $\mathcal{D}^N$ be the polytope division of P constructed by the Polytope Division Method at step $N \geq 1$. Then

$$\mathcal{D}^N = \bigcup_{\Delta \in \mathcal{D}^N} \{\Delta\} \cup \bigcup_{\square \in \mathcal{D}^N} \{\square\},$$

where Δ denotes a d-dimensional simplex and $\square$ denotes a P-boundary polytope.

Consequence of this theorem

TU/e

We claim that for both Δ and $\square$, we can determine the facets efficiently.

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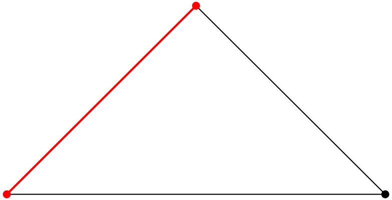

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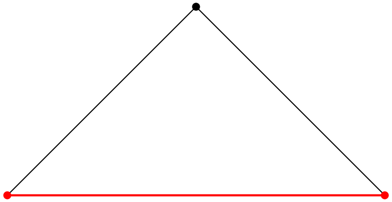

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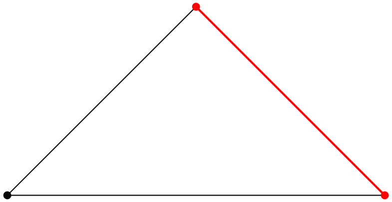

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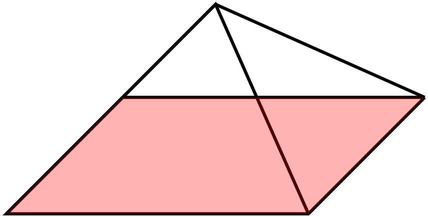

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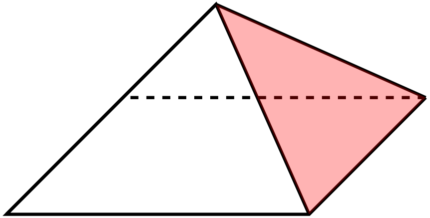

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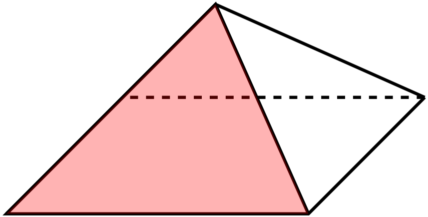


Corollary

Let P be a d-dimensional hyperrectangle, let $\mathcal{D}^N$ be the polytope division of P at step $N \geq 1$ of the Polytope Division Method, and let $D \in \mathcal{D}^N$. It then follows that $|\partial D| \leq 2d$, where $|\cdot|$ denotes the cardinality of a set.

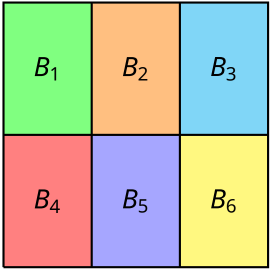
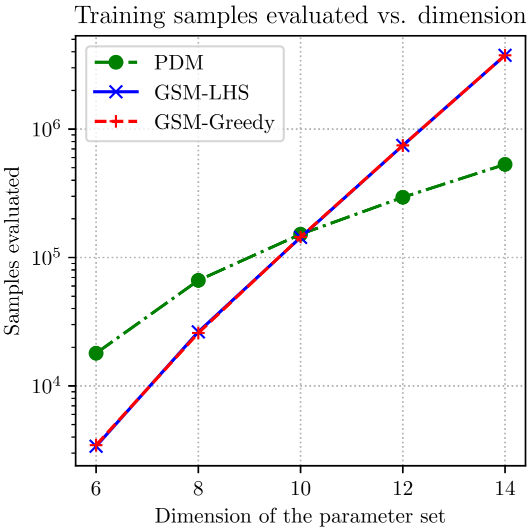
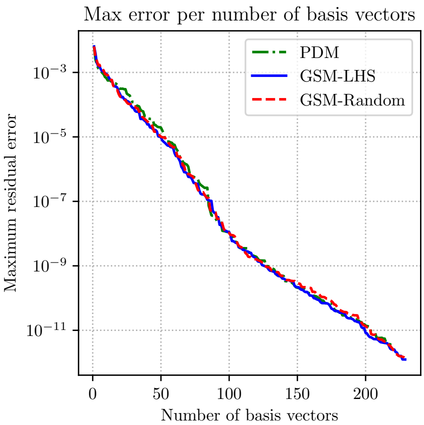


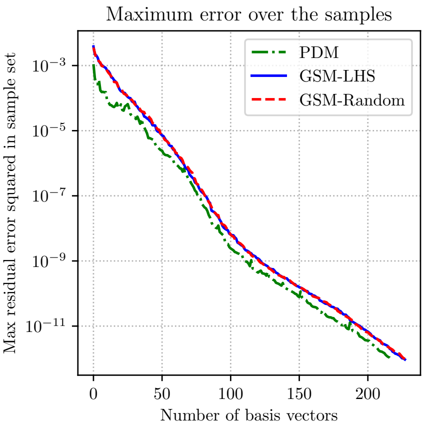
Figure: Domain Thermal Block with 6 parameters

$$\begin{cases} -\nabla \cdot [\kappa(x,\mu)\nabla u(x,\mu)] = 1 & \text{for } x \in \Omega, \\ u(x,\mu) = 0 & \text{for } x \in \partial\Omega. \end{cases}$$


Training samples evaluated vs. dimension
PDM
GSM-LHS
GSM-Greedy
10^6
10^5
10^4
Samples evaluated
6
8
10
12
14
Dimension of the parameter set

Thermal Block Example





Heat conduction with Gaussian heat source

TU/e

Let $u(x, \mu)$ be the temperature at position $x \in \Omega = (-1, 1)^2$.

$$\begin{cases} \int_\Omega \nabla u \cdot \nabla v = \int_\Omega g(x, \mu) v dx & \text{for } x \in \Omega, \\ u(x, \mu) = 0 & \text{for } x \in \partial\Omega, \end{cases}$$

where the heat source $g(x, \mu)$ is given by

$$g(x, \mu) = N(\mu) \cdot \exp\left\{ -\frac{1}{2(1-\rho^2)} \left[\left(\frac{x_1 - \mu_1}{\sigma_1} \right)^2 - 2\rho \frac{x_1 - \mu_1}{\sigma_1} \frac{x_2 - \mu_2}{\sigma_2} + \left(\frac{x_2 - \mu_2}{\sigma_2} \right)^2 \right] \right\},$$

The parameter μ is given by $\mu = (\mu_1, \mu_2, \sigma_1, \sigma_2, \rho) \in [-1, 1]^2 \times [1, 3]^2 \times [-0.8, 0.8]$.

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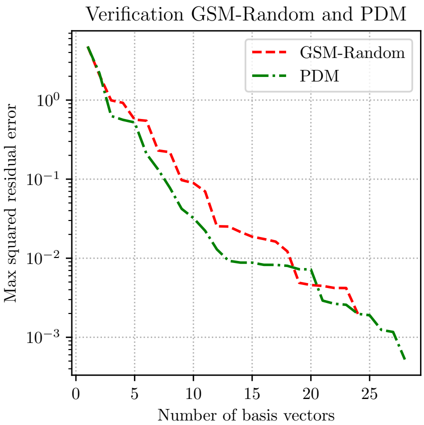

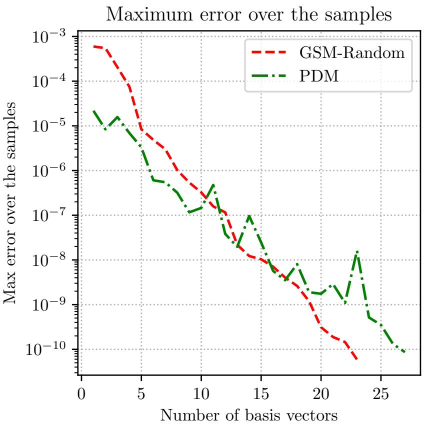

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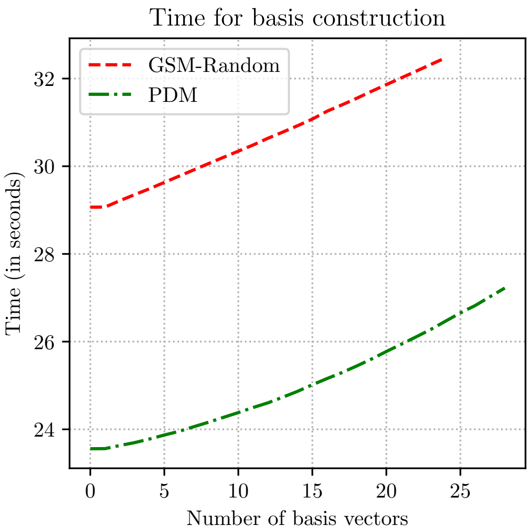

Summary

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- PDM has better scaling properties than classical Greedy Sampling methods
- To apply PDM, we don't have to choose the size of a sample set a priori. The method itself adaptively refines the sample set in each step.
- PDM could be applied in different fields, such as active learning for regression, optimal experimental design or nonlinear MOR.

PDM code and paper

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- We published code to perform PDM on Zenodo.

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- Preprint available: Nielen, E., Tse, O., & Veroy, K. (2024). Polytope Division Method: A Scalable Sampling Method for Problems with High-dimensional Parameters. arXiv preprint arXiv:2410.17938.