

Sparse polynomial chaos expansions - Benchmark of compressive sensing solvers and experimental design techniques

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SPARSE POLYNOMIAL CHAOS EXPANSIONS

BENCHMARK OF COMPRESSIVE SENSING SOLVERS
AND EXPERIMENTAL DESIGN TECHNIQUES

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SURROGATE MODELLING BY REGRESSION-BASED PCE

Our objectives

For complex and costly models from science and engineering, find a **surrogate model** that...

- approximates the model well
- requires only few model evaluations
- is nonintrusive

PCE

- **Input** random vector $\mathbf{X} = (X_1, \dots, X_d)$ with $X_k \sim f_{X_k}$ and range $\mathcal{D} \subset \mathbb{R}^d$
- **Model** $\mathcal{M} \in L^2_{f_{\mathbf{X}}}(\mathcal{D})$
- **Output** random variable $Y = \mathcal{M}(\mathbf{X})$
- **Polynomial orthonormal basis** for $L^2_{f_{\mathbf{X}}}(\mathcal{D})$: $\{\psi_{\alpha} : \alpha \in \mathbb{N}^d\}$
- **Truncation** of the **spectral expansion**: Use a subset of multi-indices $\mathcal{A} \subset \mathbb{N}^d$ to approximate

$$Y \approx Y_{\text{PCE}} = \mathcal{M}^{\text{PCE}}(\mathbf{X}) = \sum_{\alpha \in \mathcal{A}} c_{\alpha} \psi_{\alpha}(\mathbf{X}).$$

Computing a PCE by regression

- **Experimental design (ED)** $\{\mathbf{x}^{(i)}\}_{i=1}^{N_{\text{ED}}} \subset \mathcal{D}$
 - Model evaluations $\{y^{(i)} = \mathcal{M}(\mathbf{x}^{(i)})\}_{i=1}^{N_{\text{ED}}}$
 - Multi-index set \mathcal{A} defining the set of **candidate polynomials**
 - Matrix Ψ containing evaluations of the polynomials
- Solve $\mathbf{y} \approx \Psi \mathbf{c}$.

Many real-world models are compressible.

Find a sparse solution \mathbf{c} , e.g. by Basis Pursuit Denoising:

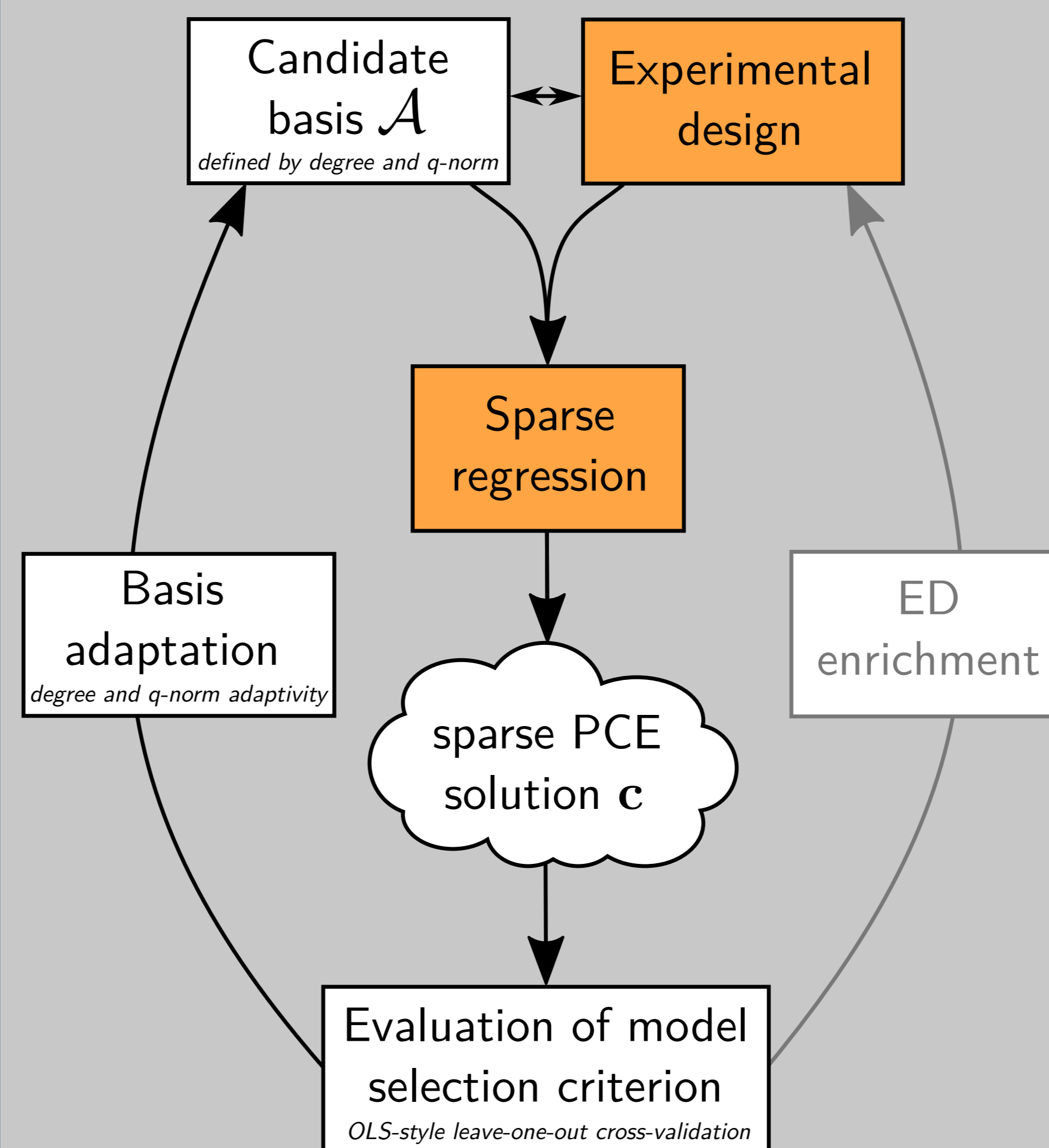
$$\min_{\mathbf{c}} \|\mathbf{c}\|_1 \text{ s.t. } \|\Psi \mathbf{c} - \mathbf{y}\|_2 \leq \epsilon$$

SPARSE REGRESSION SOLVERS

Sparse regression: Find \mathbf{c} sparse with $\|\Psi \mathbf{c} - \mathbf{y}\|_2$ small.

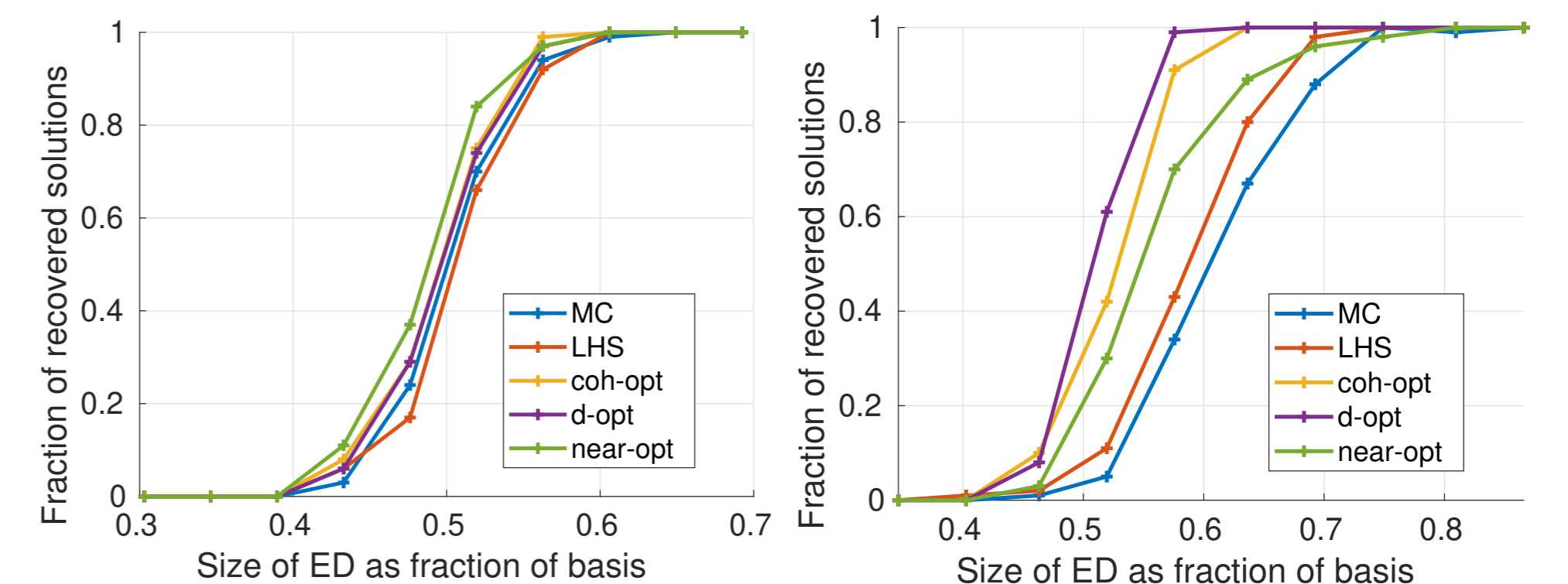
Solver options:

- **Least angle regression (LARS)** Efron, Hastie, Johnstone, Tibshirani 2003; Blatman, Sudret 2011
 - greedy method based on correlation between regressors and residual; using equiangularity
- **Orthogonal matching pursuit (OMP)** Pati, Rezaiifar, Krishnaprasad 1993; Tropp, Gilbert 2007; Berchier 2015
 - "stagewise regression": greedy method based on correlation between regressors and residual
- **Subspace pursuit** Dai, Milenkovic 2003; Diaz, Doostan, Hampton 2018
 - iterative updating of a size K regressor set based on correlation and coefficient magnitude
- **FastLaplace** (Bayesian compressive sensing) Tipping 2001; Babacan, Molina, Katsaggelos 2010
 - Hierarchical Bayesian setting: sparsity-inducing prior on coefficients
- **SPGL1** Van den Berg, Friedlander 2008
 - convex optimization: solving LASSO with spectral projected gradient descent and more.

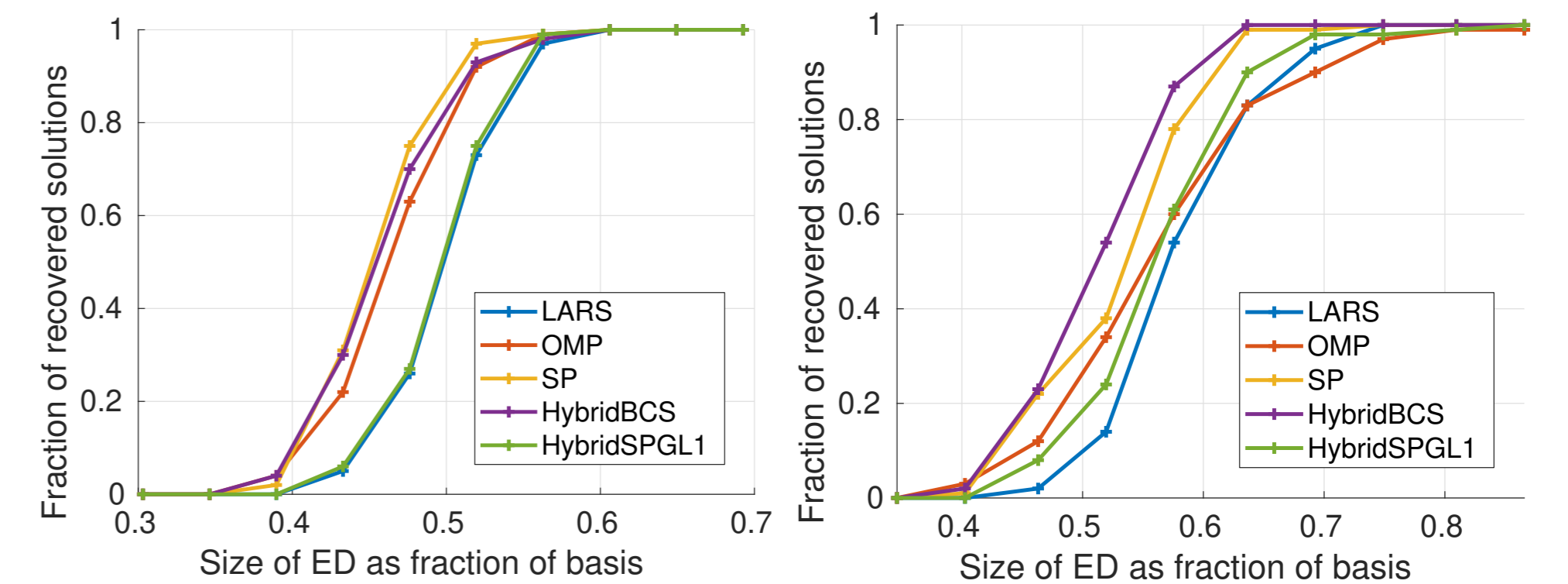


BENCHMARK RESULTS

1) Fraction of correctly identified coefficient vector for a manufactured sparse PCE (uniform input, sparsity = 20%)

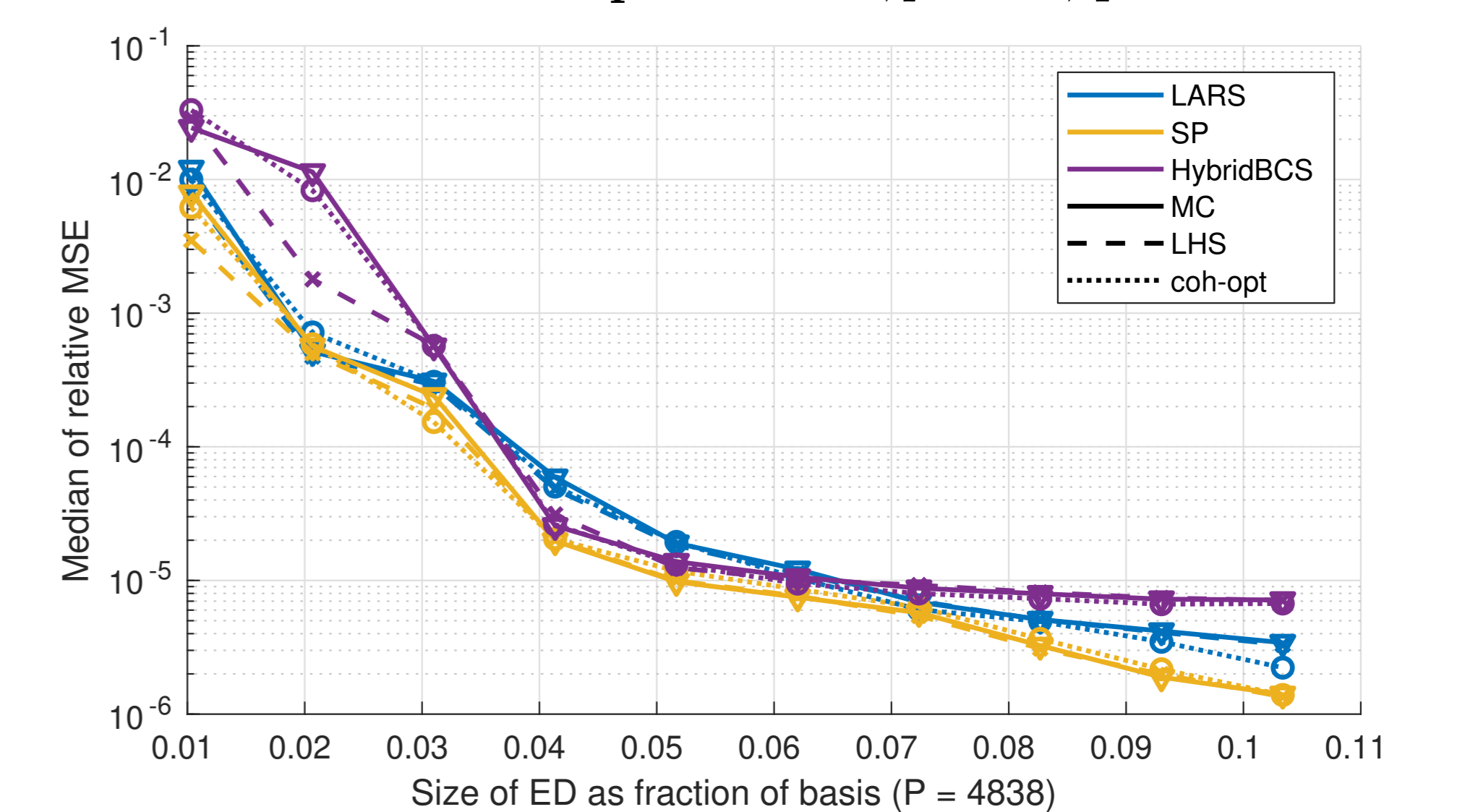


(a) ED $d = 20, p = 2$ (LARS) (b) ED $d = 2, p = 20$ (LARS)



(c) Solvers $d = 20, p = 2$ (LHS) (d) Solvers $d = 2, p = 20$ (LHS)

2) Validation error for the wingweight function (analytical model, uniform input, $d = 10, p \leq 10, q \leq 0.7$)



Conclusion

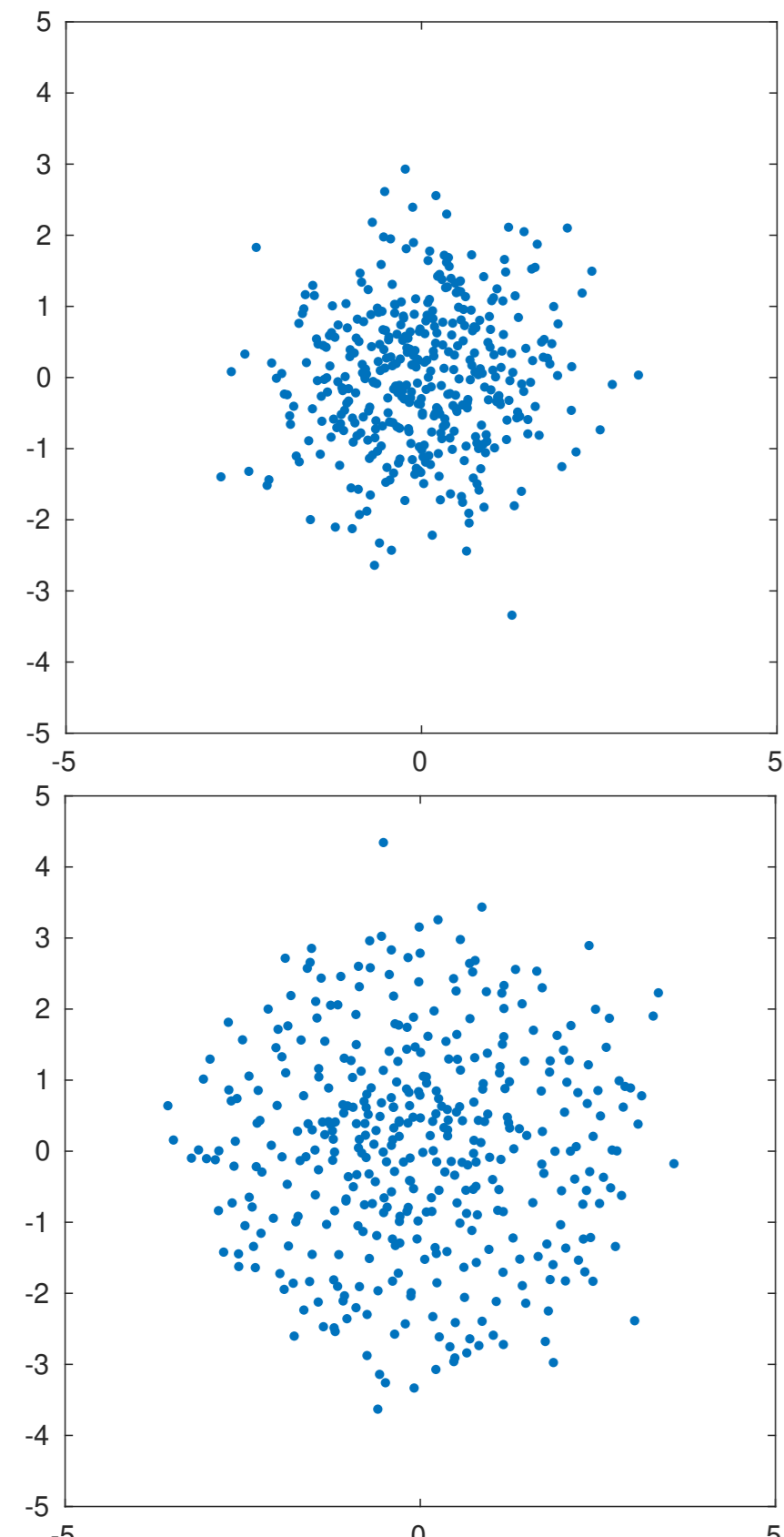
- Solver and sampling type make a difference in the quality of the solution
- Model characteristics influence the solver and sampling performance

Further work

- Characterize the influence of input and model characteristics on the choice of best components for the sparse PCE procedure
- Investigate impact of sequential ED enrichment

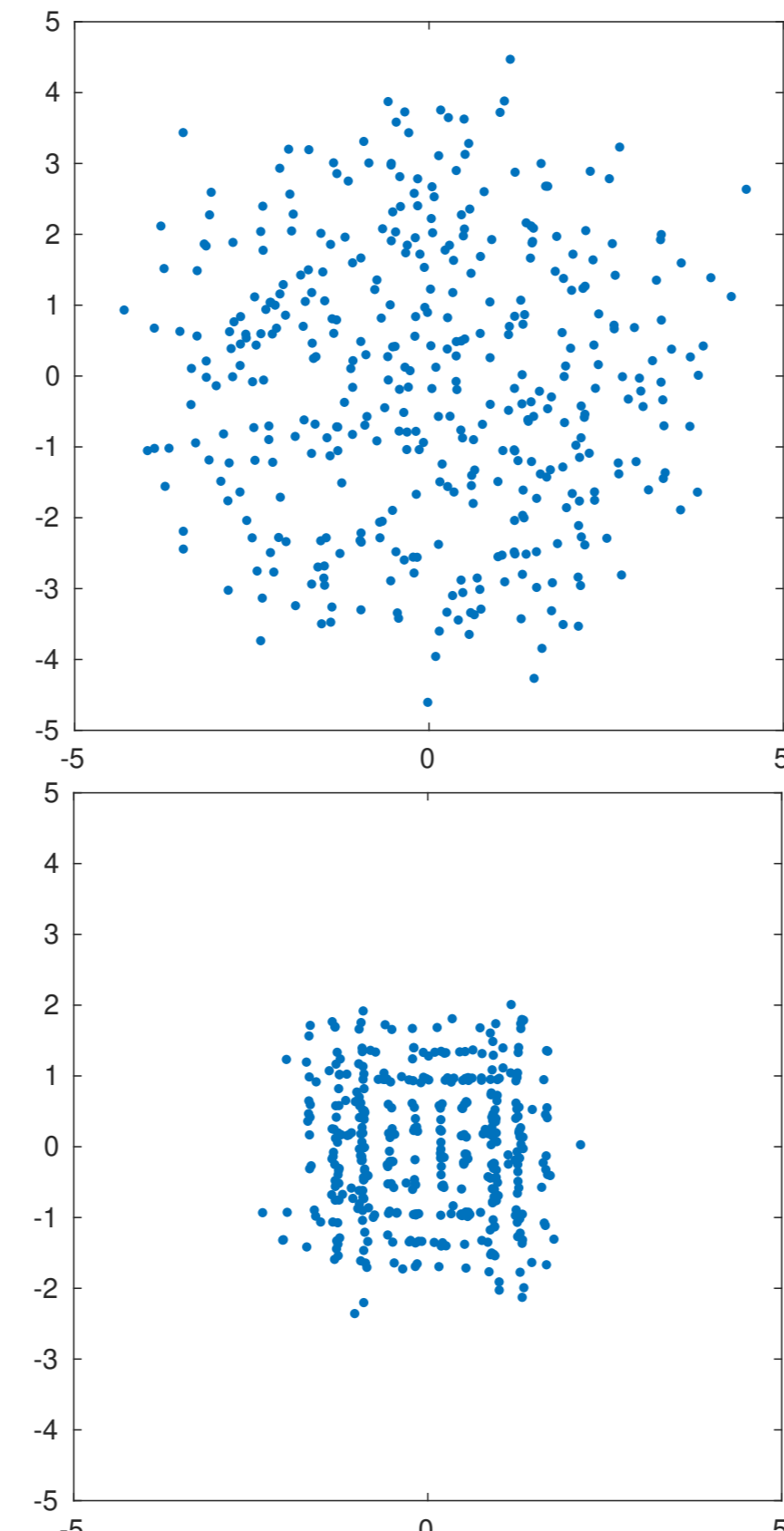
EXPERIMENTAL DESIGN SAMPLING

Illustration for $d = 2, \mathbf{X} \sim \mathcal{N}(0, \mathbf{1}), p = 20$



Latin Hypercube Sampling (LHS)

D-optimal
 $D(\Psi) = \det(\Psi^T \Psi)$
Diaz, Hampton, Doostan 2019



Coherence-optimal
 $\mu(\mathcal{A}) = \max_{\alpha \in \mathcal{A}} \sup_{\mathbf{x} \in \mathcal{D}} |\psi_{\alpha}(\mathbf{x})|$
Hampton, Doostan 2015

Near-optimal
 $\eta(\Psi) = \max_{i \neq j} \frac{|\Psi_i^{\text{col}T} \Psi_j^{\text{col}}|}{\|\Psi_i^{\text{col}}\|_2 \|\Psi_j^{\text{col}}\|_2}$
 $\gamma(\Psi) = \frac{1}{P(P-1)} \sum_{i \neq j} \frac{|\Psi_i^{\text{col}T} \Psi_j^{\text{col}}|}{\|\Psi_i^{\text{col}}\|_2 \|\Psi_j^{\text{col}}\|_2}$
Alemazkoor, Meidani 2018