

A Unified Benchmarking Platform for UQ Algorithms in UQLab

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A Unified Benchmarking Platform for UQ Algorithms in UQLAB

SIAM UQ24

A. Hlobilová, S. Marelli & B. Sudret February 29, 2024



Outline

- 1. Why is benchmarking essential?
- 2. Ingredients of a benchmark study
- 3. Demo No. 1: Live module presentation (A toy benchmark analysis)
- 4. Demo No. 2: Live module presentation (Post-processing of a real benchmark)
- 5. Summary

Why is benchmarking essential?



A **novel** sequential design strategy for global **surrogate modeling** K Crombeca, L De Tommasi... - Proceedings of the 2009 - ieeexplore.ieee.org

... Please note that global surrogate modeling differs from local surrogate modeling in the way the surrogate models are employed. In local surrogate modeling, local models are used to ... \$\phi \$\sec\$ save \$\pri\$ Cite Cited by 156 Related articles All 11 versions

INTELL Smart sampling algorithm for surrogate model development SS Garud, IA Karimi, M Kraft - Computers & Chemical Engineering, 2017 - Elsevier

... Furthermore, numerical models ... model into a computationally inexpensive surrogate model that captures its essential features with prescribed numerical accuracy. Surrogate modelling ... \$\overline{T}_{\ov

[HTML] Surrogate modelling for sustainable building design–A review <u>P Westermann, R Evins</u> - Energy and Buildings, 2019 - Elsevier

... surrogate model type. Based on the literature major research trends are extracted and useful practical aspects outlined. As surrogate modelling ... to make surrogate modelling accessible ... \u03c5 Save 59 Cite Cited by 149 Related articles All 2 versions Web of Science: 81

[HTML] An adaptive hybrid surrogate model J Zhang, S Chowdhury, A Messac - Structural and Multidisciplinary ..., 2012 - Springer



A ${\bf novel \ algorithm}$ for structural ${\bf reliability \ analysis}$ based on finite step length and Armijo line search

P Huang, HZ Huang, T Huang - Applied Sciences, 2019 - mdpi.com

... This paper presents a **novel algorithm** for structural **reliability analysis** based on the finite Rakwitz-Fiessler (HL-RF) **algorithm** that may be subjected to non-convergence in the first-order **x**² save 99 Cite Cited by 16 Related articles All 4 versions Web of Science: 11 ⊗

[HTML] **Novel algorithms** for **reliability** evaluation of remotely deployed wireless sensor networks

C Chowdhury, N Aslam, G Ahmed... - Wireless Personal ..., 2018 - Springer

... This paper investigates reliability analysis and makes two contributions. First, an algorithm based ... We propose two novel algorithms to calculate reliability. An Ordered Binary Decision ... \$\phi_S cave \$\pi_0\$ Cite Cited by 16 Related articles All 5 versions. Web of Science: 8

A novel algorithm on network reliability analysis

J Xiong, W Gong - 10th International Conference on ..., 2003 - ieeexplore.ieee.org

... a novel algorithm for network reliability analysis in this paper. The algorithm is based on rational approximation. It uses rational functions to estimate the transformed reliability function. It ... \$\phi_\$ Save \$9\$ Cite Cited by 7 Related articles

Why is benchmarking essential?



Fig. 1. RMSE of surrogate models for Ishigami function.

Fig. 3. TEST 1: Mean RMSE convergence comparison between Ordinary Kriging, sparse PDD and coupled PDD-UK metamodels, m = 5.

Shang, X. et al. (2023). An efficient multi-lidelity Kriging surrogate model-based method for global sensitivity analysis. Reliability Engineering & System Safety 229, 108858. dol 🖉 Zhang, B.-Y. & Ni, Y.-Q. (2023). A novel sparse polynomial chaos expansion technique with high adaptiveness for surrogate modelling. Applied Mathematical Modelling 121, 562-585. dol 🖉 Cortesi, A. F. Jannoun, G., & Concedo, P. M. (2019). Krigino-sparse Polynomial Dimensional Decomposition surrogate model with adaptive refinement. Journal of Computational Physics. 380, 212-242. dol 🖓

Why is benchmarking essential?

SIAM/ASA J. UNCERTAINTY QUANTIFICATION Vol. 9, No. 2, pp. 593-649 © 2021 Society for Industrial and Applied Mathematics

Sparse Polynomial Chaos Expansions: Literature Survey and Benchmark*

Nora Lüthen[†], Stefano Marelli[†], and Bruno Sudret[†]

Abstract: Sparse polynomial chaose expansions (PCE) are a popular surrogate modelling method that takes advantage of the properties of PCE. He apsaudy-cell-effects principle, and powerful sparse regression solvers to approximate computer models with many input parameters, relying on only a few model PCE has been publicled in the application that near engineering instrume. We present an extensive review of the existing methods and develop a framework for classifying the algorithms. Furthermore, we conduct: a unique benchmark on a selection of passer engineering instrume. We present an extensive review of the existing methods and develop a framework for classifying the algorithms. Furthermore, we conduct: a unique benchmark on a selection of passe regression adverse and assuppling scheme for functions. Comparing their accuracy on several benchmark models de varying illumerical applications. Comparing their accuracy on several benchmark models do varying international applications. Comparing their accuracy on several benchmark models of varying international complexity, we fit that the their does of passes regression advect and assupplications for the particular days and experimental days and experimental design atom.

Key words. uncertainty quantification, surrogate modelling, sparse regression, sparse polynomial chaos expan-



Structural Safety 96 (2022) 102124 Contents lists available at ScienceDirect Structure Structural Safety journal homepage: www.elsevier.com/locate/strusafe Active learning for structural reliability: Survey, general framework and henchmark Maliki Moustapha ', Stefano Marelli, Bruno Sudret Choir of Risk Sofety and Decentricity Doublication. FTU Parish Station-Democrat. Harr 5, 8003 Parish Station-Institutional ARTICLE INFO ABSTRACT Active learning methods have recently surged in the literature due to their ability to solve complex structural Structural reliability reliability problems within an affordable computational cost. These methods are designed by adaptively building an incompanies surrounds of the original limit state function. Examples of such surrounder include Gaussian process models which have been adopted in many contributions, the most popular ones being the efficient Benchmark tility analysis (EGRA) and the active Kriging Monte Carlo simulation (AK-MCS), two milester Structural Safety . Open Access . Volume 96 . May 2022 . Article number 102174 Active learning for structural reliability: Survey. general framework and benchmark Moustanha, Maliki 🖾 : Marelli, Stefano: Sudret, Bruno Save all to author list * Chair of Risk, Safety and Uncertainty Quantification, ETH Zurich, Stefano-Franscini-Platz 5, Zurich, 8093, 56 99th percentile 9.98 40 View all metrics > FWCI @ Views count (?) Citations in Sconus

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The UQLAB software framework



- Matlab-based high-level language
- Complete framework for uncertainty quantification
- BSD license: completely open-source for both academia and industry
- Approx. 6.8k unique users from 90+ countries
- 1500+ combined citations on Google Scholar since 2014

Continuously developed/updated by the RSUQ Chair @ETH Zurich

Marelli, S. & Sudret, B. (2014). UCLab: A framework for uncertainty quantification in Matlab. Proc. 2nd Int. Conf. on Vulnerability, Risk Analysis and Management (ICVRAM2014), Liverpool, United Kingdom, 2554-2563. doi:10.3929/ethz-a-010238238 [2]

Our proposal

- Unified, standardized, and objective way to evaluate the performance of algorithms against established standards
- Curated database containing datasets, configurations, algorithms, and performance measures
- Sets of settings of competitors tailored for specific benchmark case scenarios
- Reduce the workload and time investment for researchers

Outline

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2. Ingredients of a benchmark study

3. Demo No. 1: Live module presentation (A toy benchmark analysis)

4. Demo No. 2: Live module presentation (Post-processing of a real benchmark)

5. Summary

Ingredients of a benchmark study

- Bench cases
- Competitors
- Performance measures
- Post-processing of the results

Additional features

- Library
- Dispatch of computations (HPC)

Bench cases





Bench cases

- Described by
 - a computational model with an associated set of probability distributions, or
 - datasets
- Example: Borehole model for surrogate modeling

$$f(X) = \frac{2\pi T_u (H_u - H_l)}{\ln \left(\frac{r}{r_w}\right) \left(1 + \frac{2LT_u}{\ln \left(\frac{r}{r_w}\right) r_w^2 K_w} + \frac{T_u}{I_l}\right)} \frac{\frac{Variable \ Description \ Distribution \ Statistics}{r_w \ Radius of borehole (m) \ Normal \ \mu_w = 0.10, \sigma_*^2 = 0.0161812} \\ \frac{r_w \ Radius of borehole (m) \ Normal \ \mu_w = 0.10, \sigma_*^2 = 0.0161812}{T_v \ Tansmissivity of operaulier (m^2/ry) \ Uniform \ T_v \sim U(3070, 115600) \\ H_v \ Potentionetric head of upper aquifer (m^2/ry) \ Uniform \ T_v \sim U(0307, 115600) \\ H_v \ Potentionetric head of oper aquifer (m^2/ry) \ Uniform \ T_v \sim U(0307, 115600) \\ H_v \ Potentionetric head of oper aquifer (m^2/ry) \ Uniform \ T_v \sim U(0307, 0.115600) \\ H_v \ Potentionetric head of oper aquifer (m^2/ry) \ Uniform \ T_v \sim U(0307, 0.11680) \\ K_w \ Hydraulic conductivity of borehole (m/yr) \ Uniform \ K_w \sim U(1985, 12045) \\ \end{array}$$

sample No.	r_w	r	T_{u}	H_u	T_l	H_l	L	K_w	f(X)
1	0.096852	3778.2	90956	1106.2	104.3	733.72	1410.1	11336	87.913
2	0.078719	3186	97448	1053.8	85.501	752.81	1648.4	10488	37.185
3	0.10404	354.06	84482	1029	67.905	763.26	1477.1	11326	68.951
4	0.09882	501.17	1.0614e5	1002.7	77.196	754.89	1656.3	11377	52.024
:	:	:	:	:	:	:	:	:	:
N	0.1083	1392.1	1.0081e5	1063.3	71.228	805.04	1254.8	10004	75.399

Competitors

Potential competitors for benchmarking

- Metamodels
- Reliability analysis
- Classifiers
- Samplers
- [Robust] Optimization algorithms
- ► Bayesian inference/inversion
- ► [Sensitivity analysis (specific measures, such as ANOVA)]

Competitors Metamodels

- Configuration parameters:
 - Metamodel family
 - Smoothness (degree/covariance)
 - Sparsity
 - Optimization algorithms
 - Adaptivity
- Example: Kriging
 - Correlation families (exponential/Matern/...)
 - Optimization algorithms (BFGS, GA)
 - Regression vs interpolation





Performance measures

Why are performance measures computed?

- Comparing different algorithms
- Assessing accuracy and precision of the algorithm
- Improving algorithm development

Typical performance measures

- Accuracy prediction (e.g., RMSE, MAE, or R²)
- Convergence analysis (e.g., probability of failure or reliability index)
- Computational efficiency (costs)
- Robustness (e.g., by cross-validation)



Analysis, and aggregating & post-processing results

Let's run the benchmarking analysis!

- Assemble all combinations of bench cases and competitors
- Run the competitors to obtain performance measures

What should be included in post-processing?

- Brief overview of the analysis
- Aggregating results
- Book-keeping / Interactive results
- Ranking
- Graphical representation of results

Library

Purpose of the library

To provide a curated, standardized, and comprehensive collection of benchmark cases, settings, and results for evaluating and comparing the performance of newly implemented algorithms

What should be stored in the library?

- Bench case inputs: Input data for benchmark cases
- Competitor settings: Settings used by previously analyzed competitors during benchmark analysis
- Unified benchmark results: Exhaustive collection of benchmark results
- Curated competitor settings: Specified sets of settings for competitors, tailored for specific benchmark cases

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Demo No. 1 Run the live demo in MATLAB

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Demo No. 1 Initialization

Goal: Initialize UQLAB and the Benchmark module using the Metamodel benchmark type

```
%% 1 - INITIALIZE UQLAB
%
% Clear all variables from the workspace,
% set the random number generator for reproducible results,
% and initialize the UQLab framework:
clear, clc
rng(100,'twister')
uqlab
%% 2 - SETUP THE SURROGATE MODELLING BENCHMARK
%
% Select the benchmark tool and the benchmark type case:
BOpts.Type = 'Benchmark';
BOpts.BenchmarkType = 'Metamodel';
```

Demo No. 1 Bench case: Ishigami function

Goal: Bench case #1 with 3 different experimental designs (30, 50, and 70 samples) and 10 different replications (by using a user-defined input and model)

```
22 3 - BENCH CASES
%% 3.1 - ISHIGAMI FUNCTION
BOpts.BenchCases(1).Name = 'Ishigami function';
22 3 1 1 - COMPUTATIONAL MODEL
BOpts.BenchCases(1).Model.mFile = 'ug_ishigami';
22 3.1.2 - PROBABILISTIC INPUT MODEL
for ii = 1:3
    IshigamiInput.Marginals(ii).Type = 'Uniform';
    IshigamiInput.Marginals(ii).Parameters = [-pi pi]:
and
BOpts.BenchCases(1).Input = IshigamiInput:
%% 3.1.3 - EXPERIMENTAL DESIGN AND VALIDATION SETS
NSamples = [30, 50, 70];
Replications = 10:
BOpts.BenchCases(1).ExpDesigns = struct('NSamples', num2cell(NSamples), ...
                                        'Replications', Replications):
BOpts.BenchCases(1).ValidationSet.NSamples = 1e4:
```

Demo No. 1 Bench case: Borehole function

Goal: Bench case #2 with 3 different experimental designs (30, 50, and 70 samples) and 10 different replications (by using UQLAB-defined input and model)

```
%% 3.2 - BOREHOLE FUNCTION
uq_BoreholeInputModel;
BOpts.BenchCases(2).Name = 'Borehole function';
%% 3.2.1 - COMPUTATIONAL MODEL
BOpts.BenchCases(2).Model = myModel;
%% 3.2.2 - PROBABILISTIC INPUT MODEL
BOpts.BenchCases(2).Input = myInput;
%% 3.2.3 - EXPERIMENTAL DESIGN AND VALIDATION SETS
NSamples = [30, 50, 70];
Replications = 10;
BOpts.BenchCases(2).ExpDesigns = struct('NSamples', num2cell(NSamples), ...
'Replications', Replications);
BOpts.BenchCases(2).ValidationSet.NSamples = 1e4;
```

Demo No. 1 Competitors: PCE, Kriging

Goal: Set up PCE and Kriging competitors with (almost) default options

```
%% 4 - COMPETITORS
%% 4.1 PCE
PCEMetaOpts.Type = 'MetaModel';
PCEMetaOpts.MetaType = 'PCE';
PCEMetaOpts.Degree = 1:15;
PCEMetaOpts.Method= 'LARS';
BOpts.Competitors(1).MetaOpts = PCEMetaOpts;
BOpts.Competitors(1).Name = 'PCE (LARS, d=1:15)';
%% 4.2 Kriging
KrigingMetaOpts.Type = 'Metamodel';
KrigingMetaOpts.MetaType = 'Kriging';
KrigingMetaOpts.Corr.Family = 'Exponential';
BOpts.Competitors(2).MetaOpts = KrigingMetaOpts;
BOpts.Competitors(2).Name = 'Ordinary Kriging (Exponential corr. family)';
```

Demo No. 1 Run and post-process the analysis

```
%% 5 - GENERATE AND RUN THE BENCHMARK
myBenchmark = uq_createAnalysis(BOpts);
```

%% 6 - POSTPROCESSING
% Print a summary of the resulting analysis
uq_print(myBenchmark)

% Create a graphical representation of the results uq_display(myBenchmark, 'full')

%% 7 - STORING BENCHMARKING ANALYSIS DATA uq_saveToLibrary(myBenchmark,'myNewFancyLibrary.mat')

Demo No. 1 Results



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5. Summary

Demo No. 2: Post-processing of a real benchmark Run the live demo in MATLAB



Demo No. 2: Post-processing of a real benchmark Bench cases

Bench case	Dimension	Experimental designs (samples)	Validation set (samples)
Ishigami function	3	30, 50, 70, 90, 120, 150, 200	100 000
Borehole function	8	50, 100, 150, 200, 250, 300	100 000
Damped oscillator	8	100, 150, 200, 250, 300, 350, 400	100 000
Wingweight function	10	100, 150, 200, 250, 300	100 000
Truss model	10	100, 150, 200, 250, 300	100 000
		50 replications	1 replication

Demo No. 2: Post-processing of a real benchmark Competitors

No.	Competitor Names	Number of Hyperparameters
1	PCE (LARS)	3
2	PCE (OMP)	3
3	PCE (SP)	3
4	Ordinary Kriging	4
5	Kriging with a linear trend	4
6	PCK	7
7	XGBoost (sklearn Python module)	8
8	Multi-Layer Perceptron (torch Python module)	10

Demo No. 2: Post-processing of a real benchmark Results in MATLAB



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Summary

We propose a flexible framework to fairly and efficiently compare the performance of surrogate models:

- Selection of benchmark cases
- Selection of competitors
- Natively enabling replications
- Standardized performance measures
- Integration of data from third-party packages
- Archiving through open-source libraries of pre-computed performances

Next steps

- Finalizing the current state (external competitors called by the benchmark module, asynchronous computation, etc.)
- Release the software into UQLAB Version 2.2, scheduled for late Q2, 2024
- After populating the benchmark library, open access to contributors from different fields to cater to a larger audience
- Extend benchmarking functionality to different types of analysis (e.g., Bayesian calibration, sensitivity analysis, optimization, etc.)
- ► Post a public challenge for datasets and algorithms on our online community UQWorld C, which counts hundreds of users from different fields of applied science and engineering

Questions?



Chair of Risk, Safety & Uncertainty Quantification www.rsuq.ethz.ch

Thank you very much for your attention!

The Uncertainty Quantification Software

www.uqlab.com



www.uqpylab.uq-cloud.io



The Uncertainty Quantification Community www.uqworld.org



BACKUP SLIDES



Benchmark analysis info

>> bug_Example_Benchmark_SIAM01 Copyright 2013-2022, Stefano Marelli and Bruno Sudret, all rights reserved. This is UGLab, version 2.0 UGLab is distributed under the BSD 3-clause open source license available at: C:\Jøsers\ahlobilovs\bounderlabuslovs\bounderlabuslows\bounderlabuslovs\bounder

To request special permissions, please contact:

- Stefano Marelli (marelli@ibk.baug.ethz.ch).

Useful commands to get started with UQLab:

uglab -doc	 Access the available documentation
uqlab -help	- Additional help on how to get started with UQLab
uq_citation_help	- Information on how to cite UQLab in publications
uglab -license	- Display UQLab license information

Initialization of the Benchmark Analysis done at 14-Feb-2024 15:59:58...

Starting Benchmark Metamodel Analysis...

Analyzing bench case No. 1 (Ishigami function):

- Evaluating competitor No. 1: PCE (LARS, d=1:15)
- Evaluating competitor No. 2: Kriging (Matern 5/2)

Analyzing bench case No. 2 (Borehole function):

- Evaluating competitor No. 1: PCE (LARS, d=1:15)
- Evaluating competitor No. 2: Kriging (Matern 5/2)

Benchmark Metamodel Analysis done in 5 minutes and 12 seconds



Benchmark analysis: Analysis 1

Bench cases and experimental dealon sizes

1) Ishigami function

1) 30 samples (10 replications)

- 2) 10 samples (10 replications)
- 3) 70 samples (10 replications)

2) Borehole function

- 1) 30 samples (10 replications)
- 2) 50 samples (10 replications)
- 3) 70 pamples (10 replications)

Competitors:

1) PCE (LARS, d=1:15) 21 Eriging (Hatern 5/2)

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Agregated results:

Bench Case	Compatitor	Experimental Design Size	Re1MSE: mean (CoV)	RelCVErr: mean (CoV)	MAPE: mean (CoV)	MAE_norm: mean (CoV)
Ishigami function	PCE (LARS, d=1:15)	30	3.15e-01 (67%)	6.59e-02 (133%)	-1.38e+01 (-119%)	9.54e-02 (36%)
Ishigami function	PCE (LARS, d=1:15)	50	2.68e-02 (105%)	6.03e-03 (184%)	-2.56e+00 (-190%)	2.01e-02 (58%)
Ishigami function	PCE (LARS, d=1:15)	70	9.65e-04 (203%)	0.46e-05 (245%)	4.90e-02 (205%)	2.40e-03 (171%)
Ishigami function	Rriging (Matern 5/2)	30	8.61e-01 (95%)	3.98e-01 (38%)	-1.13e+01 (-299%)	1.69e-01 (40%)
Ishigami function	Kriging (Matern 5/2)	50	3.51e-01 (30%)	3.23e-01 (31%)	-1.14e+01 (-115%)	1.07e-01 (16%)
Ishigami function	Kriging (Matern 5/2)	70	2.38e-01 (37%)	2.24e-01 (33%)	-1.50e+01 (-73%)	0.57e-02 (13%)
Borehole function	PCE (LARS, d=1:15)	30	3.18e-02 (73%)	6.73e-03 (135%)	5.08e+00 (37%)	3.95e-03 (38%)
Borehole function	PCE (LARS, d=1:15)	50	2.27e-03 (31%)	1.11e-03 (49%)	1.37e+00 (11%)	1.02e-03 (17%)
Borehole function	PCE (LARS, d=1:15)	70	1.43e-03 (22%)	7.33e-04 (44%)	1.13e+00 (16%)	7.598-04 (14%)
Borehole function	Kriging (Matern 5/2)	30	3.31e-02 (24%)	2.22e-02 (11%)	4.26e+00 (15%)	3.66e-03 (14%)
Borehole function	Kriging (Matern 5/2)	50	1.77e-02 (43%)	7.20e-03 (20%)	2.93e+00 (20%)	2.44e-03 (19%)
Borehole function	Kriging (Matern 5/2)	70	1.01e-02 (22%)	6.99e-03 (52%)	1.81e+00 (10%)	1.59e-03 (10%)

Dasful functions for nost-processing data in Banchmark modular

ug printBenchmark - Display interactive benchmark analysis

- ug filterBenchmark Filter benchmark data
- uq getDetails Get details about a particular test case
- ug appregateResulta Appregate data from the benchmarking analysis for the replicated datasets

ug saveToLibrary - Save data to a new library or add data to an existing library

uq loadFromLibrary - Load data from a library to UGLab



Live demo No. 1: Results Benchmark analysis post-processing: uq_print, filtering

Bench Case	Competitor	Experimental Design Size	RelMSE: mean (CoV)	RelCVErr: mean (CoV)	MAPE: mean (CoV)	MAE_norm: mean (CoV)
Ishigami function	PCE (LARS, d=1:15)	30	3.15e-01 (67%)	6.59e-02 (133%)	-1.38e+01 (-119%)	9.54e-02 (36%)
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Ishigami function	PCE (LARS, d=1:15)	70	9.65e-04 (283%)	8.46e-05 (245%)	4.98e-02 (205%)	2.48e-03 (171%)
Ishigami function	Kriging (Matern 5/2)	30	8.61e-01 (95%)	3.98e-01 (38%)	-1.13e+01 (-299%)	1.69e-01 (40%)
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Ishigami function	Kriging (Matern 5/2)	70	2.38e-01 (37%)	2.24e-01 (33%)	-1.50e+01 (-73%)	8.57e-02 (13%)

Benchmark analysis: Analysis 1

Bench cases and experimental design size:

...........

1) Ishigami function

1) 30 samples (10 replications)

2) 50 samples (10 replications)

3) 70 samples (10 replications)

2) Borehole function

1) 30 samples (10 replications)

2) 50 samples (10 replications)

3) 70 samples (10 replications)

Competitors:

1) PCE (LARS, d=1:15)

2) Kriging (Matern 5/2)

Live demo No. 1: Results Benchmark analysis post-processing: uq_print, filtering

Bench Case	Competitor	Experimental Design Size	RelMSE: mean (CoV)	RelCVErr: mean (CoV)	MAPE: mean (CoV)	MAE_norm: mean (CoV)
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Benchmark analysis: Analysis 1

......

Bench cases and experimental design size:

1) Ishigami function

1) 30 samples (10 replications)

2) 50 samples (10 replications)

3) 70 samples (10 replications)

2) Borehole function

1) 30 samples (10 replications)

2) 50 samples (10 replications)

3) 70 samples (10 replications)

Competitors:

.......

1) PCE (LARS, d=1:15)

2) Kriging (Matern 5/2)



Benchmark analysis post-processing: uq_display





The analytic expression:

 $Y(\mathbf{x}) = \sin(x_1) + 7\sin^2(x_2) + 0.1x_3^4\sin(x_1)$ (1)

- ► 3 independent random variables $\mathbf{X} = \{X_1, X_2, X_3\}$
- ▶ Inputs are modelled by uniform distributions in the cube $\mathbf{X} \in [-\pi,\pi]^3$



	Number of Samples	Replications
Exp. Designs	30, 50, 70, 90, 120, 150, 200	50
Validation set	100 000	1

Live demo No. 2: Bench cases Borehole Function B2

The analytic expression:

$$f(\mathbf{X}) = \frac{2\pi T_u (H_u - H_l)}{\ln(r/r_w)(1 + \frac{2LT_u}{\ln(r/r_w)r_w^2 K_w} + \frac{T_u}{T_l})}$$
(2)

- ► 8 independent random variables $X = \{r_w, r, T_u, H_u, T_l, H_l, L, K_w\}^a$
- ► Inputs are modeled by normal (r_w), lognormal (r), and uniform distributions (T_u, H_u, T_l, H_l, L, K_w)



	Number of Samples	Replications
Exp. Designs	50, 100, 150, 200, 250, 300	50
Validation set	100 000	1

^awhere r_w : Radius of borehole, r: Radius of influence, T_u : Transmissivity of upper aquifer, H_u : Potentiometric head of upper aquifer, T_l : Transmissivity of lower aquifer, H_l : Potentiometric head of lower aquifer, L: Length of borehole, K_w : Hydraulic conductivity of borehole.

Live demo No. 2: Bench cases Damped Oscillator Function (B_3)





- 8 independent lognormal distributed random ► variables
 - $X = \{m_p, m_s, k_p, k_s, \zeta_p, \zeta_s, S_0, F_s\}^a$



	Number of Samples	Replications
Exp. Designs	100, 150, 200, 250, 300, 350, 400	50
Validation set	100 000	1

^awhere m_p : Primary mass, m_s : Secondary mass, k_p : Primary spring stiffness, k_s : Secondary spring stiffness, ζ_p : Primary damping ratio, ζ_s : Secondary damping ratio, S_0 : Intensity of the white noise, F_s : Force capacity of the secondary spring.

Live demo No. 2: Bench cases Wing weight function B_4

The analytic expression:

$$f(\mathbf{X}) = 0.035 S_w^{0.758} W_{fw}^{0.0035} \left(\frac{A}{\cos^2(\Lambda)}\right)^{0.6} q^{0.006} \\ \times \lambda^{0.04} \left(\frac{100t_c}{\cos(\Lambda)}\right)^{-0.3} \left(N_z W_{dg}\right)^{0.49} + S_w W_p$$
(3)

10 independent uniform distributed random variables

 $\mathbf{X} = \{S_w, W_{fw}, A, \Lambda, q, \lambda, t_c, N_z, W_{dg}, W_p\}^{\mathsf{a}}$



	Number of Samples	Replications	
Exp. Designs	100, 150, 200, 250, 300	50	
Validation set	100 000	1	

^awhere S_w : Wing area (ft²), W_{fw} : Weight of fuel in the wing (lb), A: Aspect ratio, Λ : Quarter-chord sweed (degrees), g: Dynamic pressure at cruise (lb/ft²), λ : Taper ratio, t_c : Aerofoil thickness to chord ratio, N_z : Ultimate load factor, W_{dg} : Flight design gross weight (lb), W_p : Paint weight (lb/ft²).

Live demo No. 2: Bench cases

Model:



- ▶ 10 independent random variables X = {E₁, E₂, A₁, A₂, P₁, P₂, P₃, P₄, P₅, P₆}^a
- ► Inputs are modeled by lognormal (E₁, E₂, A₁, A₂) and Gumbel distributions (P_i, i = 1, ..., 6)
- $\overset{a}{}$ where $A_1, A_2:$ Cross-sectional areas, $E_1, E_2:$ Young's moduli, $P_i, i=1,\ldots,6:$ applied loads.



	Number of Samples				
Exp. Designs	100, 150, 200, 250, 300	50			
Validation set	100 000	1			

Live demo No. 2: Competitors

PCE

- Regression solvers: LARS C₁, OMP C₂, and SP C₃
- ▶ Degree adaptivity: $p \in [1, 15]$ with early stop based on ϵ_{LOO}
- q-norm truncation: [0, 75, 1]

Kriging

- ordinary C_4 and with linear trend C_5
- ► Correlation family: Matérn-5/2
- Correlation type: Ellipsoidal
- HGA optimizer

Sequential PC-Kriging C6

- Kriging
 - ordinary Kriging
 - Correlation family: Matérn-5/2
 - Correlation type: Ellipsoidal
 - HGA optimizer
- ► PCE
 - Regression solver: LARS
 - Degree: 3

Live demo No. 2: Competitors

XGBoost C7

- sklearn Python module
- ▶ gamma: $3.4 \cdot 10^{-7}$
- ▶ learning_rate: 0.13
- ▶ max_depth: 3
- min_child_weight:1
- ▶ n_estimators: 900
- ▶ reg_alpha: 5.7 · 10⁻⁴
- ▶ reg_lambda:1.2
- ► subsample: 0.8

Multi-Layer Perceptron (MLP) C8

- torch Python module
- ▶ lr: 5 · 10⁻⁴
- ▶ max_epochs: 100
- ▶ batch_size: 256
- optimizer_name: adamw
- ▶ lr_scheduler:False
- ▶ es_patience: 40
- ▶ lr_patience: 30
- module__n_layers: 4
- module__d_layers: 1024
- ▶ module__dropout: 0.2

Live demo results: Example 2

Benchmark analysis post-processing: uq_print

Benchmark analysis: Analysis 1

Bench cases and experimental design size:

1) Ishigami function

- <u>30 samples</u> (50 replications)
- 2) 50 samples (50 replications)
- 3) 70 samples (50 replications)
- 90 samples (50 replications)
- <u>120 samples</u> (50 replications)
- 6) 150 samples (50 replications)
- 7) 200 samples (50 replications)

2) Borehole model

- 1) 50 samples (50 replications)
- 2) 100 samples (50 replications)
- <u>150 samples</u> (50 replications)
- 4) 200 samples (50 replications)
- 5) 250 samples (50 replications)
- 6) 300 samples (50 replications)
- 3) Damped oscillator
 - 1) 100 samples (50 replications)
 - 2) 150 samples (50 replications)
 - 3) 200 samples (50 replications)
 - 4) 250 samples (50 replications)
 - 5) 300 samples (50 replications)
 - 6) 350 samples (50 replications)
 - 7) 400 samples (50 replications)

Wingweight function

- 1) 100 samples (50 replications)
- 2) 150 samples (50 replications)
- 3) 200 samples (50 replications)
- 4) 250 samples (50 replications)
- 5) 300 samples (50 replications)

5) Truss model

- <u>100 samples</u> (50 replications)
 150 samples (50 replications)
- 3) 200 samples (50 replications)
- 4) 250 samples (50 replications)
- 5) 300 samples (50 replications)

Competitors:

.....

- 1) PCE (LARS)
- 2) PCE (OMP)
- 3) PCE (SP)
- 4) Ordinary Kriging
- 5) Kriging with linear trend
- <u>PCK</u>
- 7) XGB (ext., sklearn)
- 8) MLP (ext., torch)

Benchmark analysis post-processing: uq_print (240 aggregated combinations)

Bench Case	Competitor	Experimental Design Size	BelMSE: mean (CoV)	BelCVErr: mean (CoV)	MAPE: mean (CoV)	MAE_norm: mean (CoA
Ishigani function	FCE (LAR5)	10	2,008-01 (778)	4,458-02 (1178)	2,230+01 (628)	0.028-02 (439)
Ishigami function	FCE (LARS)	50	5.408-02 (1515)	7,456-03 (1715)	8.524+00 (91%)	2.83e-02 (82%)
Ishigani function	ICE (LARS)	70	3,916-03 (3158)	4,620-04 (3198)	1.600+00 (105%)	5,276-03 (1468)
Ishigami function	FCE (LARS)	80	1,414-04 (2794)	2,728-05 (2298)	3,338-01 (1748)	0.954-04 (1568)
Ishigami function	FCE (LARS)	130	5.50e-07 (3135)	2,988-07 (335%)	2.00e-02 (236%)	6.244-05 (2235)
Ishigami function	FCE (LAR5)	150	2.148-05 (3548)	2,42e-09 (2478)	3.064-03 (2068)	0.02e-06 (106%)
Ishigami function	FCE (LARS)	200	2.60s-11 (616)	1,076-11 (476)	3.250-04 (455)	8,644-07 (114)
Ishigami function	PCE (OHP)	30	1.198+00 (70%)	3.866-04 (363%)	5.77e+01 (61%)	1.86e-01 (45%)
Ishigani function	PCE (CREP)	50	1.61e-01 (2398)	2,05e-05 (529%)	1.15++01 (1998)	3.374-02 (1798)
Ishigami function	FCE (GKF)	70	1.09#-02 (453%)	8,976-07 (480%)	1.120+00 (280%)	3.35e-03 (2814)
Ishigami function	FCE (CREP)	90	5.656-03 (7078)	1.32e-10 (477%)	3.41e-01 (705%)	6.93e-01 (692%)
Ishigami function	FCE (CHF)	120	1.698-06 (560%)	1.016-00 (706%)	0.008-03 (572%)	2,10e-05 (4054)
Ishigami function	PCE (OOF)	180	4.02e-09 (696%)	8,36e-18 (186%)	-5.20e-05 (-6168%)	1.748-06 (197%)
Ishigami function	PCE (ONP)	200	5.494-11 (478)	7.01e-13 (91%)	4.324-04 (378)	1,17e-06 (12%)
Ishigami function	PCE (SP)	30	1.93s-01 (1216)	1,998-02 (219%)	1.950+01 (72%)	6.198-02 (60%)
Ishigami function	PCE (8P)	80	5.95e-05 (208%)	8.82e-08 (189%)	7.756-01 (121%)	2.26e-03 (99%)
Ishigami function	PCE (59)	70	6.09e-07 (3538)	0.27e-00 (360%)	1.70e-02 (202%)	3,964-05 (2468)
Ishigami function	PCE (SP)	50	1.158-10 (138%)	3.51e-11 (421%)	3.578-04 (535)	1.21e-06 (28%)
Ishigami function	ECE (5P)	120	8.62e-11 (124%)	7.57e-12 (212%)	4.104-05 (47%)	1,16e-06 (20%)
Ishigami function	PCE (59)	150	5.00e-11 (50%)	4.12e-12 (52%)	3.72e-04 (428)	1,098-06 (13%)
Ishigami function	PCE (8P)	210	4.738-11 (725)	3,97e-12 (30%)	3.430-04 (46%)	1.02e-06 (14%)
Ishigami function	Ordinary Kriging	30	7.604-01 (38%)	4.24e-01 (46%)	4.70e+01 (47%)	1.65e-01 (19%)
Ishigami function	Ordinary Kriging	50	4.668-01 (46%)	2,908-01 (43%)	4.276+01 (50%)	1,10s-01 (198)
Ishigami function	Ordinary Kriging	70	2.88e-01 (37%)	1.940-01 (82%)	3.210+01 (80%)	9.33e-02 (184)
Ishigami function	Ordrawly Kirdrad	90	1.934-01 (254)	1.416-01 (50%)	2.476+01 (398)	7.556-02 (128)
Ishigami function	Ordinary Kriging	120	1.298-01 (296)	1,026-01 (225)	1.840+01 (51%)	5,928-02 (165)
Ishigami function	Ordinary Kriging	180	8.158-02 (256)	0.800-02 (314)	1.370+01 (47%)	4,426-02 (134)
Issigant function	ordrawly wirding	210	41276-02 (314)	3,708-02 (298)	1.000+01 (408)	2.998-02 (104)
Ishigami Function	kriging with linear trend	30	7.358-01 (305)	4,350-52 (434)	5.766+01 (454)	1.040-01 (176)
Issident function	stiding with linear trend	10	41736-01 (414)	3,000-72 (454)	1.008101 1 074)	11216-01 (224)
Istigant function	wriging with linear trend	70	3.018-01 (364)	2.010-01 (234)	3.378401 (474)	9.528-02 (104)
Tabloani function	Velaina with linear brend	120	1.734-01 (254)	1.040-01 (200)	1.534401 (518)	5-03e-02 (124)
Tabioani function	Veloine with linear grand	150	8 044-03 (318)	6 844-03 4 8381	1 358401 (408)	4 344-03 (124)
Tabloant Function	Triging with linear trend	110	4.744-07 (315)	3.710-07 (198)	1.044401 / 4451	3.874-03 (104)
Tabigani function	Ery	10	6 144-01 (458)	3. 684-03. 6.8683	4 474401 (508)	1.434-01 (338)
Tablorni function	PCH .	10	4 110-01 (100)	1 808-01 4 5881	3 500001 (600)	1 144-01 (194)
Tabloant Function	100	70	3.034-03. (455)	1.610-01 (335)	7.774401 (575)	5-35e-03 (1851
Tabloani function	RCM.	10	3 110-01 (338)	1 334-01 4 5441	3 300001 4 4681	2 01=-02 (1481
Tabloant function	PCM.	130	1.244-01 (404)	1.040-01 (1951	1.784401 / 5051	5-344-02 (165)
Ishiasai function	PCR .	150	8.22#+02 (228)	6.744-02 (26%)	1.40##01 (478)	4.35e:02 (118)
Ishigani function	ECH.	210	4,218-02 (325)	3.768-02 (303)	1.088401 (458)	2.954-02 (98)
ADIANS FURITION	XIR (ext., sklearn)	30	6.468-01 (203)	8,778-01 (26%)	4.810+01 (423)	1.634-01 (105)
Tabigani function	XCB (avt., sklaarn)	50	4.248.01 (248)	5.640-03 (265)	3.09#401 (398)	1.264-01 (1181
shigsmi function	XSB (ext., sklessn)	70	3,198-01 (205)	2,910-01 (25%)	3,210+01 (275)	1,064-01 (95)
shiers! function	with laws ablanced	10	7.774-01.4.1881	3.160-01 / 2031	7.000001 (203)	5 75e-07 (5b)

Benchmark analysis post-processing: uq_filterBenchmark

RawResults_ishigami = uq_filterBenchmark(RawResults, 'Ishigami function'); AggregatedResults_ishigami = uq_aggregateResults(RawResults_ishigami, 'mean')

AggregatedResults_ishigami =

56×11 table

BenchCaseID	CompetitorID	ExpDesignID	mean_RMSE_norm	mean_MSE_norm	mean_NRMSE	mean_R2	mean_MAE_norm	mean_MAPE	mean_RelMSE	mean_RelCVErr
1	1	1	0.49167	0.28046	0.064675	0.71954	0.088833	22.301	0.28046	0.044531
1	1	2	0.17981	0.05399	0.023653	0.94601	0.028269	8.5187	0.05399	0.0074459
1	1	3	0.03547	0.0039448	0.0046658	0.99606	0.0052681	1.5968	0.0039448	0.00046906
1	1	4	0.0061094	0.00014146	0.00080364	0.99986	0.00089528	0.33343	0.00014146	2.7346e-05
1	1	5	0.00042684	9.4951e-07	5.6148e-05	1	6.2414e-05	0.020025	9.4951e-07	2.9835e-07
1	1	6	6.3117e-05	2.14e-08	8.3026e-06	1	8.0172e-06	0.0030562	2.14e-08	2.4248e-09
1	1	7	4.9407e-06	2.601e-11	6.4992e-07	1	8.6422e-07	0.0003253	2.601e-11	1.0692e-11
1	2	1	1.0105	1.1893	0.13293	-0.18925	0.18605	57.659	1.1893	0.00038583
1	2	2	0.21353	0.16141	0.028089	0.83859	0.033721	11.486	0.16141	2.8537e-05
1	2	3	0.03384	0.010917	0.0044514	0.98908	0.0033517	1.117	0.010917	8.975e-07
1	2	4	0.010645	0.0054506	0.0014003	0.99455	0.00069278	0.34119	0.0054506	1.3165e-10
1	2	5	0.0002579	1.6913e-06	3.3926e-05	1	2.1807e-05	0.0080849	1.6913e-06	1.0135e-08
1.0	1	1		1	1	1	1	1	1	1.0
1	7	з	0.56137	0.31835	0.073844	0.68165	0.10563	33.136	0.31835	0.38106
1	7	4	0.4687	0.2215	0.061654	0.7785	0.087496	26.591	0.2215	0.31628
1	7	5	0.39858	0.16025	0.05243	0.83975	0.073017	22.09	0.16025	0.22256
1	7	6	0.35996	0.13074	0.04735	0.86926	0.064542	17.685	0.13074	0.16989
1	7	7	0.30449	0.093363	0.040053	0.90664	0.053292	16.547	0.093363	0.13194
1	8	1	1.0562	1.1324	0.13893	-0.13237	0.22194	76.59	1.1324	1.5397
1	8	2	0.93773	0.88578	0.12335	0.11422	0.19704	65.929	0.88578	1.0325
1	8	3	0.87094	0.7637	0.11457	0.2363	0.18398	66.722	0.7637	0.83987
1	8	4	0.80413	0.65369	0.10578	0.34631	0.16886	55.15	0.65369	0.76533
1	8	5	0.72043	0.52592	0.094767	0.47408	0.15111	42.27	0.52592	0.603
1	8	6	0.69829	0.50004	0.091855	0.49996	0.14944	43.939	0.50004	0.51364
1	8	7	0.55491	0.32314	0.072994	0.67686	0.11602	36.606	0.32314	0.43724

Display all 56 rows.

Benchmark analysis post-processing: uq_filterBenchmark

```
RawResults_ishigami_kriging = uq_filterBenchmark(RawResults, ...
{ 'Ishigami function', 'kriging'}, '-intersection');
AggregatedResults_ishigami_kriging = uq_aggregateResults(...
RawResults_ishigami_kriging, 'mean')
```

AggregatedResults_ishigami_kriging =

14×11 table

BenchCaseID	CompetitorID	ExpDesignID	mean_RMSE_norm	mean_MSB_norm	mean_NRMSE	mean_R2	mean_MAE_norm	mean_MAPE	mean_RelMSE	mean_RelCVErr
1	4	1	0.85876	0.76026	0.11296	0.23974	0.1647	47.82	0.76026	0.42431
1	4	2	0.65517	0.44611	0.086183	0.55389	0.11797	43.73	0.44611	0.29012
1	4	3	0.53001	0.28814	0.06972	0.71186	0.093297	32.088	0.28814	0.19373
1	4	4	0.4327	0.18962	0.056919	0.81038	0.075499	24.652	0.18962	0.14088
1	4	5	0.35572	0.12895	0.046793	0.87105	0.058793	18.416	0.12895	0.10198
1	4	6	0.28371	0.081513	0.03732	0.91849	0.044159	13.689	0.081513	0.068565
1	4	7	0.20455	0.042719	0.026907	0.95728	0.029821	10.398	0.042719	0.037018
1	5	1	0.84821	0.7348	0,11158	0.2652	0.16436	57,448	0.7348	0.43932
1	5	2	0.67301	0.47329	0.08853	0.52671	0.1214	46.762	0.47329	0.30595
1	5	3	0.54216	0.30141	0.071318	0.69859	0.095244	33.72	0.30141	0.201
1	5	4	0.43876	0.19514	0.057716	0.80486	0.076345	25,184	0.19514	0.14334
1	5	5	0.36101	0.13287	0.047488	0.86713	0.059472	18,272	0.13287	0.10411
1	5	6	0,28236	0.080606	0.037143	0,91939	0.04363	13,469	0,080606	0.069371
1	5	7	0.20426	0.042604	0.026869	0.9574	0.0297	10.428	0.042604	0.037112











Benchmark analysis post-processing: uq_display



Benchmark analysis post-processing: uq_display

