MOSKopt — simulation-based stochastic black-box optimization under uncertainty

Ph.D. Resul Al

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A simulation-based stochastic black-box optimizer

A new generic black-box solver: MCSKopt

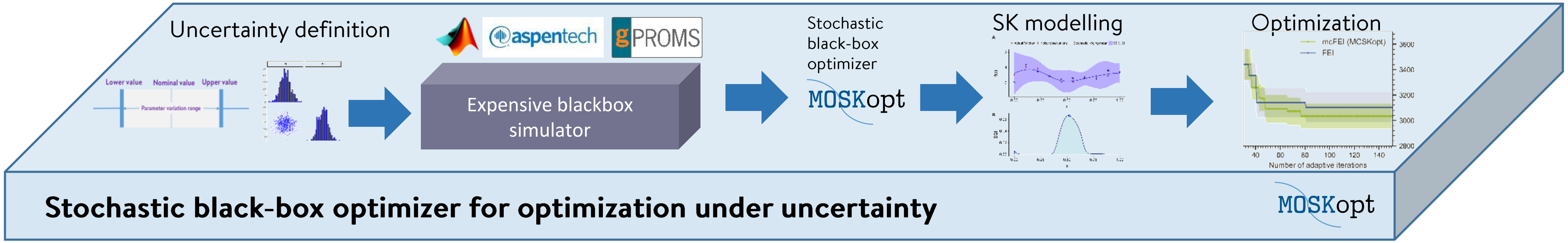
introducing

MCSKopt

Stochastic black-box optimizer for optimization under uncertainty of complex systems, e.g. digital twins.

available on GitHub

Download



> Available from a GitHub repository, documentation in preparation.
> A generic *stochastic black-box optimizer*, implements the workflow.
> *Embedded* Monte Carlo simulations for uncertainty quantification.
> Allows for multiple uncertainty *hedging* strategies.
> Implements SK modelling, infill optimization, and provides the popular as well as the newly proposed infill (mcFEI) criteria.
> Object-oriented programming → *user-extendable* infills.
> Applications to other processes (e.g., *fermentation*) underway.

Chapter 6 > Introduction

Optimization of WWTP networks under uncertainty

Chapter motivations

> WWTP design is subject to high uncertainty.

> Use the community's well-matured first principles simulation models to do design optimization (e.g., ADM1).

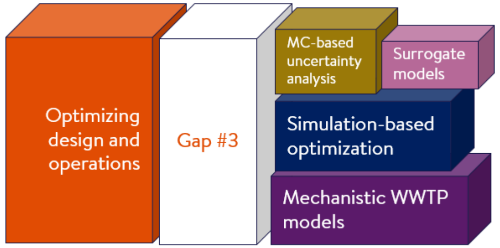
> Address Gap#3 identified in literature review.

> Further optimize WWTP layouts that are identified as *promising* in Chapter 4.

> Quantify and integrate the impacts of uncertainties (e.g., influent composition).

Gap #3

No applicable workflow for optimizing WWTPs using simulation models under uncertainty.



> The potential of simulation-based optimization is not investigated.

> Quantification and incorporation of uncertainties in optimization.

Primary goals:

> Develop/demonstrate an applicable simulation-based workflow for WWTP design *optimization under uncertainty (OUU)*.

> Automate the workflow in a generic tool.

Exhaustive sampling-based optimization

- Used as a benchmark method.
- Discretizes both the design and the uncertainty spaces using sampling.
- Allows for an exhaustive search for an optimum under uncertainty.
- Effective yet heavily suffers from the *curse of dimensionality*.
- $N_d \times N_u$ simulations needed.

Table 6.1: Pseudocode for the exhaustive sampling-based method for design space exploration.

Algorithm 1:	**Design space exploration via exhaustive sampling**
1:	**input** $S_d = \{x_i \in X_d : i = 1,\ldots,N_d\}$, and $S_u = \{u_j \in X_u : j = 1,\ldots,N_u\}$
2:	$DS \leftarrow U$
3:	**for all** $x_i \in S_d$ **do**
4:	$DS \leftarrow DS \cup \left\{x_i;\ \hat{\mathrm{P}}[G(x_i,\cdot) \leq 0 \mid S_u]\right\}$
5:	**end for**
6:	**return** DS

Hedging strategies against the uncertainties

- Tune the level of conservativeness.

Name	Explanation
Mean	The mean of constraint observations acquired from the Monte Carlo simulations is less than the constraint limit.
UCI95	The upper confidence interval for the mean of constraint observations acquired from the Monte Carlo simulations is less than the constraint limit.
PF80	The probability of the feasibility calculated from the Monte Carlo simulations is higher than 80 %.
MeanPlusSigma	The mean plus one standard deviation of constraint observations acquired from the Monte Carlo simulations is less than the constraint limit.

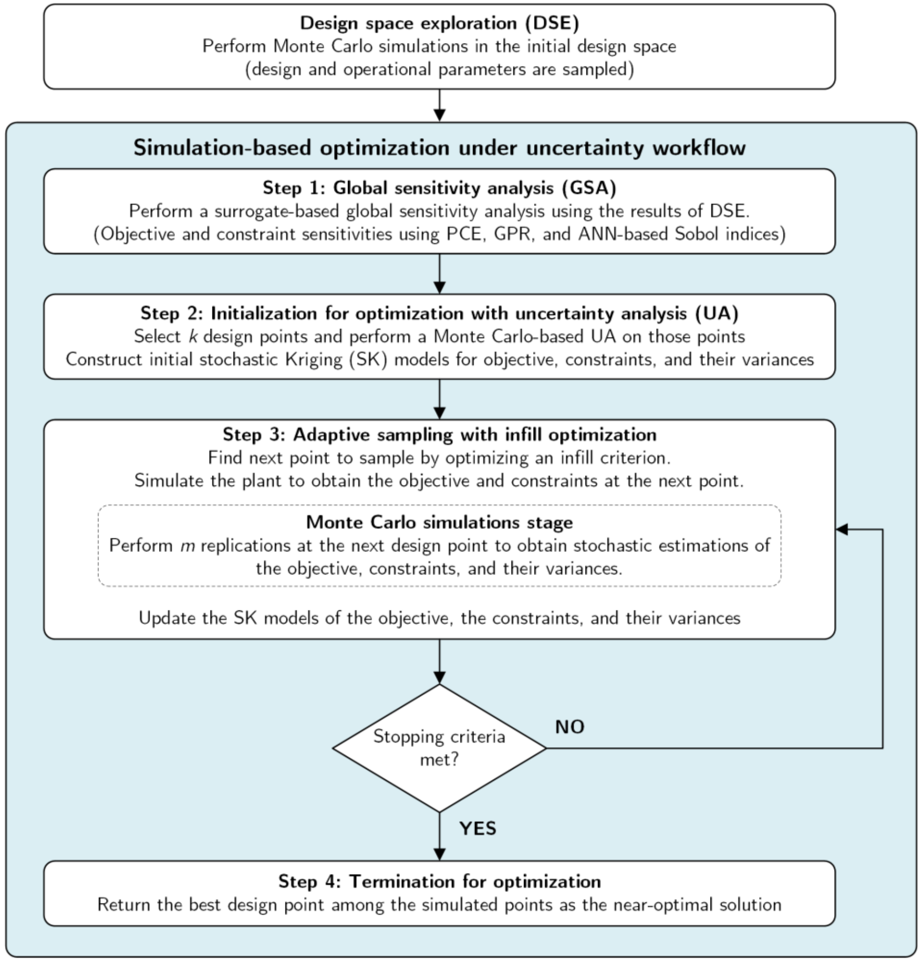
Chapter 6 > Methods

Simulation-based optimization under uncertainty

- Employs surrogate models for *a better-informed exploration* in the design space.
- Generic workflows have 3 stages: initialization, adaptive sampling, and termination.

- We integrate *2 more stages*: global sensitivity (prior to initialization) and uncertainty analysis (both in initialization and in adaptive sampling stages).

- Key to its success is the *infill criterion*,—an internal optimization of an expected improvement measure using surrogates.



Chapter 6 > Methods

Stochastic Kriging modeling

- An extension of *Kriging*,—an interpolation-based meta-model.
- Introduced by Ankenman *et al*. as a meta-modeling technique for stochastic simulations.
- Found *promising uses* in simulation optimization.

Wang and Ierapetritou, 2018. *Comput Chem Eng* 118.   Picheny *et al*., 2013. *Technometrics* 55.

Extrinsic uncertainty

- The lack of certainty of the meta-model about the simulation model's behavior at regions where no observations are obtained.

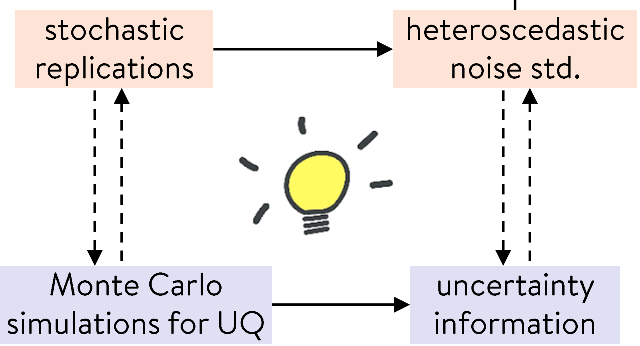
Intrinsic uncertainty

- The lack of certainty in the original simulation model's responses.

Stochastic Kriging model structure

$$\overbrace{y}^{\text{SK model}}{}^{SK}(x) = \underbrace{\mu}_{\text{a constant surface trend, i.e. mean}} + \underbrace{M(\overbrace{x}^{\text{input vector}})}_{\textit{extrinsic}\text{ uncertainty}} + \underbrace{\varepsilon_r(x)}_{\textit{intrinsic}\text{ uncertainty}}$$

Ankenman *et al*., 2010. *Oper Res* 58.



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Chapter 6 > Methods

Infill criteria for optimization

Expected Improvement

Mockus, J., 1975. *Opt Techniques* → Jones *et al.*, 1998. *J Glob Optim* 13.

$$E\left[I(x)\mid f^n\right]=\left(f_{\min}-\mu_f(x)\right)\Phi\left(\frac{f_{\min}-\mu_f(x)}{\hat{s}_f(x)}\right)+s(x)\phi\left(\frac{f_{\min}-\mu_f(x)}{\hat{s}_f(x)}\right)$$

Unconstrained deterministic

Expected Quantile Improvement

Picheny *et al.*, 2013. *Technometrics* 55.

$$EQI_n(x)=\left(q_{\min}-m_Q(x)\right)\Phi\left(\frac{q_{\min}-m_Q(x)}{s_Q(x)}\right)+s_Q(x)\phi\left(\frac{q_{\min}-m_Q(x)}{s_Q(x)}\right)$$

Unconstrained stochastic

Constrained Expected Improvement

Wang and Ierapetritou, 2018. *Comput Chem Eng* 118.

$$cAEI_f(x)=\underbrace{E\left[I_f(x)\right]}_{\text{improve objective}}\cdot\underbrace{P\left(G_i(x)\le 0\right)}_{\text{prioritize feasible regions}}\cdot\underbrace{\left(1-\tau_f\,/\sqrt{\tau_f^2+\hat{s}_f^2}\right)}_{\text{balance between explore \& exploit}}$$

Feasibility Enhanced Expected Imp. (FEI)

Wang and Ierapetritou, 2018. *Comput Chem Eng* 118.

$$FEI(x)=cAEI_f(x)+\underbrace{P(Y_f(x)\le f^{***})}_{\text{focus on areas where } f \text{ is small}}\cdot\underbrace{EQI_g(x)}_{\text{handle stochasticity in the constraint}}$$

Multiple-constrained FEI (mcFEI)

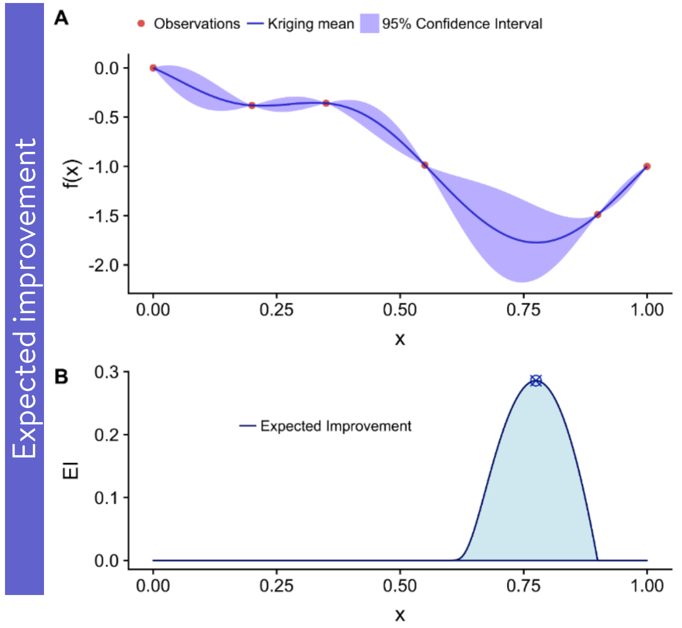
Al *et al.*, 2020. *Comput Chem Eng* (under review).

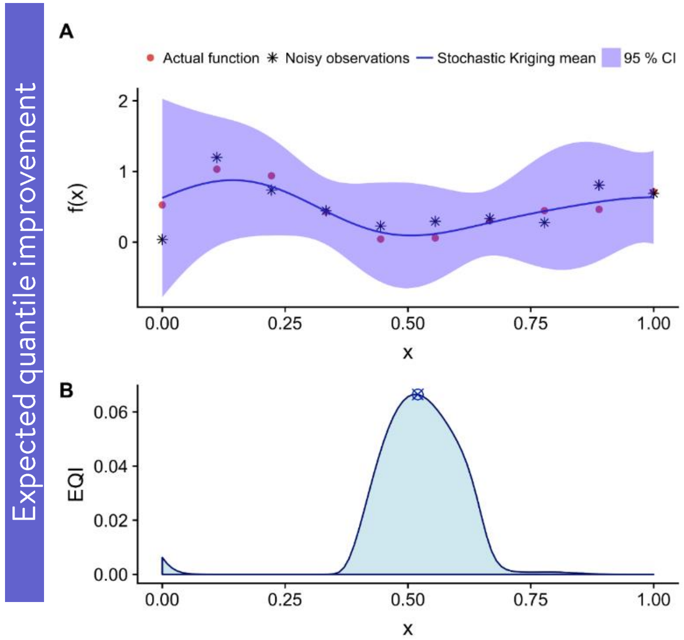
$$mcFEI(x)=mcAEI(x)+P(Y_f(x)\le f^{***})\cdot\prod_{i=1}^{c}EQI_{g_i}(x)$$

$$mcAEI(x)=E[I_f(x)]\cdot\left(1-\tau_f\,/\sqrt{\tau_f^2+\hat{s}_f^2}\right)\cdot\prod_{i=1}^{c}P[G_i(x)\le 0]$$

handle stochasticity in multiple constraints

Understanding infill optimization





Chapter 6 > Results > Case study 1

Sasena: An illustrative example

Sasena test problem

> Mathematical formulation (*modified*).

$$
\begin{aligned}
\min_{x} \quad & f(x) = -u_1(x_1-1)^2-(x_2-0.5)^2 \\
s.t. \quad & g(x) = [g_1(x),\, g_2(x),\, g_3(x)] \le 0 \\
& g_1(x) = (u_2(x_1-3)^2+(x_2+2)^2)e^{-x_2^7}-12 \\
& g_2(x) = 10u_3x_1+x_2-7 \\
& g_3(x) = (x_1-0.5)^2+u_4(x_2-0.5)^2-0.2 \\
& 0 \le x_i \le 1 \ \text{ for } i=1,\,2 \\
& \ln(u_j) \approx \mathcal{N}(\mu,\sigma) \text{ for j}=1,..,4
\end{aligned}
$$

> 2 decision variables,—visualize the design space.

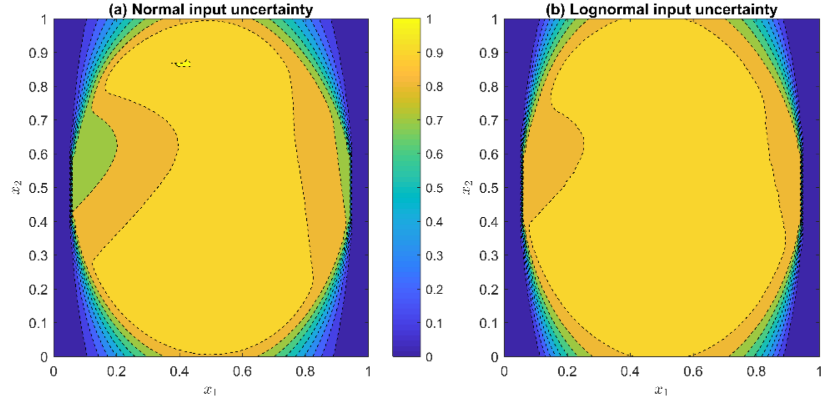
> 4 uncertain parameters,—following normal and lognormal distributions.

Solution via Exhaustive sampling

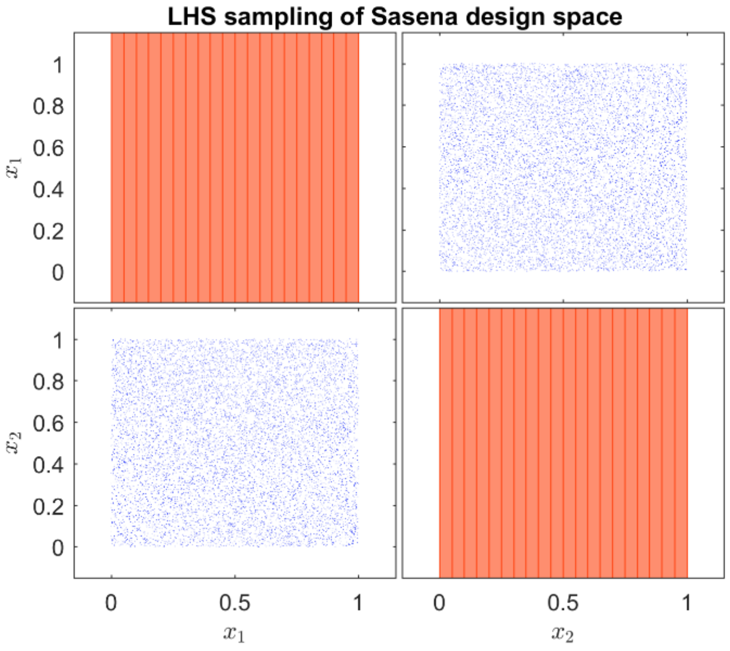
> From 10 to 10^5 LHS design samples x 10^3 LHS uncertainty samples.

> *Vectorized* Monte Carlo simulations → simultaneous exploration in both spaces.

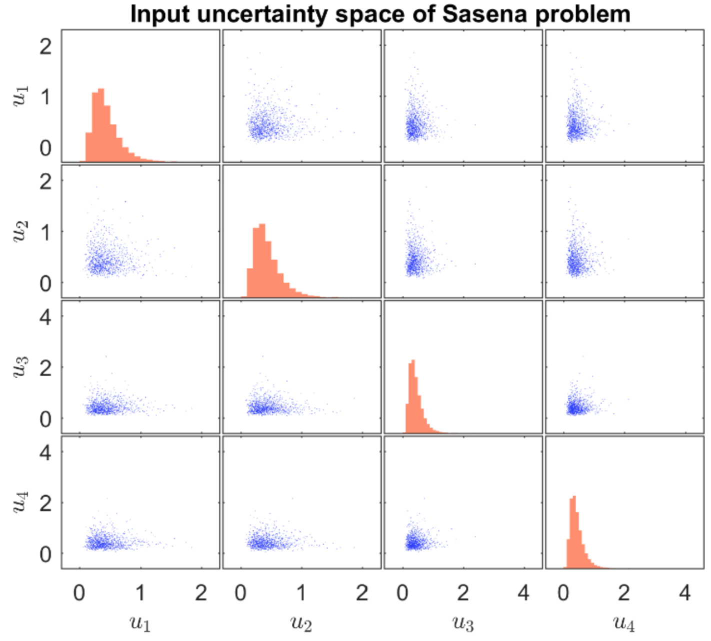
Probabilistic design spaces



Design space



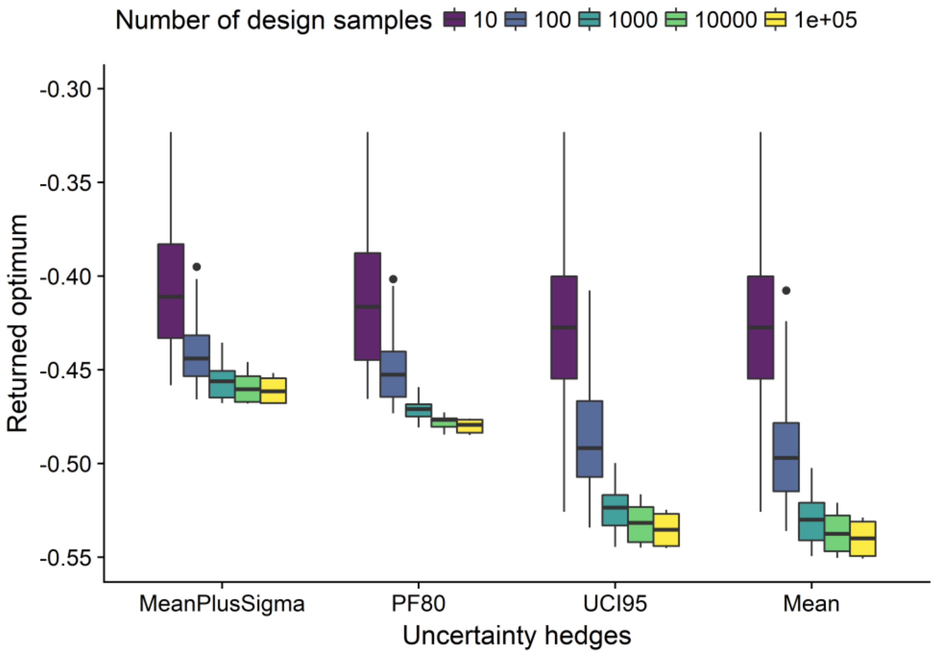
Uncertainty space



Sasena results

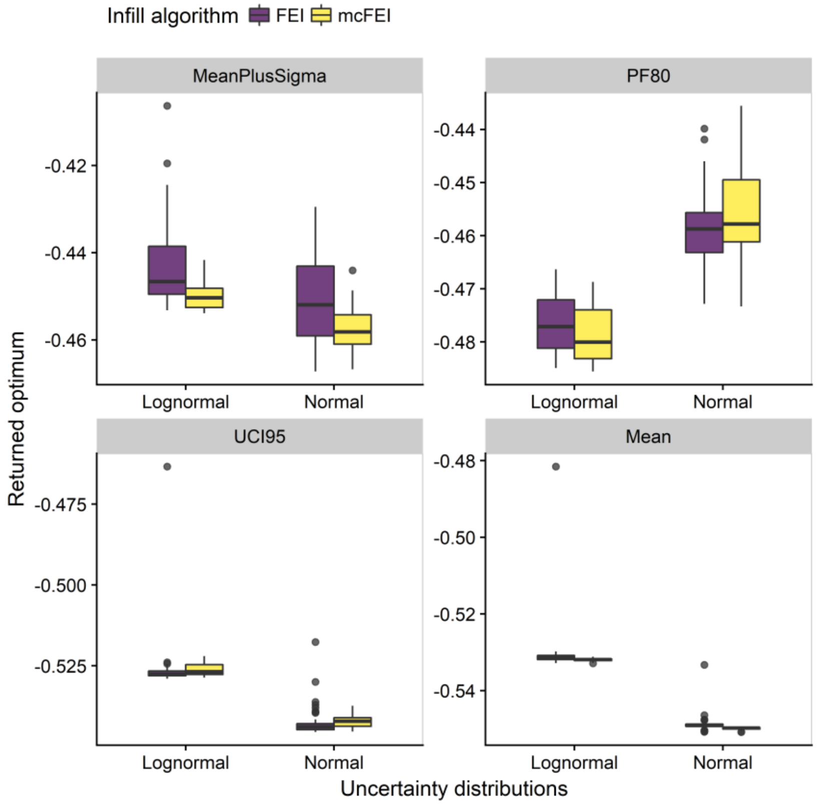
Solutions via Exhaustive sampling

> Competitive solutions already at 10^3 samples.



Solutions via simulation-based optimization

> 100 design samples, 50 independent repetitions.



Rosen Suzuki: A higher dimensional example

Rosen Suzuki test problem

> Mathematical formulation (*modified*).

$$\min_{x} \quad f(x) = x_1^2 + x_2^2 + 2u_1 x_3^2 + x_4^2 - 5x_1 - 5x_2 - 21x_3 + 7x_4$$

$$s.t. \quad g(x) = [g_1(x),\ 100g_2(x),\ 1000g_3(x)] \le 0$$

$$g_1(x) = x_1^2 + u_2 x_2^2 + x_3^2 + x_4^2 + x_1 - x_2 + x_3 - x_4 - 8$$

$$g_2(x) = x_1^2 + 2x_2^2 + x_3^2 + 2u_3 x_4^2 - x_1 - x_4 - 10$$

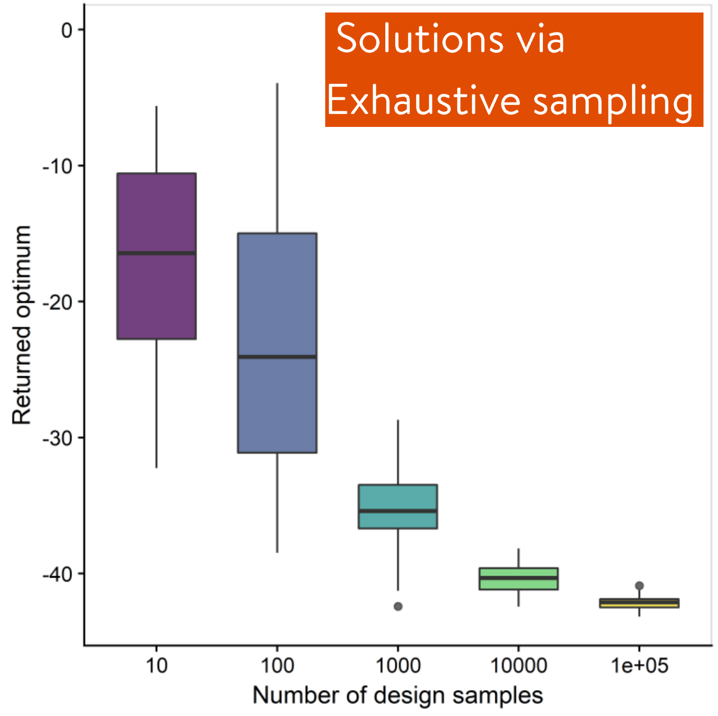
$$g_3(x) = 2x_1^2 + u_4 x_2^2 + x_3^2 + 2x_1 - x_2 - x_4 - 5$$

$$-3 \le x_i \le 3 \text{ for } i = 1,..,4$$

$$u_j \approx \mathcal{N}(\mu,\sigma) \text{ for j} = 1,..,4 \text{ and } \mu = 1,\ \sigma = 0.25$$

> 4 decision variables.

> 4 uncertain parameters,—following normal distributions.



Benchmark solution

Number of LHS design samples	Total number of calls to the model	Optimum value of the objective	Location of the optimum (x)
10^5	10^8	-42.152	[-0.026, 0.841, 1.951, -0.914]

Chapter 6 > Results > Case study 2

Rosen Suzuki

Solution via simulation-based optimization

- MOSKopt is called with two infills: FEI and mcFEI.
- 50 design samples with 50 independent runs.
- The mcFEI visibly *outperforms* FEI.
- The mcFEI solution (cost=50) is *even better* than the benchmark solution (cost=10^5). Why? → the *curse of dimensionality*.
- SK-based approach → a *better-informed* exploration.

Infill algorithm	Number of LHS design samples	Total # of calls to the model	Optimum value of the objective	Location of the optimum (x)
FEI	50	50×10^3	-24.915	[-0.368, 0.607, 1.468, 0.128]
mcFEI	50	50×10^3	-42.701	[0.028, 0.608, 1.996, -0.996]
Exhaustive	10^5	10^8	-42.152	[-0.026, 0.841, 1.951, -0.914]

Optimization progress: FEI (blue) vs mcFEI (orange)