May 23, 2017

Recent developments in metamodel based robust black-box simulation optimization: An overview

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Recent Developments in Metamodel Based Robust Black-Box Simulation Optimization: An Overview

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Abstract:

In the real world of engineering problems, in order to reduce optimization costs in physical processes, running simulation experiments in the format of computer codes have been conducted. It is desired to improve the validity of simulation-optimization results by attending the source of variability in the model's output(s). Uncertainty can increase complexity and computational costs in Designing and Analyzing of Computer Experiments (DACE). In this state-of the art review paper, a systematic qualitative and quantitative review is implemented among Metamodel Based Robust Simulation Optimization (MBRSO) for black-box and expensive simulation models under uncertainty. This context is focused on the management of uncertainty, particularly based on the Taguchi worldview on robust design and robust optimization methods in the class of dual response methodology when simulation optimization can be handled by surrogates. At the end, while both trends and gaps in the research field are highlighted, some suggestions for future research are directed.

Keywords: *Simulation Optimization, Robust Design, Metamodel, Polynomial Regression, Kriging, Computer Experiments.*

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1. Introduction

Nowadays, developing processes in an engineering world is strongly associated to computer simulations. These computer codes can collect appropriate information about characteristics of engineering problems before actually running the process. Computer simulations can help a rapid investigation of various alternative designs to decrease the required time to improve the system. In addition, most numerical analyses for engineering problems make a well-suited use of mathematical programming. Clearly, a Simulation-Optimization (SO) becomes necessary to find more interest and popularity than other optimization methods, in order to the complexity of many real world optimization problems in way of mathematical formulation analyzing (Dellino et al., 2014). The main goals of simulation can be defined as two, first what-if study of model or sensitivity analysis, and second is optimization and validation of model (van Beers & Kleijnen, 2003). The essential benefit of simulation is its ability to cover complex processes, either

(a)   (b)
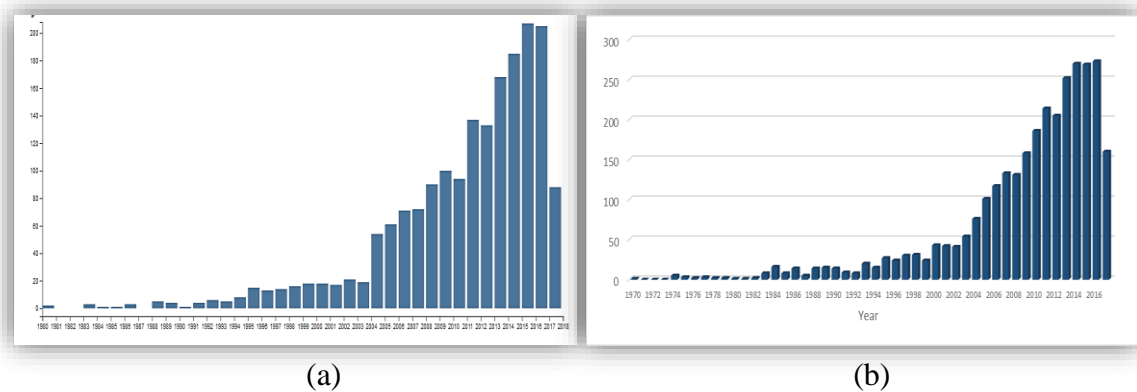
Figure 1 The trend of publications with topic of "simulation optimization" in (a) the Web of Science databases (source: WoS, Data retrieved on August 2017), and (b) SCOPUS (source: Scopus, Data retrieved August 2017).

deterministic or random while eliminating mathematical sophistication (Figueira & Almada-Lobo, 2014). In general, SO techniques are classified into model-based and metamodel-based (Mohammad Nezhad & Mahlooji, 2013; Viana et al., 2014). In the model-based, the simulation running is not expensive and model output can be used directly in optimization. Many large scales and detailed simulation models in the complex system particularly under uncertainty may be expensive to run in terms of time-consuming, computational cost, and resources. Moreover, to address such a challenge, metamodels need to be derived via combing by robust design optimization.

The trend of publications on the topic of "simulation optimization" in both Web of Science and SCOPUS databases are confirming the interest on the search term, see Figure 1. On the other hand, an internet search by using a popular web browser "Google Scholar" returns over 40,300 pages, which mainly containing scientific and technical articles, research reports, conference publications, and academic manuscript.

In this paper, we follow to review latest developments in Metamodel-Based Simulation Optimization (MBSO) and in wider scope, Metamodel-Based Robust Simulation Optimization (MBRSO) when simulation affected from uncertainty in model's parameters. MBRSO is applied in the complex simulation model under uncertainty when simulation running is expensive in terms of computational time and/or cost, therefore the just limited number of simulation running is possible.

The rest of this review is organized as follows. Section 2 covers quantitative analysis and also illustrates the survey method while highlighted method of gathering and reviewing articles. In section 3, qualitative analysis is provided including the relevant basic approaches and methodologies around the MBRSO. Section 4 discusses remarkable research findings and

provides main recommendations which are extracted throughout reviewing the literature. This paper is concluded in section 5 with summarizing important research tips.

2.   Quantitative analysis on metamodel based simulation optimization

SciVal offers quick, easy access to the research performance of 8,500 research institutions and 220 nations around the world (see "About SciVal" in Elsevier 2017[1]). Visualization of Elsevier's SCOPUS data for the selected search terms "Visibility" and "Citations" is provided by SciVal. Being the largest abstract and reference database, SCOPUS provides citation dataset of research literature and quality web sources (Aghaei Chadegani et al., 2013). Figure 2 shows the publications trend on "Metamodel" and "simulation optimization" impact 1996 to date (12 September 2017) . The number of publication on the topic has increased from one publication in the year 2006 to 65 publications in 2016. In order to forecast the trend of scholarly outputs in following years, we fit polynomial regression over data in when x is year and y is number of annual documents. In the last six years 659 papers were published, receiving over 10,503 views, 2,465 citations, 147 international collaborations, and 1.36 Field-Weighted Citation Impact (FWCI). The FWCI is a measure of citation impact that normalizes for differences in citation activity by subject field, article type, and publication year (Jang & Kim, 2014). The world's average for FWCI is indexed at 1.00, as such, values above 1.00 indicate an above average citation impact. Specifically, a citation impact of 1.36 indicates 36% of the citations are above the average citations in this same filed.

$$y = 0.3279x^2 - 3.6583x + 6.8256$$
$$R^2 = 0.9396$$
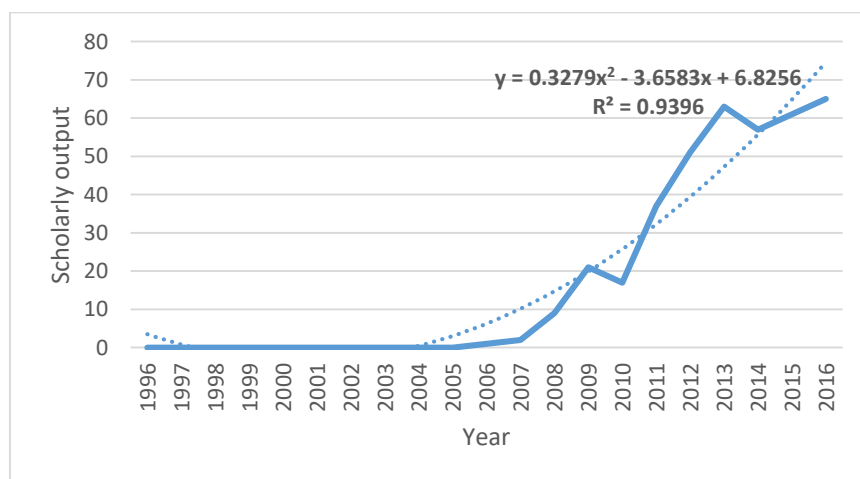
Figure 2 Trend of publications on "Metamodel and simulation optimization" impact (data from 1996 to date).
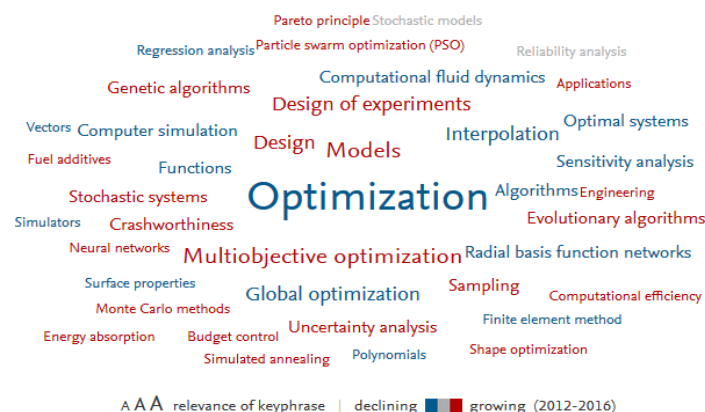
Figure 3 The top 50 key-phrases by relevance in the past five years papers (656 publication).

The top 50 key-phrases by relevance for the past five years publications (656 publication) is shown in Figure 3. Notably, the phrases "optimization" are the most repeated keyword. The highlighted importance of key phrases of "interpolation", "computer simulation", and global optimization" are obvious. In addition, the phrase of "design of experiments", "multi-objective optimization", and "uncertainty analysis" among the most repeated keywords in recent publications which gained growing attentions. The trends of publications and the top 50 key-phrases have proven the importance of current research on in scholarly publications. Therefore, there is an interest to find alternative ways to improve research on simulation optimization, such as combining design of experiments by evolutionary algorithms like expected improvement methodology which today become to be interested among academic research world, for instance see (Havinga et al., 2017; Zhang, J et al., 2017). According to associated obtained data from SciVal among search on metamodel and simulation optimization, the top ten countries, authors, and journals which ranked based on views count (views source: Scopus data up to 31 Jul 2017) are respectively sketched in Table 1, Table 2, and Table 3.

Table 1 Top ten high view counts countries in field MBSO.

No	Country	Views Count	Scholarly Output	FWCI
1	United States	2166	154	1.63
2	China	1837	145	1.04
3	France	927	58	1.52
4	Italy	907	39	3.66
5	Iran	629	30	1.19
6	United Kingdom	549	31	2.63
7	Germany	487	42	1.02
8	Netherlands	480	21	2.09
9	South Korea	422	22	1.02
10	Canada	353	22	0.81

Table 2 Top ten high view counts authors in field MBSO.

No	Author	Affiliation	Views Count	Scholarly Output	FWCI
1	Kleijnen, Jack P.C.	Tilburg University	205	7	4.34
2	Toropov, Vassili V.	University of Leeds	193	7	7.83
3	Sudret, Bruno	ETH Zurich	179	5	4.76
4	Wen, Guilin	Hunan University	176	9	2.15
5	van den Boogaard, A. H.	University of Twente	170	5	1.15
6	Wiebenga, J. H.	Materials Innovation Institute	170	5	1.15
7	Yin, Hanfeng	Hunan University	167	8	2.33
8	Qing, Qixiang	Hunan University	158	5	3.83
9	Shao, Xinyu	Huazhong University of Science and Technology	129	9	2.17
10	Jiang, Ping	Nanjing Agricultural University	122	6	2.07

Table 3 Top ten high view counts journals in field MBSO.

No	Country	Views Count	Scholarly Output	FWCI
1	Structural and Multidisciplinary Optimization	448	23	1.49
2	53rd AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference 2012	332	4	0.77
3	Advances in Intelligent Systems and Computing	274	6	7.63
4	WIT Transactions on Engineering Sciences	240	2	0
5	Advanced Materials Research	239	3	0
6	European Journal of Operational Research	217	4	4.3
7	International Journal of Impact Engineering	202	4	2.77
8	Engineering Optimization	198	10	1.22
9	Renewable Energy	196	2	1.69
10	Expert Systems with Applications	195	5	3.02

2.1 Instruction of current research

In the current systematic literature review, the search strategy was as follow steps. Some common electronic databases (Scopus indexed) were applied in search processes such as Science Direct, IEEE Xplore, Springer Link, and etc. Different keywords and their combinations were used to search relevant resources in literature from mentioned electronic databases. The SCOPUS databases cover almost two times more than the Web of Science journals (Aghaei Chadegani et al., 2013). Therefore, the SCOPUS databases selected as a reference for academic documents source. Table 4 illustrates the number of document results from Scopus by employing some relevant keywords with conjunction 'AND'. The search was conducted on each article title, abstract, and keywords. There are a different number of SO methods that discussion about most of them is beyond of this context. Instead, we focus on simulation-optimization under uncertainty by employing metamodels and robust optimization.

Table 4 Number of document results based on combination of different keywords (Scopus database).

ID	Keyword	Combination of keywords with conjunction 'AND'								
1	Simulation	*	*	*	*	*	*	*	*	*
2	Optimization	*	*	*	*	*	*	*	*	*
3	Metamodel	*	*	*						
4	Response surface				*	*	*			
5	Kriging							*	*	*
6	Uncertainty		*			*			*	
7	Robust design			*			*			*
Total results		512	86	29	2,710	279	94	1,124	208	42
Results in range of 2000 - 2017		493	86	29	2,523	270	89	1,106	205	42

Particular metamodels which concentrated are polynomial regression methodology (also called Response Surface Method (RSM)) and Kriging surrogate model. In general, whole findings were filtered based on three factors, i) selecting articles which are associated to interesting our topic (polynomial regression, Kriging, robust design, and SO), ii) recent articles are preferred (all articles were published after 2000, when around 60% of them were published between 2010-Spetember 2017, iii) number of citations are attended. Notably, there are a different number of papers and electronic resources related to the topic, but we just filtered resources which can cover need basic knowledge around simulation-optimization via robust design integrating metamodels. So, remarkable findings are concluded into 5 books (Del Castillo, 2007; Dellino & Meloni, 2015; Fang et al., 2006; Kleijnen, 2015; Myers et al., 2016), 3 Ph.D thesis (Dellino, 2008; Jurecka, 2007; Rutten, 2015), and 60 articles (16 review papers and 41 research papers and 3 chapters). Table 5 shows the identifier of articles while are sorted based on publishing year. Note that the citations were counted from Scopus leading up to April 2017. In this context, articles were reviewed based on seeking in methodology and scope of applicability, while focused on methods, techniques, and approaches which employed to achieve their relevant goal(s).

3. Qualitative analysis on MBRSO

The black-box and also computationally expensive simulation models are often found in engineering and science disciplines. Expensive simulation running and expensive analysis of processes are often considered black-box function. In general surrogate models treat the simulation model as a black-box model (Beers & Kleijnen, 2004; Kleijnen, 2005; Shan & Wang, 2010). In fact, many simulation-optimization approaches solely depend on such input-output data in investigating of optimal input settings, while in the black box feature, the simulation just permits the evaluation of the objective and constraint for a specific input (Amaran et al., 2016).

Table 5 Identifiers of articles ("Rev." means review paper, "Res." means research paper, and "Cha." means chapter).

| ID	Type	Reference	Citation	ID	Type	Reference	Citation
R1	Rev.	(Simpson, Poplinski et al., 2001)	990	R31	Res.	(Kleijnen, 2010)	3
R2	Res.	(Simpson, Mauery et al., 2001)	529	R32	Res.	(Wiebenga et al., 2012)	17
R3	Rev.	(Jin et al., 2001)	804	R33	Res.	(Chang et al., 2013)	4
R4	Res.	(Abspoel et al., 2001)	10	R34	Res.	(Kleijnen & van Beers, 2013)	5
R5	Res.	(Kleijnen & Gaury, 2003)	35	R35	Res.	(Zhang et al., 2013)	7
R6	Res.	(Truong & Azadivar, 2003)	29	R36	Res.	(Dellino et al., 2012)	26
R7	Res.	(Wang, 2003)	207	R37	Res.	(Dellino et al., 2014)	1
R8	Rev.	(Jin et al., 2003)	173	R38	Res.	(Zhang et al., 2014)	11
R9	Rev.	(Chen et al., 2003)	29	R39	Res.	(Uddameri et al., 2014)	3
R10	Res.	(van Beers & Kleijnen, 2003)	100	R40	Res.	(Cozad et al., 2014)	29
R11	Res.	(Lehman et al., 2004)	20	R41	Rev.	(Viana et al., 2014)	69
R12	Rev.	(Beers & Kleijnen, 2004)	49	R42	Rev.	(Figueira & Almada-Lobo, 2014)	31
R13	Res.	(Kleijnen & Beers, 2004)	118	R43	Cha.	(Dellino et al., 2015)	0
R14	Rev.	(Kleijnen, Jack P. C., 2005)	154	R44	Rev.	(Jalali & Van Nieuwenhuyse, 2015)	6
R15	Cha.	(Barton & Meckesheimer, 2006)	103	R45	Res.	(Taflanidis & Medina, 2015)	0
R16	Res.	(Williams et al., 2006)	31	R46	Res.	(Kamiński, 2015)	2
R17	Rev.	(Wang & Shan, 2007)	685	R47	Res.	(Sreekanth et al., 2016)	4
R18	Res.	(Jurecka et al., 2007)	13	R48	Rev.	(Amaran et al., 2016)	1
R19	Res.	(Stinstra & den Hertog, 2008)	23	R49	Res.	(Li et al., 2016)	2
R20	Res.	(Wim et al., 2008)	43	R50	Res.	(Han & Yong Tan, 2016)	0
R21	Res.	(Dellino et al., 2009)	21	R51	Rev.	(Haftka et al., 2016)	3
R22	Rev.	(Kleijnen, 2009b)	331	R52	Res.	(Leotardi et al., 2016)	0
R23	Res.	(Steenackers et al., 2009)	11	R53	Res.	(Sathishkumar & Venkateswaran, 2016)	0
R24	Cha.	(Kleijnen, 2009a)	3	R54	Res.	(Moghaddam & Mahlooji, 2016)	0
R25	Res.	(Dellino et al., 2009)	25	R55	Res.	(Javed et al., 2016)	0
R26	Res.	(Dellino et al., 2010)	43	R56	Rev.	(Kleijnen, 2017)	1
R27	Res.	(Dellino et al., 2010b)	3	R57	Res.	(Khoshnevisan et al., 2017)	0
R28	Res.	(Dellino et al., 2010a)	1	R58	Res.	(Zhou et al., 2017)	0
R29	Res.	(Kuhnt & Steinberg, 2010)	6	R59	Res.	(Havinga et al., 2017)	0
R30	Rev.	(Li et al., 2010)	44	R60	Res.	(Zhang, 2017)	0

Moreover, methodologies which are mentioned in this paper can be applied in the class of black-box problems, since it does not need to identify expression or internal structure of the system, and just analyzing output with given list of inputs. Investigating in literature particularly in recent years has been confirmed that application of metamodels in SO is more interested than other methods due to increasing complexity in real systems while they need to be approximated by cheaper methods. In this context, all studies which were investigated among reviewing of literature, are focused on SO techniques via surrogate models. This paper covered more the stochastic simulation-optimization hybrid metamodels (e.g. polynomial regression and Kriging). It is notable that all topics which are explained in continue, are presented to show recent methodological development in analyzing, optimizing and improving complex systems under uncertainty through their relevant simulation models by employing some main statistical and mathematical techniques (e.g. robust design optimization and surrogate models as two basic methodologies).
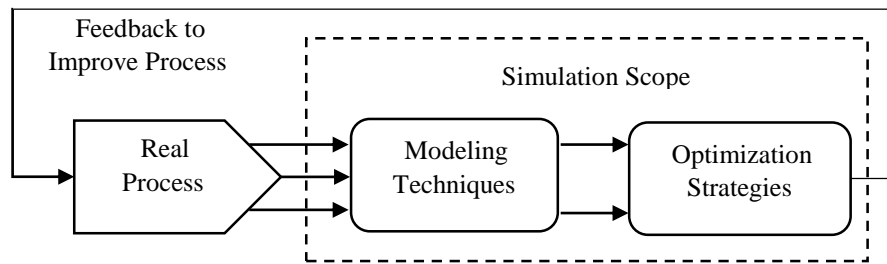
Figure 4 An overview of simulation scope.

3.1 Simulation-optimization (SO)

The process of investigating the best value of input variables among all possibilities in a simulation model is Simulation-Optimization (SO), also known as an optimization via simulation or simulation-based optimization. The objective of SO is obtaining the optimum value for output while minimizing the resource spent. Kleijnen (2015) have described simulation model as a dynamic or static model that be solved by means of experimentation. Generally, there are two types of simulation models. The first type is a physical model which describes model's characterization in a smaller dimension (for example, miniature airplane in a wind tunnel). The second type is a mathematical model which usually coded into computer programs. The term dynamic illustrates parameters of the model are variated over time while in the static model the time does not play an important role. The simulation model often is studied by a mathematical model. The system behavior is evaluated by running the simulation model for a fixed period of time. Generally, a study in simulation techniques can be concentrated into two main parts, first simulation modeling, and second simulation-optimization (see Figure 4). With optimization strategy, the feedback on the process is provided by the output of simulation model (Carson & Maria, 1997). In the modeling part, the method can be used to identify process components and select them to design simulation model (Banks et al., 2010; Neelamkavil, 1987). The SO can be attracted the attention of many researchers in improving practical engineering problems via different methods. Azadivar (1999) has compared some common SO methods included gradient based search methods, stochastic approximation methods, sample path optimization, response surface methodology, and heuristic search methods. Figueira and Almada-Lobo (2014) have reviewed recent development on SO and classified latest approaches based on four key aspects, simulation purpose, hierarchical structure, search scheme and search method. Other recent studies over SO methods can be found in two books (Dellino & Meloni, 2015; Kleijnen, 2015) and four review papers (Barton, 1992; Carson & Maria, 1997; Li et al., 2010; Simpson, Poplinski et al., 2001). In general, SO models can be divided into two types of stochastic and deterministic
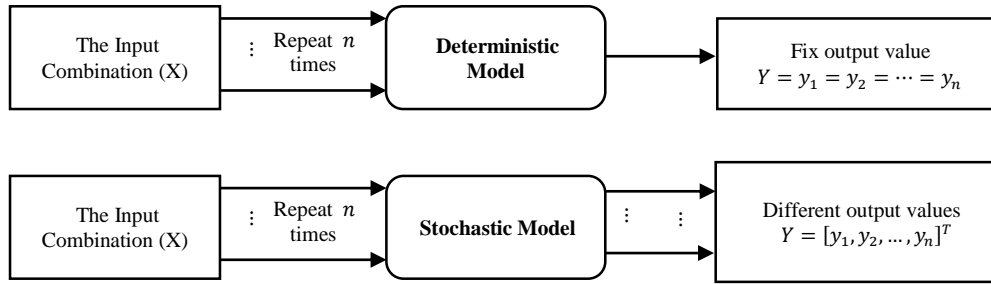
Figure 5 Deterministic and stochastic simulation models

models (Figure 5). In deterministic models, a response of model lacks random error, or in another mean, repeated runs for the same design of input parameters, the same result for the response can be gain from the model. Examples of the deterministic simulation are models of airplanes, automobiles, TV sets, and computer chips applied in Computer Aided Engineering (CAE) and Computer Aided Design (CAD) at Boeing, General Motors, Philips, etc.(Kleijnen, 2009b). On the other hand, the output in stochastic or random simulation usually follows some probability distribution which may vary around its space. So, running simulation for the same input combination gives different outputs. Examples are models of logistic and telecommunication systems (Kleijnen, 2009b). This noisy condition of output also enhances optimization challenge, while it becomes harder to distinguish the best set of input variables, and their validity in deterministic approaches are lost. In SO usually cannot distinguish the exact (deterministic) solution for the black-box system, so the mean and the variance obtained from sampling points (Amaran et al., 2016). Polynomial regression can sufficiently support both deterministic and random simulation, but Kriging has hardly been used in stochastic simulation (van Beers & Kleijnen, 2003). In other classification, Amaran et al. (2016) have categorized SO algorithms based on local or global optimal solution (Figure 6). Barton & Meckesheimer (2006) have classified SO approaches depend on the nature of design variables types. Design variables in
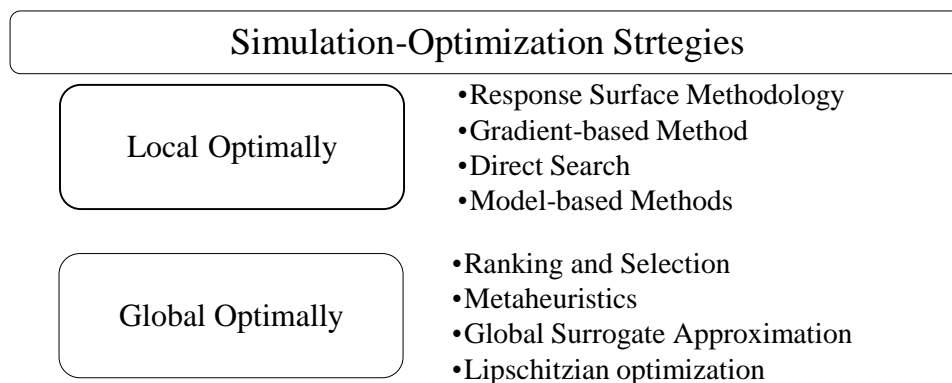
Figure 6 Simulation optimization strategies based on locally and globally solution.
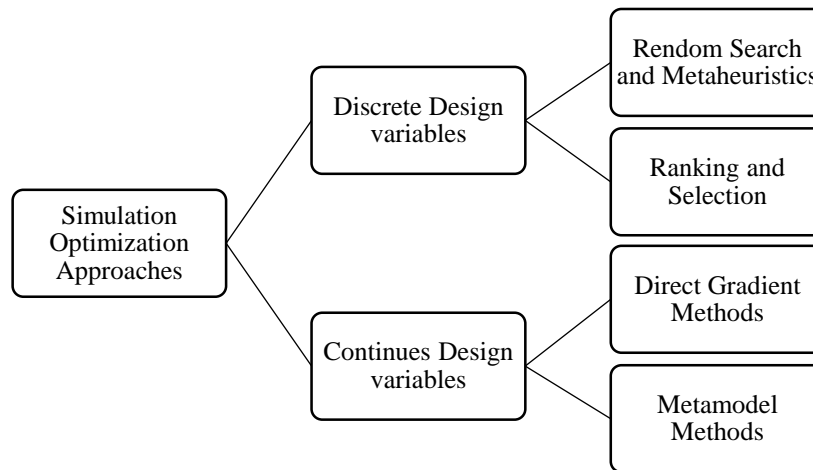
Figure 7 Simulation optimization strategies based on nature of design variables.

simulation models can be either continues and discrete, (see Figure 7). Continues variables can take any real value within a given range which is imposed by constraints. In most engineering problems, during the optimization process with approximation methods (metamodels), the discrete patterns of input variables are neglected and all variables can vary continuously due to solving continues patterns easier. Moreover, based on the optimum design in the continuous feature, the values which inherently are discrete existence, then can be adjusted to the nearest feasible discrete value (Jurecka, 2007).

3.1.1   Applications of simulation-optimization

Various types of problems in engineering design and management have been developed by application of different methods in SO (e.g. production, transportation and logistics, energy management, finance, engineering, and applied sciences). In a real case study, (Kleijnen, 1993) has applied SO methods in production planning to report practical decision support system in the Dutch company. In (Jin et al., 2001) the application of different metamodels have been studied (e.g. polynomial regression, multivariate adaptive regression splines, radial basis functions, and kriging) over 14 test SO problems in engineering design based on noisy or smooth behavior. In the other work by (Kleijnen & Gaury, 2003), four different techniques have been combined included simulation, optimization, uncertainty analysis, and bootstrapping through implementing in a real case study in production control. The appropriate review study which addressed some applications of SO in sub-communities in machine learning problems, discrete event systems such as queues, operations, and networks, manufacturing, medicine and biology, engineering, computer science, electronics, transportation, and logistics have been done by (Amaran et al., 2016).

Table 6 Application of SO (surrogate-based) in different engineering design and management problems.

ID	Application	ID	Application
R2	Aerospace engineering (design of an aerospike nozzle).	R33	Semiconductor wafer fabrication system
R3	14 test problems in engineering design based on noisy or smooth behavior.	R34	Discrete-event simulation (M/M/1)
R4	Production Planning (Four station production flow line)	R35	Wind farm power generation, product platform planning (for universal electric motors), three-pane window heat transfer, onshore wind farm cost estimation
R5	Production Planning (Kanban system)	R36	Inventory Management
R6	Supply Chain Management	R38	Nonpoint source pollution control
R7	Beam design problem	R39	Groundwater management (groundwater joint planning process)
R8	The two-bar structure	R40	Thermodynamics (modeling of steam density as a function of heat duty in a flash drum modeled)
R9	Electrical engineering, chemical engineering, mechanical engineering, and dynamic programming	R42	manufacturing system (job shop consisting of four machines and three buffers (or queues),
R10	A single server queueing, M/M/1 hyperbola,	R43	Inventory Management
R15	Network routing example	R44	Inventory management
R16	Flyer plate experiments	R45	Skyhook dampers for the suspension of a half-car nonlinear model driving on a rough road.
R17	Review different application of simulation optimization in engineering design and management.	R46	Schelling's segregation model
R18	10-bar truss under varying loads	R47	Groundwater management (injection bore field design problem)
R19	Design of two parts of the TV tube	R49	Production planning in manufacturing system (a scaled-down semiconductor wafer fabrication system)
R20	Expected steady-state waiting time of the M/M/1 queuing model, and the mean costs of a terminating (s, S) inventory simulation	R50	Design of a chemical cyclone, Manufacturing processes
R21	Inventory Management	R52	Steady two-way coupled hydro-elastic system, Racing sailboat keel fin
R23	A slat track, structural component of an aircraft wing	R53	(s,S) inventory policy
R24	Supply-chain management	R54	Well-known EOQ problem, the multi-item newsvendor problem
R25	Compressed Natural Gas (CNG) engines	R55	Compressor impellers for mass-market turbochargers are
R26	Inventory Management	R57	Soldier pile tieback anchor supported excavation in sandy and gravelly site
R28	Inventory Management	R58	Nonlinear Programming, pressure vessel design
R30	Job shop simulation problem	R59	Metal forming processes, strip bending process
R32	Metal forming processes	R60	Skyhook control for the suspension of a half car model, The dampers for a building exposed to earthquake excitation

Recently, a work based on metamodel and Monte Carlo simulation method have been done by (Li et al., 2016) applied in production planning of manufacturing system and compared their proposed model with other approaches (e.g. mathematical programming). The application of robust design hybrid metamodeling in management science and engineering problems has been reviewed by (Parnianifard et al., 2018).

The application of SO in inventory management has been significantly interested in different studies such as (Dellino et al., 2015, 2010a) and review papers (Jalali & Van Nieuwenhuyse, 2015; Kleijnen, 2017). However, in this context among a review of the literature, the application of SO methods in different types of engineering design and management problems were considered that results are represented in Table 6. Notable, we just targeted SO methods based on surrogates and robust design optimization in black–box and expensive simulation models under uncertainty. For such cases, computer experiments are conducted as main supplementary of metamodel based robust simulation optimization.

3.2   Uncertainty management in SO via robust design optimization

In practice, most engineering problems have been affected by different sources of variations. One of the main challenges of SO is address uncertainty in the model, by a variety of approaches, such as robust optimization, stochastic programming, random dynamic programming, and fuzzy programming. Uncertainty is undeniable which effect on the accuracy of simulation results while making variability on them. In uncertain condition, robust SO allows us to define the optimal set point for input variables while keeping the output as more close as possible to ideal point, also with at least variation. Robust design approaches try to make processes insensitive to uncertainty as sources of variation by investigating qualified levels of design input factors. The source of variation in output can be divided into two main types, first is variation due to variability in environmental (uncontrollable or noise) variables (Park & Antony, 2008; Phadke, 1989), and second is fluctuating of input (design) variables in their tolerance range (Anderson et al., 2015; Myers et al., 2016).

Robust design optimization is an engineering methodology to improve the performance of a model by minimizing the effects of variation without eliminating the causes since they are too difficult or too expensive to control. Robust simulation-optimization is about solving simulation model with uncertain data in a computationally tractable way. The main goal of robustness strategy is to investigate the best level of input factors setting for obtaining desirable output goal which is insensitive to the changeability of uncertain parameters.

Table 7 Applied different strategies in literature for management of uncertainty.

ID	Uncertainty management strategy	ID	Uncertainty management strategy
R1	Taguchi Approach	R32	Dual response
R4	Stochastic programming	R36	Taguchi Approach, Crossed Arrays
R5	Scenario Cases (combination of non-controllable input values), risk analysis (RA) and Monte Carlo	R38	Two-stage robust optimization
R8	Dual response methodology	R39	Fuzzy Logic
R9	Taguchi robust design	R43	Taguchi Approach-Crossed Arrays
R11	Minimax approach	R44	Mean-variance trade-off approach (Taguchi, Dual Response Surface), Worst Case.
R12	Cross-validation, Parametric bootstrapping, distribution free bootstrapping.	R45	Probability logic approach
R13	jackknifed variance	R47	Stochastic Optimization
R16	Calibration of simulation model, trade-offs among parameters	R48	Squared Loss Function
R17	Robust Design	R50	Expected quality loss
R18	Taguchi quality loss, Minimax principle, Bayes principle,	R51	Expected Improvement (EI)
R19	Robust counterpart methodology	R52	Stochastic programming
R21	Crossed array-Combined Array	R53	Uncertainty on parameters distribution (bootstrapping)
R23	Robust design (dual response surface)	R54	Minimax problem, Chance constraint definition
R24	Signal to Noise Ratio	R55	Stochastic optimization algorithm
R26	Taguchi Approach-Crossed Arrays	R56	Taguchi worldview
R27	Taguchi Approach-Crossed Arrays	R57	Robust geotechnical design
R28	Taguchi Approach-Crossed Arrays	R58	Robust optimization based on the reverse model (RMRO), Genetic Algorithms
R30	Robustness is defined as the standard deviation of one method's error values across different problems.	R59	Leave-One-Out Cross-Validation
R31	Taguchi robust optimization	R60	Stochastic approach

Table 7 illustrates a different number of strategies which have been done in reviewed literature through the management of uncertainty in SO. Most times, in robust design approach the output goal is to gain the minimum distance of mean with target point and with at least variance simultaneously. The main attention behind overall viewpoint via robust design method for designing and developing processes and products is concentrated on three aspects:

i. At least sensitivity to uncontrollable environmental conditions and robustness to any source of variation.

ii. Minimization of variability in product or process characteristics

iii. Minimizing deviance between the performance of product or process and its relevant target point.

3.2.1 Robust optimization in the class of dual response

The dual response surface approach has been successfully applied in robust process optimization. Jalali & Van Nieuwenhuyse (2015) have reviewed some methods of robust design optimization in the class of dual response which applied in simulation optimization, and concluded that the dual response surface approach is more attended among other techniques in that subject. This model has employed two metamodels separately for the process mean and another for the process variance. By combining both types of factors in process included design and noise (uncertain) variables, we can approximate the $y = f(X, Z)$ as a function of design factors (X) and uncertain factors (Z). Due to the stochastic nature of the simulation model, repeated runs of the simulation model with the same combination of input variables, lead to different outputs. Typically, as the training set to improve the metamodel, the average magnitude of repeated runs can be used (Li et al., 2010). If the stochastic simulation models is followed, each input combination $s, (s = 1, 2, …, l)$ repeat m times $(r = 1, 2, …, m)$, while in random simulation m is number of uncertainty scenarios. If $Y = (y_1, y_2, \cdots, y_l)$ is the s-dimensional vector with the simulation's output, then the mean and variance of each input combination can be computed by:

$$\bar{y}_s = \frac{\sum_{r=1}^{m} y_{sr}}{m} \qquad (s = 1, 2, …, l) \tag{1}$$

$$\sigma_{y_s}^2 = \frac{\sum_{r=1}^{m}(y_{sr} - \bar{y}_s)}{m - 1} \qquad (s = 1, 2, …, l) \tag{2}$$

Note that in deterministic simulation models, above equations have $m = 1$, for more information can see (Dellino et al., 2015; Kleijnen, 2009b, 2015). For both Eqs.(1) and (2) are assumed that all scenario of uncertainty have the same probability, else based on probability of uncertainty in a model, equations for computing mean and variance can be rewritten as below:

$$\bar{y}_s = \sum_{r=1}^{m} p(z_r) \cdot y_{sr} \qquad , for \quad (s = 1, 2, …, l) \tag{3}$$

$$\sigma_{y_s}^2 = \sum_{r=1}^{m} p(z_r) \cdot y_{sr}^2 + \left(\sum_{r=1}^{m} p(z_r) \cdot y_{sr}\right)^2 \qquad (s = 1, 2, …, l) \tag{4}$$

Where $p_r(z)$ denotes the probability of rth scenario of uncertainty. Furthermore, there are different optimization approaches available on dual response methodology which some of them are referenced in (Ardakani & Noorossana, 2008; Beyer & Sendhoff, 2007; Nha et al., 2013;

Yanikoglu et al., 2016), so here just for instance some most common robust optimization methods in class of dual response surface are mentioned:

Bi-objective model (Chen et al., 1999):

$$Min: \quad \left[\frac{\bar{y}_s}{\bar{y}_s{}^*}, \frac{\sigma_{y_s}^2}{\sigma_{y_s}^2{}^*}\right] \tag{5}$$

MSE (expected loss) model (Del Castillo & Montgomery, 1993; Phadke, 1989):

$$Min: \quad (\bar{y}_s - T)^2 + \sigma_{y_s}^2 \tag{6}$$

Relaxing the "mean at target" constraint (Yanikoglu et al., 2016):

$$Min: \quad \sigma_{y_s}^2 \; s.t. \; \bar{y}_s \leq T \tag{7}$$

Weighted metric method (Ardakani & Noorossana, 2008; Ardakani et al., 2009):

$$Min: Lp = \left[w\left(\frac{\hat{\sigma}_{y_s} - \sigma_{y_s}^{min}}{\sigma_{y_s}^{max} - \sigma_{y_s}^{min}}\right)^p + (1-w)\left(\frac{\bar{y}_s - \bar{y}_s{}^{min}}{\bar{y}_s{}^{max} - \bar{y}_s{}^{min}}\right)^p\right]^{\frac{1}{p}} \tag{8}$$

where $0 \leq Lp \leq 1$, and p, $(0 \leq p \leq \infty)$ denotes the importance of deviation for each objective function from its relevant utopia. The quantity w illustrates the importance of the mean compared to the standard deviation.

Relaxing the "variance at target"(Lehman et al., 2004):

$$Min: \quad \bar{y}_s \quad s.t. \; \sigma_{y_s}^2 \leq T \tag{9}$$

The standard deviation of the goal output (Dellino et al., 2015):

$$Min: \quad \bar{y}_s \quad s.t. \; \sigma(y) \leq T \tag{10}$$

When the probability distribution of noise (uncertain) parameters are unknown but historical data are available, some methods such as φ-divergence approach can be used to find the estimation of probability distribution (Moghaddam & Mahlooji, 2016). Attending the probability of occurrence of uncertain parameters guide to tighter uncertainty set and less conservative robust solution. Yanikoglu et al. (2016) have suggested robust optimization in the class of dual response
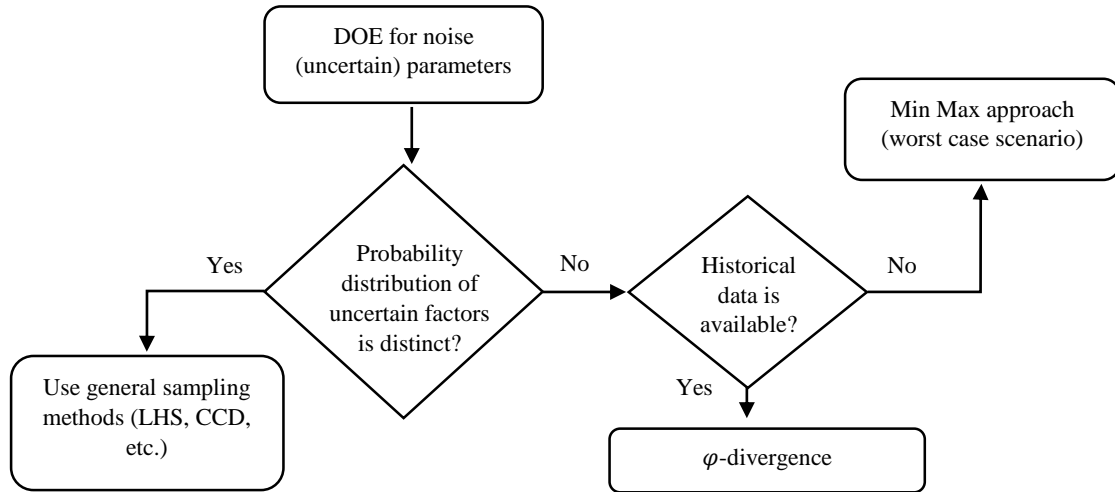
Figure 8 The strategies in faced with unknown probability distribution of uncertain variables.

for such a problem when the probability distribution of uncertain parameters is unknown, but historical data are available:

$$Min_S \ Max_{p(z)} \ \sigma^2_{y_{s\,p(z)}} \quad s.t. \quad \overline{y}_{s\,p(z)} \leq T, \qquad \forall s \epsilon \ S, \forall p(z) \epsilon \ U \qquad (11)$$

Where $p(z)$ represents the unknown true probability distribution of uncertain parameter (z), and denotes a family of distribution that is obtained from old data ($\varphi -$divergence measure). Figure 8 summarizes the strategies on facing with unknown probability of uncertain parameters.

3.3   Designing of computer experiments

In this context, we focus on experiments via computers in simulation terms. Recently, the acronym of Design and Analysis of Simulation Experiments (DASE) has been introduced which is inspired of the common acronym in deterministic simulation as Design and Analysis of Computer Experiments (DACE) (Kleijnen, 2015). In practice, most simulation models have many combinations of input factors to run which may lead to time consuming and expensive patterns, e.g. the model with 7 input factors and 10 levels per each input requires 10^7 combinations. In addition, in an uncertain environment, the analyzing of uncertain (noise) factors need extra computational efforts. Furthermore, if we wish to analyze all combinations to investigate the best set of input factors, then we need extremely long simulation runs unless the appropriate sampling methods are successfully used. As to the number of sample points to produce an accurate response surface model, using $1.5n$ to $2.5n$ sample points have been recommended in literature, see, (Giunta et al., 1994; Simpson, Mauery et al., 2001) when n is number of coefficients that need to be estimated. There are three common types of design based
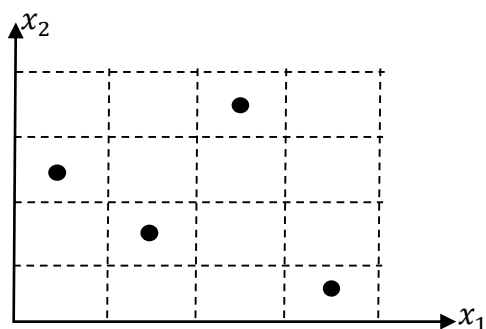
on aliasing main or interaction effects in a model. While the effect one factor depends on the levels of one or more other factors, called two of more degree of interaction between factors. A resolution-III design indicates that main effects may be aliased with two factor interactions. A resolution-IV design indicates that main effects may be aliased with three-factor interactions. Two-factor interactions may be aliased with other two-factor interactions. Resolution-V (or higher) assume that main effects and two-factor interactions can adequately model the factors. Table 8 shows some DOE methods that have been used in literature to design experimental points through analyzing and improving different engineering design problems.

Table 8 Different strategies of DOE for SO in literature.

DOE Strategy	Article ID
Monte-Carlo method, Random Sampling	R10, R49, R56, R3, R59, R53
Orthogonal array	R2, R9, R16
Central Composite Design (CCD)	R1, R9, R14, R31
Space filling, Latin Hypercube Sampling (LHS)	R1, R3, R5, R7, R8, R9, R10, R11, R14, R16, R17, R18, R21, R22, R25, R26, R27, R28, R29, R30, R32, R35, R36, R40, R43, R45, R48, R54, R58, R59, R60
Full and Fractional Factorial Designs, Optimal Designs	R8, R9, R15, R17, R24, R31
sequential design	R13, R20, R40, R52, R60, R35
Plackett-Burman	R14, R17, R56

3.3.1 Latin Hypercube Sampling (LHS)

LHS was first introduced by (McKay et al., 1979). It is a strategy to generate random sample points, while guarantee all portions of the design space is depicted. Generally, LHS is intended to develop results in SO (Kleijnen, 2015). LHS has been commonly defined for designing computer experiments based on space filling concept (Bartz-Beielstein et al., 2015; Del Castillo, 2007). In general, for n input variables, m sample points are produced randomly into m intervals or scenarios (with equal probability). For the particular instance the LHS design for $m = 4, n = 2$ is shown in Figure 9. The LHS strategy proceeds as follows:

i. In LHS, each input range divided into m subranges (integer) with equal probability magnitudes, and numbered from 1 to m. In general, the number of m is larger than total sample points in CCD (Kleijnen, 2004).

Figure 9 An example for LHS design with two input factors, and

ii. In the second step, LHS place all m intervals by random value between lower and upper bounds relevant to each interval, since each integers $1,2,\ldots,m$ appears exactly once in each row and each column of the design space. Note that, within each cell of design, the exact input value can be sampled by any distribution, e.g. uniform, Gaussian or etc.

Three common choices are available to ensure appropriate space filling of sample points in LHS design:

Minimax: This design tries to minimizing the maximum distances in design space between any location for each design point and its nearest design points.

Maximin: In this design attempt to be maximized the minimum distance between any two design points.

Desired Correlational function: Inspired by (Iman & Conover, 1982) in the case of non-independent multivariate input variables the desired correlation matrix can be used to produce distribution free sample points in LHS.

3.3.2 Orthogonal Array (OA)

The OA design can fill whole design space like LHS, and it has strength to allocate points in each corner of design space (Owen, 1992). The OA was adapted to balance an discrete experimental factors in a continues space (Koehler & Owen, 1996). The orthogonal array is matrix with n rows and p columns where n is number of experiments (input combination) and p is number of input factors. Each factor is divided into m equal size ranges (grids), and sample points are allocated to these orthogonal grid spaces. In general, the orthogonal array shows with symbol of $L_n(m^p)$, and has the following properties:

- For the input factor in any column, every level happen n/m times.

For the two input factors in any two columns, every combination of two levels happen n/m^2 times.

- For the two factors in any two columns, all n input combinations are combined by levels as belows:

$$\{(1,1),(1,2),\cdots(1,m),(2,1),(2,2),\cdots,(2,m),\cdots,(m,1),(m,2),\cdots,(m,m)\}$$

- By replacing any two columns of an orthogonal array, the remaining arrays are still orthogonal to each other.

- By removing one or some columns of an orthogonal array, the remaining arrays are orthogonal to each other, and OA is able to employ by a smaller number of factors.

3.3.3 Sequential design:

Most time in practice due to expensive simulations (i.e. a single simulation run is intensive time consuming), reducing the number of simulation runs (sample points) is interested. In mathematical statistics it is common that sequential designs are more well-organized than fixed sample size design (Wim et al., 2008). Different types of criteria can be used to sequentially define a candidate set of sample points, that most of them are based mean squared prediction error (Van Beers & Kleijnen, 2004). (Kleijnen & Beers, 2004) have proposed a customized sequential method based on cross-validation and jackknifing approaches. In SO, (Kleijnen, 2017) has suggested replacing one-shot designs by sequential designs that are customized for the given simulation models. In other similar work, (Wim et al., 2008) have employed bootstrapping technique to propose the sequential DOE with a smaller number of sample points than other alternative design like LHS, also with better results. A comparison on different sequential sampling approaches has been provided in (Jin, R. et al., 2002). Here, inspired by (Kleijnen & Beers, 2004; Wim et al., 2008) the cross-validation and jackknifing method are followed due to four reasons. First, this method is adapted for expensive simulation models. Since this model is used the cross-validation method and does not need extra simulation runs, so is appropriate for expensive simulation models. Second, evaluate I/O behavior with highest estimated variance which is desirable in robustness study. Third, smaller prediction error than other sequential design (Van Beers & Kleijnen, 2004). Fourth, this method is able to use for different types of metamodel such as polynomial regression and Kriging.

Following steps are shown the procedure of sequential design based on cross-validation and jackknifing:

- Expensive simulation runs are implemented for n_0 initial sample points, and the approximation metamodel is constructed based on initial result.

- Then select c candidate points ($j = 1,2, \dots , c$). To select candidate points can use halfway space-filling between vertices.

- To compare all candidates and select winner for expensive simulation, a jackknife variance for each candidate need to be computed separately and selected a point with maximum jackknife variance. To avoid extrapolating, do not drop the sample points on vertices, k sample on vertices doesn't drop, so n_0 is replaced by n_c when $n_c = n_0 - k$.

- Drop one point from model $-i$, $(i = 1,2, \dots, n_c)$ and construct metamodel based on $n_0 - 1$ remain points.

- Calculate the jackknife's pseudo-value for candidate j as below:

$$\tilde{y}_j^{-i} = n_c \times \hat{y}_j^{-0} - (n_c - 1) \times \hat{y}_j^{-i} \quad for \quad i = 1,2, \dots, n_c \ \ and \ \ j = 1,2, \dots, c \tag{3-12}$$

where $\hat{y}_j^{-0}$ is the original prediction for candidate j with metamodel over initial sample points, and $\hat{y}_j^{-i}$ is prediction for candidate j with metamodel over $n_0 - i$ points (delete i_{th} sample point from n_0 set of points).

- The jackknife variance is computed for candidate j by employing relevant pseudo-values:

$$\widetilde{s_j^2} = \frac{1}{n_c(n_c - 1)} \sum_{i=1}^{n_c} \left(\tilde{y}_j^{-i} - \bar{\tilde{y}}_J \right)^2 \quad with \quad \bar{\tilde{y}}_J = \frac{1}{n_c} \sum_{i=1}^{n_c} \tilde{y}_j^{-i} \tag{3-13}$$

where the candidate with maximum $\widetilde{s_j^2}$, $(arg\ max_j\{\widetilde{s_j^2}\})$ is a winner and enter in set of initial sample points after computing its relevant response with original simulation.

- All steps are repeated till stop creation is satisfied. Among literature could not be found any suggested appealing stopping criterion, see (Van Beers & Kleijnen, 2004). It can be defined based on a limitation of computational time or cost.

3.4   Metamodeling

Metamodeling techniques have been used to avoid intensive computational and numerical simulation models, which might squander time and resource for estimating model's parameters. Metamodeling has utilized variety statistical and mathematical approach for interpreting parameters and their relationship in an original model. A metamodel or surrogate model by mathematical expression $\hat{Y} = f(\widehat{X, Z})$ can replace with true functional relationship $Y = f(X, Z)$, where X and Z denotes respectively design and noise (uncertain) factors. The general overview
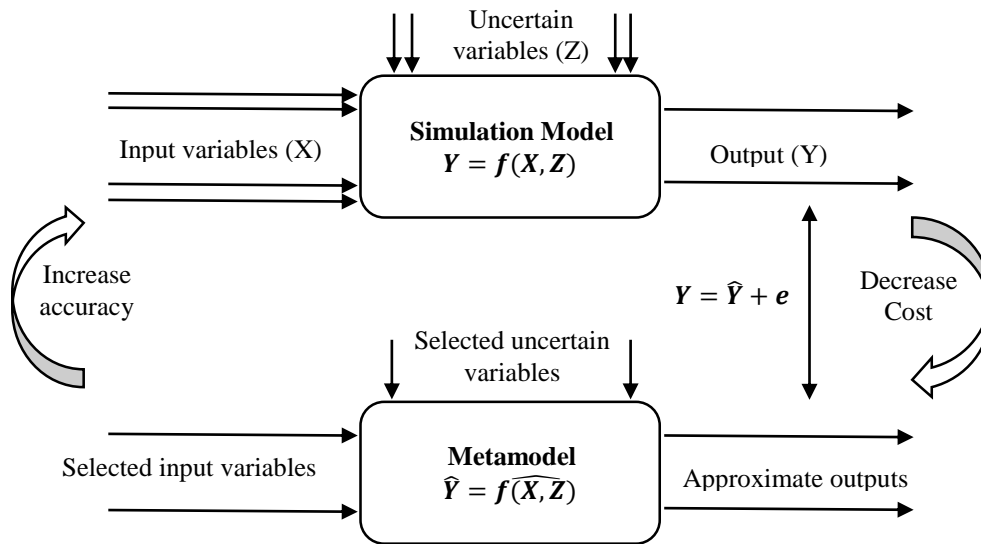
Figure 10 The viewpoint of metamodel under uncertainty (noise variables) and relationship with a simulation model.

of a metamodel with uncontrollable noise variables as uncertainty symbols is illustrated in (Figure 10).

3.4.1 Polynomial regression

Polynomial regression also called Response Surface Methodology (RSM) is a collection of statistical and mathematical techniques useful for developing, improving, and optimizing the process. The functional applicability of RSM in literature can be i) approximate the relationship between design (dependent) variables and single or multi-response (independent variables), ii) investigating and determining the best operating condition for the process, by finding the best levels of design region which can satisfy operating limits, and iii) implementing robustness in the response(s) of the process by designing the process robust against uncertainty. Barton & Meckesheimer (2006) have claimed the RSM has been successfully used in recent decades for processes with the stochastic application. Kleijnen (2017) has mentioned the RSM is sequential since it uses a sequence of local experiments and leads to the optimum input combination. He also has claimed that the RSM can achieve an appropriate track record in literature. Some of the initial applications of RSM in SO can be found in (Azadivar, 1999; Biles, 1974). Commonly, the main motivation of polynomial approximation for true response function is based on Taylor series expansion around a set of design points, see (Myers et al., 2016). The general overview of the first-order response surface model is shown as:

$$y = f(X) = \hat{\beta}_0 + \sum_{i=1}^{k} \hat{\beta}_i \, x_i + \varepsilon \tag{14}$$

where k is number of design variables. Most times, the curvature of response surface is stronger than the first model can approximate it even with the interaction terms, so a second-order model can be employed:

$$y = f(X) = \hat{\beta}_0 + \sum_{i=1}^{k} \hat{\beta}_i \, x_i + \sum_{i=1}^{k} \hat{\beta}_{ii} \, x_i^2 + \sum_{i=1}^{k} \sum_{i<i'=2}^{k} \hat{\beta}_{ii'} \, x_i x_{i'} + \varepsilon \tag{15}$$

where $\widehat{\beta}_0, \hat{\beta}_i, \hat{\beta}_{ii}$ and $\hat{\beta}_{ii'}$ are unknown regression coefficients and the term ε is the usual random error (noise) component. The number of expression in a linear polynomial regression model is $p = k + 1$, quadratic model is $p = \frac{1}{2}(k + 1)(k + 2)$, and cubic model is $p = \frac{1}{6}(k + 1)(k + 2)(k + 3)$ when n is number of input variables. By polynomial regression to fit reasonable metamodel, the sample size should be at least two or three times the number of expression (p) (Jin et al., 2003).

3.4.2   Kriging

Since Daniel G. Krige (1951) has addressed the geostatistics around six decades ago, today Kriging (also called Gaussian process) models have been used as a widespread global approximation technique (Jurecka, 2007). Kriging is an interpolation method which could cover deterministic data in a black-box presentation, and it is highly flexible due to ability in employing a various range of correlation functions. In general, Kriging has been used in deterministic simulation models, i.e. Computer Aided Engineering (CAE). Kriging is hardly any application yet in random simulation (Kleijnen, 2005; Kleijnen, 2015). The higher accuracy of Kriging models than other alternatives such as polynomial regression is confirmed via different numerical cases in literature (Dellino et al., 2015; Jin et al., 2001; Simpson, Poplinski et al., 2001). In the Kriging model, a combination of a polynomial model and realization of a stationary point are assumed by the form of:

$$y = f(X) + Z(X) + \varepsilon \tag{16}$$

$$f(X) = \sum_{p=0}^{k} \hat{\beta}_p \, f_p(X) \tag{17}$$

where the polynomial terms of $f_p(X)$ are typically first or second order response surface approach and coefficients $\widehat{\beta}_p$ are regression parameters $(p = 0,1,\dots,k)$. This types of Kriging approximation is called universal Kriging, while in ordinary Kriging instead of $f(X)$ the constant mean $\mu = E(y(x))$ is used. The term ε describes approximation error, and the term $Z(X)$ represents realization of a stochastic process, which most time normally distributed Gaussian random process with zero mean, variance σ^2 and non-zero covariance. The correlation function of $Z(X)$ is defined by:

$$Cov[Z(x_k), Z(x_j)] = \sigma^2 R(x_k, x_j) \qquad (18)$$

where σ^2 is process variance and $R(x_k, x_j)$ is the correlation function, and can be chosen from different functions which proposed in literature (e.g. exponential, Gaussian, linear, spherical, cubic, and spline). For instance, the general exponential correlation function is defined as below:

$$R_{\theta,p}(x_k, x_j) = \prod_{i=1}^{n} \exp(-\theta_i |x_{ki} - x_{ji}|^{p_i}) \qquad (19)$$

where n is dimension of input variables, and p_i determine the smoothness of the correlation function and θ_i indicates the importance of ith input factor, while the higher θ_i denotes the less effect of factor i on output. For $p_i = 1$ and $p_i = 2$ respectively the exponential and Gaussian correlation function is made.

3.4.3 Validation of metamodel

In general, to assess the predictor behavior and evaluating of the model, the techniques can be divided into two types based on the set of sampling points. The first type is evaluated model by using training data (i.e. the set of data which is used in estimating model) and second by employing validating data (i.e. new set of data except for data which used in estimation). Some different methods have been suggested for evaluating a metamodel, while among them four more applicable validation methods are chosen to discuss in follow. Notably, mentioned methods are based on employing validation data in semi-expensive models, since in expensive simulation models impose extra computational costs due to extra simulation runs. Moreover, in such a case some methods such as cross-validation or bootstrapping can be used, see (Kleijnen, 2015).

R-square Index

This method can be used to compare first order against second or above order polynomials regression, or RSM with other metamodels namely Kriging. The R^2 coefficient is defined as:

$$R^2 = 1 - \frac{\sum_{j=1}^{m}(y_j - \hat{y}_j)^2}{\sum_{j=1}^{m}(y_j - \bar{y}_j)^2} = 1 - \frac{Mean\ Square\ Error}{Variance} \tag{20}$$

where $\bar{y}_j$ is mean of observed values (y_j) and $\hat{y}_j$ is corresponding predicted values.

Adjusted R-square Index

Due to the index R^2 always increases when the terms are added to the model, some regression analysts prefer to use another statistic index which called adjusted R-square:

$$R_{Adj}^2 = 1 - \frac{n-1}{n-p}(1 - R^2) \tag{19}$$

By adding variables to the model, generally the statistic R_{Adj}^2 will not increases. In fact, the value of adjusted R-square often decrease, if unnecessary terms are added to the model.

Relative Maximum Absolute Error (RMAE)

While the larger magnitude of R-square indicates better overall accuracy, the smaller amount of RMAE indicates the smaller local error. A suitable overall accuracy does not necessarily signify a good local accuracy (Jin et al., 2003).

$$RMAE = \frac{\max\{|y_1 - \hat{y}_1|, |y_2 - \hat{y}_2|, \dots, |y_m - \hat{y}_m|\}}{\sqrt{\frac{1}{m}\sum_{j=1}^{m}(y_j - \hat{y}_j)^2}} \tag{20}$$

Cross-validation

The cross validation method can be used when collecting new data or further information about simulation model is costly. The cross validation uses an existed data and does not require to re-run of the expensive simulation. This method also called leave-k-out cross-validation to validate metamodel (i.e. in each run k sample points would be removed from an initial training sample points)(Kleijnen, 2015). The leave-one-out cross validation ($k = 1$) is briefly explained in follows that is most popular than others:

Step 1: Delete s^{th} input combination and relevant output from the complete set of l combination $(s = 1,2, ... , l)$.

Step 2: Approximate the new model by employing $l - 1$ remain rows s_{-1}.

Step 3: Predict output for left-out point (s_{-1}) with metamodel which obtained from Step 2.

Step 4: Implementing the preceding three previous steps for all input combination (sample points) and computing n predictions $(\hat{y}_s)$.

Step 5: The prediction result can be compared with the associated output in original simulation model. The total comparison can be done through a scatter plot or eyeball to decide whether or not metamodel is acceptable.

3.5 Robust metamodeling in SO

There are different number of methodologies in optimizing of deterministic simulation, but there are few number of studies have been done on random (stochastic) SO problems under uncertainty and effect of noise parameters, particularly based on combination of metamodels and robust optimization, see (Simpson, Poplinski et al., 2001) and two recent review papers by (Amaran et al., 2016; Kleijnen, 2017). Table 9 depicts a different combination of SO methods which have been applied in reviewed articles. Barton (1992) has introduced the Taguchi methods as an alternative to metamodeling strategies. Bates et al. (2006) have shown that the Taguchi crossed array was more successful than the dual response designs in its relevant numerical example. On the other side (Dellino & Meloni, 2015; Kleijnen, 2015; Myers et al., 2016; Vining & Myers, 1990) have been combined the Taguchi approach with approximation methods to be used advantages of both methods. Figure 11 illustrates a general procedure in SO method under uncertain condition based on surrogate models and Taguchi termonology (Dellino & Meloni, 2015; Kleijnen, 2015).

Table 9 Simulation optimization methods applied in literature ("M" means multi-objective, "C" means constrained problem).

| ID	Type	Methodologies	ID	Type	Methodologies
R1		RSM-Kriging-Neural Networks-Rule Induction.	R31		First-order and second-degree polynomials (RSM) and Kriging.
R2	M	Kriging, Response Surface, simulated annealing algorithm, generalized reduced gradient (GRG).	R32	C	Deterministic Sequential Approximate Optimization (SAO), finite element method, and single response surface modeling.
R3		Polynomial regression, multivariate adaptive regression splines, radial basis functions, and Kriging.	R33	M	Genetic algorithm, on-line and off-line scheduler, and RSM.

Table 9 (Continued).

ID	Type	Methodologies	ID	Type	Methodologies
R4	C	Integer linear programming and RSM.	R34		Monotonicity preserving Kriging models and distribution-free bootstrapping.
R5	M/C	Stochastic Optimization, the Genetic algorithm (GA), RSM, and bootstrapping.	R35		Adaptive hybrid functions (combination of quadratic response surface, radial basis functions, and Kriging), and Cross validation.
R6	C	Genetic Algorithm and Mixed Integer Programming.	R36		Kriging
R7	C	(Adaptive)Response Surface Method, and Simulated annealing global optimization method.	R37		Select and review 10 top articles in simulation optimization.
R8	C	Polynomial regression, Kriging, and Radial Basis Functions (RBF).	R38	C	Hydrologic simulation and Mathematical Programing.
R9		RSM, Kriging, regression splines, regression trees, and neural networks.	R39	C	RSM and fuzzy linear programming.
R10		Ordinary Kriging and classic cross validation.	R40		Integer programming formulation, low-complexity surrogate model, machine learning techniques, derivative based or algebraic solvers, reduced-order modeling, and error maximization sampling (EMS).
R11		Updated correlation parameter estimates.	R41		Multiple surrogates techniques (polynomial regression and Kriging).
R12		Low order polynomial and Kriging.	R42		Statistical Selection Methods (SSM), Metaheuristics (MH), Memory-based Metaheuristics (MMH), Random Search (RS), Stochastic Approximation (SA), Sample Path Optimization (SPO) and Metamodel-based Methods, Gradient Surface Methods (GSM), Surrogate Management Framework (SMF), Reverse Simulation Technique (RST), Retrospective Simulation Response Optimization (RSRO).
R13		Kriging, cross-validation, and jackknifing.	R43		RSM and Kriging
R14		Polynomial regression, Kriging, and cross-validation.	R44	M/C	RSM, Kriging, and neutral network.
R15		RSM, regression spline, spatial correlation (Kriging), radial basis function, and neural network.	R45		Kriging metamodel and Monte Carlo simulation.
R16		The Bayesian approach, Gaussian process based emulator, free surface velocity, and third-degree polynomial response surface.	R46		Bayesian inference and Interval metamodel.
R17	M/C	Polynomial functions, Kriging, neural networks, Radial Basis Functions (RBF), Multivariate Adaptive Regression Splines (MARS), least interpolating polynomials, and inductive learning.	R47	M/C	Monte-Carlo Simulation.

Table 9 (Continued).

ID	Type	Methodologies	ID	Type	Methodologies
R18	C	Kriging (spatial correlation metamodels) and generalized expected improvement criterion.	R48		RSM, gradient-based methods, discrete optimization via simulation, sample path optimization, direct search methods, random search methods, and model-based methods.
R19		RSM and Kriging.	R49	M	Transfer function modeling and time-series pre-specified by forecasting methods.
R20		Kriging and bootstrapping.	R50	M	A Gaussian process metamodel, Monotone cubic spline, and computer-aided IPTD (Integrated Parameter and Tolerance Gaussian process or Kriging surrogates, global optimization algorithm, surrogate-based algorithms, nature-inspired algorithms, and evolutionary algorithms.
R21		RSM and Kriging.	R51		
R22		Kriging, classic linear regression (RSM), and bootstrapping.	R52		A quasi Monte Carlo (MC) simulation, deterministic multi-resolution lattice points, thin plate spline (TPS) metamodel (which is a special case of RBF), and swarm optimization.
R23		RSM, Monte-Carlo simulations, and finite element design.	R53		Regression models (RSM).
R24		Sequential Bifurcation (SB)	R54		φ- divergence and Kriging
R25	M/C	Kriging, evolutionary optimization algorithms (EAs), Data Envelopment Analysis (DEA), adopted optimization system, and Non-dominated Sorting Genetic Algorithm-II (NSGA-II).	R55	M	Polynomial response surface, Kriging, computational fluid dynamics (CFDs) solver, and Monte Carlo simulation.
R26		RSM	R56	M	Polynomial regression and Kriging.
R27		Kriging	R57	M	Quasi-response surface approach, gradient-based robustness measure, minimum distance (MD) algorithm, and weighted sensitivity index.
R28		RSM, one layer Kriging, and two layers Kriging	R58	C	Kriging, single-loop optimization structure.
R29		Kriging	R59	C	Radial basis function, leave-one-out cross-validation, and sequential improvement criterion.
R30	C	Multivariate adaptive regression splines, Kriging, RBF, Artificial Neural Networks, and Support Vector Regression.	R60		Monte Carlo, kriging, sequential approximate optimization (SAO), and gradient realization.

3.5.1 Bootstrapping

Consequently both sensitivity analysis and optimization must be done on metamodels to interpret the observed simulation input/output data (Van Beers & Kleijnen, 2004). Sensitivity analysis can serve optimization of the simulated system (Kleijnen, 2010). The sensitivity analysis is based on a fixed condition for a system just with the variation of one factor.
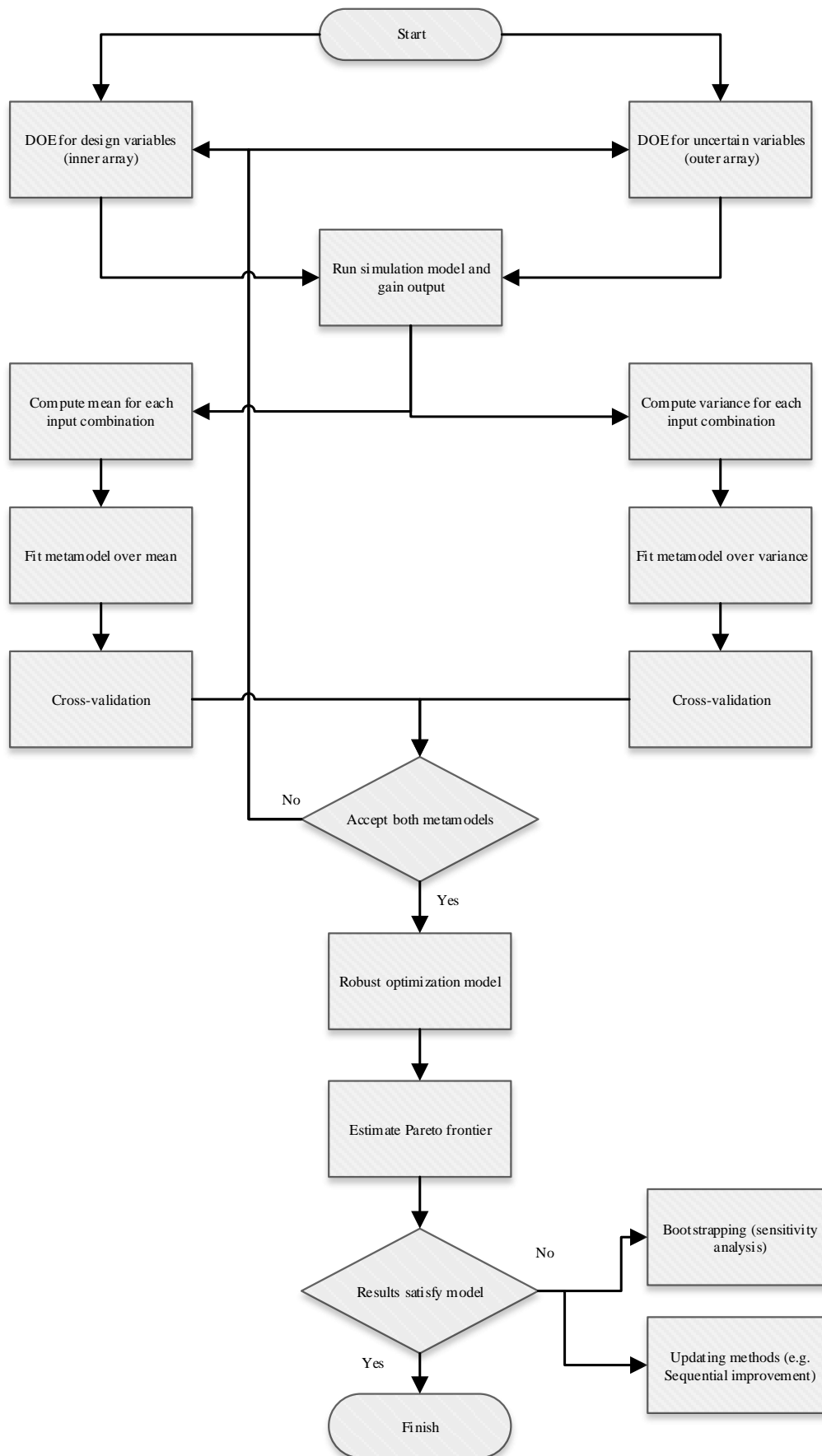
Figure 11 Main steps in MBRSO procedure.

(Kleijnen, 2009b) has recommended that the designs for sensitivity analysis and optimization need to be combined for robust optimization. The parametric bootstrapping has been suggested in such a case while assume a specific distribution type is estimated from I/O simulation data on hand. The basics of this method have been explained in (Kleijnen, 2004; Kleijnen, 2010; Kleijnen, 2009b, 2015). In stochastic simulation, each input combination X is replicated a number of times $m \geq 1$. In an expensive simulation, yet just the number of replication are less, so good results cannot be expected to gain by this types of bootstrapping (i.e. rarely can find the exact distribution of I/O simulation data). Moreover, a simple method for estimating the exact variance of predictor is distribution-free bootstrapping, see (Dellino & Meloni, 2015).

3.5.2   Sequential improvement:

The sequential improvement methods have been interested in engineering design problems to a trade-off between local and global search with the criterion of expected improvement. (Abspoel et al., 2001) have proposed a sequential approximate approach to solving SO with integer design variables. Sequential improvement can be appropriately used in different practical engineering design problems, for instance, see (Wiebenga et al., 2012) and (Havinga et al., 2017) in improving metal forming processes, (Jurecka et al., 2007) in the 10-bar truss under varying loads, and (Zhang, J et al., 2017) for optimal design of the skyhook control for the suspension of a half-car model.

These methods are combined with two main parts, first statistical part consist of DOE and metamodeling techniques, and second evolutionary algorithms. Note that, this method handles capturing the behavior of the overall design space, so the global approximation methods (e.g. Kriging) can be covered by this method while polynomial regression cannot, due to locally behavior. Sometimes due to the low correlation between predicted optimum point (which estimated by metamodel) and other points, the metamodel does not show enough accuracy in optimal point compare to the original model, for more information see (Havinga et al., 2017; Jurecka, F et al., 2007; Sóbester et al., 2004).

4.   Discussion and results:

Polynomial regression metamodel can be established by two main consecutive steps, screening and optimization. In the screening step, the significant interested levels of input factors can be identified, so in the second step, the closer interval of input factors can be studied (Kleijnen, 2010; Myers et al., 2016). Haftka et al. (2016) have considered the latest development on global-local approach. In this approach, the rough surrogate model is constructed in entire design space, and then apply it to zoom on promising regions. Wang, (2003) has developed the adaptive RSM

which instead regions with large-scale, made a new DOE through the central composite design or LHS in reduced region, for more information can also see (Peri & Tinti, 2012). On the contrary, a polynomial model is easy to establish, more distinct in the sensitivity analysis, and cheap to work (Wang & Shan, 2007). In addition comparison of different metamodel types such as polynomial regression and Kriging in practical problems also remains a challenging topic (Beers & Kleijnen, 2004; Kleijnen, 2017; Wang & Shan, 2007).

More support is currently available for implementation of polynomial regression with computer software than other types of metamodels (e.g. Design Expert (V. 10), Minitab (V. 17), SAS (V. 14.2), SPSS (V.23), and so on). For Kriging the MATLAB (DACE, free Kriging toolbox[1] can be used (Lophaven et al., 2002). In addition, ARCGIS (geostatistical analysis) and Isatis (geographical analysis) can support the Kriging surrogate model, but till the number of input factors does not exceed three (Kleijnen, 2009b).

However, a study in literature shows there is a lack software package that can cover Kriging surrogate model in the framework of practical engineering design (Jin et al., 2001; Kleijnen, 2009b), while it has been more employed for academically usage than for practical problems in the real world (Jalali & Van Nieuwenhuyse, 2015). Viana et al. (2014) have listed a number of existed commercial software (e.g. BOSS/Quattro, DAKOTA, HyperStudy, IOSO, LS-OPT, OPTIMUS, and VisualDOC) with highlighting their metamodeling and optimization capabilities, while they have claimed that for many these software systems, metamodeling is not a final goal.

In practice, most problems can be supported by polynomial regression requirements, and due to less complexity, process designers have preferred to use it than other metamodels, see (Forsberg & Nilsson, 2005; Jalali & Van Nieuwenhuyse, 2015; Jin et al., 2003; Simpson et al., 2004). However, due to strength points of Kriging, recently there is a significant increasing trend to attend more in the application of common modern metamodel namely Kriging, compared to classical metamodel techniques such as the different order of polynomial regression. Kriging is a popular method for metamodeling with simulation data (Havinga et al., 2017). The Kriging gives more accurate and flexible approximation than polynomial regression due to fit globally over whole design space (Dellino, 2015; Jin et al., 2001; Simpson, Poplinski et al., 2001). The main advantages of Kriging over polynomial regression is exact interpolating of Kriging, i.e. the predicted values and simulated output in the set of observed input values are exactly equal

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[1] http://www2.imm.dtu.dk/pubdb/views/edocdownload.php/1460/zip/imm1460.zip

(Kleijnen, 2005). In general, Kriging predicts very bad in the case of extrapolation outside observed sample data (Kleijnen & Beers, 2004).

Most methods which mentioned in this context just have been tested in theoretical settings of problems, so applying these methods in practical problems and in-depth comparing of their performance can be an interesting area for additional research (Dellino, 2009; Jalali & Van Nieuwenhuyse, 2015). Kleijnen, (2009b) has emphasized on applying metamodels particularly Kriging in practical random simulation models, which are more complicated than the academic M/M/1 queueing and (s, S) inventory models.

Another shortcoming which has been revealed by reviewing literature is that most publication assume single variable output, whereas in practice simulation models have to covered by multi-variable output methodology (Kleijnen, 2009b; Simpson, Mauery et al., 2001; Teleb & Azadivar, 1994). Yet, investigating suitable DOE for multiple outputs has been an interesting topic for researchers (Kleijnen, 2005).

To the best of our knowledge, rarely can find the study which considers variability in design variables parallel with noise variables. Most studies consider the variability of environmental factors and it influences in response variability, so they have assumed that design variables can be exactly controlled in their relevant value, while in practice this assumption may be failed, see (He et al., 2010; Sanchez, 2000). Most times in practice important uncertainty can be tolerances in nominal value of design variables (Myers et al., 2016).

5.   Conclusion:

In this paper, the latest developments on optimization of complex simulation models under uncertainty are investigated. Intensive attention is focused on surrogate based methods hybrid robust design optimization, particularly according to dual response methodology. These type of methods are being in the class of MBRSO. Main methodologies that have been used in reviewed articles are highlighted, while important methods are discussed. Outstanding shortcomings and also positive points of each method are mentioned based on discussed topics. Respect to advantages and disadvantages of both metamodels (polynomial regression and Kriging), appropriate methods which integrated both metamodels (hybrid surrogate methods) in practical problems have not been attended enough. The low-order polynomial can be used in screening and Kriging for optimizing as well. Proposing methodologies which can cover different gaps which mentioned in discussion and result section can be interesting topics for future works by researchers.

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