Robust design of optimal experiments considering consecutive re-designs ⋆

Anwesh Reddy Gottu Mukkula * **Radoslav Paulen** **

* *Process Dynamics and Operations Group, Technische Universität Dortmund, Emil-Figge-Strasse 70, Dortmund 44227, Germany*
** *Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, Radlinského 9, 812 37 Bratislava, Slovakia*

Abstract: We investigate the problem of robust design of experiments (rDoE) in the context of nonlinear maximum-likelihood parameter estimation. It is assumed that an experimenter designs a series of experiments with the possibility of a re-design after a particular experiment run. We present a novel rDoE approach that uses multi-stage decision making in order to explicitly account for the experiment re-designs. This is an extension to our previous work Gottu Mukkula et al. (2021) whereby we focus on the framework of the exact joint-confidence regions for uncertain model parameters. An over-approximation of the exact joint-confidence region is used for designing robust A-optimal experiments. We compare the presented approach with the standard robustification approaches and report the findings on a simple nonlinear case study.

Keywords: Optimal experiment design, Parameter estimation, Least-squares estimation, Robust design of experiments, Exact joint-confidence region

1. INTRODUCTION

Mathematical modeling has been at the core of engineering, physics, chemistry, etc. for many years. In process industries, mathematical models are used widely for process and control system design, process optimization, etc. Model development is usually divided into three major steps a) identification of the model structure, b) design and realization of the experiments, and c) estimation of the unknown parameters. In the latter phase, one often realizes maximum-likelihood estimation via least-squares methodology as he/she assumes that the measurement error corrupting the measured data is statistically distributed as a white Gaussian noise. Once the parameter estimates are known, the experimenter commonly determines the quality of the obtained model. This can be done either by using some validation data—if available—or by assessing the joint-confidence regions of the estimated parameters. If the model quality is unsatisfactory, it is possible to simply re-run the experiment or to re-design and run a new experiment based on the *lessons learned*.

Design of experiments (DoE) is a branch of mathematics that determines the most favorable experimental conditions that allow the most informative data to be collected during an experiment. Unlike in linear parameter models, the model nature is highly influenced by the parameter values in nonlinear models. This makes DoE for nonlinear parameter models to be heavily dependent on the a priori knowledge of the uncertain parameters. This phenomenon is commonly referred to as a chicken-and-egg problem, where one requires precise knowledge of the parameters a priori to estimate parameters with high precision.

A standard procedure of experiment design for nonlinear models is to select nominal values of the uncertain parameters in the nominal model and perform DoE. The nominal design will be suboptimal—or even infeasible to conduct in the presence of strict plant constraints—if the nominal values of the uncertain parameters are far from reality (Pronzato and Walter, 1985). Several approaches such as the robust min-max optimization (Walter and Pronzato, 1987) and stochastic (Galvanin et al., 2010; Streif et al., 2014; Mesbah and Streif, 2015; Nimmegeers et al., 2020) or scenario-based (Telen et al., 2014; Welsh and Rojas, 2009) approaches have been proposed to overcome this problem. An overview of the different approaches for robust design of experiments (rDoE) is available in Asprey and Macchietto (2002). A majority of these approaches concentrate primarily on fulfilling the process operational constraints. Additionally, they try to decrease the loss in optimality by optimizing experiments for the worst-case or the most probable model, based on some a priori information.

A series of successive experiments are often performed in the experimentation phase of model building as the initial experiment—designed with DoE or rDoE methods using a nominal model—might not be optimal (Vanaret et al., 2021). At the same time, information gained from the previous experiments can be used to design the next experiments better—based on model parameters re-estimated from the newly available data. This gives rise to the design of sequential experiments (Barz et al., 2010), which is sometimes referred to as Bayesian design of experiments because of the ability of Bayesian techniques to incorporate the a priori knowledge that can be present by historical experience or by some past experiments. Recently,

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Gottu Mukkula and Paulen (2017b); Gottu Mukkula et al. (2021) proposed a multi-stage rDoE framework in the context of guaranteed parameter estimation and linearized (maximum-likelihood) confidence regions. In the proposed rDoE framework, the whole series of experiments are optimized while explicitly accounting for the possible redesign of the successive experiments once new information becomes available.

In this paper, we study the rDoE problem and particularly address the situation, where one can plan a series of experiments ahead, considering the possibility of re-estimating the uncertain model parameters in-between the experiments. We study the rDoE using the exact (nonlinear) confidence regions (Gottu Mukkula and Paulen, 2017a, 2019). We organized the paper as follows. The concepts of nonlinear parameter estimation are introduced first. Next, the formulation for the experiment design using nonlinear (exact) confidence regions is reviewed. Further, well-known rDoE approaches are briefly shown and the proposal for robust multi-stage DoE is outlined in detail. Lastly, in the case study section, we illustrate the theoretical findings on a simple nonlinear model.

2. PRELIMINARIES

2.1 Mathematical Model

In this paper, a mathematical model of a nonlinear parameter system is represented by

$$\hat{\boldsymbol{y}}(\boldsymbol{p},\tau) = \boldsymbol{F}(\boldsymbol{p},\boldsymbol{u}_\tau), \tag{1}$$

with $\hat{\boldsymbol{y}}$ as n_y output variables, $\boldsymbol{u}_\tau$ as n_u degrees of freedom and $\hat{\boldsymbol{p}}$ as n_p uncertain parameters. Here τ represents an ordinal number of a data point taken in one or more experiments. Nonlinear function $\boldsymbol{F} : \mathbb{R}^{n_p} \times \mathbb{R}^{n_u} \to \mathbb{R}^{n_y}$ is considered to be a twice continuously differentiable mapping. Throughout the paper, we resort to the representation in (1), which considers the system model as static and explicit w.r.t. output variables. However, the presented findings can straightforwardly be extended to dynamic and implicit models.

We will assume throughout the paper that the model is not over-parameterized and that all the parameters are identifiable. We consider that, upon the realization of an experiment or several experiments, N instances are gathered of n_y-dimensional vector of plant measurements $\boldsymbol{y}_m$ and are subsequently used for the estimation of unknown parameters. Throughout the paper, we will assume a white Gaussian noise to be corrupting the measurements. In the following subsections, existing frameworks are presented for the identification of the unknown parameters and the corresponding exact confidence regions for nonlinear parameter estimation problems.

2.2 Parameter Estimation

Given a static nonlinear mathematical model (1), the expected values of parameters $\hat{\boldsymbol{p}}$ are identified by solving the following weighted least-squares estimation problem

$$\hat{\boldsymbol{p}} = \arg\min_{\boldsymbol{p}} J(\boldsymbol{p}), \tag{2}$$

with

$$J(\boldsymbol{p}) := \sum_{i=1}^{n_y} \sum_{\tau=\tau_1}^{\tau_N} \sigma_i^{-2}(y_{m,i}(\tau) - \hat{y}_i(\boldsymbol{p},\tau))^2. \tag{3}$$

Here $y_{m,i}$ and σ_i represent the plant-output measurement and the standard deviation of the measurement noise for the i^{th} measured output variable, respectively.

The exact joint-confidence region of the uncertain model parameters is defined as a set of all parameters that satisfy the implicit nonlinear inequality (Seber and Wild, 2003)

$$J(\boldsymbol{p}) - J(\hat{\boldsymbol{p}}) \leq \chi^2_{\alpha,n_p}. \tag{4}$$

Unlike in the linear parameter estimation, the exact confidence region does not generally take a shape of an ellipsoid due to nonlinearity. We also note that—despite using standard asymptotic confidence regions in this paper—there exist non-asymptotic confidence regions (Campi and Weyer, 2005; Perić et al., 2018) that can be used in nonlinear parameter estimation and also in experiment design through the developments presented here.

2.3 Model-based Design of Experiments

In this paper, we assume that the joint-confidence region of the uncertain model parameters is continuous. It is generally suggested to re-parameterize the model if the joint-confidence region is discontinuous (Bates and Watts, 1988) as this indicates (local) indetifiability issues. Without loss to generality—even for the latter rDoE—we will consider that limits of the experimental degrees of freedom $\boldsymbol{u}_\tau$ are the only constraints for the experiment. We also assume that an estimate $\hat{\boldsymbol{p}}$ is available. The final assumption—inherent to the standard experiment design techniques—is that there exists no structural plant-model mismatch and that the expected realization of the measurement noise is 0. In turn, this results in $\boldsymbol{y}_m(\tau) = \hat{\boldsymbol{y}}(\hat{\boldsymbol{p}},\tau)$, $\forall\tau$.

Several criteria for DoE such as A, D, E, Modified E, V, Q, M and so on are proposed in the literature (Franceschini and Macchietto, 2008). Each of these design criterion aims to tune a specific property of the joint-confidence region. In this study, we use the A design criterion, yet other design criteria might be considered using the ideas presented herein.

The optimization problem of the nonlinear A design can be stated as (Gottu Mukkula and Paulen, 2019)

$$\boldsymbol{u}^\star := \arg\min_{\boldsymbol{u}} \phi_A(\boldsymbol{u}) := \arg\min_{\boldsymbol{u}} \max_{\boldsymbol{\pi}} \sum_{j=1}^{n_p} p_j^U - p_j^L \tag{5a}$$

$$\text{s.t. } \forall\tau \in \{\tau_1,\dots,\tau_N\},\ \forall j \in \{1,\dots,2n_p\}:$$

$$\hat{\boldsymbol{y}}(\boldsymbol{\pi}_j,\tau) = \boldsymbol{F}(\boldsymbol{\pi}_j,\boldsymbol{u}_\tau), \tag{5b}$$

$$\boldsymbol{y}_m(\tau) = \hat{\boldsymbol{y}}(\hat{\boldsymbol{p}},\tau) = \boldsymbol{F}(\hat{\boldsymbol{p}},\boldsymbol{u}_\tau), \tag{5c}$$

$$J(\boldsymbol{\pi}_j) - J(\hat{\boldsymbol{p}}) \leq \chi^2_{\alpha,n_p}, \tag{5d}$$

$$\boldsymbol{u}^L \leq \boldsymbol{u}_\tau \leq \boldsymbol{u}^U. \tag{5e}$$

Here, the vector $\boldsymbol{\pi}$ represents $2n_p$ anchor points

$$\boldsymbol{\pi} := \left\{ \begin{pmatrix} p_1^L \\ p_2^{1,L} \\ \vdots \\ p_{n_p}^{1,L} \end{pmatrix}, \begin{pmatrix} p_1^U \\ p_2^{1,U} \\ \vdots \\ p_{n_p}^{1,U} \end{pmatrix}, \begin{pmatrix} p_1^{2,L} \\ p_2^{L} \\ \vdots \\ p_{n_p}^{2,L} \end{pmatrix}, \cdots, \begin{pmatrix} p_1^{n_p,U} \\ p_2^{n_p,U} \\ \vdots \\ p_{n_p}^{U} \end{pmatrix} \right\}, \tag{6}$$

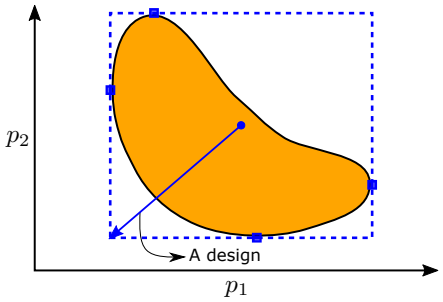

Fig. 1. Illustration of the nonlinear A design.

where each point represents a lower or an upper limit of an uncertain parameter within the exact confidence region. The idea is illustrated in Figure 1 for a two-dimensional parametric space. The anchor points—illustrated by blue squares in Figure 1—are identified by solving the maximization problem in (5), which inflates a box around the confidence region such that the box intersects the confidence at all anchor points (see (5d)) at least in one point. The experiment design objective then acts counteractively and tries to minimize the dimensions of the box. Hence this gives rise to the min-max problem.

Note that the maximization problem in (5) is well structured and separable. Besides that, the maximization problem is non-convex and the number of its optimization variables ($2n_p^2$) grows quadratically with the number of uncertain parameters. Therefore the identification of an orthotope might get challenging for the state-of-the-art solvers and high-dimensional problems.

In this work, we will refer to the presented DoE method as a nominal DoE.

3. ROBUST DESIGN OF EXPERIMENTS

The nominal DoE might be significantly suboptimal if the nominal parameters $\hat{\boldsymbol{p}}$ are far from the true values $\boldsymbol{p}^\star$. In this section, we summarize ways for robustifying the DoE with well-known robust DoE techniques and propose a methodology based on multi-stage decision making. We shall assume that a set $\boldsymbol{P}$ is available such that $\boldsymbol{p}^\star \in \boldsymbol{P}$.

3.1 Sequential Approach

If it is possible to run a series of N_e experiments (adding up to a total of N experiments), sequential design (Barz et al., 2010) is one of the simplest robustifying schemes. Here $\hat{\boldsymbol{p}}$ is iteratively adjusted based on the experiments performed and the nominal design (Section 2.3) is re-conducted. The pseudo-algorithm for the sequential approach is:

1. Set $\hat{\boldsymbol{p}}$ such that $\hat{\boldsymbol{p}} \in \boldsymbol{P}$.
2. Perform the nominal DoE (Section 2.3) for $N_e < N$ experiments using the known value for $\hat{\boldsymbol{p}}$. Get $\boldsymbol{u}^\star$.
3. Conduct the designed N_e according to $\boldsymbol{u}^\star$ and obtain the measurements $\boldsymbol{y}_m$.
4. Compute a new value of $\hat{\boldsymbol{p}}$ and the corresponding confidence region using the least-squares estimation (Section 2.2) over all the past experiments.
5. Go to step 2. unless:
   a. the maximum (user-defined) number of possible experiments was conducted, or
   b. only a marginal (user-defined) improvement of the confidence region—measured by the chosen design criterion—was reached, or
   c. only a marginal (user-defined) update of the least-squares estimates was obtained.
6. Terminate.

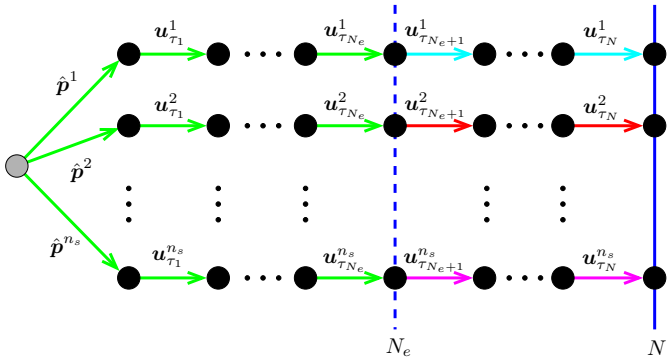

Fig. 2. Illustration of scenario-based and multi-stage DoE.

3.2 Min-max Approach

Min-max formulation of DoE (Pronzato and Walter, 1988) identifies the optimal experiment conditions $\boldsymbol{u}$ under the worst-case realization of $\hat{\boldsymbol{p}} \in \boldsymbol{P}$. For the nonlinear DoE, the formulation reads as

$$\min_{\boldsymbol{u}} \max_{\boldsymbol{\pi},\, \hat{\boldsymbol{p}} \in \boldsymbol{P}} \sum_{j=1}^{n_p} p_j^U - p_j^L \tag{7a}$$

$$\text{s.t. } \forall \tau \in \{\tau_1, \ldots, \tau_N\},\ \forall j \in \{1, \ldots, 2n_p\}:$$

$$\hat{\boldsymbol{y}}(\boldsymbol{\pi}_j, \tau) = \boldsymbol{F}(\boldsymbol{\pi}_j, \boldsymbol{u}_\tau), \tag{7b}$$

$$\boldsymbol{y}_m(\tau) = \hat{\boldsymbol{y}}(\hat{\boldsymbol{p}}, \tau) = \boldsymbol{F}(\hat{\boldsymbol{p}}, \boldsymbol{u}_\tau), \tag{7c}$$

$$J(\boldsymbol{\pi}_j) - J(\hat{\boldsymbol{p}}) \leq \chi^2_{\alpha, n_p}, \tag{7d}$$

$$\boldsymbol{u}^L \leq \boldsymbol{u}_\tau \leq \boldsymbol{u}^U. \tag{7e}$$

We note here that the optimization for the worst case can lead to overly conservative results (Lucia et al., 2013) and its benefits are mostly gained by seeking a feasible design with strict constraints on the experiments.

3.3 Scenario-based Approach

Opposed to the robust min-max design, the idea behind scenario-based DoE (Telen et al., 2014; Welsh and Rojas, 2009) is to optimize for the mean value of the objective under the stochastic realization of the uncertainty. This approach considers n_s discrete realizations (scenarios) of $\hat{\boldsymbol{p}}$ from the set $\boldsymbol{P}$ and is illustrated in Figure 2. The figure shows a scenario tree with black nodes representing N experiments in n_s branches. Each branch represents a particular realization of $\hat{\boldsymbol{p}}$.

In the simplest alternative, the scenarios can be selected as combinations of minimal, nominal and maximal parameter values from $\boldsymbol{P}$ if one assumes a uniform probability distribution of $\hat{\boldsymbol{p}}$ over $\boldsymbol{P}$. If $\boldsymbol{P}$ represents a joint-confidence region, the scenarios can be selected to represent the (approximate) sigma points of $\boldsymbol{P}$ (Nimmegeers et al., 2020). One can also consider scenarios to be the samples from the underlying probability distribution within $\boldsymbol{P}$ (Mesbah and Streif, 2015). In all the cases, one can assign a certain probability to the scenarios selected.

The optimization then seeks a common experiment policy that minimizes the average—weighted by the scenario probability—of the objectives of the individual scenarios. The associated optimization problem in the case of nonlinear DoE is given as

$$\min_{\boldsymbol{u}^s,\forall s\in\{1,\dots,n_s\}} \sum_{s=1}^{n_s} \omega^s \max_{\boldsymbol{\pi}^s} \sum_{j=1}^{n_p} p_j^{U,s} - p_j^{L,s} \tag{8a}$$

$$\text{s.t. } \boldsymbol{u}_\tau^1 = \boldsymbol{u}_\tau^2 = \dots = \boldsymbol{u}_\tau^{n_s},\ \forall \tau \in \{\tau_1,\dots,\tau_N\}, \tag{8b}$$

$$\forall \tau \in \{\tau_1,\dots,\tau_N\},\ \forall j \in \{1,\dots,2n_p\},$$

$$\forall s \in \{1,\dots,n_s\}:$$

$$\hat{\boldsymbol{y}}^s(\boldsymbol{\pi}_j^s,\tau) = \boldsymbol{F}(\boldsymbol{\pi}_j^s,\boldsymbol{u}_\tau^s), \tag{8c}$$

$$\boldsymbol{y}_m^s(\tau) = \hat{\boldsymbol{y}}(\hat{\boldsymbol{p}}^s,\tau) = \boldsymbol{F}(\hat{\boldsymbol{p}}^s,\boldsymbol{u}_\tau^s), \tag{8d}$$

$$J(\boldsymbol{\pi}_j^s) - J(\hat{\boldsymbol{p}}^s) \le \chi^2_{\alpha,n_p}, \tag{8e}$$

$$\boldsymbol{u}^L \le \boldsymbol{u}_\tau^s \le \boldsymbol{u}^U, \tag{8f}$$

where ω^s represents the weight of the sth scenario and $\hat{\boldsymbol{p}}^s$ is the particular realization of $\hat{\boldsymbol{p}}$ in the sth scenario. The problem—compared to the min-max formulation (7)—maintains a highly structured form and the maximization problems are separable. We also note that the scenario-based approach can be a viable alternative to truly robust (min-max) optimization for strictly constrained DoE problems. This is supported by possibility of identifying a worst-case scenario—in terms of feasibility—that is often present in practical applications or can be pre-identified (Holtorf et al., 2019). Such scenarios can then be added among the branches of the scenario tree to guarantee robust feasibility.

3.4 Multi-stage Approach to Robust Design of Experiments

The scenario-based and min-max DoE are one-shot (single-stage) approaches in principle, i.e., all the N experiments are conducted once the design is calculated. Of course, one can combine these approaches with sequential approach for iterative re-design. The major issue within this approach is that the aforementioned designs do not consider explicitly the possibility of re-estimation and re-design based on the available intermediate information.

The explicit consideration of the so-called recourse actions (Garstka and Wets, 1974) gives rise to a multi-stage decision making. Such scheme effectively combines elements of sequential and scenario-based DoE. We illustrate the approach in Figure 2 for a situation of two-stage decision making. The green-colored branches of the scenario tree represent the first-stage decisions, i.e., the design is essentially equivalent to scenario-based DoE. After the N_e^{th} experiment is performed, a sequential-design principle is applied for the second stage over the individual branches. This is represented by the branches of different colors (in Figure 2), which illustrates that the decisions are decoupled and that n_s individual re-designs are performed. The overall optimization takes both stages into account and finds the best conditions for initial N_e experiments, which make the successive $N-N_e$ redesigned (recourse) experiments to minimize the weighted-average performance of the outcome from N experiments. In our previous work, we suggested a similar strategy in the context of set-membership (guaranteed) estimation (Gottu Mukkula and Paulen, 2017b), which offers even more intuitive explanation of the effects of multi-stage decision making on experiment design. The optimization problem for the A optimal design with a multi-stage approach can be formulated by a slight alteration of the scenario-based approach. For completeness, we state the underlying optimization problem here in full length, despite it only requires a minor modification of the problem (8) regarding the so-called non-anticipativity constraints (8b). The problem reads as

$$\min_{\boldsymbol{u}^s,\forall s\in\{1,\dots,n_s\}} \sum_{s=1}^{n_s} \omega^s \max_{\boldsymbol{\pi}^s} \sum_{j=1}^{n_p} p_j^{U,s} - p_j^{L,s} \tag{9a}$$

$$\text{s.t. } \boldsymbol{u}_\tau^1 = \boldsymbol{u}_\tau^2 = \dots = \boldsymbol{u}_\tau^{n_s},\ \forall \tau \in \{\tau_1,\dots,\tau_{N_e}\}, \tag{9b}$$

$$\forall \tau \in \{\tau_1,\dots,\tau_N\},\ \forall j \in \{1,\dots,2n_p\},$$

$$\forall s \in \{1,\dots,n_s\}:$$

$$\hat{\boldsymbol{y}}^s(\boldsymbol{\pi}_j^s,\tau) = \boldsymbol{F}(\boldsymbol{\pi}_j^s,\boldsymbol{u}_\tau^s), \tag{9c}$$

$$\boldsymbol{y}_m^s(\tau) = \hat{\boldsymbol{y}}(\hat{\boldsymbol{p}}^s,\tau) = \boldsymbol{F}(\hat{\boldsymbol{p}}^s,\boldsymbol{u}_\tau^s), \tag{9d}$$

$$J(\boldsymbol{\pi}_j^s) - J(\hat{\boldsymbol{p}}^s) \le \chi^2_{\alpha,n_p}, \tag{9e}$$

$$\boldsymbol{u}^L \le \boldsymbol{u}_\tau^s \le \boldsymbol{u}^U. \tag{9f}$$

Allocation of the number of experiments for the first and the second stage, respectively, is an adjustable parameter. If no prior experimental results are available—i.e., one only possesses the knowledge of $\boldsymbol{P}$—he/she would naturally set N_e such that $N_e \times n_y \ge n_p$ to satisfy the standard minimal identifiability conditions. We note that there are other criteria for selecting the least number of experiments (Georgakis, 2013), yet a study of these aspects is beyond our scope in this paper. A simulation-based tuning is also in principle possible here combined with some previous plant expertise. The case, in which past experiments are available, naturally opens up wider options to tune the parameter N_e especially in situations, where N is relatively small.

The optimization problem (9) is formulated for the two-stage decision making and is thus optimistic. It assumes that a true value of the parameter is inferred once the N_e experiments are conducted. There are two possible modifications for more realistic uncertainty modeling. One represents the use of multi-stage decision making, where one continues to branch the tree after the stage N_e and the optimization thus still accounts for the uncertainty in the recourse experiments. The mathematical formulation of such problem can be derived from our earlier work (Gottu Mukkula et al., 2021). The second option lies in the usage of techniques from a so-called dual control, where the essential part of the technology is the stochastic prediction of future estimates (Filatov and Unbehauen, 2004). As an example, Thangavel et al. (2018) illustrated a dual-control approach in the framework of multi-stage NMPC, which is directly applicable here.

The application of the two-stage design can either be done in an open-loop or in a closed-loop manner. In the open-loop approach, re-estimation is performed at the stage N_e, i.e., after the designed experiments are performed. This is followed by a (nominal) re-design and realization of the remaining experiments. In the closed-loop approach, the two-stage DoE is applied in a moving-horizon fashion, i.e., it is recast from the stage N_e repetitively. The decision of performing open- or closed-loop approach is mainly connected to the number of possible experiments N and to

the quality of estimates obtained at the stage N_e. Similar approaches can be devised for the multi-stage designs.

4. CASE STUDY

We study a two-parameter kinetic model of the reaction A $\xrightarrow{p_1}$ B $\xrightarrow{p_2}$ C taken from Atkinson and Hunter (1968). The concentration of B follows

$$y_\tau = \frac{p_1}{p_1 - p_2} \left(\exp(-p_2 u_\tau) - \exp(-p_1 u_\tau)\right), \qquad (10)$$

where u_τ represents the time at which the concentration of component B is measured. We can observe that both parameters enter the model equation in a nonlinear fashion, which might foreshadow the utility of a robust design.

The true parameter values are unknown but are assumed to lie within $\boldsymbol{P} := [0.55, 0.9] \times [0.1, 0.45]$. The nominal values of parameters are taken as the midpoint of $\boldsymbol{P}$. We consider the measurement error to be a random variable distributed as zero-mean, white Gaussian noise with standard deviation $\sigma = 0.1/3$. The general structure of the designs is to repetitively take (two) measurements at $u_\tau \in [0.9, 1.6]$ to estimate p_1 and $u_\tau \in [5.4, 11.0]$ to estimate p_2.

We test the presented methodologies using the simplest possible setup regarding the number of consecutive DoEs and the number of experiments considered, i.e., $N := 4$ and $N_e := 2$ with two consecutive DoEs and two experiments in each DoE. We generate all the rDoE procedures outlined above using the numerical implementation described in our previous work (Gottu Mukkula and Paulen, 2019).

As the scenario-based designs consider discretization of the set $\boldsymbol{P}$ into finite number of scenarios, we implement the same strategy in the min-max approach to make a fair comparison among these approaches. To solve the arising bi-level programs we use the nested approach (Gottu Mukkula and Paulen, 2019) with BARON (Matlab interface) as a global solver and with *fminunc* (quasi-Newton method option) and *fmincon* (SQP method option) as local solvers. BARON is also used for all the single-level (minimization) problems. All solvers are used with default settings.

The presented rDoE methodologies are evaluated in the following setup: a) In the first stage, the parameters are only known to lie in the set $\boldsymbol{P}$. A designed experiment is executed until N_e measurements are obtained. b) After taking N_e measurements, it is assumed that the least-squares estimation reveals true values of the parameters. This serves for a fair comparison of the designs as it mitigates the effects connected to the actual noise realization. The outlined implementation naturally does not hold for the nominal design, which is evaluated in an open-loop fashion (no re-estimation) and serves as a reference case. The performance of the different designs measured by the true value of A-design criterion is evaluated using Monte Carlo simulation, where the true values of parameters for each simulation are taken from a uniform 10×10 grid discretized from $\boldsymbol{P}$.

We compare the performance of the different methods for rDoE measured by the value of the respective A-optimal design objective function. Figure 3 shows the box

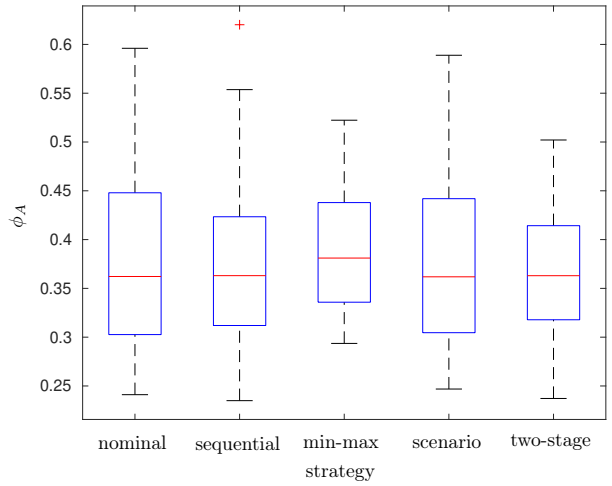

Fig. 3. A box plot of performance of the different approaches to robust nonlinear A design.

plot of performance reached over the 100 Monte Carlo simulations. The central horizontal-line marker indicates the median, the bottom and top edges of the box indicate the 25$^{\text{th}}$ and 75$^{\text{th}}$ percentiles, respectively, the whiskers extend to the most extreme data points not considered outliers, and the outliers are plotted individually using the '+' symbol. First, we can observe that the variance of the performance of the different designs is higher than the differences among them. This can be expected given the analysis concerning model nonlinearity. We can observe that

- Nominal design performs relatively poorly (largest performance variance), which can be expected given the elevated nonlinearity.
- Sequential design achieves the best performance in the best case but does not perform well w.r.t. to the worst case. Also its performance variance is not satisfactory.
- Min-max design gives the worst performance in terms of median and best case as could be expected. Its worst-case performance is very good despite not being the best, contrary to all expectations.
- Scenario-based strategy achieves the best median performance that is, however, outweighed by the large performance variance that diminishes it.
- Two-stage design is the best in terms of the median performance, very good performance w.r.t. the best and the worst case. The improvement in mean performance is around 5% compared to the nominal design. Also its performance variance is comparatively good and definitely better than the closest competitors, i.e., the sequential and scenario-based design.

5. CONCLUSIONS

In this paper, we presented and compared some well-known schemes for robust design of experiments. We have proposed and studied a novel method based on multi-stage decision making, which is found to be a viable methodology for (re-)design of experiments. We used a simple nonlinear case study for evaluation of the presented method and we have shown few interesting insights into the problem of robust DoE. The proposed multi-stage ap-

proach, in the context of the exact joint-confidence region, clearly stands for a viable alternative to more standard robustification approaches to DoE. It achieves very good performance in terms of best-case, median and worst-case performance. We note here that its performance can be even improved in more advanced rolling-horizon strategies, if one considers the setup with unknown measurement variance, or if the number of the experiments to be designed is large.

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