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Uncertainty Quantification and design optimization using multi-objective optimization techniques

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The NASA-DNV challenge problem aims to develop methodologies for Uncertainty Quantification (UQ) in safety-critical and high-consequence systems with sparse or expensive data. The challenge is designed to be discipline-independent while capturing the complexities of real-world engineered systems. It consists of two key problems: (1) quantifying both aleatory and epistemic uncertainties by integrating computational models with real system data, and (2) optimizing control variables to balance performance and risk. Given the presence of conflicting objectives in both problems, multi-objective optimization techniques provide a promising approach for simultaneously addressing these trade-offs. This paper explores the role of multi-objective optimization in UQ and control optimization within the challenge framework.

Keywords: Multiobjective optimization, uncertainty quantification, DNV Challenge.

1. Introduction

The NASA-DNV challenge problem (Agrell et al., 2024) is designed to explore methodologies for Uncertainty Quantification (UQ) in safety-critical and high-consequence systems where data is sparse or expensive to obtain. The problem formulation is intentionally discipline-independent but represents the inherent complexities of real-world engineered systems. The challenge focuses on developing robust methods that can accurately assess uncertainties in system performance under a wide range of operating conditions. The challenge problem consists of two parts. On the one hand, problem 1 is about modeling (quantifying) uncertainty aleatory and epistemic, by using the computational model together with data from the real system. On the other hand, problem 2 is about optimizing the control variables for the system, balancing performance and risk.

In both instances, conflicting objectives arise. When multiple objectives appear, multi-objective optimization techniques can be an appealing strategy due to their capability to simultaneously optimize conflicting objectives. This process leads to the approximation of the so-called Pareto front (Miettinen, 1999), where all solutions are Pareto optimal. The analyst (or designer) must then select the most preferable solution for the problem at hand, with the desired trade-off. Within this context, it could mean the possibility of analyzing different control solutions, for example, and analyzing the trade-off between performance and risk probabilities of them.

Given that, the motivation of this paper is to answer the following question: *how could multi-objective optimization techniques could be of assistance for UM quantification and for design optimization*? Therefore, we propose a multi-objective optimization approach to address the challenge of modeling uncertainty and optimizing control variables in complex systems.

The rest of this work is as follows: in Section 2 a brief theoretical framework on multi-objective optimization techniques is given, with a contextual framework about its usability for modeling and control design. In Section 3 the proposal of this work is stated, with the tools and methods to be used. Results and discussions (still in development) are commented on in Section 4 and Section 5 presents the conclusions of this work (in development).

2. Theoretical framework

Multi-objective optimization can be defined, roughly speaking, as the simultaneous optimization of more than one objective function, searching for a better solution to a mathematical problem. In general, a multi-objective problem, without loss of generality, can be defined as follows:

$$\min_{\boldsymbol{\theta}} \boldsymbol{J}(\boldsymbol{\theta}) = [J_1(\boldsymbol{\theta}), \ldots, J_m(\boldsymbol{\theta})] \tag{1}$$

subject to:

$$\begin{aligned} g(\boldsymbol{\theta}) &\leq 0 \\ h(\boldsymbol{\theta}) &= 0 \\ \underline{\theta_i} \leq \theta_i &\leq \overline{\theta_i}, i = [1, \ldots, n] \end{aligned} \tag{2}$$

where $\boldsymbol{\theta} \in \Re$ is the decision vector, $\boldsymbol{J}(\boldsymbol{\theta})$ is the objective vector, $g(\boldsymbol{\theta})$ and $h(\boldsymbol{\theta})$ are, respectively, the inequality and equality constraints and $\underline{\theta_i} \leq \theta_i \leq \overline{\theta_i}$ are the boundaries of the decision space for the variable $\boldsymbol{\theta}$ (Miettinen, 1999).

It is impossible to have a single solution that is better for all objectives, since improving one objective can worsen a second one. Therefore, a set of solutions classified as optimal is obtained; this set is defined as the Pareto front; each solution of this set defines an objective vector in the Pareto front. All solutions in the Pareto front are considered nondominated solutions; this definition is explained below, and it is depicted in Figure 1:

Pareto Dominance: Given two design objective vectors $J(\theta^1), J(\theta^2)$, objective vector $J(\theta^1)$ dominates $J(\theta^2)$, iif:

$$\begin{aligned} J_i(\theta^1) \leq J_i(\theta^2) \, \forall \, i \in [1, 2, ..., n] \quad and \\ J_j(\theta^1) < J_j(\theta^2) \, \exists \, j \in [1, 2, ..., n] \end{aligned} \tag{3}$$

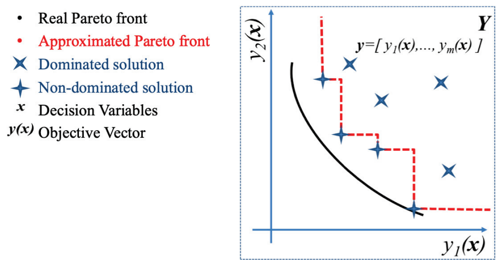

Fig. 1. Pareto optimality and dominance concepts (min-min problem) for design objective $y_1(\boldsymbol{x}), y_2(\boldsymbol{x})$ for decision variables $\boldsymbol{x}$. (Carrau et al., 2017).

In order to have success employing such ideas in engineering design, at least three fundamental steps (Reynoso Meza et al., 2017) must be carried out:

- Multi-Objective Problem (MOP) Statement: In this step, the parametric model, the cost function, the design concept (decision variables), and the constraints must be defined.
- Multi-Objective Optimization (MOO) Process: This step involves applying a multi-objective optimization algorithm to simultaneously optimize all design objectives defined in the previous step. As a result, an approximation of the Pareto front is obtained.
- Multi-Criteria Decision Making (MCDM) Analysis : This step involves analyzing and selecting the most preferable solution from the Pareto optimal set for implementation.

Next, the proposal to use such techniques in the NASA-DNV challenge will be presented.

3. Proposal, tools and methods

Here it is presented the overall pipeline proposal for the challenge, using Multi-objective Optimization Design (MOOD) techniques and Design Science Approach (DSA). Firstly, a brief description of the benchmark is given.

3.1. *Benchmark description*

The input $\boldsymbol{X}$ contains parameters that describe a physical structure and its environment. For this challenge problem, the relevant range of $\boldsymbol{X}$ is standardized, and we let $\boldsymbol{X} \in [0,1]^{n_x}$. The components of $\boldsymbol{X}$ have different characteristics as follows:

$$\boldsymbol{X} = [\boldsymbol{X_a}, \boldsymbol{X_e}, \boldsymbol{X_c}] \tag{4}$$

where:

- $\boldsymbol{X_a} \in \mathbb{R}^{n_a}$ is an **aleatory variable** whose value varies randomly. For this challenge, a given vector $\boldsymbol{X_a} = [x_{a1}, x_{a2}]$.
- $\boldsymbol{X_e} \in \mathbb{R}^{n_e}$ is the **epistemic variable** whose true value X_e^* is unknown. For this challenge, a given vector $\boldsymbol{X_e} = [x_{e1}, x_{e2}, x_{e3}]$.
- $\boldsymbol{X_c} \in \mathbb{R}^{n_c}$ is the **control variable** whose value is to be set by the analyst. For this challenge, a given vector $\boldsymbol{X_c} = [x_{c1}, x_{c2}, x_{c3}]$

The objective is on the one hand to quantify $\boldsymbol{X_a}, \boldsymbol{X_e}$ and on the other hand to determine the control variable $\boldsymbol{X_c}$ that optimizes system performance under uncertainty.

The organizers have provided a model in Matlab to run optimization tests locally and they have also made available a budget of 10 tests in the real model. Local optimizations are carried out with the model provided by the organizers and with access to the ”real model” to get new data on the system.

3.2. *Overall Methodology*

The methodology employed in this work is based on the multi-objective optimization design (MOOD) framework previously described (MOP statement, MOO process, and MCDM analysis). In particular, MCDM analysis plays a crucial role in two aspects: first, to provide an estimate of the model uncertainties and second, to enable the selection of robust decisions.

At a high level, the Design Science Approach (DSA) is used to facilitate iterative optimization cycles. The DSA is a research methodology focused on the iterative development and evaluation of entities (such as models, algorithms, and decision-making frameworks) to address complex real-world problems. Unlike purely descriptive research methods, DSA emphasizes the creation of innovative solutions through a cycle of problem identification and motivation, definition of objectives for a solution, design and development, demonstration, evaluation, and communication (Peffers et al., 2007). In the context of this study, the DSA enables a structured refinement of both optimization models and decision-making processes by integrating new insights obtained from each iteration (Ribeiro and Reynoso-Meza, 2024). This ensures that the optimization framework remains adaptable and robust as more data and experimental results become available. Similar ideas have previously been explored with multiobjective optimization techniques in Carrau et al. (2017); Reynoso-Meza et al. (2019).

Specifically, an initial MOO process is executed to quantify uncertainty $\boldsymbol{X}_a$, $\boldsymbol{X}_e$, followed by the selection of a probable operating scenario for the designed system, via MCDM analysis in the approximated Pareto front. Subsequently, another MOO is performed to assess the performance of the control subsystem $\boldsymbol{X}_c$. The results obtained are then tested in the original model, and the collected information is fed back into the process for a new iteration. This iteration may involve modifying the design objectives or adjusting the parametric models used in the optimization.

Next, the MOP, MOO and MCDM for the NASA-DNV challenge will be explained.

3.3. *Multi-objective Problem statement*

As previously mentioned, two multi-objective problems will be stated and their Pareto fronts approximated. The first MOP (5) aims to quantify uncertainty through a six-objective multi-objective identification problem. This MOP evaluates the probability of a given output $\boldsymbol{Y}(\boldsymbol{X_a}, \boldsymbol{X_e}, \hat{\boldsymbol{X}}_{\boldsymbol{c}})$ to belong to the dataset of outputs provided by the real model with a fixed $\hat{\boldsymbol{X}}_{\boldsymbol{c}}$.

$$\max_{\tilde{\boldsymbol{X}}_{\boldsymbol{a}}, \boldsymbol{X_e}} \boldsymbol{J}\left(\tilde{\boldsymbol{X}}_{\boldsymbol{a}}, \boldsymbol{X_e}, \hat{\boldsymbol{X}}_{\boldsymbol{c}}\right) = [\mathcal{L}_1\left(\tilde{\boldsymbol{X}}_{\boldsymbol{a}}, \boldsymbol{X_e}, \hat{\boldsymbol{X}}_{\boldsymbol{c}}\right), \ldots, \mathcal{L}_6\left(\tilde{\boldsymbol{X}}_{\boldsymbol{a}}, \boldsymbol{X_e}, \hat{\boldsymbol{X}}_{\boldsymbol{c}}\right)] \quad (5)$$

Where $\mathcal{L}_i\left(\boldsymbol{X_a}, \boldsymbol{X_e}, \hat{\boldsymbol{X}}_{\boldsymbol{c}}\right)$ is the the log-likelihood of a candidate solution $\hat{\boldsymbol{Y}}_i$, $i \in [1, \ldots, 6]$. $\tilde{\boldsymbol{X}}_{\boldsymbol{a}}$ represents the parameters for a beta distribution to approximate the distribution of the aleatory variables. The choice of the beta distribution to model the two aleatory uncertainty variables is justified by its flexibility in representing a wide range of behaviors over the $[0, 1]$ interval, from uniform to highly skewed shapes. Given the absence of prior knowledge about the true distributions, the beta family provides a minimal-assumption with an interpretable and flexible structure to approximate a model of such uncertainty.

In order to evaluate this likelihood of a given solution, a non-parametric probability density estimation method (KDE), is employed. The design objective is formulated as the maximization of the log-likelihood of the solution under the estimated probability distribution. To achieve this, the initial step involves utilizing the control vector $\hat{\boldsymbol{X}}_{\boldsymbol{c}} = [0.533, 0.666, 0.500]$ provided by the challenge organizers and evaluating it against the available model data.

The second MOP (6) involves parametric modeling for control. After performing the multi-criteria decision analysis on the Pareto front obtained in the previous MOP-1, the next step is to analyze the most probable values for $\boldsymbol{X_a}, \boldsymbol{X_e}$. Based on this analysis, the control vector $\boldsymbol{X_c}$ will be optimized for a specific seed instance[a]. The optimization objectives in this case will focus on the three system outputs $\hat{Y}_i, i = [1, 2, 3]$ while ensuring that the model constraints $\hat{Y}_i, i = [4, 5, 6]$ are satisfied. Following the Pareto front analysis, an optimal control vector will be selected for implementation in the real system.

$$\max_{\boldsymbol{X_c}} \boldsymbol{J}(\boldsymbol{X_c}) = [Perf(\boldsymbol{X_c}), -Var(\boldsymbol{X_c}), Ctn(\boldsymbol{X_c})] \quad (6)$$

subject to:

$$0 \leq x_i \leq 1, i = [6, \ldots, 8]$$

where $Per(\boldsymbol{X_c})$ is the performance (ad defined in the challenge) at 95 percentile given 25 scenarios; $Var(\boldsymbol{X_c})$ the difference between 5 and 95 percentile of the performance; and $Ctn(\boldsymbol{X_c})$ the worst case scenario for the constraints.

3.4. *Multi-objective optimization process*

The optimization process is carried out using the *spMODEx* algorithm[b]. *spMODEx* belongs to the family of spMODE algorithms (Reynoso-Meza et al., 2014), which have been widely applied and documented in controller tuning tasks in control systems (Reynoso-Meza et al., 2022). It is a population-based algorithm that incorporates the following key features:

- The core search mechanism of the algorithm is based on the Differential Evolution (DE) algorithm (Pant et al., 2020), which is widely documented in the scientific literature for its effectiveness in population-based optimization.
- To ensure diversity in Pareto front solutions, it employs a spherical coordinate grid mechanism. This approach guarantees that only one solution is retained within each sector of the spherical grid, preventing solution clustering and promoting a well-distributed front.

[a]It is true that this can lead to a bias in the optimization, however by performing the optimization on various scenarios we hope to adequately capture the variability in the response.

[b]Available at `https://www.mathworks.com/matlabcentral/fileexchange/65145`.

- To enhance the relevance of the solutions, it integrates a preference-based selection mechanism inspired by Physical Programming techniques (Melachrinoudis et al., 2005). This allows for a guided selection of the most pertinent region of the Pareto front according to predefined preferences.

3.5. *Multi-criteria decision making and analysis*

In both optimization problems, Pareto fronts are approximated as the result of the multi-objective optimization process. To facilitate the analysis and selection of solutions, we employ *Parallel Coordinates* (Johansson and Forsell, 2015), a well-documented technique for visualizing multidimensional Pareto fronts.

Parallel Coordinates provide an effective way to represent high-dimensional data by transforming each multidimensional point into a set of connected line segments. Formally, let $\boldsymbol{J}(\boldsymbol{\theta}))$ $= [J_1(\boldsymbol{\theta})), \ldots, J_m(\boldsymbol{\theta})]$ be a solution in the m-dimensional objective space, where $J_i(\boldsymbol{\theta}))$ represents the i-th objective function value of a given solution $\boldsymbol{\theta})$. The projection of this solution in Parallel Coordinates is defined as:

$$P(\boldsymbol{\theta}) = \{(i, S_i(\boldsymbol{\theta}) \mid i = 1, 2, \ldots, m\}, \quad (7)$$

where:

- $P(\boldsymbol{\theta})$ represents the transformed representation of $\boldsymbol{\theta}$ in Parallel Coordinates.
- Each objective $J_i(\boldsymbol{\theta})$ is mapped to a normalized scale $S_i(\boldsymbol{\theta})$, given by:

$$S_i(\boldsymbol{\theta}) = \frac{J_i(\boldsymbol{\theta}) - \min\limits_{\boldsymbol{\theta}\in\boldsymbol{\Theta}} J_i(\boldsymbol{\theta})}{\max\limits_{\boldsymbol{\theta}\in\boldsymbol{\Theta}} J_i(\boldsymbol{\theta}) - \min\limits_{\boldsymbol{\theta}\in\boldsymbol{\Theta}} J_i(\boldsymbol{\theta})}, \quad (8)$$

  ensuring that all values are normalized between 0 and 1.
- The transformed solution is plotted by connecting the points $(i, S_i(\boldsymbol{\theta}))$ for all i sequentially, creating a set of polyline segments.

4. Results and discussions

The results of applying the ideas presented in Section 3 to the Challenge are presented below. They have been divided into two subsections: one focusing on the quantification of uncertainty, and the other on the optimization of the device's performance.

In total, three cycles of Design Science Research were applied to produce the results presented in this section. The main outcome of the first cycle was the refinement of the design objective functions used in the multi-objective problems. The second cycle focused on the definition and tuning of the algorithm's hyperparameters. The third cycle yielded the final results, which are presented in the following subsections.

4.1. *Result on uncertainty model quantification*

Figure 2 shows the approximated Pareto front obtained for the uncertainty quantification problem. The magenta dashed lines represent the Pareto front approximation in parallel coordinates across the six design objectives. The blue lines indicate the solutions from the Pareto front that were selected during the decision-making process. The decision making consisted in evaluating for 100 scenarios the similarity (instead of 25) and applying a dominance filter.

In Figure 3, the Pareto front is further analyzed to estimate the uncertainty-related variables in the model, including both aleatory and epistemic uncertainty. The figure presents boxplots showing the range of the variables identified during the multi-objective optimization. The blue boxplots correspond to the original Pareto front solutions, while the red boxplots represent the filtered solutions after the decision-making step.

The first four variables in the plot refer to the parameters of the Beta distribution function, which were used to model the aleatory uncertainty. The last three variables are associated with epistemic uncertainty. These variable ranges were then used in subsequent analyses.

As the most probable value set, we selected the solution highlighted in Figure 2, which sacrifices similarity with the *exchange*-related con-

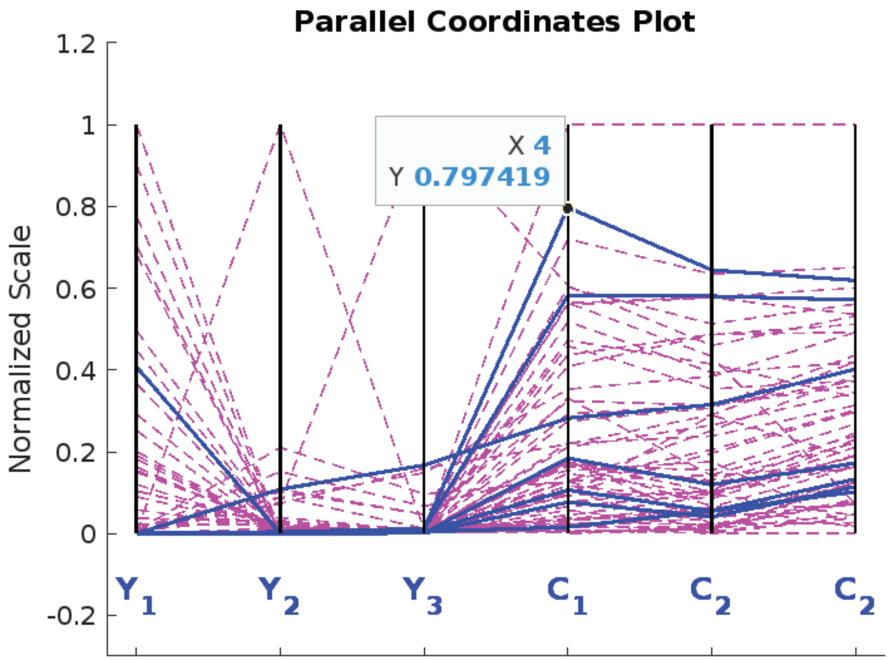

Fig. 2. Pareto front approximated for uncertainty modeling.

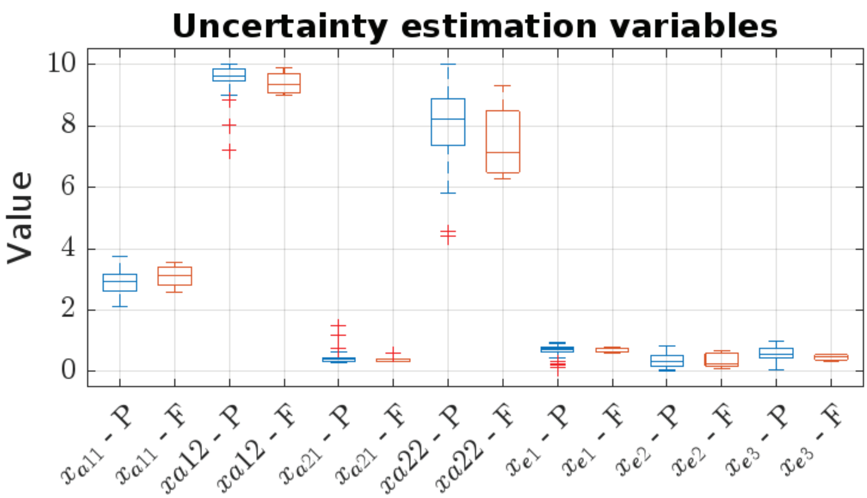

Fig. 3. Uncertainty model extracted from the Pareto front approximation fo Figure 2.

straints in favor of improved performance-related variables. The selected values for the epistemic variables (as the most probable) are $\boldsymbol{X_e} = [0.6327, 0.1751, 0.4497]$, while the intervals for each were stated as $x_{e1} \in [0.6124, 0.7948]$, $x_{e2} \in [0.0896, 0.6776]$, $x_{e3} \in [0.3365, 0.5600]$. Those values are determined by the maximum and minimum values of x_{ei}, $i \in [1, 2, 3]$ of the approximated Pareto front after the decision-making step. The variables selected for the beta distribution for the aleatory variables are $\tilde{\boldsymbol{X}}_{\boldsymbol{a}} = [3.1053, 9.0497, 0.3861, 7.1219]$.

4.2. *Results on Control design*

Figure 4 presents the results of the performance optimization process, where the control variables were treated as decision variables. The uncertainty model—comprising both aleatory and epistemic components was defined using the ranges identified in the previous subsection. For each candidate set of control variables, 25 simulations were executed using random samples of the aleatory variables to evaluate the performance.

After approximating the Pareto front shown in Figure 4, a decision-making procedure similar to the one described in the previous subsection was applied. The Pareto-optimal solutions were re-evaluated over 100 uncertainty scenarios, and any solutions that were found to be dominated under this more extensive evaluation were discarded.

In the plot, magenta dashed lines represent the original approximated Pareto front in parallel coordinates, while solid blue lines highlight the three remaining non-dominated solutions after filtering. The trade-off between constraint margin and variability is particularly evident through the crossing of lines across axes. These three robust solutions were subsequently evaluated using the high-fidelity model. Among them, solution $\boldsymbol{X_c} = [0.4828, 0.4970, 0.6601]$ demonstrated the best optimization of performance under uncertainty, and was therefore selected as the final design solution. Nevertheless, via the Pareto front approximation analysis, a different design alternative could be selected, with a more preferable balance between performance and risk for a given mission. This could be handy in incorporating the experience of decision makers (mission analysts) to select an alternative fulfilling the desirable trade-off. For the selected solution (hereafter $\boldsymbol{X_{c,DM}}$), the interval of the performance over the 100 scenarios is $Perf(\boldsymbol{X_{c,DM}}) \in [3.35, 10.05]$.

5. Conclusions

This work presented a multi-objective optimization based approach to address the DNV-NASA benchmark. By applying a structured pipeline grounded in Design Science Research methodology, it was possible to both characterize the uncertainty model and optimize the control variables of the system. The first stage focused on uncertainty quantification, while the second tackled performance optimization under uncertain conditions.

The methodology proved effective in selecting robust solutions that balance performance, variability, and fulfilling constraints. As future work, we aim to address the remaining challenges of the benchmark, as the present study focused only on the two problems: those related to uncertainty modeling and control optimization.

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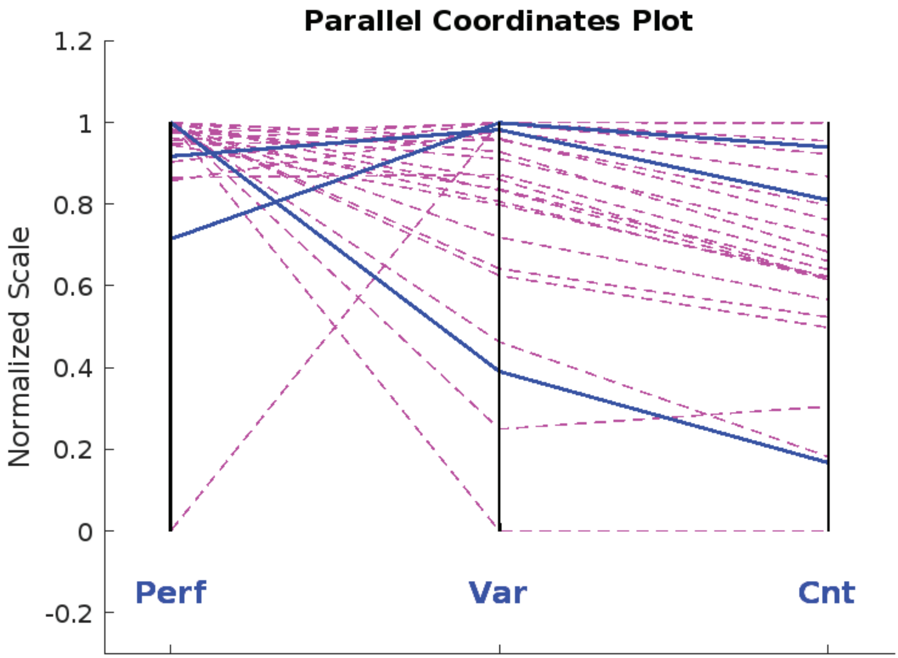

Fig. 4. Pareto front approximated for control optimization.

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