Handling uncertainty in higher dimensions with potential clouds towards robust design optimization

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Abstract Robust design optimization methods applied to real life problems face some major difficulties: how to deal with the estimation of probability densities when data are sparse, how to cope with high dimensional problems and how to use valuable information provided in the form of unformalized expert knowledge. We introduce the *clouds* formalism as means to process available uncertainty information reliably, even if limited in amount and possibly lacking a formal description. We provide a worst-case analysis with confidence regions of relevant scenarios which can be involved in an optimization problem formulation for robust design.

1 Background

Robust design is the art of safeguarding reliably against uncertain perturbations while seeking an optimal design point. In every design process an engineer faces the task to qualify the object he has designed to be robust. That means the design should not only satisfy given requirements on functionalities, but should also work under uncertain, adverse conditions that may show up during employment of the designed object.

Hence the process of robust design demands both the search of an optimal design with respect to a given design objective, and an appropriate method of handling uncertainties. In particular for early design phases, it is frequent engineering practice to assign and refine intervals or safety margins to the uncertain variables. These intervals or safety margins are propagated within the whole optimization process. Thus the design arising from this process is supposed to include robustness intrinsically. Note that the assessment of robustness is exclusively based on expert knowledge of the engineers who

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assign and refine the intervals. There is no quantification of reliability, no rigorous worst-case analysis involved.

Several methods exist to approach reliability quantification from a rigorous mathematical background, originating from classical probability theory, statistics, or fuzzy theory. However, real life applications of many methods disclose various problems. One of the most prominent is probably the fact that the dimension of many uncertain real life scenarios is very high. This can cause severe computational effort, even given the complete knowledge about the multivariate probability distributions of the uncertainties, also famous as the curse of dimensionality [Koch et al(1999)]. Often standard simulation techniques are used to tackle the dimensionality issue, as the computational effort they require seems to be independent of the dimension. Advancements have been made based on sensitivity analysis [Oberguggenberger et al(2007)], or on α-level optimization, cf. [Möller and Beer(2004)]. Moreover, if the amount of available uncertainty information is very limited, well-known current methods like Monte Carlo either do not apply at all, or are endangered to critically underestimate error probabilities, [Ferson(1996)]. A simplification of the uncertainty model, e.g., a reduction of the problem to an interval analysis after assigning intervals to the uncertainties as described before (e.g., so called 3 σ boxes), entails a loss of valuable information which would actually be available, maybe only unformalized, but not at all considered in the uncertainty model. Incomplete information supplemented by expert statements can be handled with different methods, e.g.: p-boxes [Ferson(2002)], fuzzy sets [Dubois and Prade(1986)], random sets [Molchanov(2005)]. A combination of uncertainty methods and design optimization is addressed in approaches to reliability based design optimization: based on reliability methods [Kaymaz and Marti(2007)]; based on possibility theory in [Mourelatos and Zhou(2005)]; based on evidence theory in [Mourelatos and Zhou(2006)].

This paper is organized as follows. We will start introducing our approach based on the clouds formalism and lead to the the special case of interest in this study, cf. Section 2.1: the concept of potential clouds. Several remarks on suitable potential function choices are given in Section 2.2. A short introduction how clouds can be involved in an optimization problem formulation for robust design can be studied in Section 2.3. Section 3 concludes our studies.

2 Introducing the new approach

Our work deals with a new approach based on the *clouds* formalism, cf. [Neumaier(2004)]. Clouds can process limited amounts of stochastic information in an understandable and computationally attractive way, even in higher dimensions, in order to perform a reliable worst-case analysis, reasonably safeguarded against perturbations that result from unmodeled or unavailable information. Since the strength of our new methodology lies especially in the application to real life problems with a very limited amount of uncertainty information available, we focus in particular on problem statements arising in early design phases where today's methods handling limited information are very immature. On the one hand, the information is usually available as bounds or marginal probability distributions on the uncertain variables, without any formal correlation information. On the other hand, unformalized expert knowledge will be captured to improve the uncertainty model adaptively by adding dependency constraints to exclude scenarios deemed irrelevant. The information can also be provided as real sample data, if available.

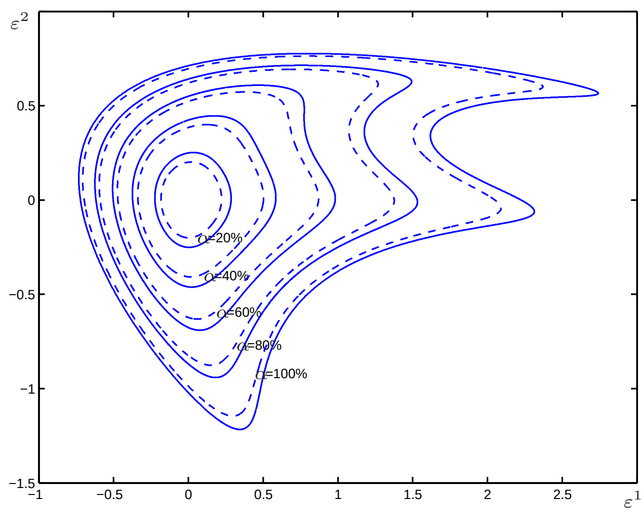

Fig. 1 Nested confidence regions in two dimensions for confidence levels $\alpha = 0.2, 0.4, 0.6, 0.8, 1$. The lower confidence regions $\underline{C}_\alpha$ plotted with dashed lines, the upper confidence regions $\overline{C}_\alpha$ with solid lines.

If we have a look at Figure 1, we see confidence levels on some two dimensional random variable ε. The curves displayed can be considered to be level sets of a function $V(\varepsilon) : \mathbb{R}^2 \to \mathbb{R}$, called the potential. The potential characterizes confidence regions $C_\alpha := \{\varepsilon \in \mathbb{R}^2 \mid V(\varepsilon) \leq V_\alpha\}$, where V_α is determined by the condition $\Pr(\varepsilon \in C_\alpha) = \alpha$. If the probability information is not precisely known nested regions are generated

$$\underline{C}_\alpha := \{\varepsilon \in \mathbb{R}^2 \mid V(\varepsilon) \leq \underline{V}_\alpha\},$$

where $\underline{V}_\alpha$ is largest such that $\Pr(\varepsilon \in \underline{C}_\alpha) \leq \alpha$, and

$$\overline{C}_\alpha := \{\varepsilon \in \mathbb{R}^2 \mid V(\varepsilon) \leq \overline{V}_\alpha\},$$

where $\overline{V}_\alpha$ is smallest such that $\Pr(\varepsilon \in \overline{C}_\alpha) \geq \alpha$. The information in $\underline{C}_\alpha$ and $\overline{C}_\alpha$ is called a *potential cloud*. The values V_α, $\underline{V}_\alpha$, $\overline{V}_\alpha$ can be found from the cumulative distribution function (CDF) of $V(\varepsilon)$ and lower and upper bounds of it. These bounds in turn can be determined empirically using the Kolmogoroff-Smirnov (KS) distribution [Kolmogoroff(1941)].

2.1 Potential cloud generation

We assume that the uncertainty information consists of given samples, boxes, non-formalized dependency constraints or continuous marginal CDFs F_i, $i \in I \subseteq \{1, 2, \dots, n\}$, on the n-dimensional vector of uncertainties ε, without any formal knowledge about correlations or joint distributions. In case there is no sample provided or the given sample is very small, a sample S has to be generated. For these cases we first use a Latin Hypercube Sampling (LHS) inspired method to generate S, i.e., the sample points $x_1, x_2, \dots, x_{N_S}$ are chosen from a grid satisfying $x_i^j \neq x_k^j\ \forall i, k \in \{1, 2, \dots, N_S\}, k \neq i, \forall j \in \{1, 2, \dots, n\}$, where x_i^j is the projection of x_i to the j^{th} coordinate. If only boxes for ε are given, then the grid is equidistant, if marginal distributions are given the grid is transformed with respect to them to ensure that each grid interval has the same marginal probability. LHS introduces some preference for a simple structure. The effect of this preference will be diminished by weighting of the sample points.

The generated sample represents the marginal distributions. However after a modification of S, e.g., by cutting off sample points as we will do later, an assignment of weights to the sample points is necessary to preserve the marginal CDFs. In order to do so the weights $\omega_1, \omega_2, \dots, \omega_{N_S} \in [0, 1]$, corresponding to the sample points $x_1, x_2, \dots, x_{N_S}$, are required to satisfy the following conditions (1)

$$\sum_{j=1}^{k} \omega_{\pi_i(j)} \in [F_i(x^i_{\pi_i(k)}) - d, F_i(x^i_{\pi_i(k)}) + d], \qquad \sum_{k=1}^{N_S} \omega_k = 1. \tag{1}$$

for all $i \in I, k = 1, \dots, N_S$, where π_j is a sorting permutation of $\{1, \dots, N_S\}$, such that $x^j_{\pi_k(1)} \leq x^j_{\pi_k(2)} \leq \cdots \leq x^j_{\pi_k(N_S)}$, and I the index set of those entries of the uncertainty vector ε where a marginal CDF $F_i, i \in I$ is given. The constraints (1) require the weights to represent the marginal CDFs with some reasonable margin d. In practice, one chooses d with KS statistics.

We determine bounds on the CDF of $V(\varepsilon)$ by $\overline{F} := \min(\widetilde{F} + D, 1)$ and $\underline{F} := \max(\widetilde{F} - D, 0)$, where $\widetilde{F}(\xi) := \sum_{\{j \mid V(x_j) \leq \xi\}} \omega_j$ the weighted empirical distribution for $V(\varepsilon)$, and D is again chosen with KS statistics. Finally we fit the two step functions $\underline{F}$, $\overline{F}$ to smooth, monotone lower bounds $\underline{\alpha}$ and upper bounds $\overline{\alpha}$. From these bounds the regions $\underline{C}_\alpha$, $\overline{C}_\alpha$ can be computed straightforward.

Lower and upper bounds of empirical CDFs remind of p-boxes. In fact a potential cloud can be considered as a p-box on the potential of a random vector. Clouds extend the p-box concept to the multivariate case without the exponential growth of work in the conventional p-box approach. Furthermore, clouds can be considered as fuzzy sets with interval valued membership function or as a special case of random sets.

2.2 Choice of the potential

We see that given a potential the corresponding potential cloud is easy to estimate, even for high dimensional data. The choice of the potential is dictated by the shape of the points set defined by the sample of available ε. We are looking for a way to find a good choice of V that gives the possibility to improve the potential iteratively and allows for a simple computational realization of the confidence regions, e.g., by linear constraints. This leads us to the investigation of polyhedron-shaped potentials. A polyhedron potential centered at $m \in \mathbb{R}^n$ can be defined as:

$$V_p(\varepsilon) := \max_k \frac{(A(\varepsilon - m))^k}{b^k}, \tag{2}$$

where $\varepsilon, b \in \mathbb{R}^n, A \in \mathbb{R}^{n \times n}$, $(A(\varepsilon - m))^k, b^k$ the k^{th} component of the vectors $A(\varepsilon - m)$ and b, respectively.

But how to achieve a polyhedron that reflects the given uncertainty information in the best way? As mentioned we assume the uncertainty information to consist of given samples, boxes or marginal distributions, and unformalized dependency constraints. After providing a sample S as described in Section 2.1 we define a box b_0 containing 100% of the sample points, and we define our potential $V_0(\varepsilon)$ box-shaped taking the value 1 on the margin of b_0. Based on expert knowledge, a user-defined variation of V_0 can be performed afterwards by cutting off sample points deemed irrelevant for the worst-case, cf. Figure 2: The optimization phase (cf. Section 2.3) provides a worst-case scenario which is highlighted in the graphical user interface. The expert can decide to exclude, e.g., the worst-case or different scenarios, based on his technical knowledge. Thus an expert can specify the uncertainty information in the form of dependency constraints adaptively, even if the expert knowledge is only little formalized, resulting in a polyhedron shaped potential.

Assume the linear constraints $A(\varepsilon - \mu) \leq b$ represent the exclusion of sample points and the box constraint from b_0, we define our polyhedron shaped potential as in (2) with $m = \mu$.

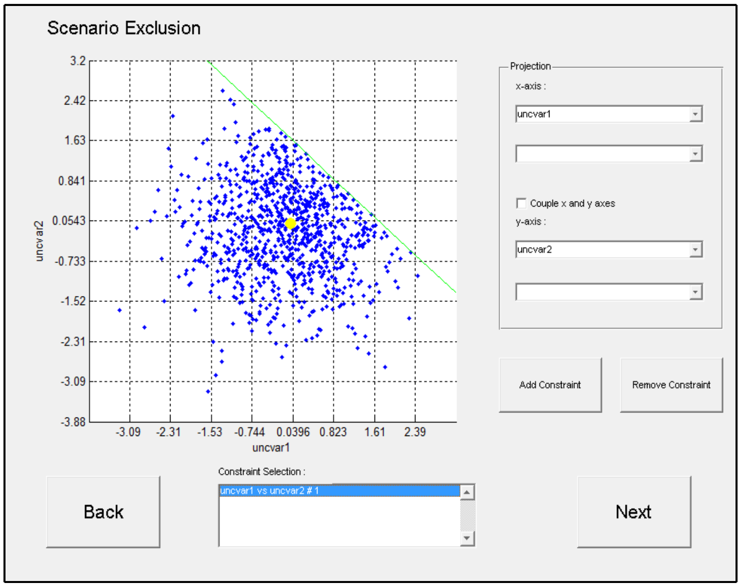

Fig. 2 Graphical user interface for an interactive scenario exclusion. The exclusion is performed in 1 and 2 dimensional projections.

Further details on the construction of potential clouds and the choice of the potential function can be studied in [Fuchs and Neumaier(2008b)].

2.3 Robust design optimization problem

In this section we give a short introduction how potential clouds can be involved in an optimization problem formulation for robust design. Provided an underlying model of a given structure to be designed, with an objective function $g(z)$ and input vector z. Let θ be a design point, i.e., it fully defines the design. Let T be the set of all allowed designs. The input variables z consist of design variables which depend on the design θ, e.g., the thrust of a thruster, and external inputs with a nominal value that cannot be controlled for the underlying model, e.g., a specific temperature. Let $Z(\theta)$ be the input vector given θ and given the external inputs at their nominal values.

The input variables are affected by uncertainties. Let ε denote the related vector of uncertain errors. One can formulate the optimization problem as a mixed-integer, bi-level problem of the following form:

$$
\begin{aligned}
&\min_{\theta}\ \max_{\varepsilon}\ g(z) && \text{(objective function)} \\
&\text{s.t.} \quad z = Z(\theta) + \varepsilon && \text{(input constraints)} \\
&\qquad\ \ \theta \in T && \text{(selection constraints)} \\
&\qquad\ \ V_p(\varepsilon) \le \underline{V}_\alpha && \text{(cloud constraint)}
\end{aligned} \tag{3}
$$

The cloud constraint involves confidence regions as level sets of the potential function $V = V_p(\varepsilon)$ as described previously. The confidence level α should be chosen to reflect the seriousness of consequences of the worst case event. In our applications from spacecraft system design we used $\alpha = 0.95$, cf. [Fuchs et al(2008)]. The cloud constraint models the embedding of the uncertainty methods into the optimization phase.

A detailed view on the optimization techniques used to solve (3) is given in [Fuchs and Neumaier(2008a)].

3 Summary

We present a new methodology based on clouds to provide confidence regions for safety constraints in robust design optimization. We can process the uncertainty information from expert knowledge towards a reliable worst-case analysis, even if the information is limited in amount and high dimensional.

We can summarize the basic concept of our methodology in three essential steps within an iterative framework. First, the expert provides the underlying system model, given as a black-box model, and all a priori available information on the input variables of the model. Second, the information is processed to generate a potential cloud thus producing safety constraints for the optimization. Third, optimization methods minimize a certain objective function subject to the functional constraints which are represented by the system model, and subject to the safety constraints from the cloud. The results of the optimization are returned to the expert, who is given an interactive possibility to provide additional information a posteriori and to rerun the procedure, adaptively improving the uncertainty model.

The adaptive nature of our uncertainty model, i.e., the possibility of manually adding dependency constraints, is one of the key features. The iteration steps significantly improve the uncertainty information and we are able to process the new information to an improved uncertainty model.

All in all, the presented approach offers an attractive novel point of view on high dimensional uncertainty handling and its involvement to robust design.

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