Simulation based uncertainty handling with polyhedral clouds

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Abstract. Past studies of uncertainty handling with polyhedral clouds have already shown strength in dealing with higher dimensional uncertainties in robust optimization, even in case of partial ignorance of statistical information. However, in thousands or more dimensions current implementations would still be computationally too expensive to be useful in real-life applications.

In this paper we propose a simulation based approach for optimization over a polyhedron, inspired by the Cauchy deviates method. Thus we achieve a computationally efficient method to use polyhedral clouds also in very high dimensions.

Keywords: clouds; robust optimization; high-dimensional uncertainty handling; Cauchy deviates method; incomplete information.

1. Introduction

Uncertainty modeling is an everyday task in human real-life: when one estimates the time to get to the workplace, when one tries to assess whether the fuel of the car suffices for that trip etc. Sometimes it can be a very difficult task, and so finding a good mathematical description for uncertainty modeling can also comprise severe difficulties. Some of the most critical issues are lack of statistical information and the well-known curse of dimensionality, see, e.g., (Koch et al., 1999).

In lower dimensions, lack of information can be handled reliably with several tools, e.g., p-boxes (Berleant and Cheng, 1998; Ferson, 2002), Dempster-Shafer structures (Shafer, 1976), however, in higher dimensions (say, greater than 10) there exist only very few. Often simulation techniques are used, but they may fail to be reliable in many cases, see, e.g., (Ferson et al., 1996). The clouds formalism (Neumaier, 2004), being a mixture of interval and fuzzy set methods, is one possibility to deal with both incomplete and higher dimensional information in a reliable and computationally tractable fashion. Still, in thousands or more dimensions current implementations would be computationally too expensive to be useful in real-life applications.

In this paper we present a method that first uses the clouds approach to determine a polyhedral representation of the uncertainties, that means, the set in which we search for worst-case scenarios with respect to the given uncertainties is a polyhedron. Methods to generate this polyhedron already exist, cf. (Fuchs and Neumaier, 2009). In the second step, to actually find the worst-case scenario, we need to solve an optimization problem subject to polyhedral constraints. For very high-dimensional problems we propose a solution approach that is computationally very attractive and can be easily parallelized, inspired by the simulation based Cauchy deviates method for interval uncertainty (Kreinovich and Trejo, 2001; Kreinovich and Ferson, 2004; Kreinovich et al., 2007).

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The new approach will be applied in the context of robust optimization. The worst-case analysis is embedded in an optimization problem formulation as additional constraints, cf. (Fuchs and Neumaier, 2009). Typical difficulties imposed by these problems are, e.g., nonlinear, or black box objective functions, or mixed integer variables. As test cases we use two applications from space system design, cf. (Fuchs et al., 2008; Neumaier et al., 2007).

This paper is organized as follows. We introduce the concept of polyhedral clouds in Section 2. The connection to robust optimization is illustrated in Section 3. The core part of the paper can be found in Section 4 presenting in detail the worst-case analysis for the robust optimization. In Section 5 we perform numerical experiments in two test cases from real-life spacecraft design.

2. Polyhedral clouds

Let ε be an n-dimensional random vector. A **potential cloud** is an interval-valued mapping $x \to [\underline{\alpha}(V(x)), \overline{\alpha}(V(x))]$, with the potential function $V : \mathbb{R}^n \to \mathbb{R}$ bounded below, and $\underline{\alpha}, \overline{\alpha} : V(\mathbb{R}^n) \to [0, 1]$ are functions constructed to be a lower and upper bound, respectively, for the cumulative distribution function (CDF) F of $V(\varepsilon)$, $\underline{\alpha}$ continuous from the left and monotone, $\overline{\alpha}$ continuous from the right and monotone.

We define the so-called **lower α-cut** $\underline{C}_\alpha := \{x \in \mathbb{R}^n \mid V(x) \leq \underline{V}_\alpha\}$ if $\underline{V}_\alpha := \min\{V_\alpha \in \mathbb{R} \mid \overline{\alpha}(V_\alpha) = \alpha\}$ exists, and $\underline{C}_\alpha := \emptyset$ otherwise; analogously we define the **upper α-cut** $\overline{C}_\alpha := \{x \in \mathbb{R}^n \mid V(x) \leq \overline{V}_\alpha\}$ if $\overline{V}_\alpha := \max\{V_\alpha \in \mathbb{R} \mid \underline{\alpha}(V_\alpha) = \alpha\}$ exists, and $\overline{C}_\alpha := \mathbb{R}^n$ otherwise. This gives a nested collection of lower and upper confidence regions in the sense that $\Pr(\varepsilon \in \underline{C}_\alpha) \leq \alpha$, $\Pr(\varepsilon \in \overline{C}_\alpha) \geq \alpha$, and $\underline{C}_\alpha \subseteq \overline{C}_\alpha$.

Note that lower and upper α-cuts $\underline{C}_\alpha, \overline{C}_\alpha$ are level sets of the potential function V. By selecting V reasonably one gets an uncertainty representation of high-dimensional, and possibly incomplete or **unformalized knowledge**, cf. (Fuchs and Neumaier, 2009). Formalized knowledge can be given, e.g., as marginal CDFs, interval bounds on single variables, or real sample data. Moreover, in real-life situations there is typically a significant amount of unformalized knowledge available based on expert experience, e.g., knowledge about the dependence of variables without any precise statistical correlation information.

In (Fuchs and Neumaier, 2009) we learn that a natural way of uncertainty elicitation given incomplete information leads to a **polyhedral** shaped cloud. This can be illustrated by the following example: First, we generate a data set from an $N(0, \Sigma)$ distribution with some 2×2 covariance matrix $\Sigma \neq \mathrm{Id}_2$, where Id_n is the $n \times n$ identity matrix, and assume that this data belongs to 2 random variables with a physical meaning. Then an expert is given the data without any information about the actual probability distribution of the random variables. The fundamental idea is that, based on his knowledge about the physical relationship between the variables, the expert is still able to provide vague, unformalized information about the dependence of the variables, modeled by polyhedral constraints on the variables, cf. Figure 1. The potential function V is constructed with respect to these constraints and can be updated by adding new constraints. Thus the lower and upper α-cuts $\underline{C}_\alpha, \overline{C}_\alpha$ become polyhedra. The polyhedra reasonably approximate confidence regions of the hidden normal distribution linearly, as shown in Figure 1, although the information given to the expert was merely vague and unformalized.

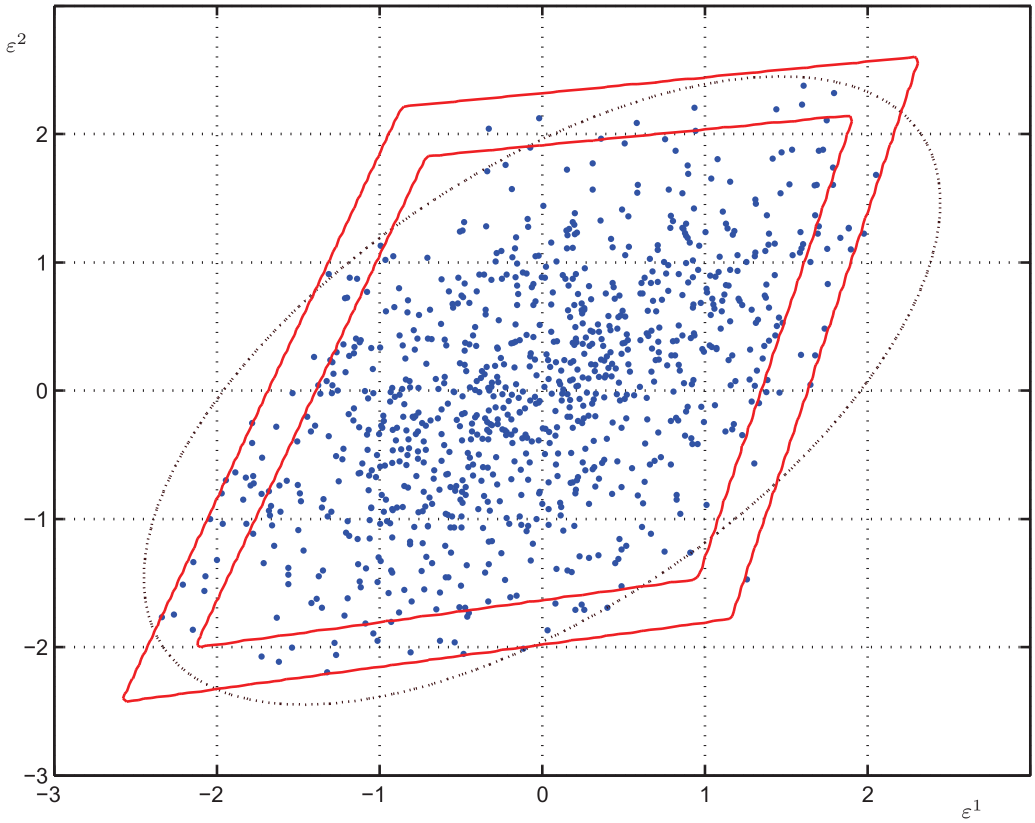

Figure 1. Approximation of a confidence region by 95% lower and upper α-cuts. The polyhedral cloud results in confidence regions that reasonably approximate confidence regions of the true $N(0, \Sigma)$ distribution although the information was given unformalized. In more than 2 dimensions the polyhedral constraints are provided for projections to 1-dimensional or 2-dimensional subspaces.

The confidence regions constructed by the polyhedral clouds based on the available uncertainty information will later become part of the search space for robust optimization, the so-called **worst-case relevant regions**, cf. Section 3. Searching for worst-case scenarios within these regions is the main scope of this paper.

There exist several relationships between clouds and other well-known uncertainty representations, cf. (Fuchs, 2009).

A ***p*-box** is a rigorous enclosure of the CDF F of a univariate random variable X, $F_l \leq F \leq F_u$, in case of partial ignorance about specifications of F, cf. (Berleant and Cheng, 1998; Ferson, 2002). The relation to potential clouds becomes evident, regarding $V(\varepsilon)$ as a 1-dimensional random variable and the functions $\underline{\alpha}$, $\overline{\alpha}$ as a p-box for $V(\varepsilon)$. Thus potential clouds extend the p-box concept to the case of multidimensional ε, without the exponential growth of work in the conventional p-box approach. Furthermore, p-boxes can be approximated discretely by **Dempster-Shafer structures** (DS structures), cf. (Ferson et al., 2003). In an analogous way one can generate a DS structure that approximates a given potential cloud.

To see an interpretation of potential clouds in terms of **fuzzy sets** one considers $\underline{C}_\alpha$, $\overline{C}_\alpha$ as α-cuts of a multidimensional interval valued membership function defined by $\underline{\alpha}$ and $\overline{\alpha}$. The major difference to clouds is the fact that clouds allow for probabilistic statements, i.e., one cannot go back and construct a cloud from a multidimensional interval valued membership function because of the lack of the probabilistic properties mentioned at the beginning of the section. If the interval valued membership function actually does have these probabilistic properties, it corresponds to consistent possibility and necessity measures (Lodwick and Jamison, 2008) which are related to interval probabilities (Weichselberger, 2000).

3. Robust optimization

Assume that we wish to find the optimum $\theta \in \mathbf{T}$ minimizing the objective function value $g(\theta, \varepsilon)$ under uncertainty of the n-dimensional random vector $\varepsilon \in \mathcal{C}$, with $\mathbf{T} = T^1 \times \ldots \times T^{n_0}$, $T^i = \{1, 2, \ldots, N_i\}$ either a finite subset of $\mathbb{N}$ or $T^i = [\underline{\theta^i}, \overline{\theta^i}]$ an interval in $\mathbb{R}$, and $\mathcal{C}$ a polyhedral α-cut from a cloud, i.e., typically

$$\mathcal{C} = \{x \mid A(x - m) \leq b\} \subseteq b_0 = [\underline{b_0}, \overline{b_0}], \tag{1}$$

with A, m, b, $[\underline{b_0}, \overline{b_0}]$ known from the generation of the cloud, $A \in \mathbb{R}^{n \times n}$, $m, b \in \mathbb{R}^n$, $[\underline{b_0}, \overline{b_0}]$ an n-dimensional box.

This problem class appears for example in robust design optimization where θ is a design point, g typically comes as a black box that computes, e.g., the cost of the design, and the uncertainty representation $\varepsilon \in \mathcal{C}$ is a safety constraint to account for the robustness of the design, cf. (Fuchs and Neumaier, 2009).

Since we seek to *minimize* g robustly, the worst-case for g is given by its *maximum* value over the uncertainties. Hence the optimization problem to be solved reads as follows

$$\begin{aligned} \min_{\theta} \ \max_{\varepsilon} \quad & g(\theta, \varepsilon) \\ \text{s.t.} \quad & \theta \in \mathbf{T}, \\ & \varepsilon \in \mathcal{C}. \end{aligned} \tag{2}$$

The main difficulties arising from (2) are imposed by the bilevel structure in the objective function, by the mixed integer formulation (since T^i can be either a discrete set or an interval), and by the fact that g may comprise strong nonlinearities, or discontinuities, or may be given as a black box.

In the remainder of the paper we particularly aim at applications in real-life situations. We assume that $g(\theta, \varepsilon)$ is given as a **computationally expensive** black box that is **linearizable** in $\mathcal{C}$ as a function of ε with fixed θ. The latter assumption is usually justified if the uncertainties are **reasonably small**. Hence we assume $\mathcal{C}$ to be a suitably small set. Also, we assume the uncertainties to be **high-dimensional**, with possibly up to thousands of uncertain parameters.

We approach a solution of (2) in two steps, regarding the inner level and the outer level of the problem separately. The **inner level** reads as follows

$$\max_{\varepsilon} \quad g(\theta, \varepsilon) \tag{3}$$

$$\text{s.t.} \quad \varepsilon \in \mathcal{C},$$

for a fixed $\theta \in \mathbf{T}$. We will refer to (3) as the **worst-case search**.

The maximizer $\widehat{\varepsilon}$ for the fixed design choice θ corresponds to the worst-case objective function value

$$\widehat{g}(\theta) := g(\theta, \widehat{\varepsilon})). \tag{4}$$

The function $\theta \to \widehat{g}(\theta)$ implicated by the solution of problem (3) is the objective function of the **outer level** of problem (2)

$$\begin{aligned} \min_{\theta} \quad & \widehat{g}(\theta) \\ \text{s.t.} \quad & \theta \in \mathbf{T}. \end{aligned} \tag{5}$$

The 1-level problem (5) can be solved with black box optimization techniques towards a robust optimum, see, e.g., (Fuchs and Neumaier, 2009).

In the following section we will focus on a method to solve the inner level (3) fast in high dimensions, so the evaluation of $\widehat{g}$ is computationally cheaper and black box optimization tools for (5) can be employed more efficiently.

4. Worst-case search

Let $f(\varepsilon) := g(\theta, \varepsilon)$ for fixed θ be a computationally expensive black box as mentioned in the last section. For a polyhedral cloud the worst-case search then becomes

$$\begin{aligned} \max_{\varepsilon} \quad & f(\varepsilon) \\ \text{s.t.} \quad & A(\varepsilon - m) \leq b. \end{aligned} \tag{6}$$

We denote the solution of (6) as $\widehat{\varepsilon}$, and $\widehat{f} := f(\widehat{\varepsilon})$.

In a classical approach one can approximate f linearly in the box b_0 that contains the polyhedron $\mathcal{C}$ by a function $f_{\text{lin}}(\varepsilon)$. Thus problem (6) becomes a linear programming problem (LP),

$$\begin{aligned} \max_{\varepsilon} \quad & f_{\text{lin}}(\varepsilon) \\ \text{s.t.} \quad & A(\varepsilon - m) \leq b. \end{aligned} \tag{7}$$

However, the cost for the linearization of f is in the order of magnitude of n evaluations of the black box f which may become prohibitively expensive for large n.

In this section we present an approach inspired by the Cauchy deviates method (CD) for interval uncertainty (Kreinovich and Trejo, 2001; Kreinovich and Ferson, 2004; Kreinovich et al., 2007), i.e.,

$$\begin{aligned} & [\min_{\varepsilon} f(\varepsilon), \max_{\varepsilon} f(\varepsilon)] \\ \text{s.t.} \quad & \varepsilon \in b_0. \end{aligned} \tag{8}$$

One avoids linearization of f and instead uses a simulation based 'trick' sampling a Cauchy distribution. We will modify this trick for the case of polyhedral uncertainty as follows.

1. The first step is the same as in CD and simply a function **evaluation at the center** m of the polyhedron, i.e., we compute $f_1 := f(m)$.

2. The second step in CD is generating a sample point $e_i \in [0,1]^n$ from a **uniform distribution**. We do the same and add a rejection step here for the case that e_i is not in a normalized version of $\mathcal{C}$. Hence, we reject and resample e_i if

$$Av > b, \tag{9}$$

with $v = (e_i - 0.5)\,.\!*(\overline{b_0} - \underline{b_0})$ in Matlab notation.

3. The third step is, as in CD, a **transformation** of e_i to a Cauchy distribution. The Cauchy distribution has the density

$$\rho_{\Delta,\ell}(x) = \frac{1}{\pi}\frac{\Delta}{\Delta^2 + (x-\ell)^2}, \tag{10}$$

with the scale parameter Δ, and the location parameter ℓ. The corresponding CDF of the Cauchy distribution is

$$F_{\text{Cauchy}}(\Delta,\ell)(x) = \frac{1}{2} + \frac{1}{\pi}\arctan\left(\frac{x-\ell}{\Delta}\right), \tag{11}$$

and the inverse CDF reads

$$F^{-1}_{\text{Cauchy}}(\Delta,\ell)(x) = \ell + \Delta\tan\left(\pi\left(x - \frac{1}{2}\right)\right). \tag{12}$$

Hence to transform e_i to a Cauchy distributed sample scaled with respect to b_0 we compute

$$x_i^j = F^{-1}_{\text{Cauchy}}((\overline{b_0}^j - \underline{b_0}^j)/2, 0)(e_i^j) = \frac{\overline{b_0}^j - \underline{b_0}^j}{2}\tan\left(\pi\left(e_i^j - \frac{1}{2}\right)\right), \tag{13}$$

where x_i^j indicates the jth coordinate of the vector x_i, $j = 1,\ldots,n$.

Thus we have simulated a sample point x_i that lies possibly outside $\{\mathcal{C} - m\} := \{x \in \mathbb{R}^n \mid x = y + m, y \in \mathcal{C}\}$.

4. So similar to CD we need a **normalization** step not to violate the constraints in (6). To this end we compute the factor

$$K = \left\|\frac{Ax_i}{b}\right\|_\infty, \tag{14}$$

thus $\frac{x_i}{K}$ lies in $\{\mathcal{C} - m\}$, and lies on the margin of $\{\mathcal{C} - m\}$ in one coordinate.

5. Evaluate

$$f\left(\frac{x_i}{K} + m\right) =: f_i \tag{15}$$

and compute the simulated deviation

$$\delta_i = K(f_i - f_1). \tag{16}$$

6. Repeat the steps 2–5 for $i = 2,\ldots,N$, where N is a user defined parameter determining the number of function evaluations of f used to solve (6). Thus we achieve the sample $\delta_2,\ldots,\delta_N$.

7. In the 7th step we **estimate** the deviation $\Delta = \widehat{f} - f_1$ from $f_1 = f(m)$ statistically thanks to the knowledge of $\delta_2, \ldots, \delta_N$. To this end we solve the following zero finding problem for Δ as in the classical CD

$$\frac{1}{1 + \left(\frac{\delta_2}{\Delta}\right)^2} + \ldots + \frac{1}{1 + \left(\frac{\delta_N}{\Delta}\right)^2} - \frac{N-1}{2} = 0. \tag{17}$$

where a zero is known to lie in the interval $\Delta \in [0, \max_i |\delta_i|]$.

Thus we find $f_1 + \Delta$ as our estimated solution $\widehat{f}$ of (6).

4.1 Remark. Note that $f_1 + \Delta$ is only a simulation based estimation of $\widehat{f}$ and not a reproducible function evaluation, so the black box $\widehat{g}(\theta)$ in the outer level problem (5) becomes noisy which may lead to a suboptimal solution which is, however, often close to the optimum in our test cases, cf. Section 5. In general the methods to solve (5) may be sensitive to a noisy worst-case function.

4.2 Remark. In (Kreinovich et al., 2007) the quality of the estimation of $\widehat{f}$ is considered with respect to the number of function evaluations N used, cf. Table I. Also the accuracy of the estimation for very small N is studied in (Kreinovich et al., 2007), cf. Table II. Based on this experience one can choose a reasonable value of N with respect to a given application. In our applications we use $N = 50$ as a default value. Note that if $N > n$ it is not reasonable to use the simulation based approach, and a linearization based approach (7) should be preferred.

Table I. Number of function evaluations N needed for a given estimation error with a given confidence.

error	95% confidence	99.9% confidence
10%	800	1800
20%	200	450
40%	50	110

Table II. Estimation error for very small N.

N	20	10	5
error	70%	110%	400%

4.3 Remark. Step 7 requires that f is linear in $\mathcal{C}$ and that the components of ε are independent random variables. Then $\widehat{f} - f_1$ is a linear combination of independent Cauchy distributed variables and thus also Cauchy distributed with the unknown parameter Δ which is determined via maximum likelihood estimation (17). The assumption that the variables are independent is violated if the polyhedral constraints arise from dependency information as described in Section 2, so Δ is actually not quite Cauchy distributed anymore. The numerical results in Section 5, however, show that this had little effect on the quality of the estimation of $\widehat{f}$ in our test cases, in particular it did not yield critical underestimation of worst-cases. In the future we need a statistically more precise estimation of Δ.

4.4 Remark. Note that the minimizer of (6), i.e., the worst-case scenario, remains unknown with the method presented.

4.5 Remark. It should be highlighted that the described method can be easily parallelized via parallel function evaluations, and that N in Table I and Table II is independent of n, so the method is computationally very efficient in high dimensions.

5. Application examples

In this section we apply the new worst-case search technique in two applications of cloud based robust design optimization in spacecraft system design: the NASAs Mars Exploration Rover (MER) mission (Fuchs et al., 2008; Erickson, 2004; MER, 2003), and the 2004 X-ray Evolving Universe Spectroscopy (XEUS) mission of the European Space Agency (ESA) (Neumaier et al., 2007; ESA CDF, 2004; ESA CDF, 2004).

Without going too much into the details of the missions, the relevant characteristics of the problems are as follows: in MER we have a 1-dimensional design problem, i.e., $n_0 = 1$, with a 34-dimensional uncertainty domain, i.e., $n = 34$. In XEUS we have a 10-dimensional design problem, i.e., $n_0 = 10$, with a 24-dimensional uncertainty domain, i.e., $n = 24$.

In the original applications there was no expert knowledge provided to generate polyhedral clouds that are not box shaped. Hence we have added artificially arbitrary polyhedral constraints in both cases in order to create a different situation from the classical interval uncertainty treated by CD.

The test cases are 24 and 34 dimensional, respectively, so actually not sufficiently high-dimensional to reveal the benefits of the new method since $n < 50$. But one can compare the results very good to the existing results found by linearization of the black box f, and the strength of the method becomes obvious by the argument that the same quality of worst-case estimation will be achieved for much higher n without additional function evaluations. Real-life applications in much higher dimensions are likely to be investigated with the presented methods in the near future.

To compare the results with the existing results for the test cases, we perform 10 full runs of robust design optimization using the new worst-case search. We regard each worst-case estimation during this process and count how often the estimated worst-case is close to the worst-case found with the previous approach based on linearization. Close here means

$$\left| \frac{\text{worstcase}_{\text{new}} - \text{worstcase}_{\text{old}}}{\text{worstcase}_{\text{old}} - f_1} \right| < 40\%. \tag{18}$$

The results are shown in Table III. They confirm the estimation quality and confidence indicated in Table I, though the requirements of CD are not perfectly met as mentioned in Remark 4.3.

Table III. Number of simulation based worst-case estimations within close range (40% error) of linearization based worst-case searches.

	number of estimations	**close results**	**percentage**
MER	400	384	96.0%
XEUS	5340	5154	96.5%

Furthermore, we have a look at the effect of the new – a bit more noisy, cf. Remark 4.1 – worst-case function on the optimal solution found. We count how often the linearization based worst-case of the new optimum (found with simulation) is close to the previously found optimal worst-case.

Table IV. Number of simulation based solutions within close range of solutions from linearization based robust optimization.

	number of optimizations	**same results**	**close results,** 5%	**close results,** 40%	**average error**
MER	10	2	6	10	7.3%
XEUS	10	0	0	9	22%

As we see in Table IV we rarely find identical results. In XEUS we find no suboptimal results that are very close to the actual optimum. In MER the suboptimal results are often very close to the actual optimum. In both test cases the suboptimal results are very often within the 40% error threshold from the actual optimum, which could be expected from Remark 4.2, since we chose $N = 50$. Especially in MER the average error is much smaller than this threshold.

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