19th International Conference
ENGINEERING MECHANICS 2013
Svratka, Czech Republic, May 13 – 16, 2013

MULTIOBJECTIVE MINIMAX DESIGNS OF EXPERIMENTS

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Summary: *Space-Filling Design Strategies known as Design of (Computer) Experiments (DoE) create an essential part of a surrogate modeling. Two main objectives are usually placed on the resulting designs - orthogonality and space-filling properties. One of the space-filling metrics, called miniMax represents very interesting research area. Given a set of n points in a d-dimensional hypercube, the miniMax is the radius of the biggest sphere with its center inside the hypercube that does not contain any point of the set. Our experiences show that majority of these spheres are located at the border of the admissible domain. However, more dangerous are spheres inside the domain. Therefore, a multiobjective procedure is proposed to take into account not only miniMax, but also the positions of the spheres with respect to the domains center. This procedure can be used for comparing different designs or can be applied as an adaptive sampling strategy based only on geometrical properties without any underlaying regression model.*

Keywords: ***Design of Experiments, space-filling, miniMax, Voronoi diagram, largest empty sphere problem, multiobjective optimization, adaptive sampling***

1. Introduction

The design of experiments (DoE) is an essential part of the development of any meta-model (surrogate) (Simpson et al., 2001; Jin, 2005). The aim is to gain maximum knowledge from a given system with a minimum number of designs. Since we assume that the final meta-model is *a priori* unknown, the design should be spread over the domain as uniformly as possible. The effectiveness of such DoE can be measured by several metrics aiming mainly at orthogonality or space-filling properties. See references Cioppa and Lucas (2007); Hofwing and Strömberg (2010) for orthogonal and sources Crombecq et al. (2009); Myšáková and Lepš (2011); Janouchová and Kučerová (2013) for space-filling criterions, respectively.

For our work, we have selected the *miniMax* (*mM*) for its simplicity and easiness in visualization. Given a set of n points in a d-dimensional hypercube, the miniMax is the radius of the biggest sphere with its center inside the hypercube that does not contain any point of the set. This problem is also known as *the largest empty sphere problem (LES)* (Dickerson and Eppstein, 1995). In other words, the miniMax serves as an estimation of the space-filling properties

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of the set of points showing the biggest unsampled space. One possible solution is to inspect all vertices forming Voronoi diagram (Okabe et al., 2000) of the given points. However, for the unbounded case the number of vertices grows as $O(n^{\lceil d/2 \rceil})$ and for bounded case, i.e. the case of points inside a hypercube, the number is even higher. The same is also valid for computational demands, see Tables 1 and 2. Although the boundary of the domain can be efficiently solved by mirroring (Pronzato and Müller, 2012), to reliably find the vertices of the Voronoi diagram in higher dimensions is not a trivial task.

Table 1. Computational demands of enumeration of miniMax value in terms of needed CPU time and allocated memory against the number of dimensions for 100 point DoE.

Dimension	Time [s]	Memory [kB]
2D	0.082	684
3D	0.085	1576
4D	0.393	9540
5D	3.885	15796
6D	150.924	71916
7D	6297.79	454236
8D	$>$ 6 d. 18 h.	$>$ 8 GB

Table 2. Prediction of computational demands of enumeration of miniMax value in terms of needed CPU time and allocated memory against the number of dimensions for 100 point DoE based on a fitted exponential function.

Dimension	Time	Memory [GB]
9D	117 days	11
10D	12,9 yrs	56
11D	521 yrs	286
12D	20977 yrs	1451
⋮	⋮	⋮

Recently, we have implemented a parallel evolutionary approach (Myšáková and Lepš, 2013) that is able to guess an approximate value of the miniMax in a reasonable time. Our work follows the paper Lee et al. (2004), where an evolution strategy has been used to find the center of the biggest empty sphere. This approach is able to find exact solutions only up to five dimensions and no more. Therefore, an improved algorithm has been proposed, where the evolution strategy is run in parallel on subdivisions of the original hypercube. This algorithm can produce a reliable estimates of miniMax in several minutes even for a problem consisting of few dozens of variables.

The availability of the miniMax value, although approximate, enables to explore properties of a particular DoE. Since the miniMax is the radius of the biggest sphere that does not contain any other point of the set, an interesting information can be the position of such a sphere. Although our experience shows that majority of these spheres are located at the border of the admissible domain, the most dangerous situation is that such spheres are inside the domain, especially in the center of the design space.

The second application is a sequential sampling strategy, that is intuitively adding next samples to the centers of the biggest spheres. This sampling strategy will not ensure some properties of the original DoE like Latin Hypercube (LH) restrictions (Sallaberry et al., 2008; Vořechovský, 2009; Crombecq et al., 2009; Myšáková and Lepš, 2012); however, it enables to adaptively refine the original DoE without the knowledge of any surrogate that is usually used, see e.g. works utilizing properties of Kriging (Jones, 2001) or Artificial Neural Networks (Devabhaktuni and Zhang, 2000).

One of the drawbacks is that the number of potential points that should be inspected is relatively huge. Therefore, we propose in this paper a multiobjective procedure that finds a trade-off between miniMax value and the distance of centers of the spheres to the domains center. Simi-

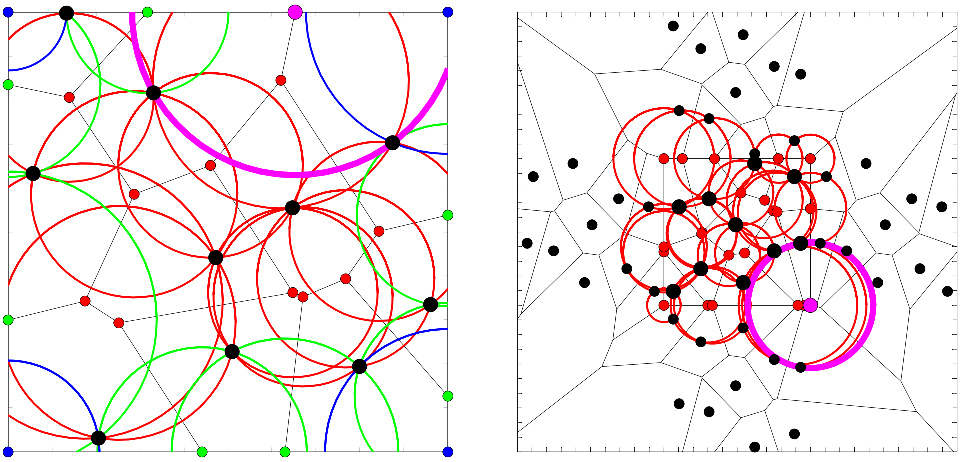

Figure 1: Exact miniMax computation - “by hand” (left) and with mirroring (right). Legend: black points - the design points; black lines - Voronoi diagram; red points - Voronoi vertices; green points - intersections of Voronoi edges and boundaries of given domain; blue points - domain vertices; red, green and blue circles - the largest empty circles with centers in red, green and blue points; magenta circle - the largest empty circle; magenta point - center of the largest empty circle.

lar procedure can be found within reliability analyses or Reliability-Based Design Optimization (RBDO) area, see e.g. works Sudret (2007); Dubourg (2011). However, these traditional approaches use Weighted Sum Method, see e.g. (Vitingerová, 2010), where each objective is multiplied by a user defined weight and their sum is then optimized. In this contribution, the exact Pareto front is computed. Presented results show that the number of points of the Pareto set grows only linearly with the number of dimensions, and therefore, the proposed methodology can be efficiently used even for multidimensional spaces. The rest of the paper is organized as follows. Next section describes the methods for enumeration of exact as well as approximate values of the miniMax metric. The description of the multiobjective methodology is accompanied with the results showing Pareto fronts of several designs. Finally, the papers is finished with the concluding remarks.

2. Enumeration of miniMax

2.1. The exact solution

We can obtain the exact value of the miniMax criterion utilizing Voronoi diagram. The center of the largest empty sphere lies in Voronoi vertex or in the intersection of Voronoi edges and a boundary of a given domain. In two dimensions it is possible to find all candidate points by hand, see Figure 1. In higher dimensions this method brings some difficulties. It is necessary to find the intersections of the Voronoi diagram with objects on boundaries of the given domain. Also we have to consider all vertices of the given domain as candidate points for center of the largest empty sphere.

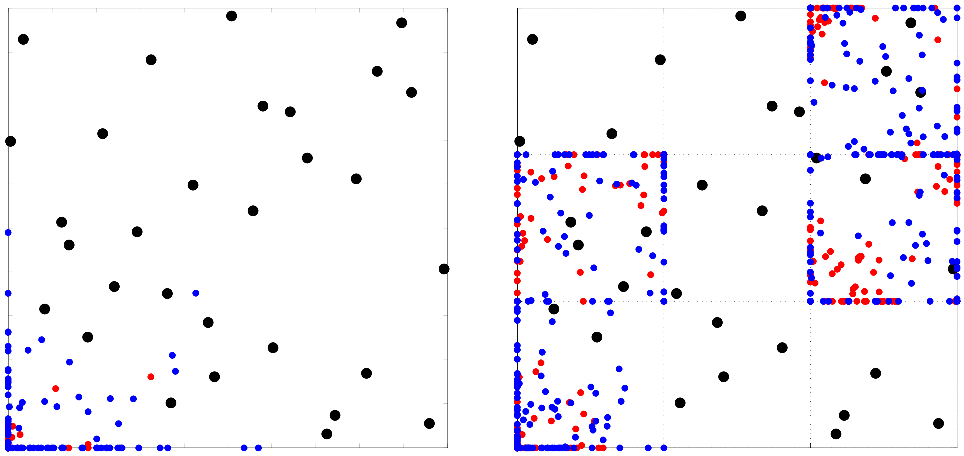

Figure 2: Serial (left) and parallel (right) evolution strategy. Legend: black points - the design points; red points -“the parents”; blue points “the offsprings”.

Extension of this method providing an exact solution is based on mirroring of the design points (Pronzato and Müller, 2012). The design points are mirrored through all $(d-1)$-facets and then Voronoi diagram is created. The mirroring guarantees presence of points on boundaries and in vertices of the domain. Unfortunately the computation of Voronoi diagram is very demanding in higher dimensions and the mirroring (each point has to be mirrored $(2d)$-times) even increases the memory demands, see again Tables 1 and 2. The problems we face in engineering practice are usually multidimensional (tens, even hundreds of input parameters), therefore a method able to work in such domains is needed.

2.2. Serial evolution strategy

One possible solution is that an estimate of the miniMax value can be computed by some heuristic or meta-heuristic method. In our case, an evolution strategy has been used. It is a method based on natural principles of adaptation, mutation, crossover and selection. The technique was created and developed in 1960s and 1970s by Rechenberg, Schwefel and co-workers, see e.g. (Rechenberg, 1973) or (Bäck and Schwefel, 1995) and references therein.

The procedure runs in a loop with iterations called generations. In each generation there is a population created by chromosomes. These are individuals spread over the solved domain. An objective function value is assigned to each chromosome. A new population (“the offsprings”) is derived from previous population (“the parents”) by mutation or crossover. There are two general types: in (μ, λ)-ES a new generation is derived from offsprings of the previous generation, in $(\mu + \lambda)$-ES a new generation is derived from the union of parents and offsprings from the previous generation. The offsprings are created by mutation - by adding a normally distributed (mean equals to zero, standard deviation decreases during the loops) random numbers to parental population. Then, the pairs from the union of “parents” and “offsprings” are selected randomly and the one with larger distance to the nearest design point is chosen to new parental population. This tournament scheme prefers better individuals for the next generation. The number of generation can be set by user or the algorithm stops when meeting a termination criterion. The procedure is depicted in Figure 2 (left). We can see how the population approximates the solution.

2.3. Parallel evolution strategy

Although the serial method is robust and user can choose a size of population and the number of generations according to the dimension of the problem, it is difficult to explore the whole given domain. Therefore we have proposed the parallel version. We can parallelize the strategy by two different ways: first, it is possible to run multiple searches over the whole domain in parallel; second we can divide the domain into multiple subdomains and run the search in parallel independently in these subdomains. Latter method is used in our computations. Figure 2 (right) shows the procedure. Several subdomains are solved in parallel on individual CPUs. We obtain candidate points from each subdomain and the point most distant from the design points is the center of the largest empty sphere and its radius is an estimation of the miniMax.

3. Results of Multiobjective selection

Here, we show the results of multiobjective procedure that finds an exact trade-off between both, exact and approximate, miniMax values and the distances of centers of the spheres to the domains center[3]. The result is Pareto front of compromising solutions that shows us where are big holes in the given design and corresponding radiuses of these holes. This procedure is visualized in Figure 3. The first line presents classical factorial design that is the most uniformly spaced design[4]. Since all possible circles share the same radius, the worst case is in this case the center of the design.

The middle and bottom line of Figure 3 represents the same 2D design. The middle line corresponds to the exact solution of the miniMax problem, i.e. all vertices of Voronoi diagram are inspected. The bottom line then represents an approximate solution found by our evolutionary algorithm. All points inspected during the evolution process are shown in the objective space. Note that the V-shape structure of points is formed by solutions lying on the boundaries of the domain. The results show that the approximate solution covers well the exact solution. Moreover, evolutionary Pareto set is reacher, visiting also smaller empty spaces in the vicinity of the domains' center.

Examples of higher dimensional spaces are shown in Figure 4. The first example is a relatively sparse design with 17 points in 6 dimensions with the exact miniMax metric. This sparsity is clearly visible; the smallest sphere's radius is almost 70% of the side of the hypercube's edge. The second example is a 65 points, 12 dimensional problem. The number of dimensions is too big, therefore, the approximate solution is used. Although more than 12000 candidate points have been investigated, only 74 points form Pareto front. Our experience shows that the size of Pareto fronts obtained by the proposed procedure does not exceed a hundred even for several dozens of dimensions.

[3] All domains are unit hypercubes in all presented examples.

[4] Note that this property is counteracted by the worst projection properties (Crombecq et al., 2011) and massive computational demands.

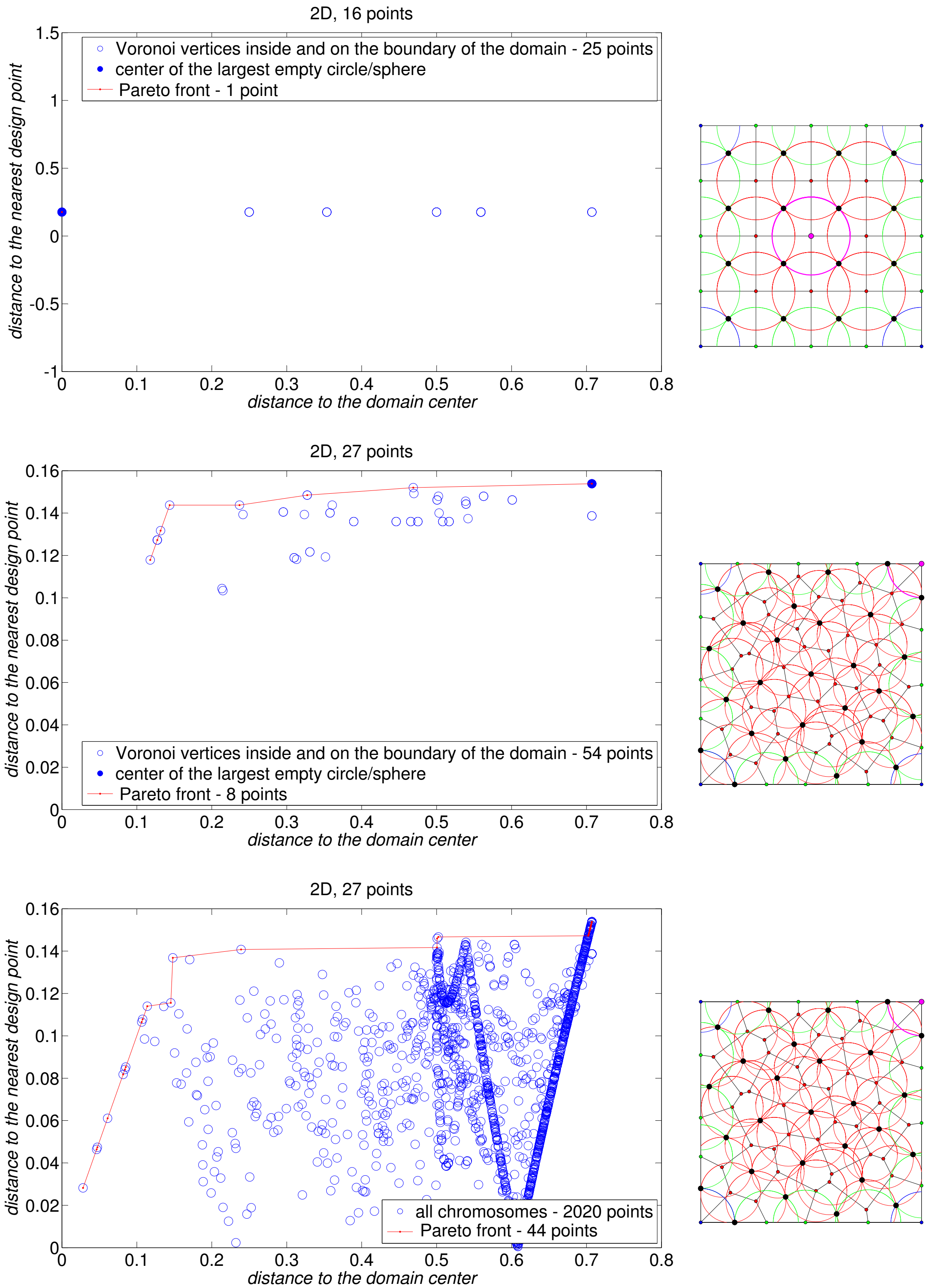

Figure 3: Pareto fronts (left) for 2D DoEs (right) with shown circles; full factorial DoE (top) and a random LHS design, same for middle and bottom line; middle line shows all exact Voronoi vertices, bottom corresponding evolutionary approximation. Legend is same as in Figure 1.

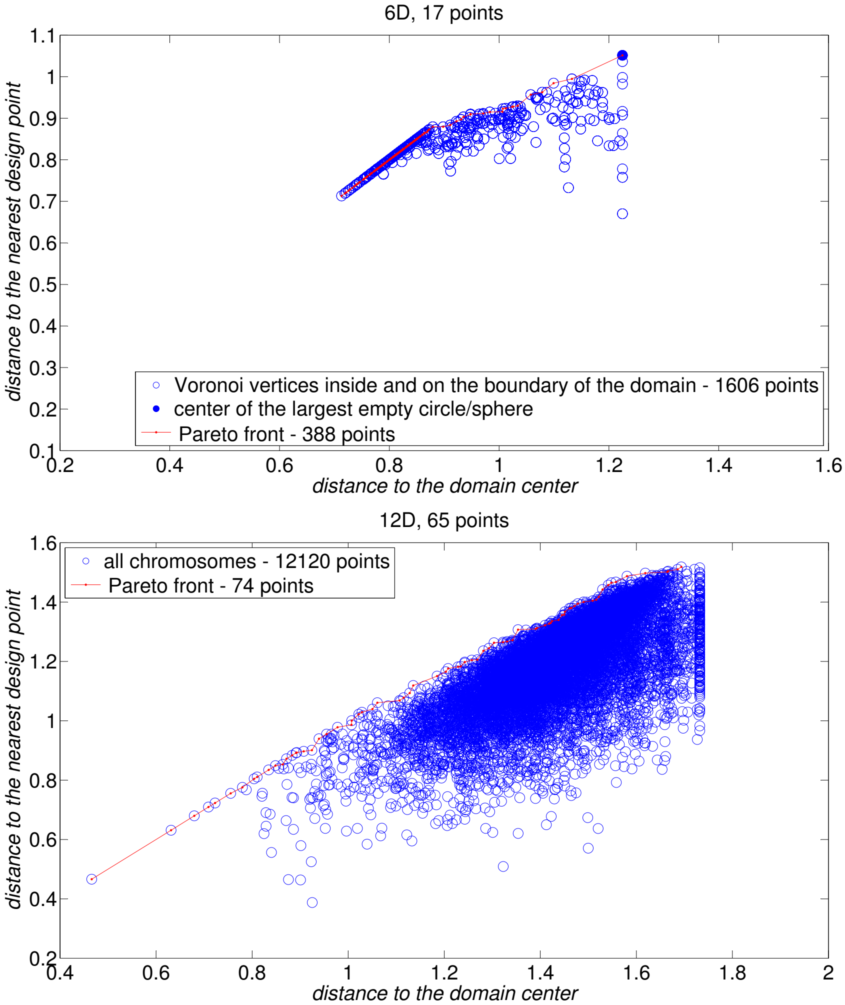

Figure 4: Pareto fronts for 6D (top) and 12D (bottom) DoEs .

4. Conclusions

The aim of this contribution is to show that the addition of another objective and therefore, the transmission of the single-objective space-filling problem to the multiobjective one can bring a new insight to the utilization of the optimization of the Designs of Experiments. Particularly, the exact and approximate computation of the miniMax metrics have been presented as the space-filling criterion. The second objective, the distance to the domains' center was used. However, any other objective can be used. For instance, for the case of Reliability-Based Design Optimization (RBDO), the distance to the Limit State Function (LSF) can be applied instead. Then, the points forming Pareto front represents ideal candidates for adaptive sampling of the LSF.

5. Acknowledgment

The authors gratefully acknowledge the financial support from the Grant Agency of the Czech Republic through the project GAČR P105/12/1146 and from the Grant Agency of the Czech Technical University in Prague, the grant SGS13/034/OHK1/1T/11.

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