Uniform Mixture Design via Evolutionary Multi-Objective Optimization

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Abstract

Design of experiments is a branch of statistics that has been employed in different areas of knowledge. A particular case of experimental designs is uniform mixture design. A uniform mixture design method aims to spread points (mixtures) uniformly distributed in the experimental region. Each mixture should meet the constraint that the sum of its components must be equal to one. In this paper, we propose a new method to approximate uniform mixture designs via evolutionary multi-objective optimization. For this task, we formulate three M-objective optimization problems whose Pareto optimal fronts correspond to a mixture design of M components (or dimensions). In order to obtain a uniform mixture design, we consider six well-known algorithms used in the area of evolutionary multi-objective optimization to solve M-objective optimization problems. Thus, a set of solutions approximates the entire Pareto front of each M-objective problem, while it implicitly approximates a uniform mixture design. We evaluate our proposed methodology by generating mixture designs in two, three, and up to eight dimensions, and we compare the results obtained concerning those produced by different methods available in the specialized literature. Our results indicate that the proposed strategy is a promising alternative to

approximate uniform mixture designs. Unlike most of the existing approaches, it obtains mixture designs for an arbitrary number of points. Moreover, the generated design points are properly distributed in the experimental region.

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1. Introduction

Design of experiments is a well-established methodology widely applied to experimental processes in the industry, process design, and science in general [1, 2, 3, 4, 5, 6, 7]. This approach has been found to be a powerful method to
identify active and unimportant effects in an experimental process. However, many challenges arise from a practical standpoint, which have encouraged the development of different designs to meet practical needs. Mixture designs are a particular case of experimental designs subject to certain constraints. In a mixture, the independent components are proportions of different ingredients
of a blend, and therefore, the sum of its components must be one. When the mixture design is only subject to the constraint that the components' sum must be one, it is called standard mixture design. Examples of these methods are the Simplex-Lattice design [8] and the Simplex-Centroid design [9]. When the mixture design is subject to additional constraints, such as a maximum
and/or minimum value for each component, it is referred to as Extreme-Vertices design (or constrained mixture design) [10].

The main goal of the uniform mixture design methods is to scatter the design points in the experimental region as uniformly as possible. Some authors have focused their studies on mixture designs from the viewpoint of classical optimal
design [8, 9, 11, 3, 12]. This type of approaches aims to find an optimal distribution of points through an $(M-1)$-dimensional simplex. However, as pointed out by some authors [13, 14, 15, 6], optimal design has several disadvantages:

1. An optimal design tends to distribute most of the design points on or near the experimental area's boundary, leaving the interior mostly devoid of

25   design points;

2. An optimal design is not a robust design to the assumed model; in most cases, the experimenter does not know the form of the model beforehand;

3. The high dimensionality of the mixtures makes it difficult for the existing methodologies to obtain an optimal design.

30   In order to address these drawbacks, researchers have developed diverse mixture designs from different nature [6, 16, 17, 18]. In this paper, we propose a new methodology for uniform mixture designs based on multi-objective evolutionary optimization. To this end, we must answer two questions: i) what multi-objective optimization problem should we solve? and ii) what evolutionary multi-objective algorithm should we use? In this research work, we formulate three M-objective problems whose Pareto optimal fronts correspond to a mixture design of M components, i.e., the Pareto front shapes describe a regular $(M-1)$-dimensional simplex. Each M-objective optimization problem is solved using a multi-objective evolutionary algorithm. This way, a set of solutions approximates the entire Pareto front of each M-objective problem while a uniform mixture design is implicitly reached. In our experimental study, we identify the M-objective problem formulation for which the evolutionary algorithm searches for the best approximation to the entire Pareto front, i.e., the best approximation of a uniform mixture design. To validate our proposed approach, we generate uniform mixture designs in two, three, and up to eight dimensions, and we compare our results with respect to those produced by different uniform design methods available in the specialized literature. As we will see later on, our proposed approach is a promising alternative to approximate uniform mixture designs because it can create mixture designs for an arbitrary number of points distributed adequately in the $(M-1)$-dimensional simplex.

The rest of the paper is organized as follows. Section 2 presents a review of different methods for mixture design. In Section 3, we introduce some basic concepts that will help to understand the rest of the paper. Section 4 introduces our proposed methodology. An experimental study of our proposed approach

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[55] is presented in Section 5. Finally, our conclusion and some possible paths for future research are drawn in Section 6.

2. Related Work

Uniform mixture design methods play an essential role in diverse areas of knowledge [1, 2, 3, 6]. According to their conceptual basis, we classify uniform [60] mixture design approaches as follows.

Methods employing geometric concepts. Scheffé [8] proposed the simplex-lattice design (SLD) technique in 1958 [1]. Let M be the dimension of the mixture and H the number of subdivisions for each dimension. SLD generates $N = \binom{M+H-1}{H}$ points uniformly distributed on a hyperplane ($\{M-1\}$ unity simplex-[65] lattice). This means that N increases quickly with respect to the number of dimensions. Years later, Scheffé [9] proposed another method called simplex-centroid design (SCD) which generates $2^M - 1$ distinct uniform points using as centroid point $(1/M, 1/M, \ldots, 1/M)$. SLD and SCD are not good options for some applications, e.g., in chemical experiments, a component cannot be [70] zero. Since both techniques generate several points at the simplex boundary, it is necessary to use another distribution type. To overcome this disadvantage, Cornell [20] proposed axial design (AD), which generates points on the simplex's inner region. For this, Cornell defines an axis as a line segment that joins a vertex of the simplex with its centroid. Then, AD generates q points on the q axes. [75] Fang and Yang [21] proposed to keep the pattern of SLD and SCD and contract the boundary points towards the centroid of the simplex. Many works have proposed different adaptations to the methods proposed by Scheffé to obtain different distributions, such as D-optimal distribution, A-optimal distribution, and I-optimal distribution. In [3], Chan described some of them. For example,

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[1]In the Evolutionary Multi-objective Optimization (EMO) field, it is common to use the method proposed by Das & Deniss [19] to generate a set of convex weights. This method and Scheffe's method are the same. The main difference is that Das & Deniss gave a tree-based algorithm to compute the weighting coefficients.

Kiefer [22] studied D-optimal designs for regression problems using SCD.

Another disadvantage of SLD and SCD is the number of points that they generate. For example, in the area of evolutionary multi-objective algorithms (EMOAs), algorithms based on decomposition require a set of well-distributed convex weights (i.e., a uniform mixture design). EMOAs work with populations, and regularly the number of weights is equal to the population size. Since using a large population size requires a high computational cost, there are proposals to decrease the number of points that are generated by the methods of Scheffé. For example, Deb et al. [23] proposed the two-layered SLD in many-objective optimization problems. Given H_1 and H_2 ($H_1 > H_2$), which are two relatively small numbers of subdivisions for the so-called outside and inside layers, two-layered SLD generates two subsets of uniform mixtures. The inside layer associated with H_2 is scaled in the interior of the hyperplane. On the other hand, Jiang and Yang [16] introduced the k-layer reference direction. This method partitions the unit simplex into k sub-simplexes. The number of sub-simplexes is equal to the number of dimensions in a multi-objective optimization problem, i.e., $k = M$.

Methods employing the minimization of discrepancy functions. In the specialized literature, it is possible to find several discrepancy indicators (or low discrepancy functions) that have been employed to generate uniform designs in different domains. Example of such discrepancy indicators are the centered L_2-discrepancy (CD) [24], the wrap-around L_2-discrepancy (WD) [25], and Mixture Discrepancy (MD) [26]. Such indicators are optimized, and consequently, a uniform design is approximated. Regarding the uniform mixture design, Fang and Wang [27] proposed the contract uniform design method, which contracts the boundary points towards the centroid of the simplex. Prescott [28], complemented this idea, employing the above method on a region of the simplex. In particular, a uniform design can be projected into the $(M - 1)$-dimensional simplex for obtaining a mixture design [13]. In this regard, several uniform design approaches can be found in the specialized literature. Based on the

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good lattice point [29] method (a method introduced to approximate multiple integrals), several methods to construct uniform designs have been proposed [30, 31, 32, 13, 33]. The main disadvantage of optimizing discrepancy functions is the computational cost to compute them, which increases as the number of design points increases. In this regard, Ma and Fang [34] suggested the cutting method to generate a larger uniform design via partitions of a region. An important issue in this approach is that the cutting method's performance does not depend on a specific measure of uniformity. Based on Lee's discrepancy [35], Ning et al. [15] proposed an algorithm that can be applied to any experimental design. Zapotecas et al. [36] employed transcendental numbers instead of prime numbers in a low-discrepancy sequence to obtain mixture designs. On the other hand, the effect of different low-discrepancy sequences in the construction of mixture designs was studied in [6].

Methods employing evolutionary computation. In the last few years, uniform mixture designs have been addressed by evolutionary computation. These approaches employ stochastic optimization algorithms, such as genetic algorithms or particle swarm optimization, to optimize a measure of uniformity and generate uniform designs. Although this type of algorithms does not guarantee an optimal solution (i.e., design), the practicality of these approaches makes it possible to obtain an arbitrary number of points with a reasonable approximation to the optimal design. In this regard, several authors have proposed different strategies based on evolutionary computation to construct near-optimal experimental designs. For example, Borkowski [37] uses $D-$, $A-$, $G-$ and $IV-$ optimality criteria, Heredia-Langner et al. [38, 39] work with $D-$ and $Q-$ optimality criteria, and Park et al. [40] use $G-$ optimality criteria. All of them use a genetic algorithm. However, the mixture designs, in their original formulation, have been much less studied. Goldfarb et al. [41] used a genetic algorithm to generate mixture-process experimental designs involving control and noise variables. The goal is to minimize the maximum scaled prediction variance over the design space, i.e., they work with the $G-$ optimality criteria. Limmun et

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al. [42] used a genetic algorithm to generate D-optimal designs for mixture experiments. D-optimality minimizes the generalized variance of the parameter estimates for a pre-specified model. In [43], a genetic algorithm to generate D_s-optimal designs for mixture experiments in a simplex region was proposed. D_s-optimality is an extension of $D-$ optimality, which focuses on a subset of model parameters. Wong et at. [44] introduced a particle swarm optimization technique to find optimal mixture designs. They consider $A-$, $D-$ and $I-$ optimal designs. Meneghini et al. [17] proposed a method based on a steady-state evolutionary algorithm to evolve a set of weight vectors (i.e., a set of mixtures) towards the desired distribution. The aim is to maximize the shortest distance between vectors. Rodríguez et al. [18] employed a parallel tabu search to obtain a uniform set of weight vectors minimizing the L_2-discrepancy. Recently, Blank et al. [45] introduced a metric for defining well-spaced set of points on a unit simplex (a uniform mixture design) and propose a number of viable methods for generating such a set. The above approaches use an indicator of dispersion to approximate uniform mixture designs. However, a multi-objective approach to approximate mixture designs has not been studied, and it is the motivation and the focus of the work reported herein. In the following section, we introduce some basic concepts to understand the rest of the work.

3. Basic Concepts

3.1. Mixture Design

Experiments with mixtures have been very useful in different engineering and scientific areas. In experiments with mixtures, a response is assumed to depend on the proportions of the mixture components, not on the total amount of the mixture. Commonly, there are some additional constraints imposed on the components.

Formally, the constraints of the proportions $(x_i, i = 1, 2 \dots, M)$ in a mixture

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design with M components (or M dimensions) are stated as:

$$\sum_{i=1}^{M} x_i = 1, \qquad x_i \geq 0, \text{ for } i = 1, 2, \ldots, M. \tag{1}$$

Therefore, the corresponding experimental region of M components forms a regular $(M-1)$-dimensional simplex.

Sometimes, besides the constraints stated in Equation (1), there are some other additional constraints, such as the single component constraints (SCCs):

$$0 \leq a_i \leq x_i \leq b_i \leq 1 \quad \text{ for } i = 1, \ldots, M$$

and multiple component constraints (MCCs):

$$L_v \leq \sum_{i=1}^{M} C_{vi} x_i \leq U_v, \qquad v = 1, \ldots, V$$

where V is the number of MCCs and C_{vi} denotes the v-th constraint for the i-th component in the mixture..

It should be noted that the unconstrained mixture experiment can be seen as a special type of SCCs experiment, by setting a_i's to all zeros and b_i's to all ones. And SCCs experiment can be seen as MCCs by setting C_{vi}s to special values. Here, we focus our investigation on generating uniform mixture designs satisfying the constraints of Equation (1) [15].

3.2. Multi-Objective Optimization

A multi-objective optimization problem (MOP) can be stated[2] as follows:

$$\textbf{minimize:} \quad \mathbf{F(x)} = (f_1(\mathbf{x}), \ldots, f_M(\mathbf{x}))^T \tag{2}$$

$$\text{s.t.} \qquad \mathbf{x} \in \Omega$$

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[2]Without loss of generality; we assume continuous minimization problems.

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where $\Omega \subset \mathbb{R}^n$ defines the decision variable space and $\mathbf{F}$ is defined as the vector of the objective functions where $f_i : \mathbb{R}^n \to \mathbb{R}$ is the function to be optimized. In this work, we consider the box-constrained case, i.e., $\Omega = \prod_{i=1}^{n}[a_j, b_j]$. Therefore, each vector $\mathbf{x} = (x_1, \ldots, x_n) \in \Omega$ is such that $a_i \le x_i \le b_i$ for all $i \in \{1, \ldots, n\}$.

In multi-objective optimization, it is desirable to obtain a set of trade-off solutions representing the best possible compromises among the objectives (i.e., solutions such that no objective can be improved without worsening another). To understand the concept of optimality referred to in this paper, the following definitions are provided [46].

Definition 1. *Let* $\mathbf{x}, \mathbf{y} \in \Omega$. *We say that* $\mathbf{x}$ *dominates* $\mathbf{y}$ *(denoted by* $\mathbf{x} \prec \mathbf{y}$*) if and only if* $f_i(\mathbf{x}) \le f_i(\mathbf{y})$, *for* $i = 1, 2, \ldots, M$, *and* $\mathbf{F}(\mathbf{x}) \ne \mathbf{F}(\mathbf{y})$.

Definition 2. *Let* $\mathbf{x}^\star \in \Omega$. *We say that* $\mathbf{x}^\star$ *is a* Pareto optimal *solution, if there is no other solution* $\mathbf{y} \in \Omega$ *such that* $\mathbf{y} \prec \mathbf{x}^\star$.

Definition 3. *The Pareto set (PS) is defined by:*

$$PS = \{\mathbf{x} \in \Omega \mid \mathbf{x} \text{ is a Pareto optimal solution}\}$$

Definition 4. *The Pareto front (PF) is defined by:*

$$PF = \{\mathbf{F}(\mathbf{x}) \mid \mathbf{x} \in PS\}$$

In multi-objective optimization, it is desirable to obtain as many (but different) elements of the Pareto optimal set as possible, while maintaining a distribution of solutions as uniform as possible along the Pareto front.

3.3. Evolutionary Multi-objective Algorithms

The development of optimization techniques is the result of the need to solve a specific real-world problem. Because of their flexibility and ease of use, evolutionary multi-objective algorithms (EMOAs) have become an alternative to solve an MOP in its most general case. Several EMOAs of different nature

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have been developed over the years (see the comprehensive reviews reported in [47, 48, 49]). EMOAs are normally classified into three main groups:

Pareto-based Approaches. Early evolutionary algorithms to solve MOPs straightforwardly integrate the Pareto dominance relation to rank the population and assess closeness to the Pareto optimal front. A suitable approximation of the Pareto front has to fulfill convergence and diversity simultaneously. Therefore, to distribute the solutions along the entire trade-off curve, Pareto dominance must be used in cooperation with a second criterion. Some methods that have been proposed to distribute solutions along the Pareto front include: *fitness sharing and niching* [50], *clustering* [51], *crowding distance* [52], among many others. In the early 2000s, Pareto-based MOEAs became one of the most commonly used strategies. However, their use has decreased because of the difficulty of properly spreading solutions and losing their discriminant property in high-dimensional objective spaces.

Decomposition-based Approaches. In the last decade, several evolutionary approaches have employed scalarizing functions, giving rise to the so-called EMOAs based on decomposition. Decomposition-based approaches rely on solving a number of scalarizing functions formulated by the same number of weight vectors. This strategy to solve MOPs has been useful to deal with complicated test problems (see, for instance, [53, 54, 55, 56]). Although the use of this principle has become a viable alternative to deal with multi-objective problems, its performance depends on the weight vectors which have to be appropriately distributed "*a priori.*"

Indicator-based Approaches. Indicator-based EMOAs (IBEAs) employ performance indicators in their environmental selection procedures. There exist several indicators to assess the performance of EMOAs (see the comprehensive review of performance indicators presented in [57, 58, 59]), which, in different ways, evaluate convergence or diversity, or both of them at the same time. In particular, a relatively good PF representation of an MOP can be achieved

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by adopting the hypervolume indicator [60] or by using performance indicators based on reference sets such as $R2$ [61], IGD [62], or Δ_p [63].

IBEAs based on reference sets depend on a proper definition of the reference set, which in most cases, is challenging to state before the search. In contrast, IBEAs based on the hypervolume only require a single reference vector to compute the hypervolume indicator. However, these approaches are limited by the high computational cost required for calculating the hypervolume indicator values, which increases exponentially with the number of objectives. Nonetheless, the advantage of using IBEAs based on hypervolume is that they can deal with different Pareto front geometries, including convex, concave, mixed, disconnected, and degenerated shapes. In particular, hypervolume-based EMOAs can obtain a uniform set of points in linear Pareto fronts [64], motivating its use to generate uniform mixture designs.

4. Our Proposed Approach

In this work, we formulated three M-objective optimization problems (MOPs). These MOPs have linear Pareto fronts, and their shapes describe a regular $(M-1)$-dimensional simplex. Each solution in the Pareto front is a mixture, i.e., all components are nonnegative, and their sum is equal to one. Therefore, to produce a uniform mixture design, we need to solve any of the formulated MOPs.

Our methodology to approximate uniform mixture designs is called "Mixtures via Evolutionary Multi-objective Optimization (MEMO[3])."

To solve these MOPs, we use two EMOAs based on Pareto dominance, one based on decomposition and two based on performance indicators. As we mention before, the EMOAs have two aims: i) To obtain as many solutions of the

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[3]The source code of this proposal, using the versions of iSMS-EMOA, is available at https://drive.google.com/file/d/1LD7g2jWtLqAGWXdH1MiL3vFumGmEFa53/view?usp=sharing. In the case of NSGA-II, SPEA2, VaEA, and 1by1EA, we use the Evolutionary Multi-objective Optimization platform (PlatEMO) available at https://github.com/BIMK/PlatEMO, and we incorporate the three MOPs defined in this work which are available at https://drive.google.com/file/d/1J1g3JvEpZZMzMAXR1Gh8dPmw7kOymVPj/view?usp=sharing

Pareto optimal set as possible and ii) to get a distribution of solutions as uniform as possible along the Pareto front. For the three MOPs proposed here, any decision space solution is indeed on the Pareto front. Therefore, we are evaluating the second aim.

It is well-known that EMOAs based on Pareto dominance have difficulties when the number of objective functions increases because the number of non-dominated solutions increases quickly. Additionally, they lose their discriminant property to converge to the Pareto front. However, in this case, we are only interested in evaluating the distribution technique of each EMOA.

Regarding EMOAs based on decomposition, we know that they need a set of well-distributed convex weights, which is the same to generate a uniform mixture design. However, the chosen EMOA adaptatively adjusts the weight vectors. Below, we list the EMOAs that were selected for our study:

1. NSGA-II [52] which is based on Pareto dominance and a concept of crowding distance;

2. SPEA2 [65] which is based on Pareto dominance and a clustering technique that preserves solutions in the extremes of the Pareto front;

3. VaEA [66], which is similar to decomposition algorithms, but in this case, the weight vectors are adaptively adjusted with respect to the distribution of the current population.

4. 1by1EA [67], which selects solutions one by one: first, only one solution with the best value on the convergence indicator is selected, and after that, solutions close to the one selected in the first step are de-emphasized according to the distribution indicator;

5. iSMS-EMOA [68], which is based on the hypervolume indicator (I_{Hv}). The main difference concerning other EMOAs based on I_{Hv} is that iSMS-EMOA only computes three contributions to I_{Hv} per iteration. The original SMS-EMOA needs to compute N contributions to I_{Hv} per iteration, where N is the population size.

6. Finally, we use a new version of iSMS-EMOA. The difference is in the crossover and mutation operators. The original version uses SBX and

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PBM. The new version uses the Differential Evolution operators (called in this paper iSMS-EMOA-DE).

The authors of VaEA, 1by1EA, and iSMS-EMOA mention that these EMOAs are designed to solve many-objective optimization problems, i.e., MOPs with more than three objective functions. We chose two hypervolume-based EMOAs because it has been shown that if the reference point is setting properly, the optimal distribution of the hypervolume indicator is uniform [69, 70]. Another interesting indicator is IGD+ because it is similar to the hypervolume indicator from the viewpoint of optimal distributions of solutions [71]. One advantage of IGD+ is its low computational cost. However, in our work, we can not use IGD+ because it needs a reference set and, in this case, is the set we are looking for (the uniform mixture design).

4.1. Multi-objective optimization problems

In this section, we present the multi-objective problems formulated to generate uniform mixture designs.

MOP1. The first MOP formulated in this paper consists in minimizing $\mathbf{F}(\mathbf{x}) = (f_1(\mathbf{x}), \ldots, f_M(\mathbf{x}))^T$ such that:

$$
\begin{aligned}
f_1(\mathbf{x}) &= \prod_{j=1}^{M-1} x_j \\
f_{i=2:M-1}(\mathbf{x}) &= (1 - x_{M-i+1}) \times \prod_{j=1}^{M-i} x_j \\
f_M(\mathbf{x}) &= 1 - x_1
\end{aligned}
\tag{3}
$$

where $\mathbf{x} \in [0,1]^{M-1}$.

The objective vector $\mathbf{F}(\mathbf{x})$ is a mixture for any decision variable $\mathbf{x} \in [0,1]^{M-1}$ (see the proof in Appendix A from the Supplementary Material). Furthermore, any decision vector $\mathbf{x}$ is a Pareto optimal solution of MOP1 (see the proof in Appendix D from the Supplementary Material).

Fig. 1 shows the Pareto fronts generated with 100, 210, and 300 random solutions for the MOP1 with three objective functions. It is worth noticing

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that by generating random solutions, i.e., $x_j = rand[0,1]$ for $j = 1, \ldots, M-1$, and evaluating them in MOP1, most of the objective vectors are biased towards the top of the Pareto front. This bias causes that an EMOA requires more iterations to obtain well-distributed points along the Pareto front. To deal with this bias and considering the formulation of the objective functions, we generate the initial random population in the following way: $x_j \in [0.5, 1.0]$ with a probability of 0.7 and $x_j \in [0, 0.5]$ with a probability of 0.3. Fig. 2 shows that considering this change, it is possible to generate more solutions on the bottom of the Pareto front.

As can be seen, the dimensionality of the decision variable space is $M-1$; this reduces the search space to find scatter points along the Pareto front of MOP1.

(a) (b) (c)
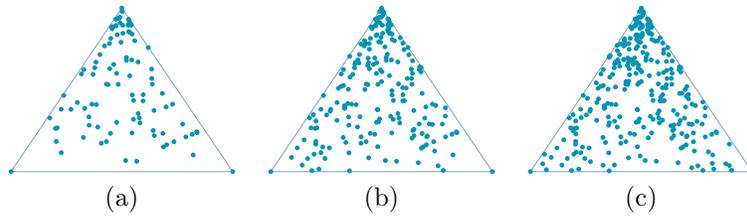
Figure 1:   MOP1 with three objective functions. We map the Pareto fronts into the two-dimensional space. In (a), (b) and (c), we use 100, 210 and 300 random solutions, respectively.


(a) (b) (c)
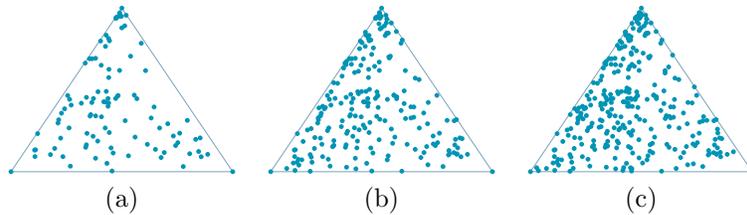
Figure 2:   MOP1 with three objective functions. We map the Pareto fronts into the two-dimensional space. In (a), (b) and (c), we use 100, 210 and 300 random solutions, respectively. To generate random solutions, we use $x_j \in [0.5, 1.0]$ with a probability of 0.7 and $x_j \in [0, 0.5]$ with a probability of 0.3.

MOP2. The second MOP formulated in this paper consists in minimizing $\mathbf{F}(\mathbf{x}) = (f_1(\mathbf{x}), \ldots, f_M(\mathbf{x}))^T$ such that:

$$
\begin{aligned}
f_1(\mathbf{x}) &= x_1 \\
f_{i=2:M-1}(\mathbf{x}) &= x_i - x_{i-1} \\
f_M(\mathbf{x}) &= 1 - x_{M-1}
\end{aligned}
\tag{4}
$$

where $\mathbf{x} \in [0,1]^{M-1}$ such that $x_1 \leq x_2 \leq \cdots \leq x_{M-1}$.

The objective vector $\mathbf{F}(\mathbf{x})$ is a mixture for any decision variable $\mathbf{x} \in [0,1]^{M-1}$ (see the proof in Appendix B from the Supplementary Material). Furthermore, any decision vector $\mathbf{x}$ is a Pareto optimal solution of MOP2 (see the proof in Appendix D from the Supplementary Material).

Fig. 3 shows the Pareto fronts generated with 100, 210, and 300 random solutions for this MOP with three objective functions. Using this formulation, random points are not biased to some regions of the Pareto front. Analogous to the previous problem, the dimensionality of the decision variable space is $M-1$. However, this formulation considers that the components of the decision variables are sorted.

(a)　　　　　(b)　　　　　(c)
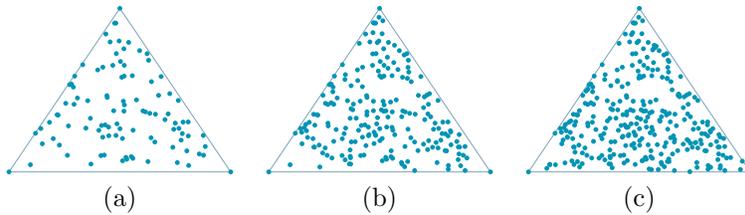
Figure 3:　MOP2 with three objective functions. We map the Pareto fronts into the two-dimensional space. In (a), (b) and (c), we use 100, 210 and 300 random solutions, respectively.

MOP3. The last MOP formulated in this paper consists in minimizing $\mathbf{F}(\mathbf{x}) = (f_1(\mathbf{x}), \ldots, f_M(\mathbf{x}))^T$ such that:

$$
f_{i=1:M}(\mathbf{x}) = \frac{|x_i|}{\|\mathbf{x}\|_1}
\tag{5}
$$

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where $\mathbf{x} \in [0,1]^M$ such that $\mathbf{x} \neq \mathbf{0}$.

335   The objective vector $\mathbf{F(x)}$ is a mixture for any decision variable $\mathbf{x} \in [0,1]^M$ (see the proof in Appendix C from the Supplementary Material). On the other hand, any decision vector $\mathbf{x}$ is a Pareto optimal solution of MOP3 (see the proof in Appendix D from the supplementary material).

Fig. 4 shows the Pareto fronts generated with 100, 210, and 300 random
340   solutions for MOP3 with three objective functions. It is worth noticing that by generating random solutions, i.e., $x_j = rand[0,1]$ for $j = 1, \ldots, M$, and evaluating them in MOP3, most of the objective vectors are biased towards the center of the Pareto front. Since the solutions cover the entire center, we hypothesize that the EMOAs can generate solutions in all the Pareto front extremes. Also,
345   note that the dimensionality of the decision variable space is M; this increases the search space to find spread points along the Pareto front of MOP3.

|		
(a)	(b)	(c)
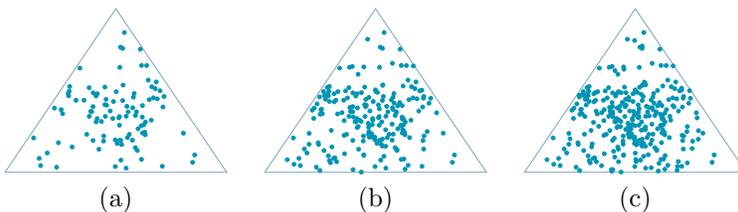
Figure 4:   MOP3 with three objective functions. We map the Pareto fronts into the two-dimensional space. In (a), (b) and (c), we use 100, 210 and 300 random solutions, respectively.

5. Experimental Results

5.1. Performance assessment

The purpose of our proposed approach is to obtain a mixture design with de-
350   sign points as uniform as possible. In the above section, we saw that the Pareto front of the formulated MOPs is a set of nondominated points that describe a mixture design, i.e., each point in the Pareto front is a mixture. Therefore, uniformity in the Pareto front implies uniformity in the mixture design. Thus, we can use a performance indicator from the evolutionary optimization community

to assess the distribution of points in a mixture design, such as inverted generational distance (IGD) [72], Δ_p-indicator [63], hypervolume indicator (I_{Hv}) [60], Schott's spacing (I_S) [73] and Deb's spread indicator [74].

The first three performance indicators do not guarantee a correct assessment of the distribution [75, 76]. For example, the IGD and Δ_p-indicator need a reference Pareto front that has to be previously defined. Therefore, if the reference Pareto front does not have well-distributed points, the measure of distribution becomes wrong. Paradoxically, IGD and Δ_p can not be used in this work as they need a reference Pareto front, i.e., the set that defines the mixture design, which is precisely the set that we are looking for. On the other hand, I_{Hv} benefits some regions depending on the geometry of the approximated Pareto front. In a convex Pareto front, I_{Hv} benefits sets with more solutions on inner regions. Conversely, in a concave Pareto front, I_{Hv} benefits sets with more solutions close to the extreme portions of the Pareto curve. However, in linear Pareto fronts (such as the Pareto fronts of the problems formulated in Section 4.1), this does not happen. In [69, 70], the authors study the reference point we should use to obtain a fair comparison when employing the hypervolume indicator. Their experiments show that in linear Pareto fronts, the optimal distribution regarding hypervolume is uniform. I_S and spread indicators only assess distribution, and it is commonly used with another indicator that assesses convergence to the Pareto front. In the proposed MOPs, all solutions are in the Pareto front. Therefore, we only need to measure the distribution. In this work, we assess the mixture design distribution by using I_{Hv} and I_S. We do not use Deb's spacing indicator because its definition contemplates "two consecutive points," and it is not clear in the case of more than two dimensions.

5.1.1. Hypervolume indicator

It was proposed by Zitzler and Thiele [60]. I_{Hv} is defined as the size of the space covered by each solution $\mathbf{z}$ in the PF approximation A. If $\mathcal{L}$ denotes the

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Lebesgue measure, I_{Hv} is defined as:

$$I_{Hv}(A, \mathbf{y}_{ref}) = \mathcal{L}\left(\bigcup_{\mathbf{z} \in A} \{\mathbf{y} \mid \mathbf{z} < \mathbf{y} < \mathbf{y}_{ref}\}\right) \tag{6}$$

where $\mathbf{y}_{ref} \in \mathbb{R}^M$ denotes a reference point that should be dominated by all solutions in A. Bigger values for I_{Hv} are better.

Ishibuchi et al. [69, 70] studied how to specify a reference point for a fair comparison. They proposed to set the reference point with $r \geq 1 + \frac{1}{(n-1)}$ in normalized linear Pareto fronts with two objective functions, where n is the number of solutions. They proposed setting the reference point with $r = 1 + \frac{1}{H}$ in normalized linear Pareto fronts with three or more objective functions. In the previous equation, H is the number of divisions in each dimension. With these reference points, the maximum hypervolume corresponds to a uniform distribution that includes extreme of the Pareto front. For this work, we calculate the above equations. We consider n as the number of weights and $H = H_2$ for the two-layered SLD. See Table 1.

5.1.2. Spacing indicator

Schott proposed I_S [73] and it is defined as follows:

$$I_S(A) = \sqrt{\frac{1}{|A| - 1} \sum_{i=1}^{|A|} \left(\overline{d} - d_i\right)^2}$$

where $d_i = \min_{j, j \neq i} \sum_k |f_k^i - f_k^j|$ and $\overline{d} = \frac{1}{|A|} \sum_{i=1}^{|A|} d_i$, $k = 1, \ldots, M$ (where M is the number of objective functions), and $i, j = 1, \cdots |A|$. When $I_S = 0$ all the solutions in A are uniformly spread. It is important to note that I_S does not measure if there are points along the entire Pareto front. If all points are uniformly distributed in a zone of the Pareto front, the value of this indicator will be zero.

5.2. Parameter settings

The chosen EMOAs need the following parameters: population size, number of generations, and genetic operators' parameters. We state the number of

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Table 1: Configurations for the simplex-lattice design and the two-layered simplex-lattice design. We consider the inside layer (H_2) for six or more objective functions to calculate the reference point.

Dimension	Number of layers	Configuration	Number of weights	Reference point (value of each component)
2	1	-	200	$1 + \frac{1}{199} = 1.005$
3	1	$H = 19$	210	$1 + \frac{1}{19} = 1.052$
4	1	$H = 9$	220	$1 + \frac{1}{9} = 1.111$
5	1	$H = 6$	210	$1 + \frac{1}{6} = 1.166$
6	2	$H_1 = 4$, $H_2 = 3$	182	$1 + \frac{1}{3} = 1.333$
7	2	$H_1 = 4$, $H_2 = 2$	238	$1 + \frac{1}{2} = 1.5$
8	2	$H_1 = 3$, $H_2 = 2$	156	$1 + \frac{1}{2} = 1.5$

points in the mixture design (population size in the EMOA) according to the simplex-lattice design (SLD) and the two-layered SLD. It is worth mentioning that our proposal can generate an arbitrary number of mixtures. However, for a fair comparison between two mixture designs, the number of points in each one must be equal. As we mentioned in Section 2, the two-layered SLD uses the SLD to generate an outside layer and an inside layer. See Figure 5. Table 1 shows the configurations used in this work for SLD and two-layered SLD.
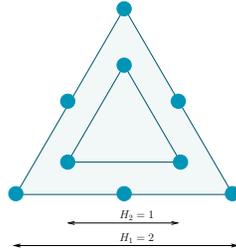
Figure 5: **Two-layered simplex-lattice design for three dimensions**. The outside layer is stated by $H_1 = 2$ (generating six points in the uniform mixture design), while the inside layer is setting by $H_2 = 1$ (generating three points in the uniform mixture design).

SPEA2, VaEA, 1by1EA, and the original iSMS-EMOA use the genetic operators of NSGA-II to create new individuals (SBX and PBM), and we use the values suggested in [52]. Only iSMS-EMOA-DE uses the genetic operators of DE. The number of generations and the parameters for DE were set experimentally. Concerning versions of iSMS-EMOA, we calculate the exact contribution

Table 2: Used parameters. M is the number of objective functions, w is the number of points in the uniform mixture design (population size), G_{max} is the number of generations, p_c and η_c are parameters required by the crossover operator of NSGA-II, p_m and η_m are parameters required by the mutation operator of NSGA-II, n is the number of decision variables, and F and p_c are parameters for the mutation and crossover operators of DE.

| | | | | SBX and PBM | | | | DE | |
M	w	G_{max}	samples	p_c	η_c	p_m	η_m	F	p_c
2	200	500	-	0.9	15	$1/n$	20	1.5	0.5
3	210	500	-	0.9	15	$1/n$	20	1.5	0.5
4	220	500	-	0.9	15	$1/n$	20	1.5	0.5
5	210	500	-	0.9	15	$1/n$	20	1.5	0.5
6	182	500	10000	0.9	15	$1/n$	20	1.5	0.5
7	238	500	10000	0.9	15	$1/n$	20	1.5	0.5
8	156	500	10000	0.9	15	$1/n$	20	1.5	0.5

to I_{Hv} for MOPs with up to five objective functions, and we approximate the contribution for MOPs with six or more objective functions. For the hypervolume contribution approximation, we employ the technique proposed by Bringmann and Friedrich in [77], which needs a set of sampling solutions. Therefore, we need to set the number of samples used for the hypervolume contribution approximation. Table 2 summarizes all parameters used in this work. The experiments were conducted on a personal computer with a 3.2GHZ CPU and 32GB in RAM.

5.3. Performance comparison of different Evolutionary Multi-Objective Algorithms

5.3.1. MOP1

Table 3 shows the results obtained by the adopted EMOAs in MOP1 regarding I_{Hv}. We elaborated a statistical analysis using Wilcoxon's rank-sum to determine if an EMOA is statistically better than another one (the null hypothesis "medians are equal" can be rejected at the 5% level, $H = 1$). Regarding results, the best algorithms are iSMS-EMOA, iSMS-EMOA-DE, and SPEA2. iSMS-EMOA occupies the sixth place in 6 dimensions; the second in 5 and 7 dimensions; the first in 3, 4, and 8 dimensions; and in 2 dimensions, iSMS-EMOA and iSMS-EMOA-DE have the same behavior. iSMS-EMOA-DE occupies the fifth place in 7 dimensions; the fourth in 8 dimensions; the second in 3 and 4

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dimensions; and the first place 5, and 6 dimensions. Finally, SPEA2 occupies
the fifth place in 8 dimensions; the third in 2, 3, 4, and 5 dimensions; the second in 6 dimensions; and the first in 7 dimensions. VaEA is competitive in 6, 7 (third place), and 8 (second place) dimensions. And, 1by1EA is competitive in 8 dimensions (third place).

Table 4 shows the results obtained by the adopted EMOAs in MOP1 regarding I_S. Also, with this indicator, the best algorithms are SPEA2, iSMS-EMOA-DE, and iSMS-EMOA. In 2 and 4 dimensions, iSMS-EMOA and iSMS-EMOA-DE have similar behavior (first place). While in 5 dimensions, SPEA2 and iSMS-EMOA-DE have similar behavior (first place). SPEA2 is third place in 2, 3, and 4 dimensions; and first in 5, 6, 7, and 8 dimensions. iSMS-EMOA-DE is second place in 3, 6, 7, and 8 dimensions; and first in 2, 4, and 5 dimensions. Finally, iSMS-EMOA is fourth place in 7 dimensions; third place in 5, 6, and 8 dimensions; and first in 2, 3, and 4 dimensions. VaEA is competitive in 7 dimensions (third place).

5.3.2. MOP2

Table 5 shows the results obtained by the adopted EMOAs in MOP2 regarding I_{Hv}. We elaborated a statistical analysis using Wilcoxon's rank-sum to determine if an EMOA is statistically better than another one (the null hypothesis "medians are equal" can be rejected at the 5% level, $H = 1$). According to the results, the best algorithms are iSMS-EMOA, iSMS-EMOA-DE, and SPEA2. In 2 dimensions, iSMS-EMOA and iSMS-EMOA-DE have similar behavior. iSMS-EMOA occupies the fifth place in 6 dimensions; the second in 7 dimensions; and the first in 2, 3, 4, 5, and 8 dimensions. iSMS-EMOA-DE occupies the sixth place in 7 and 8 dimensions; the third in 5 dimensions; the second in 3 and 4 dimensions; and the first in 2 and 6 dimensions. Finally, SPEA2 occupies the third place in 2, 3, 4, 6, and 8 dimensions; the second in 5 dimensions; and the first in 7 dimensions. VaEA is competitive in 6 and 8 dimensions (second place). And, 1by1EA is competitive in 7 dimensions (third place).

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Table 3: **Comparison of EMOAs, regarding** I_{Hv}. M is the dimensionality of the uniform mixture design (number of objective functions), and w is the number of points in the uniform mixture design (population size). We show average values over 30 independent runs. The values in parentheses correspond to the standard deviations. $P(H)$ shows the statistical analysis results applied to our experiments using Wilcoxon's rank-sum. P is the probability of observing that the null hypothesis "medians are equal" is true. $H = 1$ indicates that the null hypothesis can be rejected at the 5% level. We compare the fourth, fifth, and sixth best results of each MOP with three different shades of blue. The strongest tone corresponds to the best result, the intermediate tone to the second-best result, and the light tone is used for the third-best result.

M	w	NSGA-II	$P(H)$	SPEA2	$P(H)$	VaEA	$P(H)$	1by1EA	$P(H)$	iSMS-EMOA	$P(H)$	iSMS-EMOA DE
2	200	0.5067 (0.0001)	**0.000(1)** SPEA2	0.5074 (0.0000)	**0.000(1)** iSMS-DE	0.5072 (0.0001)	**0.000(1)** SPEA2	0.5073 (0.0000)	**0.000(1)** SPEA2	**0.5075 (0.0000)**	0.716(0) iSMS-DE	**0.5075 (0.0000)**
3	210	0.9548 (0.0025)	**0.000(1)** SPEA2	0.9691 (0.0002)	**0.000(1)** iSMS-DE	0.9679 (0.0005)	**0.000(1)** SPEA2	0.9566 (0.0027)	**0.000(1)** SPEA2	**0.9709 (0.0000)**	**0.000(1)** iSMS-DE	0.9709 (0.0000)
4	220	1.4303 (0.0023)	**0.000(1)** SPEA2	1.4470 (0.0003)	**0.000(1)** iSMS-DE	1.4440 (0.0006)	**0.000(1)** SPEA2	1.4177 (0.0045)	**0.000(1)** SPEA2	**1.4497 (0.0000)**	**0.000(1)** iSMS-DE	1.4496 (0.0000)
5	210	2.1097 (0.0010)	**0.000(1)** SPEA2	2.1225 (0.0003)	**0.000(1)** iSMS	2.1177 (0.0008)	**0.000(1)** SPEA2	2.0883 (0.0051)	**0.000(1)** SPEA2	2.1241 (0.0033)	**0.000(1)** iSMS-DE	**2.1243 (0.0011)**
6	182	5.5842 (0.0010)	**0.000(1)** VaEA	5.5923 (0.0062)	**0.000(1)** iSMS-DE	5.5887 (0.0012)	**0.000(1)** SPEA2	5.5600 (0.0047)	**0.000(1)** VaEA	5.5562 (0.0890)	**0.000(1)** VaEA	**5.5944 (0.0025)**
7	238	17.0739 (0.0023)	**0.000(1)** VaEA	**17.0782 (0.0035)**	**0.000(1)** iSMS	17.0758 (0.0005)	**0.000(1)** iSMS	17.0559 (0.0032)	**0.000(1)** VaEA	17.0768 (0.0003)	**0.000(1)** SPEA2	17.0729 (0.0200)
8	156	25.4606 (0.8389)	**0.000(1)** 1by1EA	25.5703 (0.2257)	**0.000(1)** 1by1EA	25.6049 (0.0642)	**0.000(1)** iSMS	25.5885 (0.0398)	**0.000(1)** VaEA	**25.6130 (0.0437)**	**0.000(1)** VaEA	25.5856 (0.1420)

MOP1

Table 4: **Comparison of EMOAs, regarding** I_S. M is the dimensionality of the uniform mixture design (number of objective functions), and w is the number of points in the uniform mixture design (population size). We show average values over 30 independent runs. The values in parentheses correspond to the standard deviations. $P(H)$ shows the statistical analysis results applied to our experiments using Wilcoxon's rank-sum. P is the probability of observing that the null hypothesis "medians are equal" is true. $H = 1$ indicates that the null hypothesis can be rejected at the 5% level. We compare the fourth, fifth, and sixth place against the third place, and the second place against the first place. We color the three best results of each MOP with three different shades of blue. The strongest tone corresponds to the best result, the intermediate tone to the second-best result, and the light tone is used for the third-best result.

M	w	NSGA-II	$P(H)$	SPEA2	$P(H)$	VaEA	$P(H)$	1by1EA	$P(H)$	iSMS-EMOA	$P(H)$	iSMS-EMOA DE
2	200	0.0035 (0.0003)	**0.000(1)** SPEA2	0.0016 (0.0001)	**0.000(1)** iSMS-DE	0.0031 (0.0007)	**0.000(1)** SPEA2	0.0027 (0.0002)	**0.000(1)** SPEA2	**0.0008** (0.0001)	0.574(0) iSMS-DE	**0.0008** (**0.0001**)
3	210	0.0303 (0.0019)	**0.000(1)** SPEA2	0.0109 (0.0008)	**0.000(1)** iSMS-DE	0.0209 (0.0016)	**0.000(1)** SPEA2	0.0300 (0.0041)	**0.000(1)** SPEA2	**0.0089** (**0.0007**)	**0.047(1)** iSMS-DE	0.0093 (0.0006)
4	220	0.0593 (0.0029)	**0.000(1)** SPEA2	0.0201 (0.0015)	**0.002(1)** iSMS-DE	0.0434 (0.0035)	**0.000(1)** SPEA2	0.0590 (0.0068)	**0.000(1)** SPEA2	**0.0194** (**0.0011**)	0.115(0) iSMS-DE	**0.0187** (**0.0015**)
5	210	0.0889 (0.0058)	**0.000(1)** iSMS	**0.0295** (**0.0020**)	0.417(0) iSMS-DE	0.0637 (0.0060)	**0.000(1)** iSMS	0.0859 (0.0085)	**0.000(1)** iSMS	0.0319 (0.0014)	**0.001(1)** iSMS-DE	**0.0299** (**0.0017**)
6	182	0.1200 (0.0076)	**0.000(1)** iSMS	**0.0376** (**0.0026**)	**0.000(1)** iSMS-DE	0.0917 (0.0109)	**0.000(1)** iSMS	0.1172 (0.0074)	**0.000(1)** iSMS	0.0775 (0.0051)	**0.000(1)** iSMS-DE	0.0472 (0.0034)
7	238	0.1311 (0.0047)	**0.000(1)** VaEA	**0.0417** (**0.0024**)	**0.000(1)** iSMS-DE	0.1006 (0.0058)	**0.000(1)** iSMS-DE	0.1163 (0.0097)	**0.000(1)** VaEA	0.1053 (0.0060)	**0.009(1)** VaEA	0.0607 (0.0043)
8	156	0.1649 (0.0061)	**0.000(1)** iSMS	**0.0515** (**0.0038**)	**0.000(1)** iSMS-DE	0.1417 (0.0140)	**0.000(1)** iSMS	0.1626 (0.0117)	**0.000(1)** iSMS	0.1336 (0.0115)	**0.000(1)** iSMS-DE	0.0815 (0.0072)

MOP1

Table 6 shows the results obtained by the adopted EMOAs in the MOP2 regarding I_S. SPEA2, iSMS-EMOA-DE, and iSMS-EMOA are the best algorithms. iSMS-EMOA and iSMS-EMOA-DE have similar behavior in 2, 3, 4 and 5 dimensions. SPEA2 occupies the third place in 2 and 3 dimensions; and the first in 4, 5, 6, 7, and 8 dimensions. iSMS-EMOA-DE occupies the second place in 4, 5, 6, 7 and 8 dimensions; and the first in 2 and 3 dimensions. Finally, iSMS-EMOA occupies the fourth place in 7 and 8 dimensions; the third in 6 dimensions; the second in 4 and 5 dimensions; and the first in 2 and 3 dimensions. VaEA is competitive in 7 dimensions (third place).

5.3.3. MOP3

Table 7 shows the results obtained by the adopted EMOAs in MOP3 regarding I_{Hv}. We elaborated a statistical analysis using Wilcoxon's rank-sum to determine if an EMOA is statistically better than another one (the null hypothesis "medians are equal" can be rejected at the 5% level, $H = 1$). Regarding results, NSGA-II and VaEA have similar behavior in 7 dimensions, and iSMS-EMOA and VaEA in 8 dimensions. The three best algorithms are iSMS-EMOA, iSMS-EMOA-DE, and SPEA2. iSMS-EMOA occupies the fifth place in 6 dimensions; the third in 7 dimensions; and the first place in 2, 3, 4, 5, and 8 dimensions. iSMS-EMOA-DE occupies the sixth place in 7 and 8 dimensions; and the second in 2, 3, 4, 5, and 6 dimensions. Finally, SPEA2 occupies the fifth place in 7 and 8 dimensions; the third in 2, 3, 4, and 5 dimensions; and the first in 6 dimensions. VaEA is competitive in 6 (third place), 7 (first place), and 8 (first place) dimensions.

Table 8 shows the results obtained by the adopted EMOAs in MOP3 regarding I_S. iSMS-EMOA and iSMS-EMOA-DE have similar behavior in 4 dimensions, and iSMS-EMOA-DE and SPEA2 in 5 dimensions, Again, SPEA2, iSMS-EMOA-DE, and iSMS-EMOA are the three best algorithms. SPEA2 occupies the third place in 2, 3, and 4; and the first in 5, 6, 7, and 8 dimensions. iSMS-EMOA-DE occupies the second place in 2, 6, 7, and 8 dimensions; and the first in 3, 4 and 5 dimensions. Finally, iSMS-EMOA occupies the fourth

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Table 5: **Comparison of EMOAs, regarding** I_{H_v}. M is the dimensionality of the uniform mixture design (number of objective functions), and w is the number of points in the uniform mixture design (population size). We show average values over 30 independent runs. The values in parentheses correspond to the standard deviations. $P(H)$ shows the statistical analysis results applied to our experiments using Wilcoxon's rank-sum. P is the probability of observing that the null hypothesis "medians are equal" is true. $H = 1$ indicates that the null hypothesis can be rejected at the 5% level. We compare the fourth, fifth, and sixth best results of each MOP with three different shades of blue. We compare the fourth, fifth, and sixth place against the third place, the third place against the second place, and the second place against the first place. We color the three best results of each MOP with three different shades of blue. The strongest tone corresponds to the best result, the intermediate tone to the second-best result, and the light tone is used for the third-best result.

M	w	NSGA-II	$P(H)$	SPEA2	$P(H)$	VaEA	$P(H)$	1by1EA	$P(H)$	iSMS-EMOA	$P(H)$	iSMS-EMOA DE
2	200	0.5066 (0.0001)	**0.000(1)** SPEA2	0.5074 (0.0000)	**0.000(1)** iSMS-DE	0.5073 (0.0001)	**0.000(1)** SPEA2	0.5073 (0.0000)	**0.000(1)** SPEA2	**0.5075 (0.0000)**	0.130(0) iSMS-DE	**0.5075 (0.0000)**
3	210	0.9545 (0.0023)	**0.000(1)** SPEA2	0.9686 (0.0003)	**0.000(1)** iSMS-DE	0.9677 (0.0004)	**0.000(1)** SPEA2	0.9556 (0.0041)	**0.000(1)** SPEA2	**0.9709 (0.0000)**	**0.000(1)** iSMS-DE	0.9708 (0.0000)
4	220	1.4245 (0.0026)	**0.000(1)** SPEA2	1.4454 (0.0005)	**0.000(1)** iSMS-DE	1.4429 (0.0010)	**0.000(1)** SPEA2	1.4165 (0.0041)	**0.000(1)** SPEA2	**1.4496 (0.0000)**	**0.000(1)** iSMS-DE	1.4494 (0.0000)
5	210	2.0917 (0.0410)	**0.000(1)** iSMS-DE	2.1186 (0.0104)	**0.000(1)** iSMS	2.1129 (0.0084)	**0.000(1)** iSMS-DE	2.0845 (0.0059)	**0.000(1)** iSMS-DE	**2.1245 (0.0000)**	**0.000(1)** SPEA2	2.1171 (0.0129)
6	182	5.5710 (0.0053)	**0.000(1)** SPEA2	5.5790 (0.0657)	**0.000(1)** VaEA	5.5842 (0.0016)	**0.000(1)** iSMS-DE	5.5535 (0.0082)	**0.000(1)** SPEA2	5.5648 (0.0788)	**0.000(1)** SPEA2	**5.5855 (0.0409)**
7	238	16.9229 (0.4670)	**0.000(1)** 1by1EA	**17.0680 (0.0409)**	**0.000(1)** iSMS	17.0177 (0.1799)	**0.000(1)** 1by1EA	17.0354 (0.0655)	**0.000(1)** iSMS	17.0513 (0.0698)	**0.000(1)** SPEA2	16.8833 (0.5158)
8	156	25.4770 (0.4133)	**0.000(1)** SPEA2	25.5737 (0.1595)	**0.001(1)** VaEA	25.6074 (0.0113)	**0.000(1)** iSMS	25.5643 (0.0735)	**0.000(1)** SPEA2	**25.6184 (0.0005)**	**0.000(1)** VaEA	25.4194 (0.4850)

MOP2

Table 6: **Comparison of EMOAs, regarding** I_S. M is the dimensionality of the uniform mixture design (number of objective functions), and w is the number of points in the uniform mixture design (population size). We show average values over 30 independent runs. The values in parentheses correspond to the standard deviations. $P(H)$ shows the statistical analysis results applied to our experiments using Wilcoxon's rank-sum. P is the probability of observing that the null hypothesis "medians are equal" is true. $H = 1$ indicates that the null hypothesis can be rejected at the 5% level. We compare the fourth, fifth, and sixth best results of each MOP with three different shades of blue. The strongest tone corresponds to the best result, the intermediate tone to the second-best result, and the light tone is used for the third-best result.

M	w	NSGA-II	$P(H)$	SPEA2	$P(H)$	VaEA	$P(H)$	1by1EA	$P(H)$	iSMS-EMOA	$P(H)$	iSMS-EMOA DE
2	200	0.0034 (0.0002)	**0.000(1)** SPEA2	0.0016 (0.0001)	**0.000(1)** iSMS-DE	0.0031 (0.0005)	**0.000(1)** SPEA2	0.0028 (0.0003)	**0.000(1)** SPEA2	**0.0007** (0.0001)	0.109(0) iSMS-DE	**0.0008** (0.0001)
3	210	0.0303 (0.0013)	**0.000(1)** SPEA2	0.0108 (0.0006)	**0.000(1)** iSMS-DE	0.0211 (0.0014)	**0.000(1)** SPEA2	0.0293 (0.0060)	**0.000(1)** SPEA2	**0.0092** (0.0005)	0.641(0) iSMS-DE	**0.0093** (0.0005)
4	220	0.0608 (0.0030)	**0.000(1)** iSMS	**0.0196** (0.0015)	**0.000(1)** iSMS-DE	0.0433 (0.0033)	**0.000(1)** iSMS	0.0588 (0.0065)	**0.000(1)** iSMS	0.0210 (0.0012)	0.684(0) iSMS-DE	0.0209 (0.0012)
5	210	0.0869 (0.0032)	**0.000(1)** iSMS-DE	**0.0253** (0.0026)	**0.000(1)** iSMS	0.0672 (0.0061)	**0.000(1)** iSMS-DE	0.0839 (0.0094)	**0.000(1)** iSMS-DE	0.0344 (0.0020)	0.096(0) iSMS-DE	0.0364 (0.0014)
6	182	0.1086 (0.0060)	**0.000(1)** iSMS	**0.0220** (0.0021)	**0.000(1)** iSMS-DE	0.0924 (0.0061)	**0.000(1)** iSMS	0.1099 (0.0090)	**0.000(1)** iSMS	0.0813 (0.0059)	**0.000(1)** iSMS-DE	0.0568 (0.0040)
7	238	0.1131 (0.0074)	**0.000(1)** VaEA	**0.0359** (0.0084)	**0.000(1)** iSMS-DE	0.0973 (0.0053)	**0.000(1)** iSMS-DE	0.1130 (0.0081)	**0.000(1)** VaEA	0.1048 (0.0056)	**0.000(1)** VaEA	0.0731 (0.0044)
8	156	0.1330 (0.0105)	**0.000(1)** iSMS-DE	**0.0564** (0.0139)	**0.000(1)** iSMS-DE	0.1395 (0.0127)	**0.000(1)** NSGA-II	0.1529 (0.0113)	**0.000(1)** NSGA-II	0.1382 (0.0103)	**0.000(1)** NSGA-II	0.0970 (0.0085)

MOP2

place in 7 dimensions; the third in 6, and 8 dimensions; the second in 3 and 5 dimensions; and the first in 2 and 4 dimensions. VaEA is competitive in 7 dimensions (third place).

In conclusion, for the three proposed MOPs, the best EMOAs are SPEA2, iSMS-EMOA-DE, and iSMS-EMOA. Therefore, we can say that the distributions techniques based on I_{Hv} or clustering are a good option to obtain a set of Pareto points uniformly distributed in linear Pareto fronts. If we consider I_{Hv}, iSMS-EMOA and iSMS-EMOA-DE are better than SPEA2. If we consider I_S, SPEA2 is better than the versions of iSMS-EMOA. Since I_S does not measure spread, we can consider that, in general, I_{Hv} is a fairer indicator. It is interesting to observe that VaEA tends to be a good option when increasing the number of objective functions. In the following comparisons, we only use iSMS-EMOA, iSMS-EMOA-DE, and SPEA2.

5.3.4. Difficulties in solving the formulated MOPs

This section aims to identify the MOP that is easiest to solve by iSMS-EMOA, iSMS-EMOA-DE, and SPEA2. In our comparative study, we used I_{Hv} and elaborated a statistical analysis using Wilcoxon's rank-sum to determine if an MOP is statistically easier to solve than another one (the null hypothesis "medians are equal" can be rejected at the 5% level, $H = 1$). This same analysis was also used to determine if a problem has a similar difficulty when solved by different EMOAs (the null hypothesis cannot be rejected at the 5% level, $H = 0$). This statistical test was applied to compare the performance of the EMOA, solving two different MOPs. Table 9 shows the results obtained.

For SPEA2, the degree of difficulty (from low to high) is MOP3, MOP1, and MOP2 because it obtained the best results for 2, 3, 4, 6, and 8 dimensions when solving MOP3, it obtained the best result for 5 and 7 dimensions when solving MOP1, and it obtained the best result for two dimensions when solving MOP2. Similarly, with iSMS-EMOA, it obtained the best result with MOP3 in 3, 4, 6, 7, and 8 dimensions, it obtained the best result with MOP1 in 3, 4, and 8 dimensions, and it obtained the best result with MOP2 in 2 and 5

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Table 7: **Comparison of EMOAs, regarding** I_{Hv}. M is the dimensionality of the uniform mixture design (number of objective functions), and w is the number of points in the uniform mixture design (population size). We show average values over 30 independent runs. The values in parentheses correspond to the standard deviations. $P(H)$ shows the statistical analysis results applied to our experiments using Wilcoxon's rank-sum. P is the probability of observing that the null hypothesis "medians are equal" is true. $H = 1$ indicates that the null hypothesis can be rejected at the 5% level. We compare the fourth, fifth, and sixth best results of each MOP with three different shades of blue. The strongest tone corresponds to the best result, the intermediate tone to the second-best result, and the light tone is used for the third-best result.

M	w	NSGA-II	$P(H)$	SPEA2	$P(H)$	VaEA	$P(H)$	1by1EA	$P(H)$	iSMS-EMOA	$P(H)$	iSMS-EMOA-DE
2	200	0.5067 (0.0001)	**0.000(1)** SPEA2	0.5074 (0.0000)	**0.000(1)** iSMS-DE	0.5073 (0.0001)	**0.000(1)** SPEA2	0.5073 (0.0001)	**0.000(1)** SPEA2	**0.5075** **(0.0000)**	**0.001(1)** iSMS-DE	0.5075 (0.0000)
3	210	0.9584 (0.0015)	**0.000(1)** SPEA2	0.9693 (0.0001)	**0.000(1)** iSMS-DE	0.9677 (0.0005)	**0.000(1)** SPEA2	0.9599 (0.0024)	**0.000(1)** SPEA2	**0.9709** **(0.0000)**	**0.000(1)** iSMS-DE	0.9708 (0.0000)
4	220	1.4347 (0.0014)	**0.000(1)** SPEA2	1.4475 (0.0002)	**0.000(1)** iSMS-DE	1.4431 (0.0007)	**0.000(1)** SPEA2	1.4281 (0.0031)	**0.000(1)** SPEA2	**1.4497** **(0.0000)**	**0.000(1)** iSMS-DE	1.4496 (0.0000)
5	210	2.1120 (0.0036)	**0.000(1)** SPEA2	2.1220 (0.0047)	**0.000(1)** iSMS-DE	2.1150 (0.0115)	**0.000(1)** SPEA2	2.0996 (0.0036)	**0.000(1)** SPEA2	**2.1247** **(0.0000)**	**0.000(1)** iSMS-DE	2.1246 (0.0003)
6	182	5.5871 (0.0011)	**0.000(1)** VaEA	**5.5944** **(0.0001)**	**0.000(1)** iSMS-DE	5.5889 (0.0007)	**0.000(1)** iSMS-DE	5.5704 (0.0034)	**0.000(1)** VaEA	5.5839 (0.0470)	**0.000(1)** VaEA	5.5929 (0.0088)
7	238	**17.0576** **(0.0997)**	0.695(0) VaEA	17.0452 (0.1509)	**0.000(1)** iSMS	**17.0761** **(0.0005)**	0.695(0) NSGA-II	17.0517 (0.0639)	**0.000(1)** iSMS	17.0552 (0.1182)	**0.000(1)** NSGA-II	17.0446 (0.1804)
8	156	25.6154 (0.0224)	**0.000(1)** VaEA	25.6064 (0.0926)	**0.000(1)** NSGA-II	**25.6212** **(0.0005)**	0.723(0) iSMS	25.6066 (0.0024)	**0.000(1)** NSGA-II	**25.6212** **(0.0005)**	0.723(0) VaEA	25.4283 (0.5601)

MOP3

Table 8: **Comparison of EMOAs, regarding** I_S. M is the dimensionality of the uniform mixture design (number of objective functions), and w is the number of points in the uniform mixture design (population size). We show average values over 30 independent runs. The values in parentheses correspond to the standard deviations. $P(H)$ shows the statistical analysis results applied to our experiments using Wilcoxon's rank-sum. P is the probability of observing that the null hypothesis "medians are equal" is true. $H = 1$ indicates that the null hypothesis can be rejected at the 5% level. We compare the fourth, fifth, and sixth best results of each MOP with three different shades of blue. The strongest tone corresponds to the best result, the intermediate tone to the second-best result, and the light tone is used for the third-best result.

M	w	NSGA-II	$P(H)$	SPEA2	$P(H)$	VaEA	$P(H)$	1by1EA	$P(H)$	iSMS-EMOA	$P(H)$	iSMS-EMOA DE
2	200	0.0036 (0.0003)	**0.000(1)** SPEA2	0.0016 (0.0001)	**0.000(1)** iSMS-DE	0.0030 (0.0008)	**0.000(1)** SPEA2	0.0028 (0.0004)	**0.000(1)** SPEA2	**0.0009** **(0.0002)**	**0.003(1)** iSMS-DE	0.0010 (0.0001)
3	210	0.0300 (0.0015)	**0.000(1)** SPEA2	0.0103 (0.0007)	**0.000(1)** iSMS	0.0224 (0.0018)	**0.000(1)** SPEA2	0.0272 (0.0038)	**0.000(1)** SPEA2	0.0091 (0.0005)	**0.009(1)** iSMS-DE	**0.0087** **(0.0006)**
4	220	0.0616 (0.0033)	**0.000(1)** SPEA2	0.0199 (0.0016)	**0.000(1)** iSMS	0.0434 (0.0038)	**0.000(1)** SPEA2	0.0551 (0.0052)	**0.000(1)** SPEA2	**0.0194** **(0.0010)**	0.122(0) iSMS-DE	**0.0191** **(0.0010)**
5	210	0.0911 (0.0046)	**0.000(1)** iSMS	**0.0296** **(0.0017)**	0.109(0) iSMS-DE	0.0630 (0.0048)	**0.000(1)** iSMS	0.0792 (0.0056)	**0.000(1)** iSMS	0.0318 (0.0017)	**0.002(1)** iSMS-DE	**0.0302** **(0.0018)**
6	182	0.1237 (0.0074)	**0.000(1)** iSMS	**0.0396** **(0.0020)**	**0.000(1)** iSMS-DE	0.0848 (0.0087)	**0.000(1)** iSMS	0.1056 (0.0074)	**0.000(1)** iSMS	0.0762 (0.0058)	**0.000(1)** iSMS-DE	0.0475 (0.0033)
7	238	0.1345 (0.0054)	**0.000(1)** VaEA	**0.0437** **(0.0024)**	**0.000(1)** iSMS-DE	0.0903 (0.0056)	**0.000(1)** iSMS-DE	0.1060 (0.0051)	**0.000(1)** VaEA	0.0918 (0.0053)	**0.000(1)** iSMS-DE	0.0615 (0.0048)
8	156	0.1690 (0.0076)	**0.000(1)** iSMS	**0.0578** **(0.0025)**	**0.000(1)** iSMS-DE	0.1320 (0.0124)	**0.001(1)** iSMS	0.1451 (0.0105)	**0.000(1)** iSMS	0.1205 (0.0085)	**0.000(1)** iSMS-DE	0.0900 (0.0069)

MOP3

dimensions. Finally, iSMS-EMOA-DE obtained the best results with MOP1 in all dimensions, with MOP3 in 4, 5, 6, 7, and 8 dimensions. When dealing with MOP2, it only obtained the best results for two dimensions. For this reason, in the following sections, we use SPEA2 and iSMS-EMOA with MOP3 and iSMS-EMOA-DE with MOP1.

5.4. Performance comparison of different uniform mixture design techniques

Now, we compare the results obtained by iSMS-EMOA, iSMS-EMOA-DE, and SPEA2 regarding four techniques for uniform mixture design:

1. RANDOM: We generate a set of uniform random points in the range $[0, 1]$, and we evaluate them in the MOP1. We use MOP1 because in Section 4.1, we saw that it generates solutions better distributed than those generated by MOP3.

2. Simplex-lattice design [8]: We use this technique for two, three, four, and five dimensions. For more than five dimensions, this technique generates a huge number of design points being a disadvantage from a practical viewpoint in some real-life applications.

3. Two-layered SLD [23]: This technique addresses the disadvantage of SLD. Therefore, it is possible to generate a small number of mixtures. We use this technique for six, seven, and eight dimensions.

4. Low-discrepancy-sequence-based mixture design [6]: This method is based on the Sobol sequence, which is able to generate an arbitrary number of design points in arbitrary dimensionality.

The motivation to choose these methods is that we identify two main disadvantages in the current methods to generate uniform mixture designs:

1. Methods employing geometric concepts, like simplex-lattice design and two-layered SLD, achieve a set of well-distributed mixtures. Even, they can obtain the optimal distribution. However, they cannot generate an arbitrary number of points, and

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Table 9: Obtained results with the three proposed MOPs regarding I_{Hv}. M is the dimensionality of the uniform mixture design (number of objective functions), and C is the pair of MOPs considered for the statistical analysis. We show average values over 30 independent runs. The values in parentheses correspond to the standard deviations. $P(H)$ shows the statistical analysis results applied to our experiments using Wilcoxon's rank-sum. P is the probability of observing that the null hypothesis "medians are equal" is true. $H = 1$ indicates that the null hypothesis can be rejected at the 5% level. We used three different shades of blue to highlight the results. The strongest tone corresponds to the best result, the intermediate tone is used for the second-best result, and the light tone is used for the third-best result.

M	MOP	SPEA2	C	$P(H)$	iSMS-EMOA	$P(H)$	iSMS-EMOA-DE	$P(H)$
2	1	0.507387 (0.000012)	1,2	0.190(0)	0.507495 (0.000006)	0.017(1)	**0.507496 (0.000005)**	0.229(0)
	2	**0.507391 (0.000011)**	2,3	0.061(0)	**0.507498 (0.000005)**	0.001(1)	0.507497 (0.000003)	0.000(1)
	3	**0.507396 (0.000009)**	1,3	0.003(1)	0.507492 (0.000007)	0.106(0)	0.507484 (0.000007)	0.000(1)
3	1	0.969081 (0.000208)	1,2	0.000(1)	**0.970900 (0.000043)**	0.061(0)	**0.970856 (0.000034)**	0.000(1)
	2	0.968625 (0.000260)	2,3	0.000(1)	0.970881 (0.000031)	0.000(1)	0.970789 (0.000031)	0.000(1)
	3	**0.969313 (0.000133)**	1,3	0.000(1)	**0.970919 (0.000041)**	0.214(0)	0.970828 (0.000027)	0.003(1)
4	1	1.447046 (0.000253)	1,2	0.000(1)	**1.449710 (0.000026)**	0.000(1)	**1.449591 (0.000023)**	0.000(1)
	2	1.445380 (0.000489))	2,3	0.000(1)	1.449629 (0.000026)	0.000(1)	1.449434 (0.000029	0.000(1)
	3	**1.447499 (0.000202)**	1,3	0.000(1)	**1.449714 (0.000026)**	0.515(0)	**1.449598 (0.000026)**	0.383(0)
5	1	**2.122464 (0.000281)**	1,2	0.000(1)	2.124067 (0.003345)	0.000(1)	**2.124331 (0.001088)**	0.000(1)
	2	2.118627 (0.010444)	2,3	0.000(1)	**2.124549 (0.000039)**	0.000(1)	2.117120 (0.012947)	0.000(1)
	3	2.121960 (0.004677)	1,3	0.000(1)	2.124715 (0.000025)	0.702(0)	**2.124560 (0.000254)**	0.299(0)
6	1	5.592334 (0.006189)	1,2	0.000(1)	5.556215 (0.089000)	0.000(1)	**5.594364 (0.002516)**	0.000(1)
	2	5.579036 (0.065711)	2,3	0.000(1)	5.564826 (0.078838)	0.000(1)	5.585507 (0.040869)	0.000(1)
	3	**5.594390 (0.000132)**	1,3	0.000(1)	**5.583881 (0.047038)**	0.011(1)	**5.592879 (0.008800)**	0.865(0)
7	1	**17.078234 (0.003480)**	1,2	0.000(1)	17.076830 (0.000280)	0.000(1)	**17.072856 (0.019952)**	0.000(1)
	2	17.067971 (0.040876)	2,3	0.000(1)	17.051342 (0.069815)	0.000(1)	16.883273 (0.515820)	0.000(1)
	3	17.045241 (0.150904)	1,3	0.000(1)	**17.055157 (0.118186)**	0.002(1)	**17.044591 (0.180409)**	0.137(0)
8	1	25.570263 (0.225698)	1,2	0.000(1)	**25.613044 (0.043696)**	0.000(1)	**25.585636 (0.141989)**	0.004(1)
	2	25.573655 (0.159507)	2,3	0.000(1)	25.618364 (0.000545)	0.000(1)	25.419374 (0.484984)	0.007(1)
	3	**25.606387 (0.092610)**	1,3	0.001(1)	**25.621229 (0.000487)**	0.438(0)	**25.428312 (0.560060)**	0.853(0)

2. Methods based on discrepancy functions can generate an arbitrary number of points. However, they cannot achieve the optimal distribution.

Therefore, our proposal aims to obtain a mixture design with an arbitrary number of points well-distributed. For this reason, it is important to compare our proposal against these two approaches. Our aims are:

i) The distribution obtained in the mixture designs should be competitive regarding SLD and two-layered SLD, and

ii) The distribution obtained in the mixture designs should outperform the distribution obtained by methods based on discrepancy functions.

Regarding I_{Hv}, Table 10 shows that our proposal using iSMS-EMOA and MOP3 outperformed the other approaches in four (of seven) cases (3, 4, 5, and 8 dimensions). For six dimensions, SPEA2 outperformed the other approaches. Only, in 2 and 7 dimensions, SLD was able to overcome our proposal. Moreover, if we consider the best run, iSMS-EMOA using MOP3 and iSMS-EMOA-DE using MOP1 outperformed the other techniques in six (of seven) cases.

5.5. Parallel-Coordinates graphs of the best distributions

In Fig. 6 and Fig. 7, we plot the best distributions of the uniform mixture designs obtained by SLD, SPEA2, iSMS-EMOA, and iSMS-EMOA-DE. Fig. 6(a) shows that in the two-dimensional case, these four techniques obtained well-distributed mixture designs. We corroborate this with their corresponding Parallel-Coordinates graphs. In the three-dimensional case, see Fig. 6(b), we can see that the distribution accomplished by the versions of iSMS-EMOA is similar to that obtained by SLD. This can show that maximizing the hypervolume indicator in linear Pareto fronts (at least for two and three dimensions) implies obtaining a uniform distribution of Pareto points. The Parallel-Coordinates graphs show that SPEA2, iSMS-EMOA, and iSMS-EMOA-DE cover a more significant part of the design space for four dimensions or more. This is probably because the design space grows quickly, and thus, SLD leaves huge gaps between solutions.

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Table 10: Results obtained by the six different techniques for generating uniform mixture designs regarding I_{Hv}. M is the dimensionality of the uniform mixture design (number of objective functions), and w is the number of points in the uniform mixture design (population size). For the random technique and our proposals (iSMS-EMOA and iSMS-EMOA-DE), we show average values over 30 independent runs. The values in parentheses correspond to the standard deviations. Also, we show the worst and the best value found in the 30 independent runs. SLD and SOBOL are deterministic techniques. Therefore, they found a unique uniform mixture design.

| M	w	RANDOM	SLD	two-layer SLD	SOBOL	SPEA2 MOP3	iSMS-EMOA MOP3	iSMS-EMOA-DE MOP1
2	200	0.505064 (0.000304) worst 0.504484 best 0.505594	**0.507512**	-	0.507202	0.507396 (0.000010) worst 0.507380 best 0.507417	0.507492 (0.000007) worst 0.507480 best 0.507503	0.507496 (0.000005) worst 0.507486 best 0.507506
3	210	0.948537 (0.003994) worst 0.940189 best 0.957068	0.970347	-	0.968598	0.969313 (0.000136) worst 0.968978 best 0.969550	**0.970919** (0.000042) worst **0.970848** best **0.971028**	**0.970856** (0.000034) worst **0.970800** best **0.970948**
4	220	1.404639 (0.004164) worst 1.396886 best 1.412313	1.448103	-	1.447059	1.447499 (0.000205) worst 1.447082 best 1.447841	**1.449714** (0.000026) worst **1.449662** best **1.449750**	**1.449591** (0.000023) worst **1.449536** best **1.449630**
5	210	2.057323 (0.005559) worst 2.047057 best 2.067987	2.122047	-	2.120376	2.121960 (0.004757) worst 2.096785 best **2.123132**	**2.124715** (0.000026) worst **2.124647** best **2.124763**	**2.124353** (0.001120) worst 2.118607 best **2.124649**
6	182	5.444818 (0.014505) worst 5.410405 best 5.483957	5.591748	-	5.591659	**5.594390** (0.000134) worst **5.593911** best **5.594561**	5.583881 (0.047842) worst 5.330578 best 5.593212	**5.594364** (0.002559) worst 5.585057 best **5.595389**
7	238	16.789542 (0.032717) worst 16.704197 best 16.842936	**17.076283**	-	17.076222	17.045241 (0.153484) worst 16.258828 best **17.079795**	17.055157 (0.120207) worst 16.418705 best **17.077465**	17.072856 (0.020293) worst 16.995924 best **17.080050**
8	156	25.061462 (0.047741) worst 24.976547 best 25.190708	**25.614576**	-	25.620158	25.606387 (0.094194) worst 25.107710 best **25.624353**	**25.621229** (0.000495) worst **25.618980** best **25.621770**	25.585636 (0.144416) worst 24.832231 best **25.624534**

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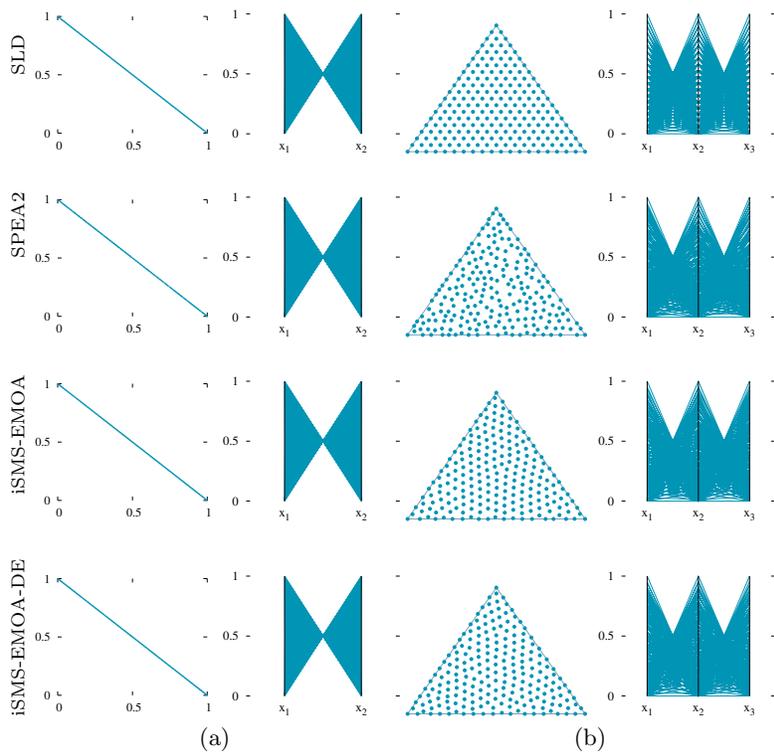
Figure 6: We show the distributions of uniform mixture designs obtained by SLD, SPEA2, iSMS-EMOA, and iSMS-EMOA-DE for two dimensions in (a) and three dimensions in (b). We also plot their corresponding Parallel-Coordinates graph.
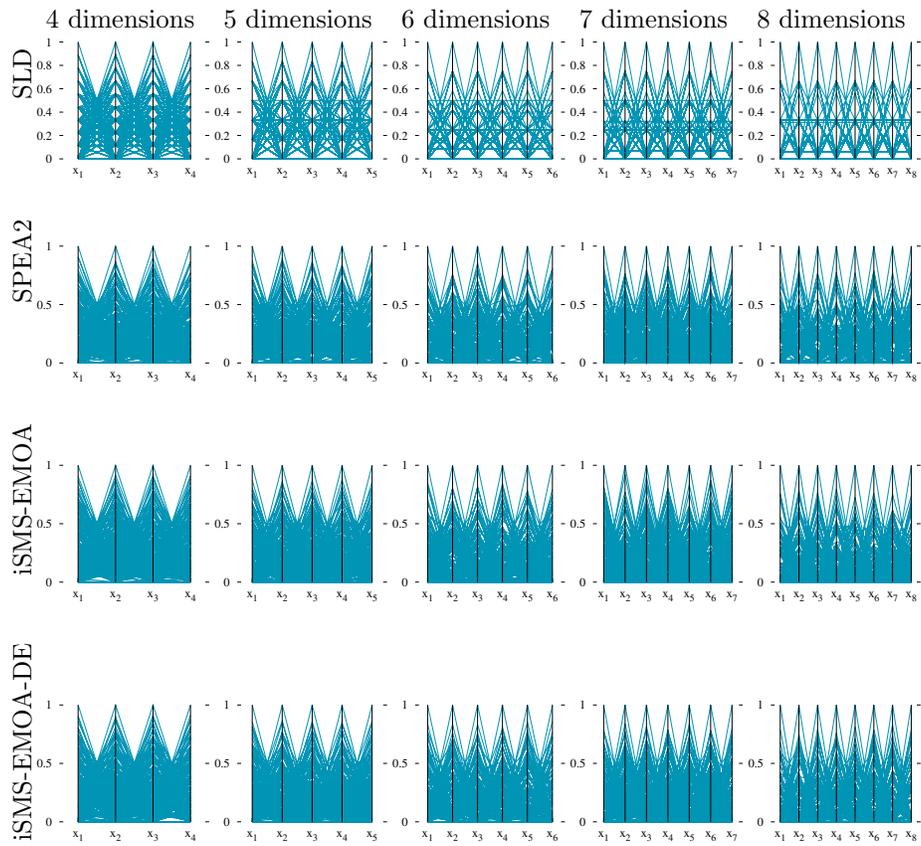
Figure 7: Distributions of the uniform mixture designs, for four, five, six, seven, and eight dimensions, obtained by SLD, SPEA2, iSMS-EMOA, and iSMS-EMOA-DE. We use Parallel-Coordinates graphs.

We conclude that our proposal is a good option if we need to generate uniform mixture designs. Moreover, different from most of the existing mixture design methods, our proposal allows generating an arbitrary number of mixtures.

6. Conclusions

In this paper, we studied different methods to generate uniform mixture designs from the most classical approaches, such as the simplex-lattice design (SLD) and the simplex-centroid design (SCD), to the most recent approaches, such as the two-layered SLD, k-layer reference direction, and an approach based on low-discrepancy sequences. Perhaps, the most frequently used method for uniform mixture designs is the SLD. However, when the dimensionality of the mixture increases, the number of design points quickly increases. In some applications, it is not desirable to have many design points because their use becomes impractical. Two-layered SLD, k-layer reference direction, and the low-discrepancy-sequence-based methods address this problem. Two-layered SLD and k-layer reference direction generate a smaller number of design points than SLD, but they cannot generate an arbitrary number of points. On the other hand, the low-discrepancy-sequence-based method can generate an arbitrary number of mixtures. However, the distribution obtained by this method does not outperform SLD or two-layered SLD.

In this paper, we have introduced a new methodology for generating uniform mixture designs via multi-objective optimization. This methodology is called "Mixtures via Evolutionary Multi-objective Optimization (MEMO)." For this task, we formulated three M-objective optimization problems (MOPs) whose Pareto fronts describe a regular $(M - 1)$-dimensional simplex. Such problems are solved by using six Evolutionary Multi-Objective Algorithms: NSGA-II, SPEA2, VaEA, 1by1EA, iSMS-EMOA, and iSMS-EMOA-DE. This way, the concerned multi-objective optimization problems are solved while a uniform design mixture is obtained. SPEA2, iSMS-EMOA, and iSMS-EMOA-DE obtained

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the best results. Particularly, the versions of iSMS-EMOA are an excellent option.

Our results indicate that our proposed method is a promising alternative for generating uniform mixture designs because it can create an arbitrary number of points, which are adequately distributed in the $(M-1)$-dimensional simplex (it outperforms a low-discrepancy-sequence-based method based on the Sobol sequence).

As part of our future work, we would like to study in-depth the parameters of SPEA2, iSMS-EMOA, and iSMS-EMOA-DE when solving the formulated MOPs. Notably, we consider investigating the reference point's impact on computing the hypervolume in iSMS-EMOA and iSMS-EMOA-DE. Additionally, we want to solve the formulated MOPs with an indicator-based EMOA using the s-energy quality indicator. This idea arises from the results reported in [78], which mention that the hypervolume and s-energy indicators converge to uniformly distributed Pareto fronts. On the other hand, we focus on studying the formulation of alternative multi-objective optimization problems for constructing mixture designs. The goal is that the new MOPs have two main features: (i) its Pareto front must be a $M-1$-dimensional simplex, and (ii) it should be easy to solve for EMOAs.Particularly, we are interested in constrained mixtures design by restricting the search space of EMOAs defining specific constraint functions. Finally, we also aim to investigate the use of preferences in EMOAs to generate extreme-vertice mixtures. Nonetheless, the above ideas remain as possible paths for future research.

Acknowledgment

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