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A new class of projected mixture designs

Walter TINSSON

Laboratoire de Mathématiques et de leurs Application de Pau, CNRS UMR 5142
Universite de Pau et des Pays de l'Adour, Pau, France

Abstract. *This paper is devoted to the construction of mixture designs obtained by projecting small size response surface designs. Such designs are then numerically obtained with the aim of finding D-optimal configurations.*

Keywords. Augmented pair designs, projected mixture designs, D-optimality.

Mathematics Subject Classification. 62K05, 62K20, 62K99.

1 Introduction

Mixture experiments are well known since the initial paper of Scheffe (1958). In this situation we assume that the response is a function only of the proportions of the components which are present in the mixture. Classical designs for mixtures are simplex lattice designs, simple centroid designs or axial designs. We are interested in this paper by a method proposed by Prescott (2000) in order to derive mixture designs from the projection of a response surface design.

The main problem of such a method is the size of response surface designs which is often too large for mixture designs (because models for fitting mixtures are submodels of classical polynomial models). Our idea in this paper is then to use small-size designs for response surfaces and more precisely saturated designs obtained by augmenting simplex designs for fitting order one model. In the class of such designs we are then looking numerically for D-optimal configurations.

This paper is organized as follows. A first part is devoted to recalls, notations and general results about augmented pair designs and projected design. A second part deals with the application of projected methods in order to obtain new mixtures designs and how to consider optimal configurations. Extensions of this method to constrained domains is presented in the last section.

2 Augmented and projected designs

2.1 Augmented pair designs

Consider a random phenomenon depending on m quantitative factors and n experimental units. We denote by $Y_{u,x}$ the observed value of the response when the treatment $x = (x_1, \dots, x_m)'$ is applied to the experimental unit u and by $\mathcal{E} \subset \mathbb{R}^m$ the experimental domain. An augmented design is firstly constituted by an initial design for fitting the order one classical model:

$$\forall x \in \mathcal{E}, Y_{u,x} = \beta_0 + \sum_{i=1}^m \beta_i x_i + \varepsilon_{u,x}.$$

In the following n_1 denotes the number of runs of this initial design and D_1 its design matrix (that is the $n_1 \times m$ matrix such that its rows are made up by the design point's coordinates). The goal is then to add some runs to the initial design in order to fit the response surface model (see, for example, Khuri and Cornell (1996) for the general subject of response surfaces methodology):

$$\forall x \in \mathcal{E}, Y_{u,x} = \beta_0 + \sum_{i=1}^m \beta_i x_i + \sum_{i=1}^m \beta_{ii} x_i^2 + \sum_{i < j} \beta_{ij} x_i x_j + \varepsilon_{u,x}. \quad (1)$$

For an augmented pair design (introduced by Morris (2000)) the idea is to consider each pair of runs (x_s, x_t) , $s < t$, of the initial design and then add the run αx_{st} with $\alpha \in \mathbb{R}$ and $x_{st} = x_s + x_t$. In other words the design matrix of the augmented design is D_{rsm} given by:

$$D'_{rsm} = [D'_1 \mid \alpha D'_2]$$

with D_2 the $n_2 \times m(m-1)/2$ matrix of the augmented part (its rows are made up by the design point's x_{st} coordinates). Note also that $n_2 = \binom{n_1}{2} = n_1(n_1-1)/2$. Two points are essential in the construction of an augmented design: the initial design and the value of α .

For the choice of the initial design it is possible to use a factorial design or a regular fraction of resolution III adapted to the first order model as proposed by Fand and Mukerjee (2004). Such designs have simple levels but are not necessarily saturated. On the other side the goal may be to consider a small initial design. Such design can be saturated using, for example, a simplex design. The matrix D_1 for a simplex design can be constructed in different ways: with a upper triangular block (see Khuri and Cornell (1996)), with cyclic permutations (see Crosier (1996)), etc. But these methods lead in general to a large number of different levels for the factors. An alternative method, suggested by Mee (2002), is to consider initial designs with only three different levels (a , b and c) such that (with $J_m = \mathbb{I}_m \mathbb{I}'_m$ the $m \times m$ matrix of ones):

$$D_1 = D_1(a, b, c) = \begin{pmatrix} a \mathbb{I}'_m \\ (b-c) I_m + c J_m \end{pmatrix} \quad (2)$$

It is easy to check that such design is saturated ($n_1 = m + 1$) and is also a simplex orthogonal design (that is $(1/\sqrt{m+1})X$ is an orthogonal matrix) if and only if $a = \pm 1$ and the choices for b and c are given by:

$$\begin{cases} a = -1 \\ b = (1 - (m-1)\sqrt{m+1})/m \\ c = (1 + \sqrt{m+1})/m \end{cases} \quad \text{or} \quad \begin{cases} a = -1 \\ b = (1 + (m-1)\sqrt{m+1})/m \\ c = (1 - \sqrt{m+1})/m \end{cases} \quad (3)$$

Two other alternatives when $a = 1$ are possible, they are obtained by reversing all the signs in the previous relations.

For the choice of the scale parameter α several ‘‘optimal’’ values have been proposed. Augmented pair design are particular case of a general theoretical method proposed by Box and Behnken (1960) for simplex-sum designs. For these designs they have suggested to take $\alpha = 1/2$ (see also Spendley et al. (1962)) that is to add to the initial design all the midpoints of its edges. More recently, Morris (2000) or Fang and Mukerjee (2004) have proved that taking $\alpha = -1/2$ lead us to more efficient designs. But for an initial design given by the matrix (2) and a spherical experimental region the choice $\alpha = -\sqrt{m/2(m-1)}$ leads in most cases to more efficient designs than those proposed by Morris (2000), see the paper of Tinsson (2007).

2.2 Projected designs

The aim of this method (see Prescott (2000)) is to derive mixture designs from response surface designs. Recall that mixture experiments involve m components and we are interested by the **proportion** x_i of each of them so $0 \leq x_i \leq 1$ for $i = 1, \dots, m$ and

$$\sum_{i=1}^m x_i = 1 \quad (4)$$

The classical second-order model for mixture is (under the constraint (4)):

$$\forall x \in \mathcal{E}, Y_{u,x} = \sum_{i=1}^m b_i x_i + \sum_{i < j} b_{ij} x_i x_j + \varepsilon_{u,x}. \quad (5)$$

The procedure to obtain a projected mixture design from an initial response surface design is given by the following steps:

- 1) use a response surface design in n runs and m factors given by the matrix D_{rsm} ,
- 2) construct the corrected matrix D_{rsm}^* such that its rows sum to zero, so:

$$D_{rsm}^* = D_{rsm} \left(I_n - \frac{1}{n} J_n \right).$$

3) transform the matrix D_{rsm}^* into matrix D such that its rows sum now to one (with $\delta \in \mathbb{R}$ and $J_{n,m} = \mathbb{I}_n \mathbb{I}'_m$ the $n \times m$ matrix of ones):

$$D = \delta D_{rsm}^* + \frac{1}{m} J_{n,m}.$$

4) find the values for the parameter δ in order to identify the matrix D to a mixture design matrix (that is all its values d_{ij} must be such that $0 \leq d_{ij} \leq 1$).

3 Application to mixture experiments

3.1 Actual context

Papers concerning projected designs are based on the projection of response surfaces designs like central composite designs (see Prescott (2000)) or on the projection of augmented pair designs with a full factorial design or a regular fraction for the initial design (see Prescott (2004)). The main problem with such methods is the size of these designs and the fact that second order models for mixtures are **submodels** of the classical response surface models. More precisely the number of unknown parameters are given by:

$$p_{rsm} = \frac{(m+1)(m+2)}{2} \text{ for model (1) and } p_{mix} = \frac{m(m+1)}{2} \text{ for model (5)}$$

so $p_{rsm} = p_{mix} + (m+1)$ and designs for response surfaces have in general too many runs in order to become “economical” projected mixture designs. For example in Prescott (2004) a projected mixture design for $m = 3$ components is obtained from an augmented pair design made with the full factorial design. In such a situation the initial full factorial design has $n_1 = 8$ runs so $n_2 = 28$ augmented runs are added and the final projected mixture design is in $n = 36$ runs. When all the experiments are expensive it is clear that such a design is not appropriate (we have here $p_{rsm} = 10$ and $p_{mix} = 6$). In a second time the author explains that the initial design can be reduced to a resolution III regular fraction of the full factorial design and then $n_1 = 4$ so $n_2 = 6$ and the final projected mixture design has just $n = 10$ runs which is a more suitable size. But such a situation works well because we are in a special case where the regular fraction is a saturated first-order design, or in other words the regular fraction is also a Plackett and Burman design (see Plackett and Burman (1946)) but such experimental designs don’t always exist (it is necessary that $m \equiv 3 \pmod{4}$). For example the same method applied to $m = 4$ factors with the smallest regular fraction is such that $n_1 = 2^{4-1} = 8$ so $n_2 = 28$ and then the final projected mixture design has $n = 36$ runs. It is not economically usable since $p_{mix} = 10$ here.

This construction method, based on full or fractional factorial designs is very efficient in the situation of **blocked** designs because as Prescott says (see Prescott (2004)): *“the orthogonal blocking property is preserved when the response surface design is projected into the mixture*

space". So such projected designs work well, and aren't too big, when heterogeneous experimental conditions require the use of two or more blocks. We'll now turn our attention to the case without blocks and look for a class of projected designs for mixtures of acceptable size.

3.2 New designs constructions

Our first goal is to obtain projected mixture design from **saturated** response surface designs. This can be done using three-levels simplex orthogonal designs presented in point (2). These designs are saturated for the first order model so the resulting augmented pair designs are also saturated for the response surface model (so constituted by $n = (m + 1)(m + 2)/2$ runs). The second goal is to have a large class of projected designs and this will be achieved by the choice of the two parameters α for the augmented pair design and δ for the projected method (see section 2). We denote in the following by $PMD_m(\alpha, \delta)$ such "projected mixture design".

We describe in the following the construction method for the particular case where $m = 3$ components are used for a mixture formulation. We start with the construction of the initial simplex orthogonal saturated design ($n_1 = 4$) with three levels presented in (2) so (using the second relation in (3)):

$$D_1 = \begin{pmatrix} -1 & -1 & -1 \\ 5/3 & -1/3 & -1/3 \\ -1/3 & 5/3 & -1/3 \\ -1/3 & -1/3 & 5/3 \end{pmatrix}$$

Adding the $n_2 = n_1(n_1 - 1)/2 = 6$ augmented runs on the form $x_{st} = \alpha(x_s + x_t)$ we obtain the following matrix for the augmented pair design:

$$D_{rsm} = \begin{pmatrix} -1 & -1 & -1 \\ 5/3 & -1/3 & -1/3 \\ -1/3 & 5/3 & -1/3 \\ -1/3 & -1/3 & 5/3 \\ \hline 2\alpha/3 & -4\alpha/3 & -4\alpha/3 \\ -4\alpha/3 & 2\alpha/3 & -4\alpha/3 \\ -4\alpha/3 & -4\alpha/3 & 2\alpha/3 \\ 4\alpha/3 & 4\alpha/3 & -2\alpha/3 \\ 4\alpha/3 & -2\alpha/3 & 4\alpha/3 \\ -2\alpha/3 & 4\alpha/3 & 4\alpha/3 \end{pmatrix}$$

The corrected projected matrix D_{rsm}^* (with rows sum to zero) and the final matrix $D = \delta D_{rsm}^* + (1/3)J_{10,3}$ are then respectively given by:

$$D_{rsm}^* = \begin{pmatrix} 0 & 0 & 0 \\ 4/3 & -2/3 & -2/3 \\ -2/3 & 4/3 & -2/3 \\ -2/3 & -2/3 & 4/3 \\ \hline 4\alpha/3 & -2\alpha/3 & -2\alpha/3 \\ -2\alpha/3 & 4\alpha/3 & -2\alpha/3 \\ -2\alpha/3 & -2\alpha/3 & 4\alpha/3 \\ 2\alpha/3 & 2\alpha/3 & -4\alpha/3 \\ 2\alpha/3 & -4\alpha/3 & 2\alpha/3 \\ -4\alpha/3 & 2\alpha/3 & 2\alpha/3 \end{pmatrix} \text{ and } D = \frac{1}{3} \begin{pmatrix} 1 & 1 & 1 \\ 4\delta + 1 & -2\delta + 1 & -2\delta + 1 \\ -2\delta + 1 & 4\delta + 1 & -2\delta + 1 \\ -2\delta + 1 & -2\delta + 1 & 4\delta + 1 \\ \hline 4\alpha\delta + 1 & -2\alpha\delta + 1 & -2\alpha\delta + 1 \\ -2\alpha\delta + 1 & 4\alpha\delta + 1 & -2\alpha\delta + 1 \\ -2\alpha\delta + 1 & -2\alpha\delta + 1 & 4\alpha\delta + 1 \\ 2\alpha\delta + 1 & 2\alpha\delta + 1 & -4\alpha\delta + 1 \\ 2\alpha\delta + 1 & -4\alpha\delta + 1 & 2\alpha\delta + 1 \\ -4\alpha\delta + 1 & 2\alpha\delta + 1 & 2\alpha\delta + 1 \end{pmatrix}$$

Now we have to select values for the parameter δ in order that the matrix D be the design matrix of a $PMD_3(\alpha, \delta)$ mixture design. If, for example, the augmented design is build with an α such that $-0.5 \leq \alpha \leq 0.5$ it is easy to check that the extremal values in the matrix D are $4\delta + 1$ and $-2\delta + 1$ so it is necessary that $0 \leq 4\delta + 1 \leq 1$ and $0 \leq -2\delta + 1 \leq 1$ so:

$$-0.25 \leq \delta \leq 0.5.$$

More generally, for m components and $\alpha \in \mathbb{R}$, denoting x the smallest value in the matrix D_{rsm}^* and y its largest value all the terms in the final matrix D are mixture propostions if and only if $0 \leq \delta a + 1/m \leq 1$ and $0 \leq \delta b + 1/m \leq 1$ that is (note that x is always negative):

$$\text{Max} \left(\frac{-1}{my}, \frac{(m-1)}{mx} \right) \leq \delta \leq \text{Min} \left(\frac{-1}{mx}, \frac{(m-1)}{my} \right).$$

3.3 Results : optimal designs

In this section the goal is to find optimal designs for the classical criteria of D-efficiency so denoting $X_{\alpha, \delta}$ the mixture model matrix obtained with the previous method we try to minimize the quantity $\left(\det \left[({}^t X X)^{-1} \right] \right)^{1/p}$ or equivalently maximize the value of $(\det ({}^t X X))^{1/p}$ (denoting now ‘‘Deff’’ in the following figures).

Firstly, all numerical results show that **large values** must be used for the parameter δ , that is $\text{Max}(-1/mb, (m-1)/ma)$ if $|\text{Max}(-1/mb, (m-1)/ma)| > |\text{Min}(-1/ma, (m-1)/mb)|$, $\text{Min}(-1/ma, (m-1)/mb)$ otherwise. Figure 1 shows some examples for $m = 4$ components. Note that this result is logical since low values for δ (close to zero) lead to low-efficiency mixture designs because all the design’s points are then close to the centroid of the experimental domain (from the relation $D = \delta D_{rsm}^* + (1/m)J_{n,m}$).

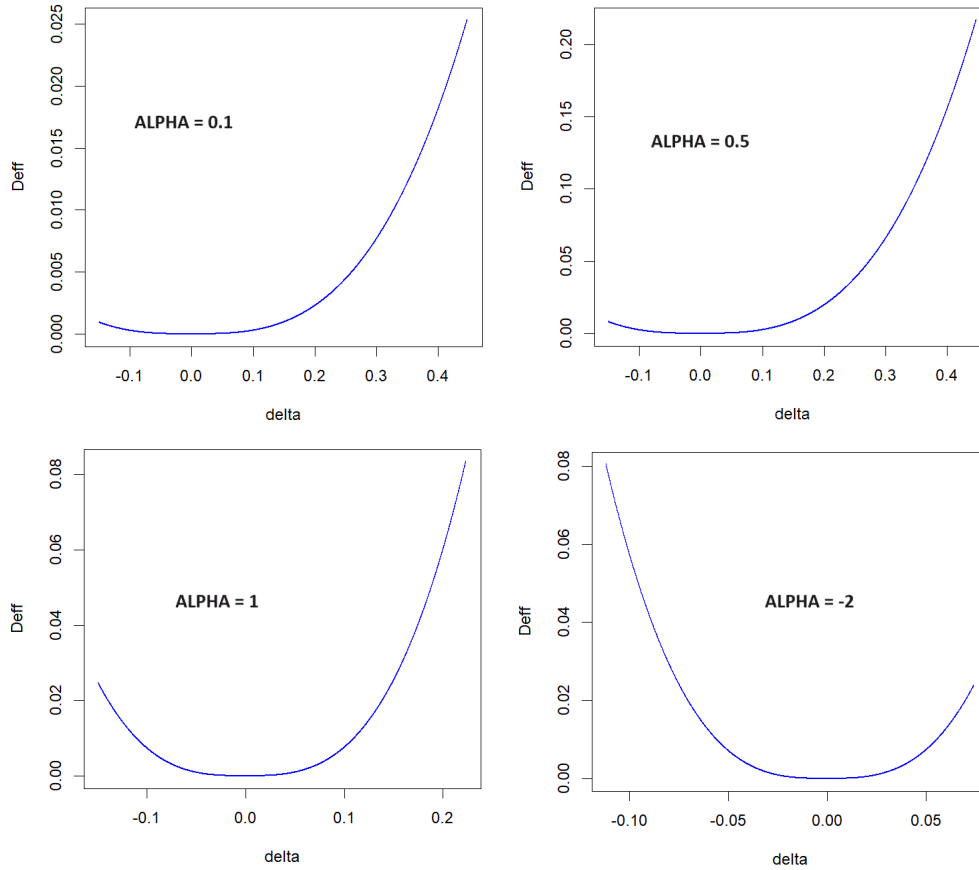


Figure 1

D-efficiencies for $m = 4$ components and several fixed values of α

We now simply denote by $PMD_m(\alpha)$ every projected mixture design obtained with the preceding optimal choice for the parameter δ . Now it is possible to compute the D-efficiencies of these designs as a function of α . Several examples are given below and lead to the same constation, that is:

Proposition 1. *For every projected mixture design $PMD_m(\alpha)$ the D-optimal configuration is obtained for $\alpha = 1/2$.*

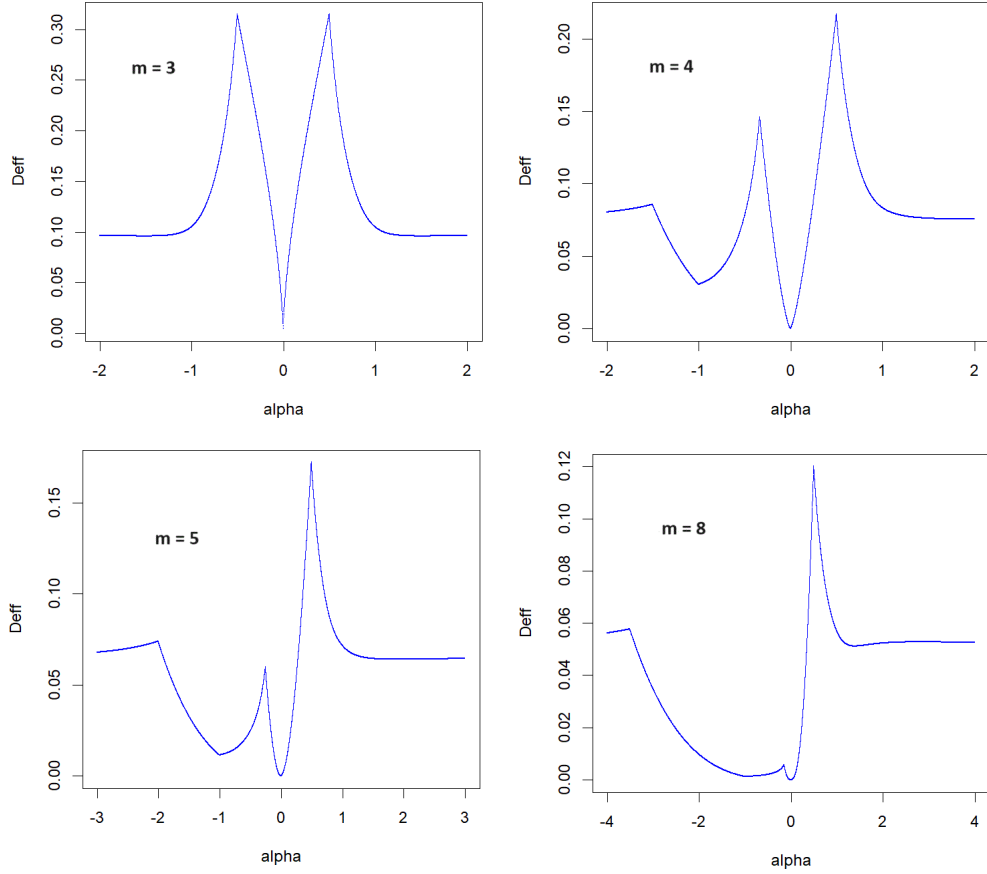


Figure 2

D-efficiencies depending on the value of α

We give in the following explicitly design matrices of these design from $m = 3$ components to $m = 8$ components. On order to simplify the presentation of large matrices we introduce the notation $\mathcal{P}_s(u)$, for every vector $u \in \mathbb{R}^n$, for the s permutations (often with repetitions) of the elements of u . For $m = 3$ components the optimal design $PMD_3(1/2)$ is given by:

$$D = \begin{pmatrix} 1/3 & 1/3 & 1/3 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 2/3 & 1/3 & 1/3 \\ 1/3 & 2/3 & 1/3 \\ 1/3 & 1/3 & 2/3 \\ 1/2 & 1/2 & 0 \\ 1/2 & 0 & 1/2 \\ 0 & 1/2 & 1/2 \end{pmatrix} = \begin{pmatrix} \mathcal{P}_1(1/3, 1/3, 1/3) \\ \mathcal{P}_3(1, 0, 0) \\ \mathcal{P}_3(2/3, 1/3, 1/3) \\ \mathcal{P}_3(1/2, 1/2, 0) \end{pmatrix}$$

Note that for $\alpha = -1/2$ we obtain in this case exactly the same design. For $m = 4$ components the optimal design $PMD_4(1/2)$ is given by:

$$D = \begin{pmatrix} 0.25 & 0.25 & 0.25 & 0.25 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0.625 & 0.125 & 0.125 & 0.125 \\ 0.125 & 0.625 & 0.125 & 0.125 \\ 0.125 & 0.125 & 0.625 & 0.125 \\ 0.125 & 0.125 & 0.125 & 0.625 \\ 0.5 & 0.5 & 0 & 0 \\ 0.5 & 0 & 0.5 & 0 \\ 0.5 & 0 & 0 & 0.5 \\ 0 & 0.5 & 0.5 & 0 \\ 0 & 0.5 & 0 & 0.5 \\ 0 & 0 & 0.5 & 0.5 \end{pmatrix} = \begin{pmatrix} \mathcal{P}_1(0.25, 0.25, 0.25, 0.25) \\ \mathcal{P}_4(1, 0, 0, 0) \\ \mathcal{P}_4(0.625, 0.125, 0.125, 0.125) \\ \mathcal{P}_6(0.5, 0.5, 0, 0) \end{pmatrix}$$

For $m = 5, 6, 7, 8$ components the optimal designs $PMD_m(1/2)$ are respectively given by:

$$D = \begin{pmatrix} \mathcal{P}_1(0.2, 0.2, 0.2, 0.2, 0.2) \\ \mathcal{P}_5(1, 0, 0, 0, 0) \\ \mathcal{P}_5(0.6, 0.1, 0.1, 0.1, 0.1) \\ \mathcal{P}_{10}(0.5, 0.5, 0, 0, 0) \end{pmatrix}, D = \begin{pmatrix} \mathcal{P}_1(0.167, 0.167, 0.167, 0.167, 0.167) \\ \mathcal{P}_6(1, 0, 0, 0, 0) \\ \mathcal{P}_6(0.583, 0.083, 0.083, 0.083, 0.083) \\ \mathcal{P}_{15}(0.5, 0.5, 0, 0, 0) \end{pmatrix}$$

$$D = \begin{pmatrix} \mathcal{P}_1(0.143, 0.143, 0.143, 0.143, 0.143, 0.143) \\ \mathcal{P}_7(1, 0, 0, 0, 0, 0) \\ \mathcal{P}_7(0.571, 0.071, 0.071, 0.071, 0.071, 0.071) \\ \mathcal{P}_{21}(0.5, 0.5, 0, 0, 0, 0) \end{pmatrix}$$

$$D = \begin{pmatrix} \mathcal{P}_1(0.125, 0.125, 0.125, 0.125, 0.125, 0.125, 0.125) \\ \mathcal{P}_8(1, 0, 0, 0, 0, 0, 0) \\ \mathcal{P}_8(0.562, 0.062, 0.062, 0.062, 0.062, 0.062, 0.062) \\ \mathcal{P}_{28}(0.5, 0.5, 0, 0, 0, 0) \end{pmatrix}$$

3.4 Discussion

We can see from the previous results that optimal projected mixture design for m components is always made up of:

- 1) one balanced mixture in m components (at the center of the centroid),

- 2) all the m single-component (at the vertices of the centroid),
- 3) m true mixtures in m components (on the Cox-axis),
- 4) $m(m-1)/2$ balanced mixtures in 2 components (at the middle of each edge).

The sizes of these designs are given below (with also the number p of unknown parameters of the mixture model).

	n	p		n	p
$m = 3$	10	6	$m = 6$	28	21
$m = 4$	15	10	$m = 7$	36	28
$m = 5$	21	15	$m = 8$	45	36

Note that parts 2 and 4 form a classical simplex lattice design $\{m, 2\}$. Part 3 is sometimes used in "axial" mixture design adding runs on the Cox-axes (the i -th Cox-axis is the line extending between single-component i and the mixture such that $x_i = 0$ and $x_j = 1/(m-1)$ for $j \neq i$). So projected method applied to an initial saturated augmented pair design for response surface lead us to a class of "augmented" simplex lattice designs. The lattice design $\{m, 2\}$ is economical but has the disadvantage of offering very simple mixtures (single-component or mixtures with only two components). Designs $PDM_m(1/2)$ are better in the sense that they offer a few more complex mixtures, while remaining relatively economical (with only $m+1$ additional runs). Note also that if the budget allows this, we can also carry out more central experiments and, for example, have a more precise decomposition of SSE with pure error and lack of fit error.

Note. *The optimal choice $\alpha = 1/2$ may seem surprising because from Morris (2000) or Fang and Mukerjee (2004) $\alpha = -1/2$ lead to more efficient designs. But the result of Morris or Fang and Mukerjee is true for "classical" designs, that is for polynomial models that are not those used with mixtures.*

Note. *The initial simplex orthogonal saturated designs used here always have the matrix formulation presented in (2) with the second relation in (3) concerning the values of a, b and c . The other choice for a, b and c does not lead to a symmetrical situation but to less efficient designs.*

4 Derivated designs

Classical simplex lattice designs or "augmented" simplex lattice designs have the practical drawback that they are not always adapted to the needs of the customers because some of their runs are too simple (or, in other words, they have too much points at the boundaries of the experimental domain). We assume in this part that all the runs must be true m -components mixtures that is:

$$\forall i = 1, \dots, m, x_i \geq p_{min} \text{ with } p_{min} > 0. \quad (6)$$

It is then easy to generalise the method proposed in section 2.2 in order to obtain efficient projected mixture designs satisfying such conditions. The last point (point 4) of this method just needs to be replaced by : find the values of the parameter δ in order to identify the matrix

$$D = \delta D_{rsm}^* + \frac{1}{m} J_{n,m}.$$

to a matrix mixture design under the constraint (6), that is all its values d_{ij} must be such that $p_{min} \leq d_{ij} \leq 1$. The admissible field of variations for the scale parameter δ is therefore more restricted than what we had before. Consider, for example, the construction of a projected mixture design for $m = 4$ components with the restriction that all of them must have a concentration such that $x_i \geq 0.05$. Using the value $a = 1/2$ (from proposition 1) for the construction of the augmented pair design the variations of the parameter δ lead to the following figure for the D-efficiency of the projected mixture design.

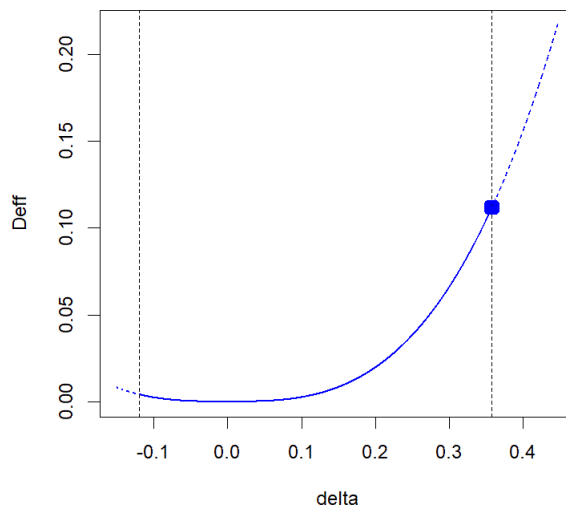


Figure 3

D-efficiencies depending on δ and restricted domain for $m = 4$ and $p_{min} = 0.05$

This figure is like one the representation of figure 1 but now the dashed parts of the curve are no longer usable. Numerical results show that the parameter δ must be such that $-0.119 \leq \delta \leq 0.358$ in order to obtain a projected mixture design with all the proportions greater than 0.05. The D-optimal design is obtained for $\delta = 0.358$ and has the following matrix D :

$$D = \begin{pmatrix} 0.25 & 0.25 & 0.25 & 0.25 \\ 0.85 & 0.05 & 0.05 & 0.05 \\ 0.05 & 0.85 & 0.05 & 0.05 \\ 0.05 & 0.05 & 0.85 & 0.05 \\ 0.05 & 0.05 & 0.05 & 0.85 \\ 0.55 & 0.15 & 0.15 & 0.15 \\ 0.15 & 0.55 & 0.15 & 0.15 \\ 0.15 & 0.15 & 0.55 & 0.15 \\ 0.15 & 0.15 & 0.15 & 0.55 \\ 0.45 & 0.45 & 0.05 & 0.05 \\ 0.45 & 0.05 & 0.45 & 0.05 \\ 0.45 & 0.05 & 0.05 & 0.45 \\ 0.05 & 0.45 & 0.45 & 0.05 \\ 0.05 & 0.45 & 0.05 & 0.45 \\ 0.05 & 0.05 & 0.45 & 0.45 \end{pmatrix} = \begin{pmatrix} \mathcal{P}_1(0.25, 0.25, 0.25, 0.25) \\ \mathcal{P}_4(0.85, 0.05, 0.05, 0.05) \\ \mathcal{P}_4(0.55, 0.15, 0.15, 0.15) \\ \mathcal{P}_6(0.45, 0.45, 0.05, 0.05) \end{pmatrix}$$

As for designs without constraints we had to carry out $n = 15$ runs in order to fit a mixture model in $p = 10$ unknown parameters. Concerning the structure of these runs we find again the centroid of the simplex. The four vertices of the projected mixture design without constraint are then replaced by four points on the Cox axes (one proportion at 0.85 and the three other at 0.15). The following four points of projected mixture design without constraint $PDM_4(1/2)$ (see part 3.3) were on the Cox axes with one proportion at 0.625 and the three other at 0.125. They satisfy the constraints but they are replaced in the optimal design by the points on the Cox axes with one proportion at 0.55 and the three other at 0.15. And finally the six points of the projected mixture design without constraint at the center of each edge are replaced with six points using two proportions at 0.45 and the two other at 0.05.

5 Conclusion

We have seen in this paper that small size mixture optimal designs can be obtained from saturated response surface designs. These projected mixture designs have a more complex structure than the classical lattice or centroid designs. Moreover they are small but not saturated designs so it is possible to estimate other effects than model's components. We have seen also that numerical generalisations can be easily obtained in order to satisfy some other constraints. At the end of this paper we have implemented constructions of such designs for constraints on the form $x_i \geq p_{min}$ but it can be easily extended to more complicated constraints like $x_i \leq p_{max}$ or $p_{min} \leq x_i \leq p_{max}$.

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