Optimal Robust Design for Mixture Experiments

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Abstract

Techniques for handling the optimal design problems related to the area of mixture models, while reducing the dependence of the assumed model, are considered in this paper. The nature of mixture experiments requires specific types of regression models and standard designs are proposed in the literature for them. Prior to running the experiment, practitioners have little information about model adequacy and optimal designs are strongly model dependent. In order to reduce this dependency, we investigate the problem of designing when the response varies over a neighbourhood of the considered model fitted by the experimenter. Optimal robust designs are computed in this work for binary and ternary blends. Techniques of construction given by Daemi and Wiens (2013) [2] are properly set for mixture problems. Nevertheless, the analytical treatment of the problem for more than two ingredients is not feasible due to the presented complexity. Two methodologies are provided in this paper for overcoming the encountered difficulties. First one is a general numerical technique based on genetic algorithm. The other consists on considering a class of restricted designs over a subregion of the simplex. The use of these restricted designs is motivated by often finding that the optimal robust designs verify certain geometrical property of symmetry. Designs verifying this property on the simplex will be named exchangeable designs. Different classes of exchangeable designs are investigated in this work for comparison purposes.

Keywords: Optimum Experimental Design; Robustness; Mixture experiments; D-optimality; Genetic algorithm;

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1 State of the art

Many experimental fields are especially interested in analysing how one or several characteristics of an end-product vary depending on its composition. Thus, the aim of mixture design is to identify the proportions of different blends which suitably describe the property under study. This kind of problems is characterized by having a constrained-shaped experimental region, which is a $(q-1)-$dimensional simplex $\mathcal{S}$ in a mixture experiment involving q ingredients.

Scheffé was a pioneer in studying mixture experiments from the design point of view [6]. His main contribution was defining mixture models, *Scheffé's canonical polynomials* and standard designs for these models, *simplex-lattice* and *simplex-centroid* designs [6], [7]. Following this idea, mixture design background has received a classical design approach and emphasis on finding optimal mixture experiments has been relatively less pronounced (see [8] for an updated review). Although other types of regression models are available in the literature, Scheffé's polynomials are the most widely used since they are sufficiently flexible for a large number of practical situations [3]. On the other hand, a general criticism of OED is that the designs are strongly model dependent at a stage when there are not observations yet. This criticism was first made by Box and Draper [1] who warned that to consider an inexact model may invalidate results from classical OED theory. Deviances from the considered model typically occur in mixture experiments, particularly when these cannot be conduced under uniform conditions and the response depends not only on the mixture ingredients but also on processing conditions [5].

Model-robustness may be classified into several streams of research. In mixture context, all contributions have been aimed at developing methods for practical scenarios. This research line focuses on considering a set of user-specified models and the optimal design is achieved optimising a modified criterion function which depends on all candidate models. Under this framework, the literature is modest, being the only existing works [4], [9]. Heredia-Langner et al. [4] provided a genetic algorithm to solve the problem whereas Smucker et al. [9] generalized an exchange algorithm. Another approach of the model-robustness is based on continuous design theory. Designs must optimize a function of a potential model subject to a contamination function which is unknown but continuous and bounded function [1], [10], [2]. It requires an analytical treatment of the bias and asymptotic designs are derived. In spite of this approach has been studied in multitude of regression contexts, it has been unexplored for mixture settings.

Regarding restricted designs, no similar study has been carried out according to exchangeable optimal robust designs for mixture models as far as the authors' knowledge.

2 Contributions

Main contributions of this work are to provide D-optimal robust designs for mixture experiments as well as techniques for the construction of these designs. The problem is set for binary and ternary blends using second-order Scheffé polynomials as potential models. Model-robustness is addressed allowing the "true" response to vary over a L_2-neighbourhood Ψ as large as the experimenter judges in a minimax sense.

Strategies followed for solving the problem under study depend on number of ingredients. In order to compute continuous designs for **binary blends**, theoretical results were obtained to set the techniques of construction [2] in mixture problems:

1. Establishing optimality conditions under which a symmetrical design $\xi \in \Xi_s$ is the global $D-$optimal robust design.

   Theorem 1 *If there exists* $\xi^* = \inf_{\xi \in \Xi_s} \max_{\psi \in \Psi_s} \mathcal{L}_D(\psi, \xi)$ *and* $\psi^* = \max_{\psi \in \Psi} \mathcal{L}_D(\psi, \xi^*)$ *belongs to* Ψ_s*, then* $\xi^* = \inf_{\xi \in \Xi} \max_{\psi \in \Psi} \mathcal{L}_D(\psi, \xi)$*,*

   where Ψ_s is the subset of Ψ of symmetrical contamination functions and $\mathcal{L}_D(\psi, \xi)$ is the loss function to minimize for D-optimality criterion.

2. The absolutely continuous design ξ with density

   $$m\left(x; \boldsymbol{\omega}\right) = \left(\frac{a + bx^2 + cx^4}{d + x^2 + ex^4}\right)^+, \ x \in \mathcal{S} \tag{1}$$

   is the minimizer of $\mathcal{L}_D(\psi, \xi)$, where $\boldsymbol{\omega}$ is a vector with constant values. Discrete designs are derived from (1) for practitioners.

Regarding **ternary blends**, previous results cannot be extended since it is not possible to achieve an algebraic expression of the eigenvalues required to compute $\mathcal{L}_D(\psi, \xi)$. Under this framework, we provide

3. A new methodology based on Genetic Algorithms (GAs) in order to numerically minimize the loss. It is noteworthy this technique may be applied to any mixture problem regardless of regression function and number of ingredients in the mixture.

4. A new class of restricted designs which efficiently perform in many study cases. Exchangeable designs have useful design properties for experimenters since they do not favour any ingredient in the mixture. Moreover, these take the advantage of significantly reducing the computational cost.

5. A more stringent class of restricted designs to obtain optimal densities from continuous approach. The minimizer density is

$$m\left(x,y;\boldsymbol{\omega}\right)=\left(\frac{a+b(x^2+y^2)+c(x^4+y^4)+dx^2y^2}{e+(x^2+y^2)+f(x^4+y^4)+gx^2y^2}\right)^+,\ (x,y)\in\mathcal{S} \quad (2)$$

which is analytically achieved. Discrete designs were calculated so that empirical moments matched up as closely with the theoretical moments (derived from the optimal densities (2)) to a sufficiently high order.

Several examples illustrate the efficiency of the computed designs through previous results. Focusing on the convergence of proposed method based on GAs, it is remarkable it converged for all study cases in spite of heuristic nature of this kind of optimization techniques.

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