

Mixture experiments: from D- to I-optimality

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Mixture experiments, which are commonly used in the chemical, food and pharmaceutical industries, are special types of response surface experiments where the response of interest is a function of the proportion of the ingredients of a mixture, but not on the total amount of the mixture. In recent years, prediction-based optimality criteria have gained substantial popularity for generating response surface designs. The best-known prediction-based optimality criteria are the G-optimality criterion, which seeks designs that minimize the maximum prediction variance over the experimental region, and the I-optimality criterion, which seeks designs that minimize the average prediction variance over the experimental region. Because it is often necessary to accept larger prediction variances over most of the region of interest to minimize the maximum prediction variance, the I-optimality criterion has become substantially more popular than the G-optimality criterion. However, despite the increasing use of the I-optimality criterion for response surface designs, little is known concerning I-optimal designs for mixture experiments. This is surprising because, in 1958, Scheffé already suggested selecting designs for mixture experiments based for two reasons, and, in 1968, Lambrakis defined the I-optimality criterion for designs for mixture experiments. We provide an overview of the published work on the optimal design of mixture experiments. Additionally, we discuss the construction of continuous and exact I-optimal designs, and we compare them to their well-known D-optimal counterparts, which focus on a precise estimation, using fraction of design space plots.

Key Words: average prediction variance, D-optimality, general equivalence theorem, I-optimality, simplex-centroid design, simplex-lattice design, V-optimality