Categorical Responses in Mixture Experiments

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Abstract

Mixture or formulation experiments are useful in cases where settings of experimental factors cannot be changed independently because of a constraint imposed on a linear combination of the factors. Applications of mixture experiments abound in the chemical, pharmaceutical, and biomedical sciences.

The focus of this talk is on mixture experiments with categorical responses namely, the binary and ordinal type. First, I present some real cases in the industry that motivated this research, such as a mixture experiment where the response of interest, fragrance intensity, is measured in an ordinal scale. I briefly discuss how these responses are modeled using Generalized Linear Models (GLMs). I also present a novel modeling approach for the fragrance intensity case that highlights the specific nuances of ordinal data.

The rest of the seminar focuses on finding optimal mixture designs for binary and ordinal responses. So far, research in this area is sparse and there are no definitive recommendations in literature that address the design of mixture experiments when the response is binary or ordinal. In this talk, I discuss the unique properties of mixture experiments and categorical data that make finding optimal designs more challenging than the linear model and unconstrained cases. Finally, I present D-optimal designs for binary and ordinal data using a point-exchange algorithm. The D-optimality properties of these designs are compared with mixture designs available in commercial software.

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