

Wanida Limmun 2012: Examining Model Robustness in Mixture Experiments. Doctor of Philosophy (Statistics), Major Field: Statistics, Department of Statistics. Thesis Advisor: Assistant Professor Boonorm Chomtee, Ph.D. 362 pages.

In this dissertation, the major objective is to develop a genetic algorithm (GA) for generating weighted  $D$ - and  $G$ -optimal exact designs for mixture experiments having model robustness properties where the experimental mixture region is defined by only single-component constraints or by single and multiple component constraints. For the GA, new versions of two crossover operators and a mutation operator are developed to handle the component constraints when generating mixture designs for an irregularly-shape polyhedron region. Two new objective functions which are the weighted  $D$ - and  $G$ - design optimality criteria are developed for evaluating the fitness of a design over sets of reduced models based on weak and strong heredity principles. This approach allows exploration and searching for points through a highly-constrained continuous mixture region and does not require selection of points from a user-defined candidate set of mixtures which is a limitation for current design-generating algorithms.

The results are focused on the examination of model robustness properties of the GA-generated mixture designs. The weighted optimal exact designs which have interior points and a point near the overall centroid have good prediction variance properties. However, not all of the weighted  $D$ -optimal exact designs have good prediction variance properties, whereas all of the weighted  $G$ -optimal exact designs have good prediction variance properties. The designs which have good prediction variance properties also appear to have good robustness properties. The weighted  $G$ -optimal exact designs are superior to the weighted  $D$ -optimal exact designs in terms of the scaled prediction variance and appear to be more robust designs than the weighted  $D$ -optimal exact designs.

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Thesis Advisor's signature

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