Algorithms for i-optimal designs for ordinal response: a literature approach

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Abstract. In many cases, the researchers face the problem how to design the experiment which deal with the real situation. This is because the designs on literature do not suit the case. To solve the problem, optimal design can be an alternative. There are two approaches on optimal design: an analytical and a computational approach. An algorithm in the computational approach is needed to find an optimal design. The optimal design is a part of experimental design which seek the design based on a certain criterion. The criterion which focuses on precision of prediction variance is I-optimality criterion. Limited literatures address the I-optimality criterion for ordinal response. Most of literatures address to developing algorithms of other optimality criteria for General Linear Model. As the response is ordinal, hence the ordinal response belongs to non-linear model.

1. Introduction
Mixture of ingredients are usually implemented in food industries, such as making cookies. Cookies consist of proportional components in order to get cookies with delicious taste. Cookies are usually with a fixed proportion of components. In order to find an optimal mixture, these cookies ingredients need to be designed based on a mixture experiment.

In mixture experiments, some proportional components are mixed together. The proportion of each component is between zero and one and the sum of proportions of all components in mixture is equal to one. The difficulty in the experiment is how to determine the proportion of each component when there are constraints. An optimal design is necessary to find an optimal mixture design [1].

Mixture designs are parts of response surface designs based the optimization process. The process is important to construct optimal designs that correspond to a criterion, such as I-optimality suggested by Scheffé [2]. The criterion which is the minimum average prediction variance over experimental region is used to construct the I-optimal designs. Therefore, regression models are needed to predict variance of all responses of every composition based on the estimation of parameters in the model.

The assumptions based on regression models that can be used to find the I-optimal designs are linear models for continuous responses and generalized linear models for categorical (ordinal) responses [3]. In the case of ordinal responses, logistic regression model can be appropriate even though with first, second, or higher order model [3].

Constraints in mixture experiment necessitate to develop an algorithm to find optimal designs. The algorithm is used to define a set of composition candidates, to estimate the parameters of the model...
and the average prediction variance. The algorithm can also evaluate the set of candidates whether or not the set fulfills the criterion.

The algorithms usually used to construct exact optimal designs are exchange algorithm (point and coordinate). Some commercial softwares use either point or coordinate exchange algorithm. In other side, Wynn algorithm, multiplicative algorithm, and cocktail algorithm are used to find continuous optimal design. This paper presents the development of algorithms for finding I-optimal designs based on ordinal response models.

2. Models for Mixture Experiments
Models of mixture experiments depend on the number of ingredients which are explanatory variables in the models. If an experiment involves \( q \) ingredients then there are \( q \) explanatory variables, \( x_1, x_2, \ldots, x_q \), in the model. The variables are components proportions with the constraint of \( \sum_{i=1}^{q} x_i = 1 \). This constraint defines an experimental region.

The Scheffé mixture models [2] are usually for mixture experiments. One of the models is the second-order models which is given by

\[
y = \sum_{i=1}^{q} \beta_i x_i + \sum_{i=1}^{q-1} \sum_{j=i+1}^{q} \beta_{ij} x_i x_j + \epsilon
\]

\( \beta \) is the coefficient. The response variables can be categoric, such as biner or ordinal variables. The model in (1) will not be fit for this kind of variables. The models for ordinal response variables are ordinal logistic model in the class of general linear models [3]. The model is the following

\[
\logit[P(y = 1)] = \sum_{i=1}^{q} \beta_i x_i + \sum_{i=1}^{q-1} \sum_{j=i+1}^{q} \beta_{ij} x_i x_j + \epsilon
\]

where the logit function represents the log of the odds ratio.

These models are used as basis to construct a set of mixture candidates. Finding optimal designs, such as I-optimal designs, are based on the mixture candidates. An intensive and efficient algorithm is necessary to search the optimal mixture candidates.

3. Algorithm for I-Optimal Designs
I-optimal designs focus on minimizing the prediction average variance appropriate for mixture designs. In the context of GLM, I-optimal design is seeking a design that minimizing Integrated Mean Square Error (IMSE) which is defined as [3]:

\[
IMSE = \text{tr} \left[ \left( \int_{\mathcal{X}} cc^T dF_{IMSE} \right) I(\epsilon, \beta)^{-1} \right]
\]

Minimizing IMSE is an optimization problem which needs computational approaches. In the computational approach, it is necessary to develop algorithms for finding the optimal or nearly optimal designs [5].

Two types of designs are continuous and exact designs. The continuous designs involve a set of distinct points and a weight for each point. The weight of each point indicates the proportion of the point to be experimental tested. These designs need larger number of points. The algorithms categorized to the continuous designs are (1) Wynn algorithm in which adding a point to a candidate set [7], (2) Multiplicative algorithm in which weights all points are updated simultaneously [6], and (3) Cocktail algorithm is an extended Wynn and multiplicative algorithms [8]. The multiplicative algorithm is faster than the Wynn algorithm to find I-optimal designs of linear model [5]. Furthermore,
the multiplicative algorithm and the sequential algorithm for finding I-optimal design of continuos design of GLM were proposed by [3].

Many literatures discussed about D-optimality criterion which is focused on precision of parameter model rather than I-optimality criterion for GLM. Finding optimal design based on the D-optimality criterion is widely used and developed in many fields [4, 9, 10, 11].

The exact designs involve \( n \) design points not necessary distinct and not need larger number of observations or runs. Two algorithms widely used for exact optimal designs and implemented in commercial softwares are (1) Point-exchange algorithm introduced by [12] and (2) Coordinate exchange algorithm introduced by [13].

The point-exchange algorithm needs to determine a candidate set, to specify a model, to specify the number of experimental runs, and to define the optimality criterion [12]. The candidate set is required but the larger the candidate set, the longer the computation time. This is the weakness of the point-exchange algorithms. In general, three steps in the point-exchange algorithms are:

1. To generate a starting design with \( n \) runs which is less than \( n \) of experimental runs
2. To augment the initial design or to delete several runs in order to get a starting design of size \( n \)
3. To improve the starting design iteratively by exchanging design points with candidate points from the candidate list. The size of the design remains fixed.

The coordinate-exchange algorithm introduced by [13] was with the assumption that the combinations of the proportions in a mixture experiment are independent even though with the mixture constraint. The algorithm was modified by [15] to cope with that every time the proportion of an ingredient is changed, the proportions of the other ingredients have to change as well because of point proportion dependency. The steps in the coordinate-exchange algorithms are:

1. To check the first proportion of the first point; if this point improves the certain optimality criterion then the point is replaced by the new one.
2. To check the second proportion of the first point; if this point improves the certain optimality criterion then the point is replaced by the new one.
3. To repeat the procedure until the \( q \)-th proportion of the first point.

The three steps of this algorithm are executed for the second point and continued execution until all proportions of ingredients have been changed. This sequential process will stop when it meets a stopping criterion.

A difficulty in mixture experiments is there is multicolllinearity among the components or ingredients. This is because sum of all ingredient proportions is unity. If a proportion is increasing, other proportions must be decreasing. A mixture-exchange algorithm was developed by [4]. However, he worked based on D-optimality criterion. The best of our knowledge, no literature addressed to I-optimality criterion for exact design of mixture experiment for ordinal response.

4. Conclusion

Many algorithms have been developed in order to construct D-optimal design of GLM compared to I-optimal design. Only limited literature addressed to develop algorithms of I-optimality criterion of GLM in general and in mixture experiments in particular. This is because there are special features on mixture experiments that they are needed to accommodate in the model. This is a challenge to develop an algorithm to find I-optimal design of mixture experiments of ordinal response.

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