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The Compromise Optimal Design Considering D-, G-, and V-optimality by Fuzzy Set Approach

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Abstract

The problem of constructing the compromise design chosen which does will on the three criteria(i.e., *D*-, *G*-, and *V*-optimality) is very important when the number of observations is not large relative to the number of parameters. It is modelled as a multiobjective optimization problem. A solution method is proposed for this optimization problem using the fuzzy-set approach which has become accepted as a tool for dealing with a certain form of imprecision inherent to multiobjective decision making environments. An example of finding an optimal compromise design in a moderate sized design problem is presented.

I. Introduction

Exact *D*- and *G*-optimum designs can be appreciably different, because the General Equivalent Theorem does not hold for exact design. In this way, Atkinson(1988) emphasizes the construction of the compromise design chosen which does well on the *D*-, *G*-, and *V*-optimality. The compromise design is studied by Welch(1982,1984). He describes the extension of algorithm of the DETMAX type to the calculation of *V*- and *G*-optimum design, and provides a list of a specified number of the best designs according to the primary criterion, for example, *D*-optimality. However, if no design simultaneously optimize the a

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bove three criteria, the choice of the compromise design from his list is subjective. So we suggest a compromise design by the fuzzy set approch. This is intuitively is not chosen in the list as Welch(1984).

We are concerned with designs when the expected value of the response Y is related to k explanatory variable x by the linear model $E(Y)=X\beta$. The experiment contains n runs or trials with the values of experimental conditions given by the n rows of $n\times k$ design matrix X. The k elements of the vector of parameters β are to be estimated from the results of the expeiment. We start with a short description of the theory when it is assumed that the errors of observation are independent and identically distributed with variance σ^2. For the moment it is appropriate to estimate β by least squares to give $\beta=(X'X)^{-1}X'y$. The variance of this estimate from an n trial design is $Var(\beta)=\sigma^2(X'X)^{-1}$. Unless otherwise stated the $k\times k$ information matrix X'X will be taken to be full rank. The predicted response at x is $\hat{y}(x)$ and

$$Var\{\hat{y}(x)\}=\sigma^2 x'(X'X)^{-1}x. \tag{1}$$

Optimum design theory (see Kiefer 1959) is concerned with the choice of X to minimize various functions of the matrix valued variance of β.

The set of possible experimental conditions is given by the design region Ξ comprising r candidate points $x_1, x_2, \cdots, x_r$. The design matrix can be thought of as a probability distribution giving weight $1/n$ to n not necessarily distinct sets of conditions in Ξ. Such a design is called 'exact' because it can be realized exactly in practice. For an exact design, the measure is denoted by ξ_n, so that $M(\xi_n)=X'X$. It is also mathematically convenient to replace $Var\{\hat{y}(x)\}$ in (1) by $d(x,\xi_n)=x'M^{-1}(\xi_n)x$.

One design criterion which has been much studied is that of D-optimality in which the determinant $det\ M(\xi_n)$ is maximized. This minimizes the variance of the parameter estimates. Another criterion, G-optimalty, is concerned with the variance of the predicted response. If we let $\bar{d}(\xi_n)=\max_{x\in\Xi} d(x,\xi_n)$, a G-optimality design is one which minimizes $\bar{d}(\xi_n)$, the maximum of the variance of the predicted response over the design region Ξ. The other criterion is that of V-optimality in which the design is found to minimize

$$d_{ave}(\xi_n)=\frac{1}{r}\sum_{i=1}^{r}d(x_i,\xi_n). \tag{2}$$

The equation (2) represents the average of the variance at r candidate points.

Then the problem of constucting the design which compromises the D-, G-, and V-optimalty above mentioned is formulated in this paper as the following multiobjective optimization model:

$$minimize \begin{bmatrix} D(\xi_n) \\ G(\xi_n) \\ V(\xi_n) \end{bmatrix} \tag{3}$$

where $D(\xi_n)$, $G(\xi_n)$, and $V(\xi_n)$ denote det $det\ M(\xi_n)$, $\bar{d}(\xi_n)$, and $d_{ave}(\xi_n)$ respectively. The model (3) is a simple multiobjective optimization model with integer varibles. Our concern is thus the determination of an optimal compromise design, taking into account the multicriteria. Fuzzy set approach, gaining recognition as a tool for handing the imprecision nature of decision making environments without undue simplification, is chosen as our solution technique over other major methods in multiobjective optimization(see Zimmermann 1985). Another benefit coming from its adaptation would be in the case of application of Mitchell's(1974) efficient DETMAX algorithm.

In section 2, we introduce the fuzzy set approach and the solution method presented in section 3 is the DETMAX which is modified in the excursion and the criteria of adding or subtacting a point. An example in section 4 suggests a good compromise design which is not given by Welch(1984).

Ⅱ. Fuzzy set approach

Ⅱ-1 Some Fundamental concepts of fuzzy sets

Fuzzy set theory is to deal quantitatively with 'imprecision' which can not be equated with 'randomness', thus for which the probability analysis is inappropriate. Consider a *set* F of objects (decisions, alternatives). A fuzzy set is a group of objects in which there is no clear(sharp) boundary between those objects that belong to the subset and those that do not. A membership function $\mu(f)$ of a fuzzy set is defined to be the mapping from F onto the closed interval [0,1], which represents the degree of likelihood that object x belongs to the subset.

In multiobjective decision environment, each goal can be represented by a fuzzy set on the universe of the associated real-valued measurement. For our study, three such fuzzy sets are in order, one on the determinant, $D(\xi_n)$, for D-optimality and another on the maximum variance, $G(\xi_n)$, for G-optimality and the other on the average variance, $V(\xi_n)$, for V-optimality. Define $\mu_D(D)$, $\mu_G(G)$, and $\mu_V(V)$ to be the membership functions of the fuzzy sets corresponding to the D-, G-, and V-optimality respectively. Then $\mu_D(D)$, $\mu_G(G)$, and $\mu_V(V)$, indicate the degree of the satisfaction with the measured $D(\xi_n)$, $G(\xi_n)$, and $V(\xi_n)$ respectively.

For each goal, there exists another fuzzy set defined directly on the set of decision alternatives. Define $\mu_D(\xi_n)$, $\mu_G(\xi_n)$, and $\mu_V(\xi_n)$ as the membership functions for the fuzzy sets associated with D-(G-,V-) optimality to the exact design ξ_n. The relationship between the membership functions for these two types of fuzzy sets can be mathematically represented by

$$\begin{aligned} \mu_D(\xi_n) &= \mu_D(D(\xi_n)) \text{ for all } \xi_n, \\ \mu_G(\xi_n) &= \mu_G(G(\xi_n)) \text{ for all } \xi_n, \\ \mu_V(\xi_n) &= \mu_V(V(\xi_n)) \text{ for all } \xi_n, \end{aligned} \qquad (4)$$

In fuzzy set theory the intersection of sets normally correponds to the logical 'and'. The fuzzy set of decisions compatible with the overall goal can therefore be defined as the intersection of those fuzzy sets, one for each partial goal. The membership function of the intersection is normally calculated by applying the min-operator to the membership functions of all fuzzy sets involved (see Zimmermann 1985). Then the membership function $\mu_C(\xi_n)$ of our design problem can be characterized as simple as

$$\mu_C(\xi_n) == min\{1-\mu_D(\xi_n),\ \mu_G(\xi_n),\ \mu_V(\xi_n)\} \qquad (5)$$

The optimal compromise design is then the one having the highest value of the above membership function μ_C.

Ⅱ-2 Fuzzy optimization model

Now back to our original multiobjective model, recall that the experiment designer has not specified his preferences on the three criteria, specially $(1-\mu_D)$, μ_G and μ_V. Also assumed for the moment is the unavailability of even the upper and lower bounds on the target level he aspires for each performance measure, such that he does not accept a level higher than the upper bound and he is fully satisfied whenever the level is equal to or lower than the lower bound. If these are available, the fuzzy objectives on the scales of performance measures can be obtained by the construction of membership functions which decrease monotonically from 1 at the lower bound to 0 at the upper bound.

As such we shall construct the membership functions according to the suggestion by Zimmermann(1978), of using 'least justifiable' solutions by as lower bounds and upper bounds which is easily specified through the execution of the DETMAX algorithm. Let D_L and D_U denote the lower bound and the upper bound of D-optimality respectively. Similarly, G_L G_U and V_L V_U are same above. Also define the following

$$
\begin{aligned}
d_D &= D_U - D_L (> 0)\\
d_G &= G_U - G_L (> 0)\\
d_V &= V_U - V_L (> 0)
\end{aligned}
\tag{6}
$$

Follwing the common practice in fuzzy mathematical programming, we assume that μ_D, μ_G, and μ_V have the simplest membership funtions of linear form over the tolerance intervals of $[D_L\ D_U]$, $[G_L\ G_U]$, and $[V_L\ V_U]$ respectively:

$$
\mu_D(D) = \begin{cases} 0 & D \le D_L \\ (D - D_L)/d_D & D_L \le D \le D_U \\ 1 & D \ge D_U \end{cases}
$$

$$
\mu_G(G) = \begin{cases} 0 & G \ge G_U \\ (G_U - G)/d_G & G_L \le G \le G_U \\ 1 & G \le G_L \end{cases}
$$

$$
\mu_V(V) = \begin{cases} 0 & V \ge V_U \\ (V_U - V)/d_V & V_L \le V \le V_U \\ 1 & V \le V_L \end{cases}
\tag{7}
$$

where the variables D, G, and V represent the objective value of D–, G–, and V–optimality to the design ξ_n respectively. The graphical description of these funtions is given in Figure 1. Now from (4), (5), and (7), we formally state the 'fuzzy' version of the multiobjective model (3) as follows:

$$
Maximize\{min(\mu_D(\xi_n),\ \mu_G(\xi_n),\ \mu_V(\xi_n))\}. \tag{8}
$$

That is, our problem of constructing the compromise design is to find the exact design ξ_n satisfying the above (8).

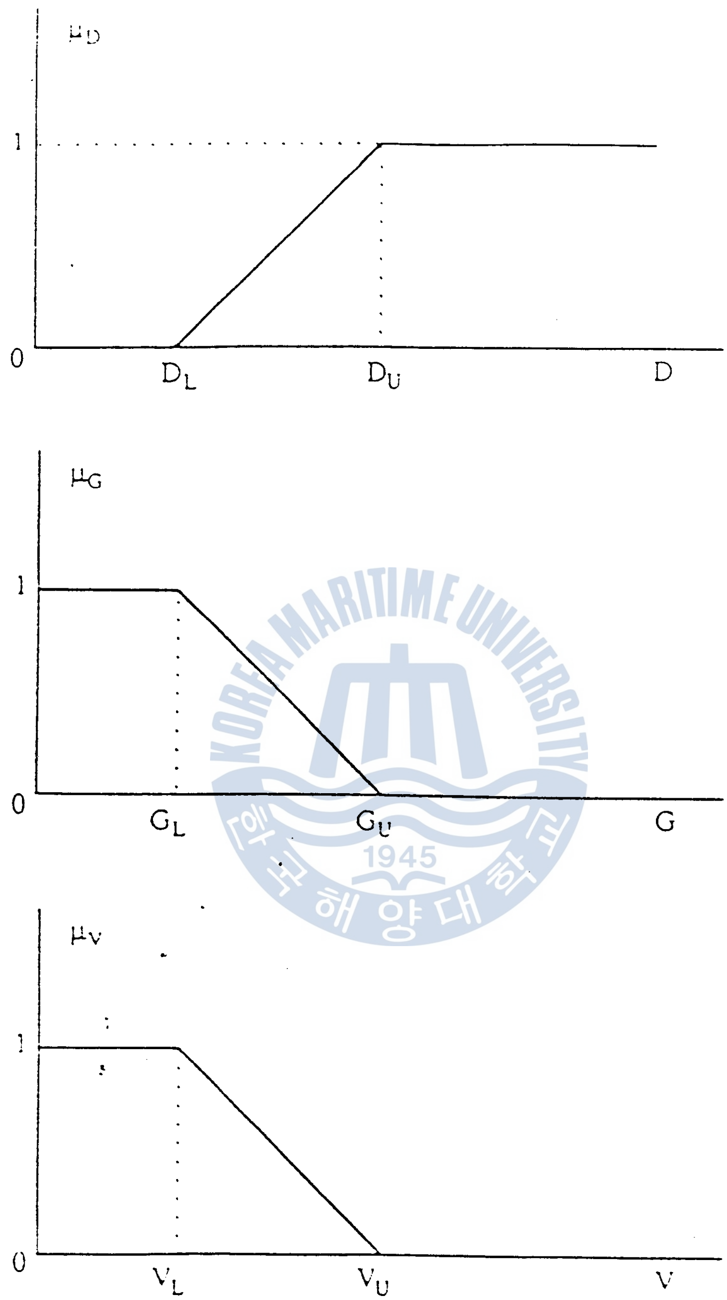

Figure 1. Membership functions

Ⅱ. Solution method

The model (8) is a nonlinear integer programming problem with the discrete variables for which no efficient solution technique is known in general. The close inspection of the model suggests the applicability of Mitchell's DETMAX algorithm. Welch(1984) suggests that the DETMAX algorithm can be generalized to minimize an arbitrary design criterion $C(\xi_n)$ over the set of exact designs. For *D*-optimality, $C(\xi_n)=det\ M(\xi_n)$ and DETMAX is recovered. Alternatively, we with to maximize the compromise design criterion, $C(\xi_n)=min(\mu_D(\xi_n),\mu_G(\xi_n),\mu_V(\xi_n))$ in (8).

Like DETMAX we attempt to improve an initial n-point design by a series of excursions. An excursion starts by adding or subtracting a point from the current n-point design $\xi_n^{(1)}$ and then performs a number of additions or subtractions of a single point, eventually returning to a possibley new n-point design $\xi_n^{(2)}$. If $C(\xi_n^{(2)}) > C(\xi_n^{(1)})$, then the excursion has succeeded and $\xi_n^{(2)}$ is used as the start for the next excursion, whereas if $C(\xi_n^{(2)}) \leq (\xi_n^{(1)})$, a failure has occurred and $\xi_n^{(1)}$ is again starting design. At each step within an excursion, two decisions ard made: whether to add or subtract a point and which design point to add or subtract accordingly. The values for the first decision follow DETMAX and are described by Mitchell(1974) and Galil and Kiefer(1980).

The algorithm to maximize the compromise design criteria $C(\xi_n)$ deviates from DETMAX in the choice of a promising point to add or subtract as required. If the adjustment involves candidate x_j, then element ξ_n of the current design is increased or decreased to ξ_{n+1} or ξ_{n-1} respectively. The obvious generalization of DETMAX is to add a point x_j, satisfying.

$$C(\xi_{n+1})=\max\{D(\xi_{n+1}) - G(\xi_{n+1}) - V(\xi_{n+1})\}$$

$$=\max_{j=1,\cdots,r}\{x_j^{1}M^{-1}(\xi_n)x_j - \bar{d}(x_j, \xi_{n+1}) - d_{ave}(x_j, \xi_{n+1})\} \quad (9)$$

or when subtracting, select x_j to satisfy

$$C(\xi_{n-1})=\max\{D(\xi_{n-1}) - G(\xi_{n-1}) - V(\xi_{n-1})\}$$

$$=\max_{j=1,\cdots,r}\{x_j^{1}M^{-1}(\xi_n)x_j + \bar{d}(x_j, \xi_{n-1}) + d_{ave}(x_j, \xi_{n-1})\} \qquad (10)$$

where $\bar{d}(x_j, \xi_{n+1})$ and $d_{ave}(x_j, \xi_{n+1})$ denote the maximum of the variance of the predicted response and the average of the variance respectively, when x_j is added to ξ_n.

By Welch(1984), *G*-optimality would be prohibitively expensive in computational consideration, and the results can also be disappointing: paradoxically the *D*- or *V*-optimal designs often possess smaller values of *G*-optimality than those generated by the *G*-optimality algorithm intended to minimize $\bar{d}(\xi_n)$.

Fortunately, though, simple modification reduces time yet further, in the criterion to add or subtract a point, the term $\bar{d}(x_j, \xi_{n+1})$ is temporarily ignored at all other steps of an excursion. At the final step of excursions, the term $\bar{d}(x_j, \xi_{n+1})$ is considered.

Ⅳ. An Exmaple

Experiments with mixtures have received much attention in the literature; Lornell(1981) provides a review. They involves explanatory variables with nonnegative levels summing to one to represent the proportions of components in a mixture. Vuchkov, Damgaliev, and Yontchev(1981) (VDY) describe the sequential generation of *D*-optimal designs for mixture experiments that also include independent process variables.

We test the example such as Welch(1984). The example applies the modified excursion algorithm for the construction of the comprise design to the case three mixture variables and one process variable. A design point $x_{(i)1},\cdots,$

$x_{(i)4}$ is therefore constrained such that

$$x_{(i)1} + x_{(i)2} + x_{(i)3} = 1;$$
$$x_{(i)s} \geq 0, \quad s = 1,\ 2,\ 3. \qquad (11)$$

The second-order model canonical parameterization given by VDY is

$$E(Y_{(i)}) \sum_{s=1}^{3} \beta_s x_{(i)s} + \sum_{s=1}^{3} \sum_{t=s+}^{4} \beta_{si} x_{(i)s} x_{(i)t} + \beta_{44} x^2_{(i)4}.$$

This model has $k=10$ parameters. As a design region suppose that the mixture proportions are continuous between zero and one, and approximate their ranges by the seven levels $x_{(i)s}=0(1/6)1$ $(s=1,2,3)$. In contrast, assume that the process variable is confined to only three values coded -1, 0, and 1. With three are 84 combinations of levels satisfying the constraints (11) to comprise the design region.

To compare the compromise design of Welch's approach and our solution approach, the designs generated by both methods are given in Table 1. In table 1, we find the compromise design chosen which does well on the D-, G-, and V-criteria without the list of Welch(1984).

Table 1. Design Properties for the Example with Three Mixture Variables and One Process Variable

n	Criterion $r=84$	$G(\xi_n)$	$V(\xi_n)$	$D(\xi_n)$
	D	1.0	0.5488	2.6367
	V	1.0	0.5235	2.6367
15	G	0.8917	0.5436	2.2236
	C	0.9518	0.5555	2.5499

NOTE: C represents the compromise design generated by our method.

V. Conclusions

We formulated the multiobjective optimization model to construct a compromise design. Then a fuzzy set theoretic solution approach was presented, which has become accepted as a tool for dealing with a certain form of imprecision inherent to multiobjective decision making environments. In order to solve the problem, the proposed procedure utilizes the DETMAX algorithm which is modified in the excursion and the criterion to add or subtract a point.

In Welch(1984), after excuting the generalized DETMAX algorithm for the each criterion, a list of a specified member of the best designs was provided. However, it is very cumbersome to find the list of best designs. And from the list, the choice of a compromise design is subjective if no design simultaneously optimizes the three criteria. So, we use the modified DETMAX, considering all the criteria(i,e, *D*-, *G*-, and *V*-optimality) at each step of excursions, And a good compromise design is systematically suggested by the fuzzy set approach.

References

1. Atkinson, A. A.(1988), Recent Developments in the methods of optimum and Related experimental designs, International Statistical Review, 56,99～115.
2. Cornell, J. A(1981). Experiments With Mixtures, New York:John Wiley.
3. Galil, Z. and Kiefer, J.(1980). Time and Space-Saving Computer Methods, Related to Mitchell's DETMAX, for Finding D-optimum Designs,Technometrics, 22, 301～313.
4. Kiefer, J.(1959), Optimal experimental designs, J. R. Statist. Soc, B21, 272～319.
5. Kiefer,J. and Wolfowitz,J.(1960). the equivalence of two extrema problems, Can. J. Math., 12, 363～366.
6. Mitchell, T. J.(1974), An Algorithm for the Construction of D-optimal Exp-

erimental Designs, Technometrics, 16, 203~210.

7. Vuchkov, I. N., Damgaliev, D. L. and Youtchev, C. A. (1981), Sequentially Generated Second order Quasi D-optimal Designs for experiments with mixture and process variable,s Technometrics, 23, 233~238.

8. Welch, W.J.(1982). Branch and Bound Search for experimental designs Based on D-optimality and other criteria, Technometrics, 24, 41~48.

9. ———————— (1984), Computer Aided Design of Experiments for Response Estimation, Technometrics, 26, 217~224.

10. Zimmermann, H. J.(1978). Fuzzy programming and linear programming with sever objective functions, Fuzzy sets and Systems, 1, 45~55.

11. ———————— (1985), applications of Fuzzy set theory to mathematical programming, Information Science, 36, 29~58.