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DISCUSSION

of the Stanley N. Deming paper, Optimization

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I appreciate the opportunity to make comments on Dr. Deming's paper. I will confine my comments to three areas: 1) optmization applications; 2) strategies for screening experiments; and 3) the steepest ascent method.

1. Optimization Applications

In 1971, Rubin, Mitchell, and Goldstein [1][1] surveyed the previous 25 years of major English language journals of analytical chemistry under the index heading of "statistics." This survey uncovered few papers in which experiments were statistically designed. Similar results were found by Morgan and Deming in 1974 [2] in their literature search under the heading "Optim/" in *Chemical Abstract* and *Chemical Titles* covering eight previous years. Nine years later, Deming and Morgan [3] found 189 titles for the years 1962-1982 listed in *Chemical Abstracts* and *Science Citation Index* related to sequential simplex optimization. About 156 papers in this search are direct applications to chemical problems. In a recent survey by Rubin and Bayne [4] for the years 1974-1984, 65 applications of optimizations and response surface methods were found to be related just to analytical chemistry. These recent literature surveys indicate that statistically designed experiments are becoming an important part of chemical experiments.

Dr. Deming deserves a large share of credit for this increased use of statistically designed experiments in chemistry. He has promoted experimental design by his many publications, seminars, and lectures. The fact that he is a chemist who has championed the statistical cause is to be admired.

[1]Figures in brackets indicate literature references.

2. Screening Experiments

The strategy for using screening experiments is influenced by the cost of an experimental run. Here cost can be interpreted as price of material, time required for an experimental run, etc. For a high cost experiment, the strategy is to run a screening experiment to identify the important factors followed by an optimization experiment using these factors. An additional screening experiment is sometimes performed to confirm that the important factors have been properly identified. Dr. Deming is correct in stating that the error rate for rejecting significant factors should have more emphasis than the error rate for accepting non-significant factors in the initial screening experiment. This conservative approach can be accomplished by testing at a 0.20 or 0.25 significance level rather than the usual 0.05 significance level.

The low cost experimental run situations may require a different strategy. Dr. Deming advocates that first an optimization using all factors be performed using a sequential simplex method followed by a screening experiment to identify important factors at optimum conditions. For additional factors, he points out that only a small increase is required for the number of initial experiments which require $K+1$ experiments for K factors, and no increase in the number of experiments is needed to move into an adjacent region of the factor space. However, the number of experiments for convergence may increase rapidly with an increase in the number factors. Nelder and Mead [6] reported that the mean number of experiments needed for convergence increases as a second-order function of the number of factors. Even for low cost experimental runs, the total number of experiments required for optimization may be impractical.

When dealing with a large number of factors, two adjustments to the sequential methods are suggested. First, use small screening experiments for initial experiments; and secondly, discard more then one vertex when moving into a different factor region.

Using small screening designs for initial experiments is suggested because execution of the initial regular simplex can be tedious. For example, the step size fraction required for one of the vertices in a four-factor regular simplex is (0.500, 0.289, 0.204, 0.791) [6]. In practice, running an experiment at the simplex vertices may either be difficult or impossible. By allowing the factor levels to be either a low or high level, initial screening designs can be easily run. Screening experiments for initial designs are given in table 1.

Changing only one vertex per experimental move may be too slow when there are many factors. For these cases, more than one vertex can be discarded to increase the rate of convergence. The rule for simplex moves is modified to delete more than one vertex by:

Table 1. Screening Experiments for Initial Designs.

Factors	Runs	Initial Design
2 or 3	3 or 4	Simplex
$4 \leq K \leq 7$	8	Fractional Factorial
$8 \leq K \leq 11$	12	Plackett-Burman
$12 \leq K \leq 15$	16	Fractional Factorial
$K > 16$		Fractional Factorial or Plackett-Burman

$$2 \times (\text{average of best vertices}) - \text{worst } \textit{vertices}.$$

To decide which are the best vertices and the worst vertices, first rank the response from lowest to highest value. Next, divide the responses into two groups with the lowest values in one group and the highest values in the second group. This division can be done K ways for K-factors. For each division, calculate the average response for each group and then take their difference. The division that has the largest difference will indicate the best and the worst vertices. By this method, the difference between the average responses for the best and the worst vertices is maximized.

3. Steepest Ascent

In a literature search by Rubin and Bayne [4], few applications were found of the steepest ascent method advocated by Box and Wilson [7] for optimization. This method maximizes the gain in the reponse and performs better than fixed step size simplex method [8]. The main arguments against the steepest ascent method are: the initial experiments require too many experiments, and the calculations are too complex.

Although the steepest ascent method does require more initial experiments, the total number of experiments may not be as many as those for the simplex method. Worksheets similar to those used for the simplex methods can be used to alleviate calculation difficulties. Because steepest ascent has the potential of out performing the simplex method, its use should be encouraged.

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