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Simulation with too many factors

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RESEARCH MEMORANDUM

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SIMULATION WITH TOO MANY FACTORS:
REVIEW OF RANDOM AND GROUP-SCREENING DESIGNS

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Abstract

Experiments with real systems, but especially with simulated systems, may involve hundreds of factors. Only a few factors are really important. Detecting these important factors requires special designs like random and group-screening designs. Random designs are simple but they yield biased estimators. Group-screening is based on aggregation. The assumptions of group-screening are discussed in detail, and turn out not to be very restrictive. Applications of both design types are given.

Keywords: Simulation, Statistics: experiment, regression.

1. Introduction

In the present paper we discuss designs for experiments with real or simulated systems involving a great many factors. Through these designs we hope to detect the few factors which are really important: screening. Such designs are useful in the preliminary, exploratory phase of an investigation.

At the beginning of an investigation, there may be extremely many conceivably important factors, for example, a thousand factors ($k = 1000$). Actually we assume that only a few, say k' , factors are really important, for instance, ten factors ($k' = 10$). We emphasize that we do not know the exact value of k' nor do we know which factors are really important. We assume that only a few factors are important, because we look for a parsimonious explanation, i.e., we do not wish to report that "everything depends on everything else". (Or as Levinthal, quoted in Pratt (1964, pp. 348-349), put it "Well, there are two kinds of biologists, those who are looking to see if there is one thing that can be understood, and those who keep saying it is very complicated and that nothing can be understood....".)

In simulation we are able to perform experiments with a great many factors, because we are in full control of all factors: we have the computer program read in its inputs. In expe-

periments with non-simulated systems it is virtually impossible to control a thousand factors, and little attention is paid to screening designs. In simulation, however, applications of such designs do exist; see Section 3.3. We note that in academic studies the system is often so small that screening is not necessary; in practical studies the system is often large but the statistical know-how is missing.

A following step (with which we have no experience yet) is as follows. Once we have executed the screening design and its (regression or Analysis of Variance) analysis, we may change the underlying simulation model. That is, the screening phase suggests that certain factors are unimportant. Consequently we might simplify the simulation model, eliminating certain factors and processes. We can check the validity of this simplification by running both the original and the simplified simulation model, and comparing their responses. Actually we already have available the inputs and outputs of the original model. We can run the simplified simulation model with the same input (possibly including the same random number seeds). We can test the difference between the outputs of the original and the simplified simulation model, using standard statistical techniques (for example, the t test and the sign test combined with the Bonferroni approach; see Kleijnen, 1975, 1986).

If we have (say) a thousand potentially important factors ($k = 1000$), then standard design like 2^{k-p} designs and one-factor-at-a-time designs would require at least a thousand and one combinations of factor levels: $n > 1001$ (see Kleijnen 1975, 1986). It is impossible to run so many combinations, because of a limited computer budget and other constraints. So in the present paper we add the condition: $n < k$.

There are several approaches to the problem of too many factors. A degenerated solution assumes that the output is insensitive to most inputs and concentrates on a few factors selected intuitively. Such an approach means that the limitations of the conclusions are unknown. Two other approaches are random designs and group-screening, which we shall discuss in the next two sections.

2. Random Designs

Random designs have been known for many years (an elaborate discussion was presented in Technometrics in 1959). In random designs we specify the $n \times k$ design matrix X or (x_{ij}) by sampling the plus (On) and minus (Off) values, with equal probabilities:

$$\begin{aligned}
 P(x_{ij} = +1) &= 0.5 & (i = 1, \dots, n) \quad (j = 1, \dots, k) \quad (n < k) \\
 P(x_{ij} = -1) &= 0.5 & (1)
 \end{aligned}$$

Obviously, this solution is extremely simple, and it has indeed been applied in simulation experiments; see Cyert and March (1963), Maas et al. (1962), Rosenkranz and Bürgisser (1976).

We may refine eq. (1) as follows. We may impose the condition that each column of the design matrix has an equal number of On and Off levels:

$$\sum_{i=1}^n x_{ij} = 0 \quad (j = 1, \dots, k) \quad (2)$$

We realize this condition by sampling without replacement, using eq. (1) and specifying n to be an even number. (Eq. (2) is also met by the classical designs such as 2^{k-p} designs.)

We may happen to sample two identical columns, for example, x_{i1} equals x_{i2} for all i values. Obviously, if we vary the factors 1 and 2 simultaneously, then we cannot estimate their (individual) effects. Algebraically we find that the matrix of independent variables (X) is collinear, because two columns are identical; hence Least Squares estimators $\hat{\beta}$ do not exist (moreover, X is collinear because $n < k+1$; see the comment below eq. 4). Of course we can compute the following intuitive estimators where y_i denotes the response of run i :

$$\tilde{\beta}_j = \frac{\sum_{i=1}^n x_{ij} y_i}{n} \quad (j = 1, \dots, k) \quad (n < k) \quad (3)$$

It is simple to derive that this estimator has the following expected value:

$$E(\tilde{\beta}_j | X) = \beta_j + \frac{1}{n} \sum_{j' \neq j} \beta_{j'} \sum_i x_{ij} x_{ij'}, \quad (4)$$

From linear algebra we know that an $n \times k$ matrix with n smaller than k has no more than n orthogonal columns. Consequently, in eq. (4) $\sum_i x_{ij} x_{ij'}$, can not be zero for all pairs (j, j') , i.e., the intuitive estimators $(\tilde{\beta}_j)$ are biased.

The intuitive estimator $\tilde{\beta}_j$ of eq. (3) is unbiased, if we do not condition on X (that is, $E(\tilde{\beta}_j)$ equals β_j), in other words, if we repeated the experiment (i.e. if we sampled X more than once, with given n and k values), then $\tilde{\beta}_j$ would be unbiased. Actually the basic assumption is that we cannot afford such extensive experimentation, in other words, we sample X once with n smaller than k , and for any realization of X the estimator $\tilde{\beta}_j$ is biased.

The older literature (see Kleijnen, 1974, pp. 378-382) gives several significance tests per factor. However, since the

intuitive estimators $\tilde{\beta}_j$ are biased, we do not discuss these tests.

We started with the assumption that two columns are identical. Then their estimated correlation coefficient r equals plus one: because we sample without replacement, we have $\bar{x}$ is zero and $\hat{\text{var}}(x)$ is one, so that the correlation estimator becomes

$$r_{jj'} = \frac{\sum_{i=1}^n x_{ij} x_{ij'}}{n} \quad (j \neq j') \quad (j, j' = 1, \dots, k). \quad (5)$$

Obviously, if r is equal to minus one, than the design is equally bad: $E(\tilde{\beta}_1|X) = -E(\tilde{\beta}_2|X) = \beta_1 - \beta_2$. In general, we may add the following condition to sampling without replacement from $P(x)$ in eq. (1): we reject any sampled column j , if the correlation with a preceding column j' is too high in absolute value, i.e., we sample from eq. (1) until $|r_{jj'}| \ll 1$.

In a design with the condition $n \leq k$ not all $k+1$ columns of the matrix of independent variables X can be orthogonal, i.e., $r_{jj'}$ cannot be zero for all pairs (j, j') . Therefore, we may formulate the criterion: minimize the maximum correlation between any two columns of the $n \times (k+1)$ matrix of independent variables X with $n \leq k$. This criterion leads to the supersaturated designs of Booth and Cox (1962) (also see Morris and

Mitchell, 1983, p. 348). These authors derived non-random designs, using a computerized search procedure to specify X for seven combinations (k,n) ranging from $(16,12)$ to $(30,24)$. We do not further discuss their designs, because the designs yield biased estimators, and we do not know any applications.

Summarizing, random designs are extremely simple: we sample (without replacement) the elements of the design matrix. Unfortunately if the number of runs does not exceed the number of factors, then bias results. Therefore we proceed to a different type of design.

3. Group-screening Designs

Group-screening was proposed in several publications in the early sixties (see Kleijnen, 1975, for references). In group screening we aggregate individual factors into groups of factors; if a group is not significant, then we conclude that all its members are unimportant. We consider an example in Table 1 and FIG. 1; in Section 3.2 we shall return to the assumptions of this example.

3.1. Example

In the example we have one hundred (individual) factors, and we form two groups of fifty factors each. Hence the number of group factors is two or, in symbols, $g = 2$. We investigate

TABLE 1

Group-screening Example

Run i	Group factor		Individual factor						Response $E(y)$
	w_1	w_2	x_1	$\dots$	x_{50}	x_{51}	$\dots$	x_{100}	
1	-	-	-	$\dots$	-	-	$\dots$	-	$-\beta_1 - \beta_2$
2	-	+	-	$\dots$	-	+	$\dots$	+	$-\beta_1 - \beta_2$
3	+	-	+	$\dots$	+	-	$\dots$	-	$\beta_1 + \beta_2$
4	+	+	+	$\dots$	+	+	$\dots$	+	$\beta_1 + \beta_2$

FIG. 1. Group screening.

the two groups (say) w_1 and w_2 in a 2^2 design. A group factor is at its Off level (or -1 level), if all its members are at their Off levels; and if the group factor is switched On, then all its members are On. The last column of Table 1 follows from the assumption that all effects are zero, except for the effects β_1 and β_2 (obviously in practice we do not know that only β_1 and β_2 are non-zero).

The expected values of the usual (least squares) estimators of the main effects of the group factors 1 and 2 are

$$E(\hat{\gamma}_1) = E\left(\frac{-y_1 - y_2 + y_3 + y_4}{4}\right) = \beta_1 + \beta_2 \quad (6)$$

and

$$E(\hat{\gamma}_2) = E\left(\frac{\sum_{i=1}^n w_{i2} y_i}{n}\right) = 0 \quad (7)$$

In eq. (6) the individual effects do not cancel out, because of the following assumptions. We assume that we know the signs of the main effects, i.e., if the factor does have an effect then we know the direction of the effect. For example, if the number of servers is important in a queuing system, then that number has a negative effect on the waiting times. Hence we can define the On and Off levels of the factors such that all effects are either positive or zero: $\beta_j > 0$ for $j = 1, \dots, k$. Moreover we assume that the k (individual) factors x_j have main effects

only. Consequently, the effects of the (individual) factors within a group cannot compensate each other. So after a pilot experiment with only four runs, we expect to eliminate all fifty (individual) factors of the non-significant group factor w_2 . In a following phase of the experiment (not shown in Table 1 and FIG. 1) we can further investigate the fifty factors of the significant group factor (w_1). We emphasize that after the four runs we do not know that the factors 1 and 2 caused the significance of group factor 1; all we know is that one or more factors within group 1 are important.

If in the first phase of the experiment we declare (many) factors to be unimportant, which levels should these factors have in the next phase of the experiment? If the factors have exactly zero effects, then the choice of their levels has zero effect. Actually their effects are so small, that these effects are masked by the important effects plus the error term. We recommend to keep the "unimportant" factors at fixed levels during future experimentation, provided our main goal is to estimate the effects of the important factors: if these non-significant factors happen to be important (β error of test), then their effects are confounded with the grand mean and not with the effects of the other individual factors. However, we randomly vary the levels of the non-significant-factors, if we wish to predict the response variable y . In general, however, the primary goal of screening is to identify the important factors, and

therefore we recommend keeping the unimportant factors at fixed levels. This recommendation implies that we can use some old runs in the next phase. For example, if we further investigate group factor 1, then we can again use run 1 of Table 1 if in the second phase we include a combination where all (fifty) factors are at their Off levels (and the other fifty factors remain at their Off levels in all runs of the second experiment). Also see Kleijnen (1975, pp. 395, 417-419), Olivi (1984).

To test the significance of group factors we need variance estimators. In simulation we obtain estimates $\hat{\sigma}_i^2$ (with $i = 1, \dots, n$) through the use of replications, subruns, and so on; see Kleijnen (1975, 1986).

3.2. Assumptions

Now we examine the assumptions of group-screening. One assumption is that we know the signs of the main effects. How restrictive is this assumption?

- In some applications we have so much qualitative insight into the system that we do know these signs; see the queuing example below eq. (7).
- Alternatively we may wish to rely on the small probability of "pathological" behavior. For example, eq. (6) proves that we miss the important factors 1 and 2, only if they belong to the same group, if their effects have opposite signs, and if these effects are of the same magnitude, so that the experimental

noise masks the effects. The smaller the group size, the smaller the chances of such pathological behavior. (Mauro and Smith, 1982, p. 83, assume that "factors are grouped randomly"; in practice, however, we have some knowledge about the system, and we use that knowledge to group factors; also see Shubik, 1975, p. 108.)

- We can place individual factors into groups of size one, i.e., if we believe apriori that a specific factor is important, then we can test that factor individually.

A second assumption was that the individual factors have main effects only. Now we consider a regression model with two-factor interactions, i.e., in the example of Table 1 factor 1 interacts with factor 2 and with factor 100: $\beta_{1,2} \neq 0$, $\beta_{1,100} \neq 0$ (and $\beta_1 > 0$, $\beta_2 > 0$). Using eq. (2) and $\sum_i x_{1j}^2 = n$ we obtain the following result, which is analogous to eqs. (6) and (7):

$$\begin{aligned}
 E(\hat{\gamma}_1) &= E\left(\frac{\sum_{i=1}^n w_{i1} y_i}{n}\right) = \frac{1}{n} \sum_i w_{i1} (\beta_1 w_{i1} + \\
 &+ \beta_2 w_{i1} + \dots + \beta_{1,2} w_{i1} w_{i1} + \dots + \beta_{1,100} w_{i1} w_{i2}) \\
 &= \frac{1}{n} (\beta_1 \sum_i w_{i1}^2 + \beta_2 \sum_i w_{i1}^2 + \dots + \beta_{1,2} \sum_i w_{i1}^3 + \dots \\
 &+ \beta_{1,100} \sum_i w_{i1}^2 w_{i2}) = \beta_1 + \beta_2 + \beta_{1,2} \cdot 0 + \beta_{1,100} \cdot 0 \\
 &= \beta_1 + \beta_2
 \end{aligned} \tag{8}$$

In general, Kleijnen (1975, p. 398) proved the following:

- Two-factor interactions do not bias the main effects, if we use a so-called design of "resolution IV" or higher for the group factors; these designs require $n > 2g$. Table 1 is an example of such a design.
- If we examine the group factors in a design of lower "resolution" ($n < 2g$) then a two-factor interaction $\beta_{jj'}$ creates bias for the estimator of a main effect β_j only if the factors j , j' and j'' belong to three different groups. Consequently, if all factors interact, then main effect estimators are biased indeed. And if not all factors interact, then we should place these "related" factors within the same group. (Pure quadratic effects of quantitative factors would not cause bias; however, in group screening the factors are qualitative.) We are misled through a resolution IV design (for the group factors), if all effects are zero except for the interactions between two factors belonging to the same group (in a case study such a situation did exist; see Kleijnen, Van den Burg, Van der Ham, 1979).

The literature gives some more assumptions for group-screening designs. These assumptions, however, are not essential, since they are used only to derive the 'optimal' size of the groups. Optimal group sizes mean that the number of runs taken over all stages of screening, is minimal. For example, if p denotes the prior probability of a factor being effective (that is, p equals the likely number of important factors

divided by the total number of factors), then the optimal group size is

$$f = \{(1-\alpha) p\}^{-\frac{1}{2}} \quad (9)$$

where α is the type I error rate used in the first stage of the two stages. This equation shows that the group size decreases, as p increases. High p values ($p > 0.25$) mean that the group size becomes one. High p values, however, conflict with the basic assumption of screening, namely, only relatively few factors are important. Obviously, if α increases, then we declare some unimportant groups to be important so that we have to observe more combinations in the next stage; see Kleijnen (1975, p. 396), Samuels (1978).

After the first stage of group screening, we may again apply group screening to the non-eliminated individual factors. If we have s stages ($s > 2$), then the formula for the optimal group size does no longer equal eq. (9). Because we wish to emphasize the principles and feasibility of group screening and not the technical details of "optimal" designs, we refer to the literature for more details; Mauro (1984), Ottieno and Patel (1984). In practice we have prior knowledge about the (simulated) system and we use that knowledge to form groups of related factors; such a procedure implicitly determines the

group sizes; we stop screening when all groups have reduced to size one.

3.3. Applications

Applications of group screening in simulation are rare yet. As we mentioned in the beginning of this paper, we conjecture that the cause is the lack of statistical know-how among simulation practitioners. Nevertheless we think that, especially in experiments with simulated systems (as opposed to real systems), this design type is very useful. Therefore we briefly describe all simulation applications we know of:

- Rooda and Van der Schilde (1982) apply two-stage group screening to a case with twenty-nine factors. They examine eight groups in a 2^{8-4} design, analyze the results through Estimated Weighted Least Squares (EWLS), and validate the first-order regression model expressed in the eight group factors (the regression model is a metamodel of the simulation model; see Kleijnen, 1986). Significance tests lead to the elimination of four groups. In the second stage they investigate the remaining twelve individual factors in a 2^{12-8} design. They again use EWLS, and so on. Their case study concerns the simulation of maritime transport and distribution by seagoing barges.
- Mihram (1972) and Nolan and Mastroberti (1972) simulate a strategic airlift system. Mihram (1972, pp. 399-400) states that interactions "would tend to conceal the true significance of other factors in the subset". However, Kleijnen (1975, p. 398)

proved that in a resolution IV design interactions do not conceal the additive main effects of the factors within a subset or group.

- Schatzoff and Tillman (1975) examine a computer system.
- De Hoogh (1982) studies a dike (storm-surge barrier) in the Netherlands.

All these applications concern simulations of systems so complicated that we do not know which factors are really important. Therefore we cannot prove that group screening works in these applications. To remedy this situation, we perform the following limited Monte Carlo experiment. We create the "real system"

$$y = \beta_0 + \sum_{j=1}^{88} \beta_j x_j + e \quad (10)$$

and all effects are zero except for seven factors. Next we apply group screening to this system. And the screening technique indeed detects the seven important effects. Mauro and Burns (1984) perform a similar Monte Carlo experiment with one hundred individual factors and they vary the total number of runs between twenty and eighty-four.

4. Conclusion

Group screening is based on the aggregation principle. The assumption of known signs (or directions) is not very restrictive, because we may rely on the low probability of pathological behavior (important factors occur within the same group and have effects of equal magnitude with opposite signs) and we may examine some factors individually (group size one). Two-factor interactions do not bias main effects, if we examine the group factors in a resolution IV design.

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