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ON THE USE OF STAGEWISE REGRESSION IN RANDOM BALANCE SCREENING EXPERIMENTS

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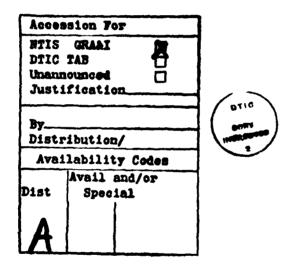
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1. INTRODUCTION AND BACKGROUND

Random Balance (RB) is a design technique that may have much to offer the researcher planning a factor screening experiment. The RB concept is most useful, however, in the design of supersaturated screening experiments. An experiment is supersaturated when the number of factors (i.e., design variables) under investigation exceeds the number of runs available. As it is, screening experiments are often handicapped by the scarcity of experimental runs because of time, budget, and/or resource The cotherslimitations. We are concerned in this paper with the supersaturated situation.

In RB designs, unlike more conventional designs, no mathematical relation or restriction need exist (except that an even number of runs be used) between the sample size N and the number of factors K under consideration. Because of this flexibility, the RB techniqe permits the researcher to screen a large (or small) number of possible contributing factors in an experiment involving a limited (N<K) number of test runs. Another advantage is that RB designs are easy to prepare for any combination of N and K.

A major concern with RB experimental design is that there are no specific or unique statistical techniques for analyzing RB designs. (See [5] and [6] for a more complete discussion.) There is no one particular method, therefore, that ought to be used to analyze RB screening experiments. Satterthwaite [5] has remarked that practically any technique used to analyze data without RB properties can be applied to any (suitably small) subset of factors in an RB design. The simplest approach, then, would be to consider each factor separately and apply some standard test of significance. Accordingly, Mauro and Smith [4] have considered the use of a standard F--1-

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test applied separately to each factor as the method of analysis for RB designs.

A more sophisticated means of analysis which is considered by Anscombe [1] and Budne [2] is as follows. We first determine the factor, say x_i , most highly correlated with the response variable Y. After a simple regression equation in x_i has been fit, the residuals $Y - \hat{Y}(x_i)$ are found. These residuals are now considered as response values and the process is repeated. We stop when we reach the stage where the regression on the most correlated variable is not significant. Of course, once a factor has been adjusted for (i.e., entered), it is not considered as part of the variable pool in subsequent stages.

The analysis procedure just described has been known under a variety of descriptive titles. We will refer to it here as "stagewise regression," which is the terminology used by Draper and Smith [3]. We should emphasize that the stagewise regression (SR) solution is not the multiple least squares solution for the variables involved. This is because at each stage of the SR procedure the remaining factors are not adjusted for previously entered factors.

The purpose of this technical report is to investigate the use of GR as a method of analysis for RB screening experiments. Our approach is to determine the efficiency of the first two stages in order to obtain an indication of what can occur between consecutive stages. In doing so, the SR method is compared with the individual F-test approach, as considered previously by Mauro and Smith. Finally, two Monte Carlo case studies are conducted.

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II. A SCREENING MODEL

When evaluating the performance of a screening strategy, one must consider both how many runs are required and how accurately factors are identified. Although the factors may range in importance from highly critical to negligible, we generally classify factors as either "important" or "unimportant". The factors deemed important are usually investigated more intensively in subsequent experimentation.

In order to provide a common statistical basis to evaluate and compare screening methods, we must make some assumptions regarding a general screening model. First of all, we assume that each factor is assigned or has two levels, high (+1) and low (-1). Using two levels for each factor is generally sufficient for screening purposes. Second, for detecting the factors having major effects it is usually reasonable to assume an additive model. Thus, we assume the model:

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$$y_{i} = \beta_{0} + \sum_{j=1}^{K} x_{ij} + \varepsilon_{i}, \qquad (2.1)$$

where y_i is the value of the response in the ith run; $x_{ij} = \pm 1$ depending upon the level of the jth factor in the ith run; β_j is the (linear) effect of the jth factor; and the error terms ε_i are independent and normally distributed with zero mean and variance σ^2 .

In essence, model (2.1) is a first-order Taylor series approximation to the actual relationship between the response and the experimental factors; ordinarily, we would assume model (2.1) over a relatively small region of the factor space. We will restrict performance assessment to this model.

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In matrix terms we can write model (2.1) compactly as $\underline{y} = \beta_0 \underline{1} + \underline{X\beta} + \underline{\epsilon}$ where $\underline{1}$ is an Nxl vector of +1's, $\underline{y} = (\underline{y}_1)$ is an Nxl vector of responses, $\underline{\epsilon} = (\epsilon_1)$ is an Nxl vector of error terms, $\underline{\beta} = (\beta_1)$ is a Kxl vector of factor effects, and $\underline{X} = (\underline{x}_{1j})$ is an NxK design matrix.

In an RB design, the design matrix \underline{X} is stochastic. Specifically, in a two-level (±1) RB design each column of the design matrix consists of N/2 +1's and N/2 -1's where N (an even number) denotes the number of runs. The +1's and -1's in each column are assigned randomly, making all possible combinations of N/2 +1's and N/2 -1's (there are $C_{N/2}^{N}$ in all) equally likely, with each column receiving an independent randomization. Factors are therefore confounded to a random degree. Moreover, we cannot generally control the amount of confounding or interdependence between factors.

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111. THE STAGEWISE REGRESSION METHOD

In this section we attempt to gain some understanding of the behavior of SR when used as the method of analysis for RB screening experiments. To obtain an indication of the possible benefits of SR, we derive an expression for the relative efficiency of the second-stage to the first-stage estimator of a factor effect. A comparison of the first two stages should provide some indication of what can happen in SR and what might be gained (or lost) in general by the stagewise procedure.

To begin, the first-stage estimator of β_j is denoted by $\hat{\beta}_j$ and is given by

$$\hat{\beta}_{j} = \underline{x}_{j} \underline{y} / N , \qquad (3.1)$$

where \underline{x}_{j} denotes the jth column vector of the design matrix. Correspondingly, the second-stage estimator of β_{j} is denoted by $\hat{\beta}_{j}(i_{1})$, for $j \neq i_{1}$, and is given by

$$\hat{\beta}_{j}(i_{1}) \approx \underline{x}_{j} \underline{y}(i_{1}) / \mathbb{N} , \qquad (3.2)$$

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$$\underline{y(i_1)} = \underline{y} - \overline{y} - \hat{\beta}_{i_1} - \hat{\beta}_{i_1} - \hat{\beta}_{i_1}$$
(3.3)

and i_1 denotes the index of the factor showing the largest effect in the first stage of the procedure. The vector $\underline{y}(i_1)$ is the vector of first-stage residuals.

Substituting (3.3) into (3.2), we see that

$$\hat{\beta}_{j}(i_{1}) = \hat{\beta}_{j} - \hat{\beta}_{i_{1}}r_{ji_{1}}$$
(3.4)

where $r_{ij} = \underline{x}_{i-j}^{\prime} / N$. In RB designs the variable r_{ij} is the sample correlation coefficient for \underline{x}_i and \underline{x}_i and is a measure of the orthogonality between the two respective design columns.

The estimator of β_1 as defined in (3.1) is precisely the estimator considered by Mauro and Smith [4] under the individual F-test approach for analyzing RB experiments. Mauro and Smith have shown that

 $V(\hat{\beta}_{1}) = (\tau^{2} - \beta_{1}^{2})/(N-1) + \sigma^{2}/N$,

$$E(\hat{\beta}_{j}) = \beta_{j}$$
(3.5)

and

where

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where
$$\tau^2 = \Sigma \beta_m^2$$
. Although $\hat{\beta}_j$ is an unbiased estimator of β_j , its variance
can be seriously inflated. The basic idea behind the use of SR is to re-
duce the effect of the inflation by adjusting for those factors which appear

to have large effects.

Regarding the estimator $\hat{\beta}_{i}(i_{1})$, we have from (3.4) and (3.5) that

$$E[\hat{\beta}_{j}(i_{1})] = \beta_{j} - E[\hat{\beta}_{i_{1}}r_{ji_{1}}]. \qquad (3.7)$$

In the Appendix we show for $i_1 \neq j$ that $E[\hat{\beta}_{i_1}, r_{ji_1}] = \beta_j/(N-1)$, so that

$$E[\hat{\beta}_{j}(1_{1})] = \beta_{j}[(N-2)/(N-1)]. \qquad (3.8)$$

The estimator $\hat{\beta}_j(i_1)$ is therefore slightly biased for β_j . We can easily remove the bias by considering the modified estimator

$$\hat{\beta}_{j}^{*}(i_{1}) = \hat{\beta}_{j}(i_{1})[(N-1)/(N-2)]. \qquad (3.9)$$

Since $\hat{\beta}_{i}^{*}(i_{1})$ and $\hat{\beta}_{i}$ are both unbiased estimators of β_{i} , it is meaningful to compare their respective variances. That is, we wish to calculate the efficiency of $\hat{\beta}_i^*(i_1)$ relative to $\hat{\beta}_i$. Accordingly, we define the

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(3.6)

measure

$$EFF = V[\hat{\beta}_{j}^{*}(i_{l})]/V[\hat{\beta}_{j}]. \qquad (3.10)$$

This ratio measures the amount of information supplied by $\hat{\beta}_j$ relative to that supplied by $\hat{\beta}_j^*(i_1)$.

Applying the results given in the Appendix, it is easily shown that the variance of $\hat{\beta}_{i}^{*}(i_{1})$, conditional on $i_{1} = i$, is given by

$$v_{i_{1}=i}[\beta_{j}^{*}(i_{1})] = (\tau^{2} - \beta_{i}^{2} - \beta_{j}^{2})/(N-2) + 2\beta_{j}^{2}/N(N-3) + \sigma^{2}(N-1)/N(N-2).$$
(3.11)

The efficiency measure defined in (3.10) requires the unconditional variance of $\hat{\beta}_j^*(i_1)$, however. In other words, we must evaluate (3.11) over variation in i_1 . Unfortunately, we have found this problem to be intractable. Nevertheless, equation (3.11) is still useful to our analysis of the first two stages of the SR method.

With some algebraic manipulation we can show that, given $i_1 = i$,

$$EFF = [(N-1)/(N-2)][1+\phi]$$
 (3.12)

where

$$\frac{2\beta_{j}^{2}(N-2) - \beta_{j}^{2}N(N-3)}{N(N-1)(N-3)V(\hat{\beta}_{j})}$$
 (3.13)

Thus, given $i_1 = i$ and for N large, EFF is approximately

EFF
$$\approx 1 + (2\beta_j^2/N - \beta_i^2)/(\tau^2 - \beta_j^2 + \sigma^2)$$
. (3.14)

We see from (3.14) that EFF<1, if and only if,

$$|\beta_{j}/\beta_{i_{1}}| \leq (N/2)^{\frac{1}{2}}$$
 (3.15)

That is, $\hat{\beta}_{i}^{\dagger}(i_{1})$ is a more efficient estimator of β_{i} than $\hat{\beta}_{j}$ as long as

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(3.15) holds. If $\hat{\beta}_{j}^{*}(i_{1})$ is to be uniformly more efficient than $\hat{\beta}_{j}$, then (3.15) must hold for every j; equivalently, we require

$$(2/N)^{\frac{1}{2}} \max_{j} |\beta_{j}| \leq |\beta_{1}| \qquad (3.16)$$

The term

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$$\frac{2\beta_{j}^{2}/N - \beta_{i}^{2}}{\tau^{2} - \beta_{j}^{2} + \sigma^{2}}$$
(3.17)

appearing in (3.14) represents the gain (if (3.17) is negative) or loss (if (3.17) is positive) of efficiency in the second stage given that $i_1 = i$. Most likely the denominator in (3.17) will be dominated by $\tau^2 = \Sigma \beta_m^2$. When (3.15) holds, the numerator in (3.17) is likely dominated by $\beta_{i_1}^2$, thus the gain in efficiency is roughly

$$\beta_{1}^{2}/\tau^{2}$$
. (3.18)

It is apparent from (3.18) that unless the contribution of $\beta_{i_1}^2$ is large relative to the total effect (τ^2) , there is little gain in efficiency.

It is interesting to note that the maximum loss of efficiency occurs when $\beta_{i_1} = 0$, that is, when the factor showing the largest effect in the first stage actually has no effect whatsoever. In this case, the loss of efficiency is roughly

$$2\beta_{j}^{2}/[N(\tau^{2}-\beta_{j}^{2})]$$
 (3.19)

In summary, our analysis indicates that if the actual effect of the factor showing the largest effect (in the first stage) is sufficiently large, then we can obtain improved estimates of factor effects in the second stage. This observation is clear from equations (3.15) and (3.16).

The extent of the improvement, however, may be slight depending on the relative contribution of the apparently largest effect to the total effect.

Our analysis takes on additional meaning considering that the (SR) first-stage estimation procedure is identical to the separate F-test estimation procedure considered by Mauro and Smith [4]. Our discussion, then, provides some preliminary indication of how these two alternative analysis techniques would compare. Admittedly, the results derived in this section do not completely answer the question of which procedure is preferable, nor do they provide a conclusive overall picture of the multistage SR method. However, the results do indicate in which situations the difference is likely to be worth considering. To gain further insight into this problem we conducted two Monte Carlo case studies, the results of which are presented and discussed in the next section.

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IV. MONTE CARLO RESULTS

In this section we consider two synthesized examples in which all the true effects are known beforehand. In both examples we assume that K=20 factors are to be screened in an RB screening experiment having N=12 runs. We simulated each test case 300 times and analyzed the test results of each simulation with both the SR and the separate F-test (SFT) methods. The distributions of factor effects used in each case study are given in Figures 1 and 2.

The absolute effects selected for Case Study I are basically (negligible effects were grouped) the expected order statistics from a sample of 20 deviates from a gamma distribution having mean $.5\sigma$ and standard deviation 1.58 σ . The absolute effects selected for Case Study II are basically the expected order statistics from a sample of 20 exponential random deviates having mean and standard deviation 1.0 σ .

In applying the SFT method we conducted each F-test at the same significance level, α . We tested for significance at the following eight α levels: .05, .40 (.05). These same α levels were used for determining the stopping rules in the SR method.¹

The results of Case Study I are summarized in Table 1. We see from this table that the observed significance levels associated with the SFT method agree closely with the various α levels employed. The observed significance levels associated with the SR method, however, are significantly larger than the α levels that define the stopping rules. This problem is

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We stop at the stage where the maximum F-statistic does not exceed the upper $100(1-\alpha)$ percentage point of an F-distribution having 1 and (N-2) degrees of freedom.

not unique to the SR method, but is often found with other sequential variable selection procedures. However, it complicates the application of the SR method in that it is difficult to control the risk of declaring important a factor having negligible effect.

It is quite clear from Table 1 that for strategies (i.e., columns) having comparable empirical Type I error rate, we obtain substantially greater power with the SR method than with the SFT method, particularly for $|\beta|/\sigma = 0.7$, 1.2, and 2.3. In detecting the largest effect, $|\beta|/\sigma = 5.3$, both methods were highly accurate. In fact, from Table 2 we see that this particular effect was entered at the first stage of the SR method in each of the 300 simulations. The next largest effect, $|\beta|/\sigma = 2.3$, was entered at the second stage in 242 of the 300 simulations.

The results of Case Study II are summarized in Table 3. We note that the same observations made in Case Study I regarding the observed significance levels also apply to Case Study II. We do not, however, always obtain greater power with SR strategies than with SFT strategies having comparable empirical Type I error rate. We see instead that the SFT method is more powerful for detecting the larger effects $(|\beta|/\sigma > 1.5)$ and the SR method is more powerful for detecting the moderate to smaller effects. We can offer two reasons for this based on our analysis made in Section III. First, we can expect the SR method to be more sensitive to the relatively small effects than the SFT method (and this is true in general) because the chance that (3.15) is true is greater for smaller effects. Thus, a gain in efficiency will, more often than not, be propagated through the stagewise procedure. Second, for the particular set of effects used in the second case study, the larger effects are not always entered early in the SR procedure. This is evident from Table 4. We see from this table that there -11-

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is a one-in-three chance that the effect showing the largest effect in the first stage will actually be less than 1.5σ in absolute magnitude. In the second stage the chance of this occurring is one in two. Thus, for the larger effects a loss of efficiency is often being propagated. As a consequence, the SFT method shows greater power for detecting the relatively large effects.

One final observation may be made. An easy calculation shows that $\tau^2 = 35.51$ and $\tau^2 = 35.77$ in Case Studies I and II, respectively. The relative contribution of the largest absolute effect to the total effect is therefore $(5.3)^2/35.51 = .79$ in Case Study I and $(3.55)^2/35.77 = .35$ in Case Study II. The larger relative contribution of the largest effect in Case Study I implies there is a greater chance in Case Study I than in Case Study II of selecting the largest effect in the first stage of the SR method. Moreover, it indicates that there is greater potential gain in efficiency.

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V. CONCLUSIONS

Although SR is a more sophisticated analysis technique than the SFT method, there are situations in which the SFT method has greater power for detecting the larger effects. Computationally, both methods are relatively quick and easy to apply. The key to SR is early detection of the relatively large effects. If the most critical factors are not entered early in the stagewise procedure, the possibility of their nondetection is increased. It is precisely this type of scenario where SR will be less efficient than the SFT analysis method.

The most favorable situation to the SR method is when only a relatively small number of factors are responsible for all or much of the total effect. In such cases the difference in effectiveness between the SR and SFT methods is likely to be large. A drawback to the SR method, as in most sequential selection procedures, is that it is difficult to control the true significance level of the test. For example, in the Monte Carlo case studies presented in Section IV, the actual value of α was roughly 50% greater than the "entry α ."

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VI. APPENDIX

In this section we state three key results that were used to establish equations (3.8) and (3.11). A proof is provided for the first result only. Result #1: For $i_1 \neq j$, $E[\hat{\beta}_{i_1}r_{j_1}] = \beta_j/(N-1)$. Proof. Note that $\hat{\beta}_i r_{ij} = \underline{x}_i^i \underline{y} \underline{x}_i^i \underline{x}_j/N^2 = \sum_{m=1}^k \beta_m \underline{x}_i^i \underline{x}_i^j \underline{x}_j/N^2 + \underline{x}_i^i \underline{c} \underline{x}_i^i \underline{x}_j/N^2$. Now, $E[\hat{\beta}_i r_{ij}] = (1/N^2) \sum_{m=1}^k \beta_m E[\underline{x}_i^i \underline{x}_i^i \underline{x}_j]$, since $E[\underline{x}_i^i \underline{c} \underline{x}_i^i \underline{x}_j] = 0$. For $i \neq j$, $E[\underline{x}_i^i \underline{x}_i^i \underline{x}_j] = 0$ unless m = j. Thus, $E[\hat{\beta}_i r_{ij}] = (1/N^2) \beta_j E[\underline{x}_i^i \underline{x}_j]^2 = (1/N^2) \beta_j (N^2/(N-1)) = \beta_j/(N-1)$. To obtain the desired result, observe that for $j \neq i_1$, $E[\hat{\beta}_{i_1}r_{j_1}] = E[E[\hat{\beta}_{i_1}r_{j_1}]i_1] = E[\beta_j/(N-1)] = \beta_j/(N-1)$.

Result #2: For $i \neq j$, $E[\hat{\beta}_{i}\hat{\beta}_{j}r_{ij}] = (\beta_{i}^{2} + \beta_{j}^{2})/(N-1) + (\tau^{2} - \beta_{i}^{2} - \beta_{j}^{2})/(N-1)^{2} + \sigma^{2}/N(N-1)$.

Result #3: For $i \neq j$, $E[\hat{\beta}_{i}^{2}r_{ij}^{2}] = \sigma^{2}/N(N-1) + \beta_{i}^{2}/(N-1) + (\tau^{2} - \beta_{i}^{2} - \beta_{j}^{2})/(N-1)^{2} + \theta_{N}\beta_{j}^{2}$, where

$$\theta_{N} = (3N - 8) / N(N-1)(N-3)$$
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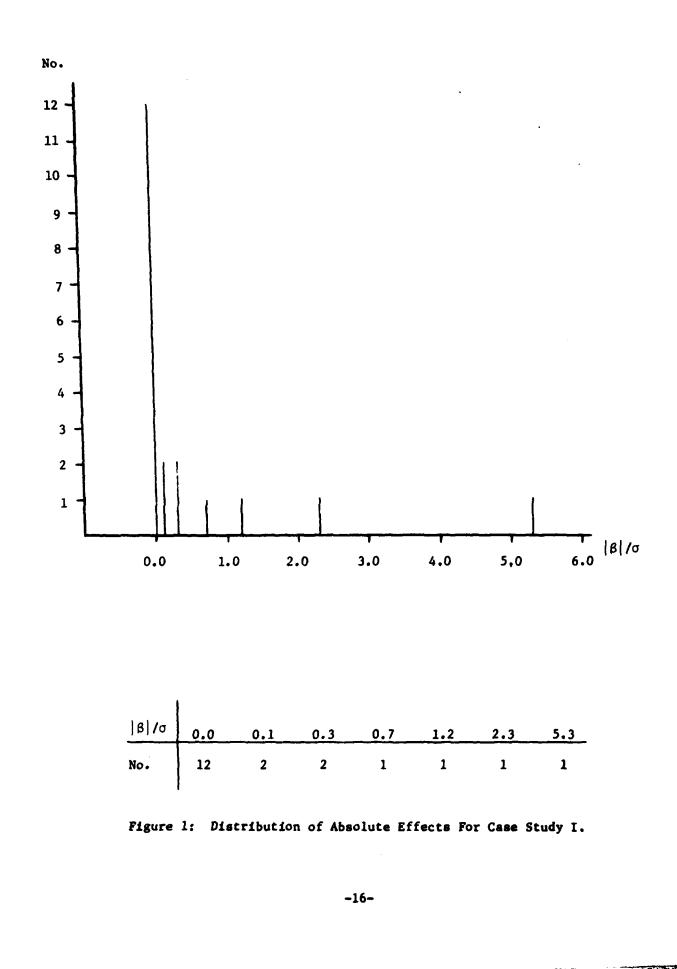
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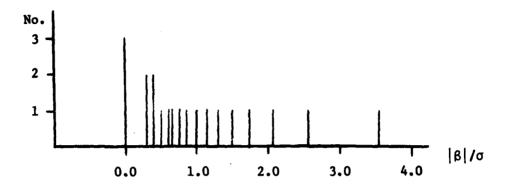
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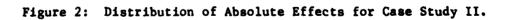
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0.0	12	.050	•00*	.142	.193	.246	.294	.340	.393
0.1	2	.052	060*	.123	.167	.200	.255	.305	.353
0.3	2	.068	•095	.143	.192	.243	.298	.342	.398
0.7	1	.050	.080	.140	.177	.230	.303	.357	.427
1.2	П	.093	.143	.220	.283	.340	.390	.437	.483
2.3	1	.213	.293	.370	.480	.553	.623	.683	.713
5.3	1	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
				a Level					
8 /a	No.	.05	.10	.15	.20	.25	.30	.35	.40
0.0	12	.078	.166	.238	.313	.379	464.	.480	.525
0.1	2	.087	.153	.227	.310	.387	.447	.505	.540
0.3	2	.105	.190	.262	.337	•400	.453	.515	.547
0.7	~	.223	.340	.423	.490	.573	.617	.643	.680
1.2	T	.473	.580	.610	.643	.673	.720	.753	.770
2.3	1	.853	.883	.917	.927	.937	.953	.960	• 963
5.3	7	1,000	1,000	1.000	1.000	1.000	1.000	1.000	1.000

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Estimate (p) That Given Effect Is Declared Important By Method. Standard Error of Each Estimate Is Given By [p(1-p)/300(No.)]³.

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β /σ	No.	Number of Simulations Entered at First Stage	Number of Simulations Entered at Second Stage
0.0	12	0	25
0.1	2	0	5
0.3	2	0	6
0.7	1	0	9
1.2	1	0	13
2.3	1	0	242
5.3	1	300	0

Table 2: Observed Counts for Entering (i.e., showing largest effect) at First and Second Stages of SR Method for Case Study I.

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181/g	No.	.05	.10	.15	.20	.25	.30	.35	.40
0.00	3	.043	.091	.153	.209	.258	.303	. 352	.403
0.30	2	.067	.117	.170	.220	.260	.312	.352	. 388
0.40	2	.077	.117	.165	.220	.275	.312	.363	.410
0.50	1	.043	,100	.150	.197	.257	.303	. 360	.413
0.60	1	.073	,127	.177	.230	.287	.327	.377	.447
0.66	1	047	.113	.173	.237	.277	.313	.357	.427
0.76	1	.077	.140	.203	.230	.277	.327	.373	.430
0.87	1	.083	.147	.200	.247	.317	.410 .	.467	.510
1.00	1	.083	.140	.210	.270	. 320	. 363	.413	.473
1.14	1	.073	.143	.203	.257	.317	. 363	.410	.470
1.31	1	.100	.163	.230	.280	.353	.410	.473	.513
1.51	1	.133	.207	.267	.3 3 3	. 397	.443	.507	.540
1.75	1	.103	.193	.253	.303	.360	.413	.480	.510
2.08	1	.210	.313	.373	.443	.517	.593	.647	.690
2.57	1	. 330	.477	.557	.613	.663	.713	.750	.780
3.55	1	.530	.663	.743	.810	.847	.893	.907	.933

SR METHOD

				a Leve	1				
B /a	No.	.05	.10	.15	.20	.25	.30	.35	.40
0.00	3	.084	.169	.227	.296	. 364	.408	.451	. 508
0.30	2	.102	.185	.263	.325	.383	.420	.495	. 540
0.40	2	.092	.198	.273	. 362	.417	.482	.527	. 568
0.50	1	.080	.200	.287	.373	.433	.493	.527	.570
0.60	1	.087	.183	.253	.310	.407	.500	.550	.607
0.66	1	,090	.193	.263	.330	.423	.493	.543	.600
0.76	1	.083	.173	.243	.310	.370	.423	.467	.547
0.87	1	.113	.247	. 350	.437	.497	.530	.570	.600
1.00	1	.153	.277	.370	.430	.483	.527	.577	.633
1.14	1	.110	.233	.330	.410	.480	.507	.553	. 597
1.31	1	.133	.287	.343	.407	.490	.527	.557	•60 7
1.51	1	.120	.243	.303	.393	.453	.487	.557	.617
1.75	1	.173	.313	.403	.473	.547	.573	.613	.653
2.08	1	.233	.357	.417	.510	.553	. 593	.630	.677
2.57	1	.280	.420	.503	.563	.630	.683	.737	.780
3.55	1	.520	.687	.747	.790	.810	.827	.850	.873

Table 3: Summary of Results for Case Study II. Table Entry Represents The Empirical Probability Estimate (\hat{p}) That Given Effect Is Declared Important By Method. Standard Error of Each Estimate Is Given By $[\hat{p}(1-\hat{p})/300(\text{No.})]^{\frac{1}{2}}$.

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B /o	No.	Number of Simulations Entered at First Stage	Number of Simulations Entered at Second Stage
<u><</u> 0.66	10	52	87
0.76	1	9	6
0.87	1	8	11
1.00	1	9	20
1.14	1	9	10
1.31	1	12	13
1.51	1	13	16
1.75	1	15	19
2.08	1	28	28
2.57	1	46	33
3.55	1	99	57

Table 4: Observed Counts for Entering (i.e., showing largest effect) at First and Second Stages of SR Method for Case Study II.

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