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REGRESSION ANALYSIS OF FACTORIAL DESIGNS WITH SEQUENTIAL REPLICATION

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ABSTRACT

In experimental designs with unequal response variances, the number of replications per factor-level combination may be selected such that the variances of the average responses become equal, i.e., combinations with high variability are more often replicated. Then Weighted Least Squares becomes identical to Ordinary Least Squares applied to the average responses. If the response variances are unknown, they can be estimated through replication. These estimated response variances yield estimates of the number of replications required to realize approximately equal variances per average response. This sequential procedure is evaluated through a Monte Carlo experiment.

1. INTRODUCTION

We consider classical experimental designs - especially 2^{k-p} factorial designs (with integers $k \ge 1$ and $p \ge 0$) - in which we sequentially determine the number of replications \underline{m}_{-1} (with i=1,...,n where n is the number of factor-level combinations, i.e., in factorials $n = 2^{k-p}$). In other words, during the experiment we analyze the responses \underline{y}_{ij} (j=1,..., \underline{m}_i) and use their variance estimators s_i^2 in a stopping rule. Once we stop the experiment we analyze its data, applying Least Squares. In the foregoing we underlined random variables, because the random character of the number of replications (\underline{m}_i) is essential and becomes explicit in this notation. (We further use the term "estimate")

becomes explicit in this notation. (We further use the term "estimate" to denote the value of an "estimator".)

The literature investigates stopping rules primarily in situations with one or two populations (n=1,2); see the textbooks by Govindarajulu (1981) and Wetherill (1975) and also Kleijnen (1936). In experimental designs the number of replications must often be prespecified. An important exception, however, are simulation experiments, i.e., experiments with a computer model (or "code") of some real system (for instance, a nuclear reactor, a company, an insect population). In simulation experiments all observations are obtained successively. Therefore sequential statistical procedures are certainly relevant to simulation.

We further assume that the response variances σ_i^2 may differ substantially. For example, Kleijnen, Van den Burg, Van der Ham (1979, p. 60) report a 2^{6-2} experiment where s_i^2 ranges between 64 and 93,228. Variance heterogeneity is further discussed in Kleijnen (1985).

2. KNOWN VARIANCES σ_i^2

In the present section we assume that the response variances σ_i^2 are known. Intuitively it seems wise to obtain more replications of those experimental conditions that have high variability. More specifically, if we take

$$m_i = c \sigma_i^2$$
 (i=1,...,n) (2.1)

where c is a (common) positive constant such that m_i becomes integer, then

 $\operatorname{var}\left(\overline{y}_{i}\right) = \frac{1}{c} \tag{2.2}$

where $\overline{\underline{y}}_{i} = \sum_{j=1}^{m_{i}} \underline{y}_{ij}/m_{i}$.

We can analyze the experimental data, applying Weighted Least Squares (WLS) to the individual responses \underline{y}_{ij} . It is simple to prove that the WLS estimate $\tilde{\beta}$ follows from

$$\min \sum_{i=1}^{n} \{ m_{i}(\bar{y}_{i} - \hat{y}_{i})^{2} \frac{1}{\sigma_{i}^{2}} \}$$
(2.3)

The Ordinary Least Squares (OLS) estimate $\hat{\beta}$ follows from

$$\min \sum_{i=1}^{n} \{ m_{i} (\bar{y}_{i} - \hat{y}_{i})^{2} \}$$
(2.4)

Under condition (2.1), or $m_i/\sigma_i^2 = c$, the WLS estimate follows from

$$\min \sum_{i=1}^{n} (\bar{y}_{i} - \bar{y}_{i})^{2}$$
(2.5)

In general, WLS gives little weight to responses with high variability; OLS gives more weight to conditions replicated often. Now condition (2.1) means that the optimal WLS estimator based on the individual responses is identical to the OLS estimator based on the average responses while ignoring the number of replications on which those averages are based. Computationally this OLS estimator is simpler, so that we shall concentrate on the OLS estimator $\hat{\beta}$ following from (2.5).

3. ESTIMATING
$$\sigma_i^2$$
 and m_i

Because the response variances are unknown, we have to estimate σ_1^2 and hence m_1 in eq. (2.1). Many estimation schemes are conceivable: two-stage (Stein estimators), multistage, sequential schemes. We concentrate on the following sequential procedure.

(1) We start with a <u>pilot</u> sample of $m_i = m_0$ responses from each of the n populations (or combinations), and compute

$$\underline{s}_{i}^{2} = \frac{\underbrace{j=1}^{m_{i}} (y_{ij} - \overline{y}_{i})^{2}}{(m_{i} - 1)} \quad (i=1, \dots, n) \quad (3.1)$$

In the Monte Carlo experiment of Section 5 we take $m_0 = 4$, 9, and 25.

(2) We use these estimators s_i^2 to obtain the estimators of the required number of replications. Straightforward application of eq. (2.1) yields:

$$\hat{\underline{m}}_{i} = \left[\frac{\underline{s}_{i}^{2}}{\min(\underline{s}_{i}^{2},)} \underline{m}_{0} \right]$$
(3.2)

where [x] denotes the integer closest to x. A refinement of eq. (3.2) is as follows. If the response variances differ greatly, then impractically many replications would be taken from the population with the maximum variance. Therefore we define the ratio

$$\underline{r} = \frac{\max_{i} (\underline{s}_{1}^{2})}{\min_{i} (\underline{s}_{1}^{2})}$$
(3.3)

and in order to control

$$\max_{i} (\underline{m}_{i}) = \underline{r} \, \underline{m}_{0} \tag{3.4}$$

we replace m_0 in eq. (3.2) - not in eq. (3.1) - by the value 1, iff r is "big":

 $\underline{m}_{0} = 1 \text{ if } \underline{r} > rmax \tag{3.5}$

In the Monte Carlo experiment we take rmax = 3000. This refinement means that, if r is big, then for the population with the smallest variance estimate $\overline{s_i^2}$, we compute the average \overline{y}_i from only 1 replication; its va-

riance, however, we compute from all replications. In this way, we obtain the most accurate variance estimator possible, while we still apply OLS to average responses with approximately constant variances.

(3) For each population with $\hat{m_i} > m_0$ we obtain one new response (i.e., our procedure is sequential, not two-stage or multi-stage). We use all available responses to re-estimate σ_i^2 : we replace eq. (3.1) (with a deterministic $m_i = m_0$) by

$$\underline{s}_{i}^{2}(\underline{m}) = \frac{\underbrace{j=1}^{\underline{m}_{i}} (\underline{y}_{ij} - \overline{y}_{i(\underline{m}_{it})})^{2}}{(\underline{m}_{-it} - 1)}$$
(3.6)

where \underline{m}_{it} denotes the number of responses from population i available after iteration t (t=1,2,...,T); $\underline{\hat{m}}$ denotes the number of responses necessary to realize constant response variances (see eq. 3.2) and

$$\overline{\overline{Y}}_{i} (\widehat{m}_{it}) = \frac{\underbrace{j=1}^{\underline{m}_{it}}}{\underbrace{\overline{m}}_{it}} (i=1,\ldots,n)$$
(3.7)

(4) We return to step (2) until (for the first time) the desired number of replications m does not exceed the available number m, for all populations:

$$\forall i: \underline{m}_{it} < \underline{m}_{it}$$
(3.8)

We let \underline{T} denote the minimum number of iterations for which (3.8) holds. Once we stop the experiment, we analyze the experimental data, as described in the next section.

4. REGRESSION ANALYSIS

We estimate the response for population i from $\underline{m}_{i\underline{T}}$ responses; see eq. (3.7) with t replaced by T. (Remember: if $\underline{r} > rmax$ then $\exists i:$ $\hat{\underline{m}}_{i\underline{T}} = 1$.) From these averages we derive the OLS point estimator $\hat{\underline{\beta}}$:

$$\hat{\underline{\beta}} = (\bar{x}'\bar{x})^{-1} \bar{x}' \bar{y} (\hat{\underline{m}}_{\underline{i}\underline{T}})$$
(4.1)

where \overline{X} is the n x Q matrix of Q independent variables obtained from the N x Q matrix X by eliminating all identical rows in X, where

$$\underline{N} = \sum_{i=1}^{n} \widehat{\underline{m}}_{i\underline{T}}$$
(4.2)

We approximate the standard errors of $\underline{\beta}$ as follows; also see eq. (2.2). Let $\underline{\hat{p}}$ be a diagonal matrix with the following elements on the main-diagonal:

$$\underline{d}_{ii} \equiv \frac{1}{\underline{c}_{i}} \equiv \hat{var} (\bar{y}_{i}) = \frac{\overset{\underline{m}_{iI}}{\underline{r}}}{\overset{\underline{j=1}}{\underline{r}}} (\underbrace{y_{ij}}_{\underline{j=1}}, \underbrace{\overline{p}_{iI}}_{\underline{m}_{iI}})^{2} \frac{1}{\underline{m}_{iI}} \frac{1}{\underline{m}_{iI}} (\underbrace{u_{iI}}_{\underline{m}_{iI}}, \underbrace{u_{iI}}_{\underline{m}_{iI}}, \underbrace{u_{iI}}_{\underline{m}_{iI}})^{2}$$

$$(i=1, \dots, n) \quad (4.3)$$

where m and \hat{m} denote the available and the desired number of responses respectively (m > \hat{m}); the first factor is the estimator of var (y) that uses all available information; the second factor corresponds to the number of responses on which \bar{y} is based. Eq. (4.1) yields:

$$\widehat{\underline{\alpha}}_{\widehat{\beta}} = (\overline{x}'\overline{x})^{-1} \overline{x}' \widehat{\underline{p}} \overline{x} (\overline{x}'\overline{x})^{-1}$$

$$(4.4)$$

If our sequential procedure works as expected, then $1/\hat{c_1} \approx 1/\hat{c} \equiv \bar{s}^2$ where (see eqs. 4.3 and 3.6)

$$\overline{\underline{s}}^{2} = \frac{\underbrace{1}_{\Sigma}^{n} \underline{s}_{i}^{2} (\underline{m}_{i\underline{T}}) / \underline{m}_{i\underline{T}}}{n}$$

$$(4.5)$$

so that eq. (4.4) reduces to

$$\hat{\Omega}_{\hat{R}} \approx \bar{s}^2 (\bar{X}'\bar{X})^{-1} \tag{4.6}$$

And if \overline{X} is orthogonal, then the estimators $\underline{\beta}_q$ are uncorrelated. If \overline{X} is a 2^{k-p} design, then var $(\underline{\beta}_q)$ becomes a constant, namely \overline{s}^2/n . The square roots of the main-diagonal elements of $\underline{\Omega}_{\beta}$ are the standard errors of $\underline{\beta}_q$; we denote these standard errors by $\underline{\sigma}_q$ (q=1,...,Q).

To obtain confidence intervals for β_q we use Student's t statistic. Kleijnen, Cremers, Van Belle (1985) investigated different degrees of freedom ν , namely min(m_i -1), $\Sigma(m_i$ -1) and infinity (so that t becomes standard normal). In sequential experiments $\Sigma(m_i - 1)$ is high; therei fore we restrict ourselves to min(m_i -1) = m_0 - 1 = ν_1 and ν_2 = ∞ (so that ν becomes non-stochastic). In the next section we investigate whether the statistic

$$\underline{t}_{\nu,q} = \frac{\underline{\beta}_{q} - \beta_{q}}{\underline{\sigma}_{q}} \qquad (q=1,\dots,Q) \qquad (4.7)$$

behaves like a Student t statistic. To study t we use Monte Carlo $-\nu,q$

5. MONTE CARLO INPUTS

We use nearly the same inputs as did Kleijnen, Cremers, Van Belle (1985). So we have 4 different \overline{X} matrices:

<u>Case 1</u>: \bar{X} is a 16 x 13 matrix, namely a 2^{6-2} design including 6 main effects, 6 two-factor interactions and a grand mean β_0 .

<u>Case 2</u>: \overline{X} is an 8 x 4 matrix following from a 2³ design (with 3 main effects). In case 2 \overline{X} is a submatrix of \overline{X} in case 1.

<u>Case 3</u>: \overline{x} is a 4 x 3 matrix following from a 2² design. \overline{x} is again a submatrix of \overline{x} in case 1.

<u>Case 4</u>: \overline{X} is again a 4 x 3 matrix as in case 3; however, \overline{X} is non-orthogonal. Kleijnen et al. (1985) studied only the first 3 cases.

We combine the above 4 matrices with different degrees of heterogeneity of response variance, measured - as in Kleijner et al. (1985, p. 88) - by

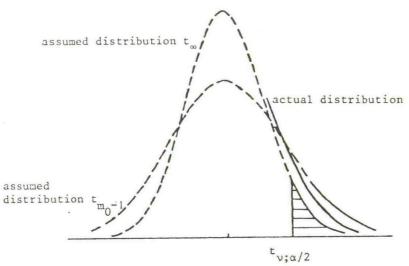
$$H = \frac{\max (\sigma_{i}^{2}) - \min (\sigma_{i}^{2})}{\min (\sigma_{i}^{2})}$$
(5.1)

We fix H at the values 0, 4, and 11.84. Kleijnen et al. (1985) varied H between 0 and 1,458; the latter value, however, means that \underline{m}_i may be so high that computer time becomes prohibitive. The individual σ_i^2 values are shown in the appendix.

Besides \bar{X} and the diagonal matrix Ω_y with elements σ_i^2 , we must specify β . We use the β values of Kleijnen et al. (1985, p. 95). The precise values of β do not affect the interpretation of the Monte Carlo experiment, so that we refer to the appendix.

We study different sizes of the pilot-sample m_0 , namely 4, 9 and 25. Kleijnen et al. (1985, p. 89) varied $m_1 = m$ between 2 and 25; the value 2, however, gave bad results. We further take rmax = 3000 in eq. (3.5), which is so high that r never exceeds rmax. We repeat each Monte Carlo situation (specified by \overline{X} , Ω_y , β , and m_0) 150 times, since Kleijnen et al. (1985) found that 150 repetitions reduce noise so much that clear patterns emerge from the Monte Carlo experiment.

We use the same multiplicative random number generator as in Kleijnen et al. (1985, p. 96). (Even though the ICL 2960 has been replaced by a VAX 785, the NAG generator was maintained.) Each of the 4 "cases" (combined with different degrees of variance heterogeneity) starts with the same random number seed. Since the random number streams get out of step, the dependence between cases is probably weak (anyhow, in our analysis we do not need to assume independence).



6. MONTE CARLO OUTPUT

We first repeat some situations also investigated in Kleijnen et al. (1985), in order to verify the correctness of our computer program. We also checked that the estimators of β remain unbiased.

As Kleijnen et al. (1985, p. 90) did, we derive two-sided confidence intervals for β_q , now using \underline{t}_v with $v = v_1 = \min_i \underline{m}_{i1} - 1 = \lim_i \underline{m}_0 - 1$ and $v = v_2 = \infty$ respectively. We again test the tails of the resulting \underline{t}_v distribution [see eq. (4.7) where $\underline{\sigma}_q \equiv var(\underline{\beta}_q)$]:

$$P\left\{\frac{\hat{\underline{\beta}}_{q} - \beta_{q}}{\hat{\underline{\sigma}}_{q}}\right\} > t_{\nu, q; \alpha/2} = \hat{\alpha} \quad (q=1,...,Q) \quad (6.1)$$

where t $v,q;\alpha/2$ denotes the tabulated 1- $\alpha/2$ quantile of Student's t v with $v = v_1$ and $v = v_2$ respectively. We estimate α from the Monte Carlo experiment (see next paragraph), and formulate 2 slightly different null-hypotheses:

$$H_{0}: E(\underline{\hat{\alpha}}) = \alpha \text{ versus } H_{1}: E(\underline{\hat{\alpha}}) \neq \alpha$$

$$H_{0}': E(\underline{\hat{\alpha}}) \leq \alpha \text{ versus } H_{1}': E(\underline{\hat{\alpha}}) \geq \alpha.$$
(6.3)

and

H₀ requires a two-sided test, while H₀ corresponds to a one-sided test.

The test statistic is the binomial variable \hat{p} based on 150 observations (Monte Carlo repetitions). Under H_0 we know that $E(\hat{p}) = \alpha$ where α is defined in eq. (6.1). We approximate the binomial distribution by the normal distribution $N(\hat{p}, \hat{p}(1-\hat{p})/150)$. Since we have Q parameters β , we apply the Bonferroni inequality, i.e., we test H_0 and H'_0 with a type I error rate of 0.05/Q (so that the experimentwise error rate is 0.05 at most). For α in eq. (6.1) (the error rate used to derive a confidence interval per parameter β_q) we use 1%, 5%, and 10%, as did Kleijnen et al. (1985).

	α =	1%	$\alpha = 5\%$		$\alpha = 10\%$		
	$v = v_1$	v = ∞	$v = v_1$	ν = ∞	$v = v_1$	$v = \infty$.	
	1		1		1		
C1H11M04*	*	*	*	*	*	*	
C1H04M04	*	*		*		*	
C1H00M04		*		*		*	
C2H10M04	*	*		*	*	*	
C2H04M04	*		*	*	*		
C2HOOMO4	*	*	*	*		*	
C3H10M04			*	*	*	*	
C3H04M04	*	*		*		*	
C3H00M04		*		*		*	
C1H11M09	*	*	*				
C1H04M09	*	*	*		*		
C1H00M09	*	*	*				
C2H10M09	*						
C2H04M09	*	*	*		*		
C2H00M09	*			*	*		
C3H10M09	*	*		*			
C3H04M09	*		*				
C3H00M09	*						
C1H11M25	*	*	*	*	*		
C1H04M25	*	*	*		*	*	
C1H00M25	*	*					
C2H10M25							
C2H04M25	*	*		*		*	
C2H00M25	*						
C3H10M25	*	*			*		
C3H04M25							
C3H00M25	*		*		*		
C4H10M04	*	*	*	*	*	*	
C4H04M04	*	*		*		*	
C4HOOMO4	*	*		*		*	
C4H10M09	*						
C4H04M09	*					*	
C4H00M09	*		*				
C4H10M25	*	*	*	*			
C4H04M25							
C4H00M25	*						
0411001120							

Table I Testing the tail of the \underline{t}_v distribution; H_0 : $E(\underline{\alpha}) = \alpha$.

* Notation: Cl refers to case 1 of Section 5; Hll means H \approx ll in eq. (5.1); M04 means a pilot sampling m_0 = 4.

	$\alpha = 1\%$		$\alpha = 5\%$	$\alpha = 10\%$	
	$v = v_1$	$v = \infty$	$v = v_1 v = \infty$	$v = v_1$	$v = \infty$
C1H11M04*		*	*		*
C1H04M04		*	*		*
C1H00M04		*	*		*
C2H10M04		*	*	*	*
C2H04M04					
C2HOOMO4		*	*		*
C3H10M04		*	*		*
C3H04M04		*	*		*
СЗНООМО4		*	*	*	*
C1H11M09					
C1H04M09					*
C1H00M09					*
C2H10M09					
C2H04M09					*
C2HOOMO9		*	*	*	*
C3H10M09					*
C3H04M09					*
C3H00M09					
C1H11M25		ne dalle subre des ha		- 2-5-4 mark - 12-24 22-25	*
C1H04M25					
C1H00M25					
C2H10M25					
C2H04M25		*	*		*
C2H00M25					
C3H10M25					
C3H04M25			*		
C3H00M25					
C4H10M04		*	*		*
C4H04M04		*	*		*
C4HOOMO4		*	*		*
C4H10M09					
C4H04M09					*
C4H00M09					*
C4H10M25					
C4H04M25					
C4HOOM25					

Testing the tail of the \underline{t}_{v} distribution; $H_{0}': E(\hat{\underline{\alpha}}) \leq \alpha$.

* Notation: C1 refers to case 1 of Section 5; H11 means H \approx 11 in eq. (5.1); M04 means a pilot sample m_0 = 4.

Table II

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The binomial test results in Tables I and II. We interpret these tables as follows; also see Fig. 1. Table I shows many asterisks-denoting rejection of H_0 : $E(\alpha) = \alpha$ - even if the pilot sample is big $(m_0 = \alpha)$ 25). The next question then is: in which direction does α deviate from a? Table II shows that if we use the standard normal distribution (or $t_{\infty; \alpha/2}$) then we accept $H'_1 : E(\hat{\alpha}) > \alpha$ (the smaller the pilot sample m_0 , the higher $\hat{\alpha}$ is). Fig. 1 demonstrates that such a high $\hat{\alpha}$ means a "fat" tail. Such a tail implies that we reject the true value β_{α} "too often", i.e. more often than the nominal α suggests. In other words, our confidence intervals around β_q are too tight. Instead of the normal distribution we can use the Student distribution with degrees of freedom $v_1 = \min(m_1 - 1) = m_0 - 1$. Obviously we have $t_{v_1; \alpha} > t_{\infty; \alpha}$ so that our confidence intervals become less tight (conservative intervals). Consequently we no longer reject the true value β "too often", i.e., α decreases and no longer do we reject $H'_0: E(\alpha) < \alpha$. Using v_1 degrees of freedom does not yield conservative confidence intervals, if we use small sample sizes and a "high" nominal α (α =0.10).

Note that we found that the estimated variances of the average responses (see eq. 4.3) are indeed approximately constant. The averaged estimated variance \overline{s}^2 (see eq. 4.5) has an empirical distribution (computed from 150 replications) which is skew with a long tail to the right. As we may expect, the variability of \overline{s}^2 increases, as the pilot-sample size m₀ decreases.

7. CONCLUSIONS AND FUTURE RESEARCH

We examined a heuristic sequential procedure for determining the number of replications per factor-level combination, such that the variances of the average responses become approximately constant. The resulting Least Squares estimator $\hat{\underline{\beta}}$ remains unbiased. Confidence intervals around $\hat{\underline{\beta}}$ (two-sided intervals) are not exact, even if the pilot sample size is as high as 25. These intervals are too tight if we use the standard normal variable. These intervals become conservative, if we use the Student statistic with degrees of freedom equal to $\min(\underset{i=1}{\min(\underline{m_i}-1)} = \underset{i=1}{\min(\underline{m_i}-1)} = \underset{i=1}{\min($

We concentrated on a purely sequential approach using as many responses \underline{y} as possible, when estimating means and variances. Many variations on this approach are conceivable which seem less efficient but might have better coverage (true type I or α error). Also see Section 3.

We did not discuss computational issues. For example, we saved all individual responses (not only sums of responses and squared responses) because in the sequential procedure we sometimes throw away responses when estimating the means (namely when $\underline{m}_{i\underline{T}} < \underline{m}_{i\underline{T}}$; we estimate the variances from all $\underline{m}_{-i\underline{T}}$ responses).

A well-known disadvantage of sequential procdures is that it is impossible to know how much computer time will be needed to execute the total number of runs $\underline{N} = \sum_{i=1}^{n} \underline{m}_{ii}$. Moreover, if the experiment has R (> 2) types of response, each type with its own variance, then our procedure needs adjustment (we might replace eq. 2.1 by $\underline{m}_i = \max_{r} c \sigma_{ir}^2 - where r = 1,...,R$). If the total computer time is prespecified, then the sequential procedure might be replaced by a fixed sample procedure (with $\underline{m}_i = \underline{m}_0$) accounting for unequal variances; see Kleijnen (1985).

We examined two-sided confidence intervals for β . On hindsight it is obvious that with negligible extra computer time we could also have studied one-sided confidence intervals for β .

APPENDIX: DETAILS OF MONTE CARLO INPUT

In this appendix we add some details not already mentioned in the main text. Most values are taken from Kleijnen et al. (1985).

 $\begin{array}{l} \underline{Case \ 1}: \ \beta' = \ (-1.42, -0.769, 13.4, -11.508, 3.5, -1.375, 140.918, \\ 15.391, 0.046, 281.098, 21.25, 11.875, -49.483). \end{array}$ H = 0: $\sigma_{\mathbf{i}}^2$ = 1 for all i. H = 4: $\sigma_{\mathbf{i}}^2$ = (4,4.5,5,6,8,9,10,11,12,13.5, 14,14.5, 16,18,19.5, 20). H = 11.84: $\sigma_{\mathbf{i}}^2$ = (1,2,3,4,4.5,5,6,7,7.5,8,9,9.5,10,11,12,12.84).

$$\frac{\text{Case 2: } \beta' = (-1.42, -0.769, 13.44, -11.508).}{\sigma_1^2 = 1 \text{ for all } 1.}$$

$$H = 4: \sigma_1^2 = (4, 6, 8, 10, 12, 14, 16, 20).$$

$$H = 10.83: \sigma_1^2 = (1, 2, 4, 5, 6, 7, 9, 11.83).$$

$$\begin{array}{r} \begin{array}{r} \begin{array}{c} \text{Case 3: } \beta' = (1,1,1) \\ \mu = 0: \\ \sigma_{1}^{2} = 1 \\ \text{for all } i \\ \mu = 4: \\ \sigma_{1}^{2} = (4,10,16,20) \\ \mu = 10.38: \\ \sigma_{1}^{2} = (1,4,8,11.38) \end{array}$$

Case 4: See case 3 for β and σ_i^2 .

	1	1	-1]	
X =	1	-1	-1 .	
	1	-1	1	
	1	-1	1	

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