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ON THE IDENTIFICATION OF ACTIVE CONTRASTS IN UNREPLICATED FRACTIONAL FACTORIALS

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Abstract: Lenth (1989) introduced a very simple method for identification of active contrasts in unreplicated factorial and fractional factorial experiments. This article gives another method which is as simple as Lenth's method. The method is compared with that of Lenth in both theoretical study and simulation experiments. Also, the method is illustrated with examples from Box and Meyer (1986) and compared with other existing methods.

Key words and phrases: Unreplicated fractional factorials, active contrasts.

1. Introduction

In the screening stage of industrial experimentation, people usually try to consider as many factors as possible from the information available. Therefore a large number of factors are considered and little information is left for estimating the variance. This is the case in unreplicated fractional factorial experiments, where there is no reliable estimate of the standard deviation τ of the contrasts. This make it difficult to identify the "active" contrasts, defined as those contrasts having large mean effects.

One way to deal with this is to construct a half-normal plot or a normal plot of the contrasts (Box, Hunter and Hunter (1978), Daniel (1959,1976)). A disadvantage of the normal-plot method is that its interpretation is somewhat subjective. The plotted points will not lie perfectly on a straight line even when all the contrasts (or residuals) are noise. An idea of the extent of nonlinearity to be expected may be obtained by looking at the forty pages of plots of pure noise given in Daniel (1976, pp.84-123). Also there is a problem of non-uniqueness for a normal plot. For a fractional factorial experiment, there can be many different normal plots of estimated contrasts for the same set of observations since the set of estimated contrasts is not unique in the sense that their signs are dependent on the experimenter's choice of labels for the "+" and "−" levels of each factor (see Loh (1992)).

A Bayesian solution was given by Box and Meyer (1986) which consists of modeling the contrasts as a sample from a scale-contaminated normal distribution. The prior information is summarized in two parameters, α (the probability that a contrast is active) and k (the inflation in the standard deviation produced by an active contrast). The authors suggested using $\alpha = 0.2$ and $k = 10$ which is based on an empirical study of published examples.

Another method, which is the simplest to apply up to now, is proposed in Lenth (1989). Lenth's method first computes an initial estimate of τ and uses this to re-estimate τ using a trimmed median procedure.

Loh (1992) proposed a method which is an extension of Daniel's normal probability plot technique. It eliminates the non-uniqueness of the normal plots. Based on a simulation experiment, Loh showed that this method is more likely to identify the correct number of active contrasts than Lenth's method.

In the present paper we propose to use a trimmed mean procedure instead of trimmed median in Lenth's method. The methods are described in Section 2. Monte Carlo comparisons of the level and power of our method versus Lenth's method are reported in Section 3. The estimated asymptotic mean square errors for Lenth's pseudo standard error (PSE) and our estimate are derived and analyzed in Section 4. In Section 5, four examples in Box and Meyer (1986) are considered.

2. The Methods

Given a set of responses from an unreplicated 2^{k-p} fractional factorial experiment, let $\hat{\beta}_1, \ldots, \hat{\beta}_n$ denote the set of estimated contrasts. Here $n = 2^{k-p} - 1$. Assume the responses are *iid* with $N(0, \sigma^2)$. Then the estimated contrasts are also independent and normally distributed with constant variance $\tau^2 = \sigma^2/2^{k-p}$.

Lenth proposed using $s_0 = 1.5 \times \text{median}\{|\hat{\beta}_j|;\ j = 1, \ldots, n\}$ as the initial estimate of τ, and the pseudo standard error (PSE), defined as $1.5 \times \text{median}$ $\{|\hat{\beta}_j|;\ j \in J\}$ where $J = \{j : |\hat{\beta}_j| \le 2.5 s_0\}$, as the final estimate of τ. He then defined the simultaneous margin of error SME$= t(\gamma, d)$PSE, where $t(\gamma, d)$ is the γth quantile of the t distribution with d degrees of freedom and $\gamma = [1 + 0.95^{1/n}]/2$, $d = n/3$. One of Lenth's suggestions is to use the simultaneous confidence interval $\hat{\beta}_i \pm$SME to determine whether a contrast β_i is active or not. The relationship $d = n/3$ was recommended by Lenth after he fitted the empirical distribution of PSE^2 with scaled chi-squared distributions by matching the first two moments. The degrees of freedom d is usually not an integer. Although Lenth used a simultaneous 95% confidence interval in his method, we will see, in the simulation study later, that his actual error rate level is closer to 3% than 5%.

In our method, we use s_1 instead of PSE where $s_1^2 = m^{-1} \sum_{|\hat{\beta}_j| \le 2.5 s_0} \hat{\beta}_j^2$ and

$m = \#\{j : |\hat{\beta}_j| \le 2.5s_0\}$. Instead of using a t distribution with fractional degrees of freedom we use $t(\gamma, m)$, the γth quantile of the t distribution, where $\gamma = [1+0.98^{1/n}]/2$; and we use the 98% simultaneous confidence interval $\hat{\beta}_j \pm t(\gamma, m)s_1$ to determine whether a contrast β_j is active or not. We choose 0.98 because it will make the actual α-levels closer to those of Lenth's procedure. Because ordinary t tables may be used, our method is simpler to use than Lenth's. To make our method work well when the percentage of active contrasts is large, we iterate, i.e. treat s_1 as s_0 and go through the 2nd step again. The iteration is used in the simulation study reported in the next section.

We shall see that our method works better than Lenth's when the hypothesis of effect sparsity is true, i.e. when the percentage of active contrasts is not large, say less than 20% and the size of the active contrasts are not too small.

3. Simulation Experiments

A simulation experiment was conducted to evaluate the power of the proposed procedure for identifying the correct number of active contrasts and to compare it with Lenth's (1989) method. The nominal level of significance used was 0.03. The values of n used were $n = 7, 15, 31$; and 0%, 5%, 20% and 40% active contrasts were employed. The experiment was performed as follows. Given n and p% active contrasts, n pseudo standard normals $(z_1, \ldots, z_n)$ were first generated in each trial. Let n_1 be the nearest integer to $np/100$ and define $\hat{\beta}_i$ to be $z_i + 4 + i$ when $i = 1, \ldots, n_1$ and z_i when $i = n_1+1, \ldots, n$. That is, the means of the active contrasts start from 5 and increment by 1 for each additional active contrast.

The results reported in Table 1 are based on 10,000 Monte Carlo trials. The column labeled "n" gives the number of contrasts in the design. The column labeled "active" gives the number of active contrasts found. A box around a number in this column indicates that it is the true number of active contrasts. The column labeled "Initial" gives the frequencies of detection of active contrasts using s_0 as the final estimate of τ and the simultaneous confidence interval $\hat{\beta}_j \pm t(\gamma, n)s_0$, where $\gamma = [1 + 0.97^{1/n}]/2$, to determine whether a contrast β_j is active or not. Here we choose 0.97 because it will make the actual α-levels closer to those of Lenth's. The columns labeled "Lenth" and "Proposed" give the frequencies of detection of active contrasts using Lenth's (1989) and the proposed methods.

The results in Table 1 show that for low percentages of active contrasts (e.g. 0%, 5%), the initial method is more likely to identify the correct number of active contrasts than Lenth's method and the proposed method is more likely to identify them than the initial method except for the case that $n = 7$ and 0% active. For higher percentages of active contrasts (e.g. 20%, 40%), Lenth's method is much better than the initial method and the proposed method is better than Lenth's. A similar conclusion was reached for other levels of significance.

Table 1. Frequencies of correct selection of the number of active contrasts by 10,000 Monte Carlo Experiments (Standard errors $\leq$ 0.005). Boxed numbers denote the true numbers of active contrasts.

n	active	Initial	Lenth	Proposed
	0% active			
7	[0]	0.978	0.975	0.968
	1	0.020	0.019	0.027
	≥ 2	0.002	0.006	0.005
15	[0]	0.975	0.972	0.971
	1	0.023	0.021	0.025
	≥ 2	0.002	0.007	0.004
31	[0]	0.974	0.970	0.974
	1	0.024	0.024	0.023
	≥ 2	0.002	0.006	0.003
	5% active			
n	active	Initial	Lenth	Proposed
15	0	0.287	0.463	0.164
	[1]	0.698	0.510	0.813
	≥ 2	0.015	0.007	0.003
31	0	0.034	0.041	0.005
	1	0.207	0.201	0.120
	[2]	0.746	0.733	0.854
	3	0.012	0.021	0.019
	≥ 4	0.001	0.004	0.002
	20% active			
n	active	Initial	Lenth	Proposed
15	0	0.084	0.108	0.024
	1	0.169	0.153	0.038
	2	0.288	0.241	0.182
	[3]	0.456	0.479	0.742
	≥ 4	0.003	0.019	0.014
31	≤ 4	0.168	0.057	0.012
	5	0.326	0.193	0.144
	[6]	0.504	0.727	0.832
	7	0.002	0.020	0.011
	≥ 8	0.000	0.003	0.001
	40% active			
n	active	Initial	Lenth	Proposed
7	0	0.668	0.581	0.588
	1	0.123	0.079	0.026
	2	0.099	0.101	0.055
	[3]	0.110	0.230	0.331
	≥ 4	0.000	0.009	0.000
15	≤ 3	0.591	0.220	0.194
	4	0.170	0.124	0.036
	5	0.143	0.178	0.117
	[6]	0.096	0.458	0.548
	7	0.000	0.017	0.005
	≥ 8	0.000	0.003	0.000
31	≤ 8	0.305	0.007	0.026
	9	0.236	0.026	0.024
	10	0.237	0.083	0.068
	11	0.157	0.221	0.148
	[12]	0.065	0.643	0.729
	13	0.000	0.018	0.005
	≥ 14	0.000	0.002	0.000

To help understand why our method is better, estimates of the precision of the various estimates of τ are given in Table 2. The columns labeled "s_0", "PSE" and "s_1" give the Monte Carlo means, variances and MSEs for s_0, PSE and s_1 respectively.

We see that when the percentage of active contrasts is not too large, the MSE of PSE is smaller than that of s_0, and the MSE of s_1 is in turn smaller than that of PSE. In the next section we give some theoretical support for this.

Table 2. Means, variances and MSEs of s_0, PSE and s_1 by 10,000 Monte Carlo Experiments with τ =1.

			0% active		
n	active		s_0	PSE	s_1
7	0	mean	1.054±0.004	0.759±0.004	0.890±0.003
		var	0.182±0.003	0.139±0.002	0.096±0.001
		MSE	0.185±0.003	0.198±0.002	0.108±0.001
15	0	mean	1.031±0.003	0.873±0.003	0.915±0.002
		var	0.089±0.001	0.083±0.001	0.047±0.000
		MSE	0.090±0.001	0.099±0.001	0.054±0.000
31	0	mean	1.022±0.002	0.941±0.002	0.930±0.002
		var	0.044±0.000	0.045±0.000	0.023±0.000
		MSE	0.044±0.000	0.049±0.000	0.028±0.000
			5% active		
n	active		s_0	PSE	s_1
15	1	mean	1.114±0.003	0.932±0.003	0.934±0.002
		var	0.104±0.002	0.101±0.001	0.052±0.000
		MSE	0.117±0.002	0.106±0.001	0.057±0.000
31	2	mean	1.106±0.002	0.944±0.002	0.941±0.002
		var	0.051±0.000	0.047±0.000	0.023±0.000
		MSE	0.062±0.000	0.051±0.000	0.027±0.000
			20% active		
n	active		s_0	PSE	s_1
15	3	mean	1.341±0.004	0.942±0.003	0.978±0.003
		var	0.139±0.002	0.113±0.002	0.085±0.002
		MSE	0.255±0.002	0.117±0.002	0.085±0.002
31	6	mean	1.324±0.003	0.944±0.002	0.955±0.002
		var	0.071±0.001	0.055±0.000	0.026±0.000
		MSE	0.176±0.001	0.059±0.000	0.028±0.000
			40% active		
n	active		s_0	PSE	s_1
7	3	mean	2.185±0.009	1.097±0.007	2.203±0.015
		var	0.732±0.012	0.500±0.008	2.200±0.015
		MSE	2.135±0.012	0.509±0.008	3.647±0.015
15	6	mean	2.051±0.006	1.005±0.005	1.468±0.010
		var	0.327±0.005	0.234±0.004	1.030±0.020
		MSE	1.431±0.005	0.234±0.004	1.250±0.020
31	12	mean	1.987±0.004	0.988±0.003	1.036±0.003
		var	0.154±0.002	0.085±0.001	0.108±0.004
		MSE	1.127±0.002	0.085±0.001	0.110±0.004

4. Theoretical Study

In this section we will give some theoretical justification for why the MSE of PSE is smaller than that of s_0 and the MSE of s_1 is smaller than that of PSE when the percentage of active contrasts is not too large.

Let n_a denote the number of active contrasts among the contrasts we consider. Theorems 4.1, 4.2 and 4.3 give the asymptotic distributions and the asymptotic mean square errors for s_0, PSE and s_1 respectively, as n increases. The proofs are omitted, they are given in Dong (1990).

Theorem 4.1. *Let μ be the median of the half normal distribution and suppose*

$$n_a = o(n^{1/2}) \text{ as } n \to \infty. \tag{1}$$

Then

$$\sqrt{n}[s_0 - 1.5\mu\tau] \xrightarrow{d} N\Big(0, (1/8)(1.5)^2\pi e^{\mu^2}\tau^2\Big)$$

and

$$\widehat{\text{MSE}}(s_0) = \tau^2\Big[(1/8n)(1.5)^2\pi e^{\mu^2} + (1.5\mu - 1)^2\Big] \tag{2}$$

$$\approx \tau^2\Big[1.393/n + (0.012)^2\Big]. \tag{3}$$

Now consider the PSE. Let

$$\widehat{\text{PSE}} = 1.5 \text{ median }_{|\hat\beta_j| \le (2.5)\tau} |\hat\beta_j|$$

$$\xi = F^{-1}\Big[(1/2)F(2.5)\Big]$$

where F is the cdf for the half normal distribution. The following theorem gives an estimate for the mean square error of the PSE.

Theorem 4.2. *If* (1) *holds for n_a, then*

$$\sqrt{n}\Big[\widehat{\text{PSE}} - (1.5)\xi\tau\Big] \xrightarrow{d} N\Big(0, (1/8)(1.5)^2\pi F(2.5)e^{\xi^2}\tau^2\Big)$$

and

$$\widehat{\text{MSE}}(\widehat{\text{PSE}}) = \tau^2\Big\{(1/8n)(1.5)^2\pi F(2.5)e^{\xi^2} + [(1.5)\xi - 1]^2\Big\} \tag{4}$$

$$\approx \tau^2\Big[1.358/n + (-0.0028)^2\Big]. \tag{5}$$

Now we derive an estimate for the mean square error of s_1. Let

$$\hat{s}_1^2(\lambda) = \lambda m^{-1} \sum_{|\hat\beta_j| \le (2.5)\tau} \hat\beta_j^2$$

where $m = \#\{j : |\hat{\beta}_j| < (2.5)\tau\}$ and λ is a coefficient to be determined later. Also let $m_0 = \int_{|x|<2.5} \phi(x)dx \approx 0.9876$, $m_2 = \int_{|x|<2.5} x^2\phi(x)dx \approx 0.8999$, and $m_4 = \int_{|x|<2.5} x^4\phi(x)dx \approx 2.1522$ where $\phi(x)$ is the pdf for the standard normal distribution. Then we have the following

Theorem 4.3. *Assume* (1) *holds for* n_a *and the means of the active contrasts are bounded. Then*

$$\sqrt{n}\left[\hat{s}_1(\lambda) - \lambda\tau m_2^{1/2} m_0^{-1/2}\right] \xrightarrow{d} N\left(0, \lambda^2\tau^2(m_0m_4 - m_2^2)/4m_2m_0^2\right)$$

and

$$\begin{aligned} \widehat{\text{MSE}}[\hat{s}_1(\lambda)] &= \tau^2\left[\frac{\lambda^2(m_0m_4 - m_2^2)}{4nm_2m_0^2} + (\lambda m_2^{1/2}m_0^{-1/2} - 1)^2\right] \\ &\approx \tau^2\left[\frac{(0.3748)\lambda^2}{n} + (0.9546\lambda - 1)^2\right]. \end{aligned}$$

If $\lambda = m_0^{1/2}m_2^{-1/2} \approx 1.048$, *and* $\hat{s}_1 = \hat{s}_1(1.048)$ *then*

$$\widehat{\text{MSE}}(\hat{s}_1) \approx \tau^2\left(0.4113/n\right). \tag{6}$$

Comparing (3), (5) and (6) we see that when the hypothesis of effect sparsity is true, the asymptotic mean square error of PSE is smaller than that of s_0, and the asymptotic mean square error of s_1 is smaller than that of PSE.

5. Examples

Four examples were given by Box and Meyer (1986). These examples are also analyzed in Loh (1992). All of them consist of 16 runs in unreplicated two-level designs. Example 1 is a 2^4 design from Daniel (1976). Example 2 is a 2^{9-5}_{III} design from Taguchi and Wu (1980). Example 3 is a 2^{8-4}_{IV} design from Box, Hunter and Hunter (1978). Example 4 is a 2^4 design from Davies (1954). The level is .05 for all examples and all methods. Normal probability plots for these examples are given in Figure 1.

Example 1. Using Box and Meyer's, or Loh's method, the conclusion is that there are 3 active contrasts. For Lenth's and our method, $s_0 = 1.5 \times .02 = .03$, PSE$= 1.5 \times .02 = .03$, SME$= 5.22 \times .03 = 0.157$, $s_1 = .026$ and $m = 12$. Using Lenth's method, the conclusion is that there are 2 active contrasts. Using our method, the conclusion is that there are 3 active contrasts.

Example 2. Box and Meyer's, Loh's and Lenth's methods all suggest that there are 2 active contrasts. For this example, $s_0 = 1.5 \times .3 = .45$, PSE$= 1.5 \times .15 =$

.225, SME= $5.22 \times .225 = 1.17$, $s_1 = .271$ and $m = 13$. Our method also suggests that there are 2 active contrasts.

Example 3. Using Box and Meyer's, or Loh's method, the conclusion is that there are 3 active contrasts. For Lenth's and our method, $s_0 = 1.5 \times .6 = .9$, PSE= .75, SME= 3.915, $s_1 = .593$ and $m = 12$. Using Lenth's method, the conclusion is that there are 2 active contrasts. Using our method, the conclusion is that there are 3 active contrasts.

Example 4. Box and Meyer were not so certain about this example. They claim that "it is impossible on the evidence of these data alone to draw reliable inferences about active and inert contrasts" and conclude that it is possible that as many as 5 of the 15 contrasts are active (see Box and Meyer (1986)). Using Lenth's or Loh's method the conclusion is that there are no active contrasts (see Lenth (1989), Loh (1992)). Using our method, the conclusion is also that there are no active contrasts. For this example, $s_0 =$ PSE $= .114$ (nothing is excluded in the 2nd step), SME= $5.22 \times .114 = 0.595$, $s_1 = .132$ and $m = 15$.

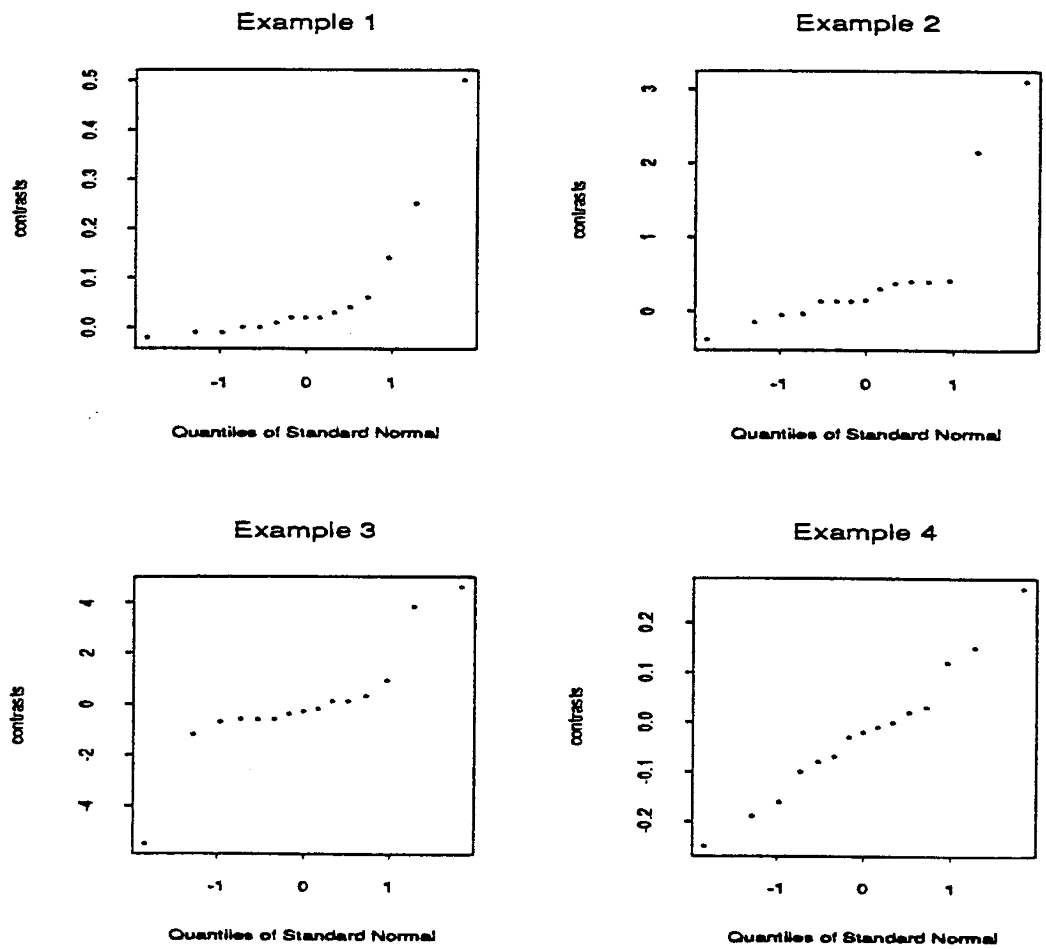

Figure 1. Normal plots for Examples 1-4

6. Discussion

The performance of both Lenth's and the proposed method depend on the success of the preliminary estimate of the standard deviation of the contrasts. Therefore the size of the active contrasts as well as their number will have an effect on the performance of the methods. In the simulation results in Section 3, the size of the active contrasts begins with 5 standard deviations and then increases by 1 for each additional active contrast. In some applications, the size of the active contrasts might be smaller. Additional simulations (not included here) show that if there are a couple of active effects with size about 3 standard deviations, both the proposed and Lenth's method are not good but neither dominates the other in detecting active contrasts.

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