Center for Quality and Productivity Improvement
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Report No. 22

FURTHER DETAILS OF AN ANALYSIS FOR UNREPLICATED FRACTIONAL FACTORIALS

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February 1987

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PRACTICAL SIGNIFICANCE

Investigators often face the challenge of identifying those few important factors--ones with the greatest impact on the design or manufacture of a product--from among many possibilities. When they can be reasonably certain there are indeed only a few important factors, investigators can use a type of designed experiment called an unreplicated fractional factorial to quickly screen the field of candidates. A formal "Bayesian-type" analysis of unreplicated fractional factorials, introduced by Box and Meyer (CQPI Report 2), makes explicit use of this factor sparsity principle, and is highly effective when used in conjunction with the normal probability plots of Daniel (1959, 1976). This report describes further implications and statistical details of Box and Meyer's approach, including computation of confidence intervals for the estimated levels of the important factors, and applications to other types of structured designs. Development of these details will allow this new method to become a general purpose tool in the use of designed experiments to improve quality.

Key Words: Unreplicated fractional factorials; Bayesian analysis; factor sparsity.

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FURTHER DETAILS OF AN ANALYSIS FOR UNREPLICATED FRACTIONAL FACTORIALS

R. Daniel Meyer*

1. Introduction

Unreplicated fractional factorials are useful experimental designs at the screening stage of an investigation, provided a condition of factor sparsity (Box & Meyer, 1986a, b) can be assumed, that is, if only a small proportion of the factors to be screened are expected to have large effects relative to noise. The Bayesian analysis of unreplicated fractional factorials introduced by Box and Meyer (1986b) makes explicit use of the factor sparsity principle and is efficacious when used in conjunction with the normal probability plots of Daniel (1959, 1976). The purpose of this article is to describe further details and implications of Box and Meyer's approach to identifying active contrasts in factorial experiments.

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2. Review of the Analysis for Unreplicated Designs

A typical fractional factorial design consists of n runs, and $n - 1$ contrasts $T_1, \ldots, T_{n-1}$ are computed from the orthogonal design array. It is assumed the T's have been standardized to have the same unknown sampling variance σ^2. The hypothesis of factor sparsity (or effect sparsity) is modeled by supposing that an effect τ_i, the expected value of T_i, is active with probability α. If an effect τ_i is not active, it is identically zero; if it is active, it has a $N(0, \sigma_\tau^2)$ (prior) distribution. Thus each T_i is the sum of an effect τ_i, which is nonzero with probability α, and an independent noise term e_i, where the e_i are i.i.d. from a $N(0, \sigma^2)$ distribution. Setting $k^2 = (\sigma^2 + \sigma_\tau^2)/\sigma^2$ and integrating over $\underset{\sim}{\tau}$, $T_1, \ldots, T_{n-1}$ are i.i.d. from the scale-contaminated normal distribution denoted by $(1 - \alpha)N(0, \sigma^2) + \alpha N(0, k^2\sigma^2)$. Let $a_{(r)}$ be the event that a particular set of r effects is active, with $\underset{\sim}{T}_{(r)}$ the vector of orthogonal contrasts corresponding to $a_{(r)}$. Then, with $p(\log \sigma)$ locally uniform, the posterior probability that $\underset{\sim}{T}_{(r)}$ comprises the active contrasts is

$$(2.1) \qquad p(a_{(r)} | \underset{\sim}{T}) \propto \left[\frac{\alpha k^{-1}}{1 - \alpha}\right]^r \left[1 - \varphi f_{(r)}\right]^{-(n-1)/2}$$

where $\varphi = 1 - 1/k^2 = \sigma_\tau^2/(\sigma^2 + \sigma_\tau^2)$, and $f_{(r)} = \underset{\sim}{T}'_{(r)}\underset{\sim}{T}_{(r)}/\underset{\sim}{T}'\underset{\sim}{T}$ is the fraction of the sum of squares associated with $\underset{\sim}{T}_{(r)}$. The constant of proportionality is that which makes the posterior probabilities of all possible $a_{(r)}$ sum to unity. The marginal probability p_i that an effect τ_i is active is

$$(2.2) \qquad p_i = P[\tau_i \text{ active} | \underset{\sim}{T}] = \sum_{(r):i \text{ active}} p(a_{(r)} | \underset{\sim}{T}) \ .$$

The sampling distribution of $\underset{\sim}{T}$ given $\{\underset{\sim}{\tau}, \sigma\}$ is

$$(2.3) \qquad p(\underset{\sim}{T} | \underset{\sim}{\tau}, \sigma) \propto \sigma^{-n} \prod_{i=0}^{n-1} \exp\left\{\frac{-(T_i - \tau_i)^2}{2\sigma^2}\right\} \ .$$

Thus each contrast T_i is independent and normally distributed. The prior distribution of each expected contrast τ_i can be written

$$(2.4)\qquad p(\tau_i|\sigma) = \alpha(2\pi)^{-1/2}(k^2 - 1)^{-1/2}\sigma^{-1}\exp\{-\frac{\tau_i^2}{2(k^2-1)\sigma^2}\} + (1-\alpha)I[\tau_i = 0]$$

with

$$(2.5)\qquad I[\tau_i = 0] = \begin{cases} 0 & \text{if } \tau_i \neq 0 \\ 1 & \text{if } \tau_i = 0 \end{cases} .$$

The prior distributions of $\log(\sigma)$ and the overall mean τ_0 are uniform in the region where the likelihood is appreciable, and are approximated by taking $p(\sigma,\tau_0) \propto 1/\sigma$. Therefore the joint posterior distribution of $\{\tau,\sigma\}$ is

$$(2.6)\qquad p(\underset{\sim}{\tau},\sigma|\underset{\sim}{T}) \propto \sigma^{-n-1}\exp\{\frac{-(T_0-\tau_0)^2}{2\sigma^2}\} \times \prod_{i=1}^{n-1}\Big[(1-\alpha)\exp\{-\frac{T_i^2}{2\sigma^2}\} + \frac{\alpha}{(2\pi(k^2-1))^{1/2}\sigma}\exp\{\frac{-1}{2\sigma^2}\Big[(T_i-\tau_i)^2 + \frac{\tau_i^2}{k^2-1}\Big]\}\Big] .$$

Integrating $\underset{\sim}{\tau}$ out of this expression gives the marginal posterior distribution of σ,

$$(2.7)\qquad p(\sigma|\underset{\sim}{T}) \propto \sigma^{-n}\prod_{i=1}^{n-1}\Big[(1-\alpha)\exp\{-\frac{T_i^2}{2\sigma^2}\} + \frac{\alpha}{k}\exp\{-\frac{T_i^2}{2k^2\sigma^2}\}\Big] .$$

The posterior probability $p_{i|\sigma}$ that τ_i is active, conditional on σ, is, by direct application of Bayes' theorem,

$$(2.8)\qquad p_{i|\sigma} = \frac{\alpha p(\underset{\sim}{T}|\sigma,\tau_i \text{ active})}{\alpha p(\underset{\sim}{T}|\sigma,\tau_i \text{ active}) + (1-\alpha)p(\underset{\sim}{T}|\sigma,\tau_i \text{ not active})}$$

$$= \frac{\frac{\alpha}{k}\exp\{-\frac{T_i^2}{2k^2\sigma^2}\}}{\frac{\alpha}{k}\exp\{-\frac{T_i^2}{2k^2\sigma^2}\} + (1-\alpha)\exp\{-\frac{T_i^2}{2\sigma^2}\}} .$$

Thus, conditional on σ, the posterior probability that τ_i is active depends only on the data through the observed contrast T_i. The unconditional probability p_i can be computed from the simple expressions for $p_{i|\sigma}$ and $p(\sigma|\underset{\sim}{T})$ by

$$(2.9) \qquad p_i = \int_0^\infty p_{i|\sigma}\, p(\sigma|\underset{\sim}{T})d\sigma \; .$$

This integral can then be computed to the desired degree of accuracy using numerical integration methods.

2.1 Parameters α and k

The parameters α and k must be specified to compute the posterior probabilities described above. Box and Meyer (1986b) examined the results of several published examples of unreplicated fractional factorials, for each example estimating α as the proportion of effects declared active and k^2 as the ratio of the mean squared active contrast over the mean squared inert contrast. This study showed a reasonable range for α to be 0.1 to 0.3, with a mean value of 0.2, and a range for k of 5 to 15 with a mean of 10. Sensitivity of the posterior probabilities to the particular choice of α and k can be assessed by repeating the calculations for various α and k within and/or beyond the above-described ranges.

2.2 Examples

Box and Meyer (1986b) illustrated the above analysis on four examples. For brevity, their Examples III and IV will be presented here as Examples 1 and 2 and used for illustration for the remainder of the article. Table 1a, b shows the design matrix, observations and observed contrasts for each example. The posterior probabilities $\{p_i\}$ calculated with $\alpha = 0.2$ and $k = 10$ are plotted as vertical lines in Figure 1a, b. In each figure, boxes are drawn to indicate the range of posterior probabilities over all possible combinations

Table 1a. Design matrix, observations, and observed contrasts for Example 1, a 2^{8-4} fractional experiment, from Box, Hunter and Hunter (1978).

	Factors								
Run	1	2	3	4	5	6	7	8	y
1	-	-	-	+	+	+	-	+	14.0
2	+	-	-	-	-	+	+	+	16.8
3	-	+	-	-	+	-	+	+	15.0
4	+	+	-	+	-	-	-	+	15.4
5	-	-	+	+	-	-	+	+	27.6
6	+	-	+	-	+	-	-	+	24.0
7	-	+	+	-	-	+	-	+	27.4
8	+	+	+	+	+	+	+	+	22.6
9	+	+	+	-	-	-	+	-	22.3
10	-	+	+	+	+	-	-	-	17.1
11	+	-	+	+	-	+	-	-	21.5
12	-	-	+	-	+	+	+	-	17.5
13	+	+	-	-	+	+	-	-	15.9
14	-	+	-	+	-	+	+	-	21.9
15	+	-	-	+	+	-	+	-	16.7
16	-	-	-	-	-	-	-	-	20.3

Column(effect)	Observed contrast	Column(effect)	Observed contrast
0(mean)	19.75	8(8)	0.60
1(1)	-0.35	9(12+37+48+56)	-0.30
2(2)	-0.05	10(13+27+46+58)	0.45
3(3)	2.75	11(14+28+36+57)	-0.20
4(4)	-0.15	12(15+26+38+47)	2.30
5(5)	-1.90	13(16+25+34+78)	-0.15
6(6)	-0.05	14(17+23+68+45)	-0.10
7(7)	0.30	15(18+24+35+67)	-0.30

of α = 0.1, 0.2, 0.3 and k = 5, 10, 15. For Example 1, there are three contrasts which receive posterior probabilities close to one and are plausibly identified as active, and conclusions are insensitive to choice of α and k. For Example 2, the situation is less clear, the choice of α and k having a much greater effect on the posterior probabilities. For a detailed discussion of implications for this example, see Box and Meyer (1986b).

Table 1b. Design matrix, observations, and observed contrasts for Example 2, a full 2^4 factorial experiment, from Davies, ed. (1954).

	Factors				
Run	A	B	C	D	y(yield)
1	-	-	-	-	6.08
2	+	-	-	-	6.04
3	-	+	-	-	6.53
4	+	+	-	-	6.43
5	-	-	+	-	6.31
6	+	-	+	-	6.09
7	-	+	+	-	6.12
8	+	+	+	-	6.36
9	-	-	-	+	6.79
10	+	-	-	+	6.68
11	-	+	-	+	6.73
12	+	+	-	+	6.08
13	-	-	+	+	6.77
14	+	-	+	+	6.38
15	-	+	+	+	6.49
16	+	+	+	+	6.23

Column(effect)	Observed contrast	Column(effect)	Observed contrast
0(mean)	6.38	8(D)	.137
1(A)	-.096	9(AD)	-.081
2(B)	-.011	10(BD)	-.126
3(AB)	-.001	11(ABD)	-.051
4(C)	-.038	12(CD)	-.013
5(AC)	.017	13(ACD)	-.003
6(BC)	-.033	14(BCD)	.062
7(ABC)	-.074	15(ABCD)	.009

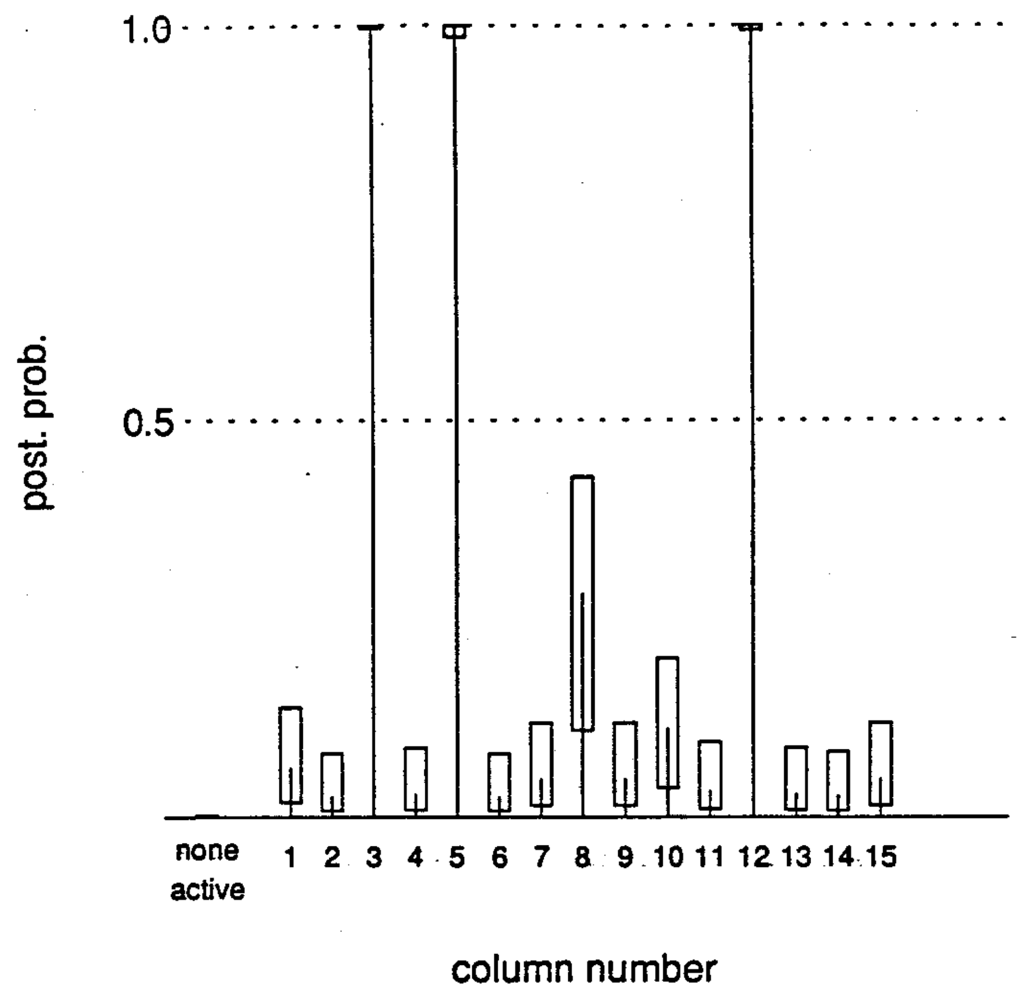

Figure 1a. Posterior probabilities $\{p_i\}$ that columns are active, Example 1. Solid vertical lines are the values for $\alpha = 0.2$ and $k = 10$; boxes indicate the range of values over $\alpha = 0.1, 0.2, 0.3$ and $k = 5, 10, 15$.

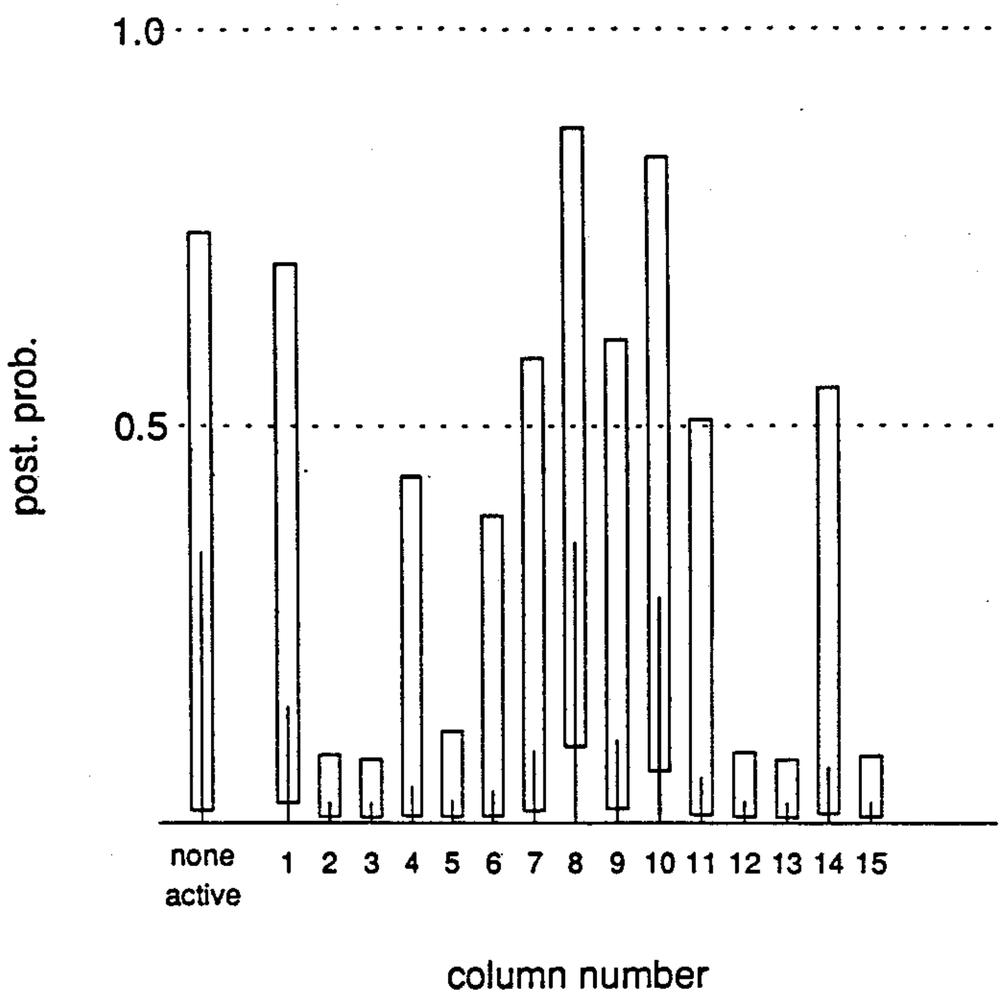

Figure 1b. Posterior probabilities $\{p_i\}$ that columns are active, Example 2. Solid vertical lines are the values for $\alpha = 0.2$ and $k = 10$; boxes indicate the range of values over $\alpha = 0.1, 0.2, 0.3$ and $k = 5, 10, 15$.

3. Further Details of the Analysis

3.1 Derivatives of the Posterior Probabilities

As illustrated by Example 2, there will be occasions when the probabilities $\{p_i\}$ will be sensitive to the choice of α and k. The partial derivatives of p_i with respect to α and k can be computed to measure the extent to which the probabilities are sensitive to the particular choice of these parameters.

First define the following quantities:

(3.1) $$p_{ij} = P[\tau_i, \tau_j \text{ active} | \underset{\sim}{T}] = \begin{cases} \int_0^\infty p_{i|\sigma}\, p_{j|\sigma}\, p(\sigma|\underset{\sim}{T})d\sigma & (i \neq j) \\ p_i & (i = j) \end{cases}$$

(3.2) $$Q_j = [\frac{T_j^2}{\sigma^2} - k^2] \; .$$

Then partial derivatives of p_i with respect to α and k are given by

(3.3) $$\frac{\partial p_i}{\partial \alpha} = \frac{1}{\alpha(1-\alpha)} [\sum_{j=1}^{n-1} (p_{ij} - p_i p_j)]$$

(3.4) $$\frac{\partial p_i}{\partial k} = \frac{1}{k^3} [\int_0^\infty (p_{i|\sigma} - p_i)(\sum_{j=1}^{n-1} Q_j p_{j|\sigma}) p(\sigma|\underset{\sim}{T}) d\sigma$$

$$+ \int_0^\infty p_{i|\sigma}(1 - p_{i|\sigma}) Q_i p(\sigma|\underset{\sim}{T}) d\sigma] \; .$$

(Recall that the quantities p_i, p_{ij}, $p_{i|\sigma}$, and $p(\sigma|\underset{\sim}{T})$ in the above expressions also depend on α and k.)

The use of derivatives to measure sensitivity relies somewhat on a low degree of curvature in p_i with respect to α and k. In Figure 2 the posterior probabilities for Examples 1 and 2 are plotted first against α for fixed $k = 10$, and then against k for fixed $\alpha = 0.2$. In all figures the relative curvature is not so extreme that the partial derivatives would not give a good measure of change.

The derivatives of the $\{p_i\}$ with respect to α and k for Examples 1 and 2 are given in Table 2, with $\alpha = 0.2$ and $k = 10$. The derivative with respect to k in the table is multiplied by 50, so that the two derivatives are roughly comparable. The values in Table 2 reflect the sensitivity illustrated by the boxes in Figure 1. For Example 1, in which contrast column 8 was most sensitive to changing α and k, the partial derivative with respect to α is 1.46, and with respect to k is -.05 (scaled by 50). This indicates much higher sensitivity to α than to k, and this is verified in Figure 2a, b, where the plot of p_8 versus k is very flat, but the plot of p_8 versus α slopes upward significantly. The remaining columns for this example were relatively insensitive to choice of α and k, and the small partial derivatives in Table 2 agree with this assessment. For Example 2, there were seven columns showing extreme sensitivity to choice of α and k in Figure 1b, corresponding to those columns in Table 2 for which the partial with respect to α is greater than one. The derivative with respect to k for columns 8 and 10 is also large (scaled by 50), indicating that the posterior probabilities for these columns are also sensitive to choice of k. This is verified by examination of Figure 2d, where the plots of p_i versus k show probabilities p_8 and p_{10} are most sensitive to change in k.

The partial derivatives are intended to be aids in interpreting the posterior probabilities by gauging local sensitivity to choice of α and k. Values greater than one tend to indicate fairly acute sensitivity, while values far below one indicate relative insensitivity. When large values occur in practice, they are a sign to investigate the dependence of the posterior probabilities on α and k more thoroughly by repeating the computations for

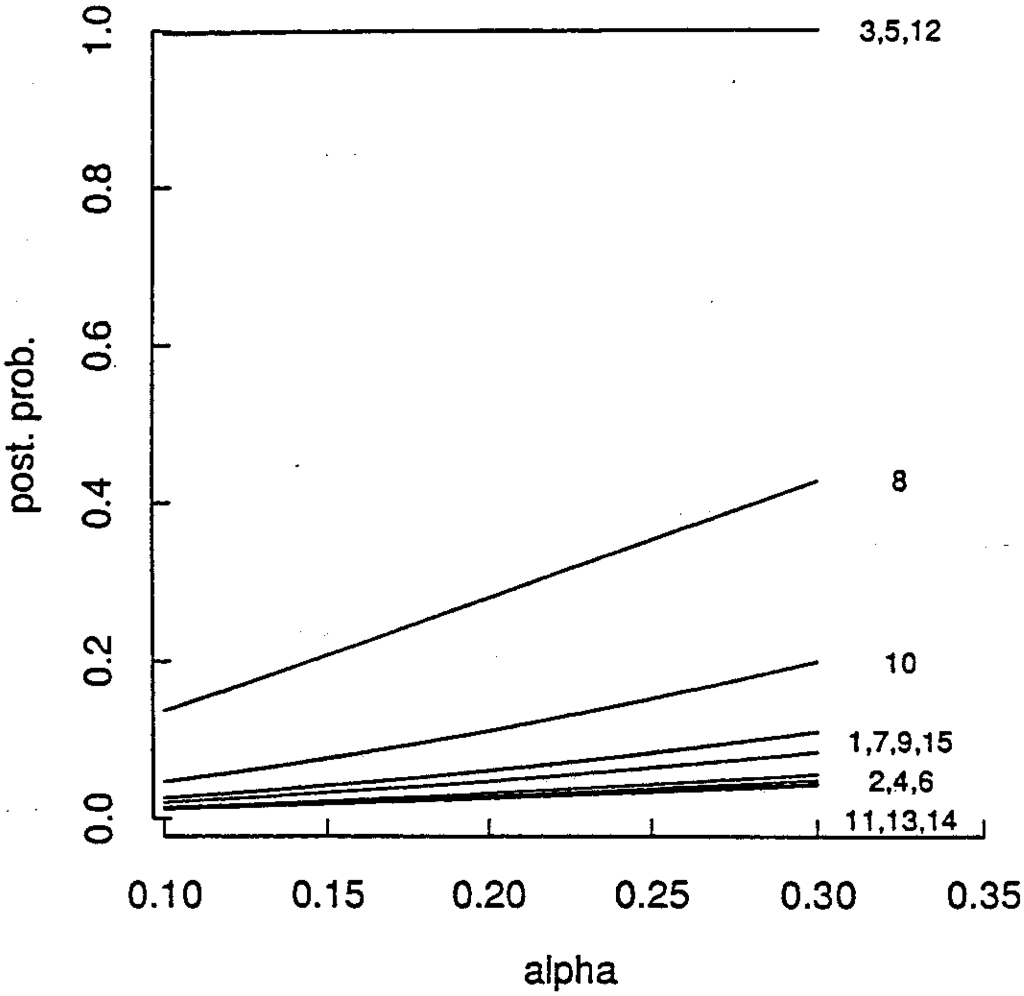

Figure 2a. Continuous plot of posterior probabilities $\{p_i\}$ versus α, k fixed at 10, Example 1. Curves are labeled on the right by their column numbers.

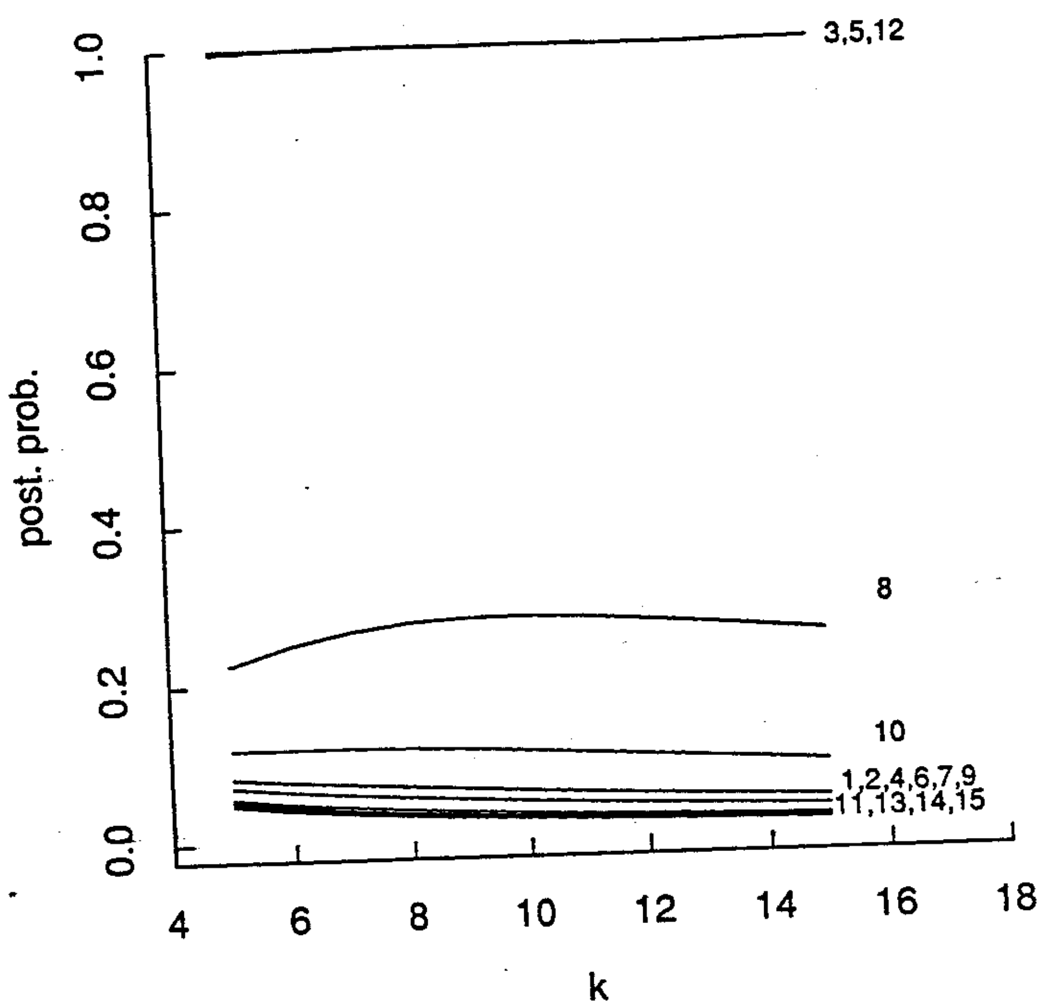

Figure 2b. Continuous plot of posterior probabilities $\{p_i\}$ versus k, α fixed at 0.2, Example 1. Curves are labeled on the right by their column numbers.

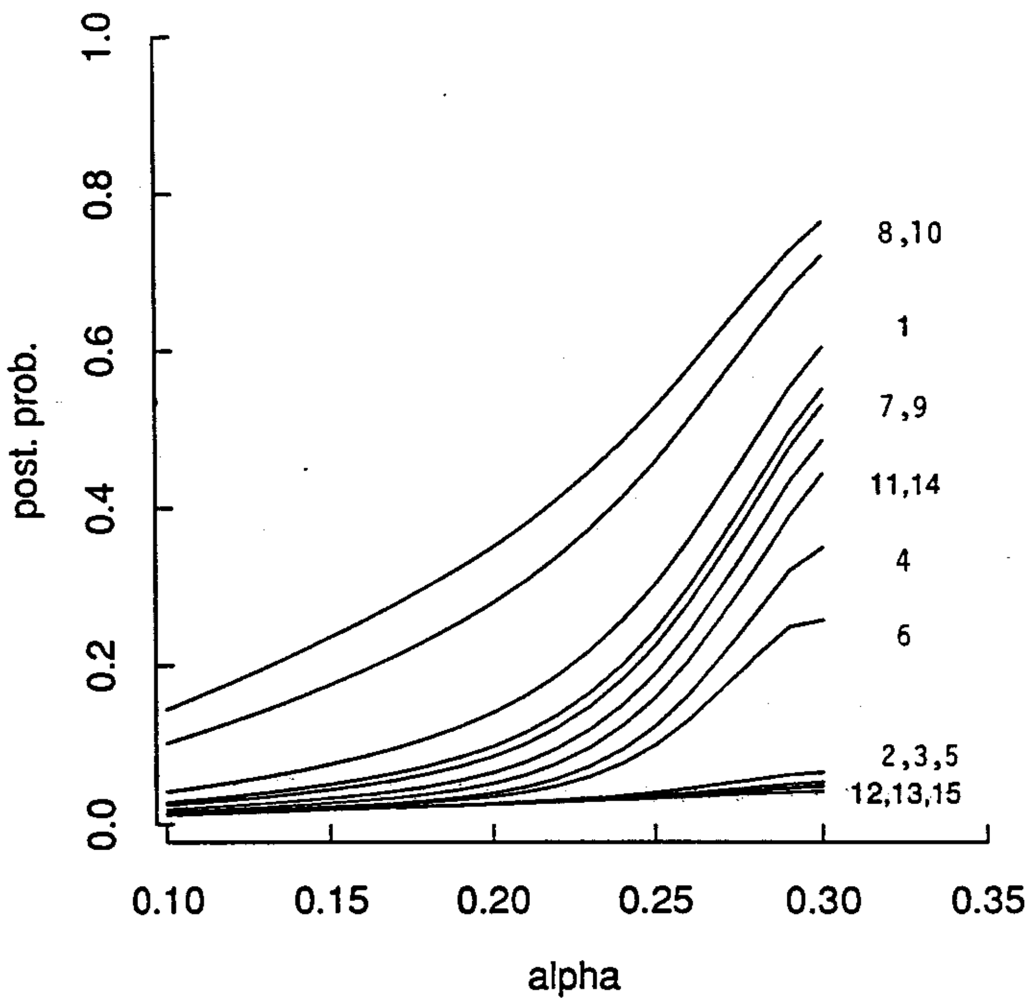

Figure 2c. Continuous plot of posterior probabilities $\{p_i\}$ versus α, k fixed at 10, Example 2. Curves are labeled on the right by their column numbers.

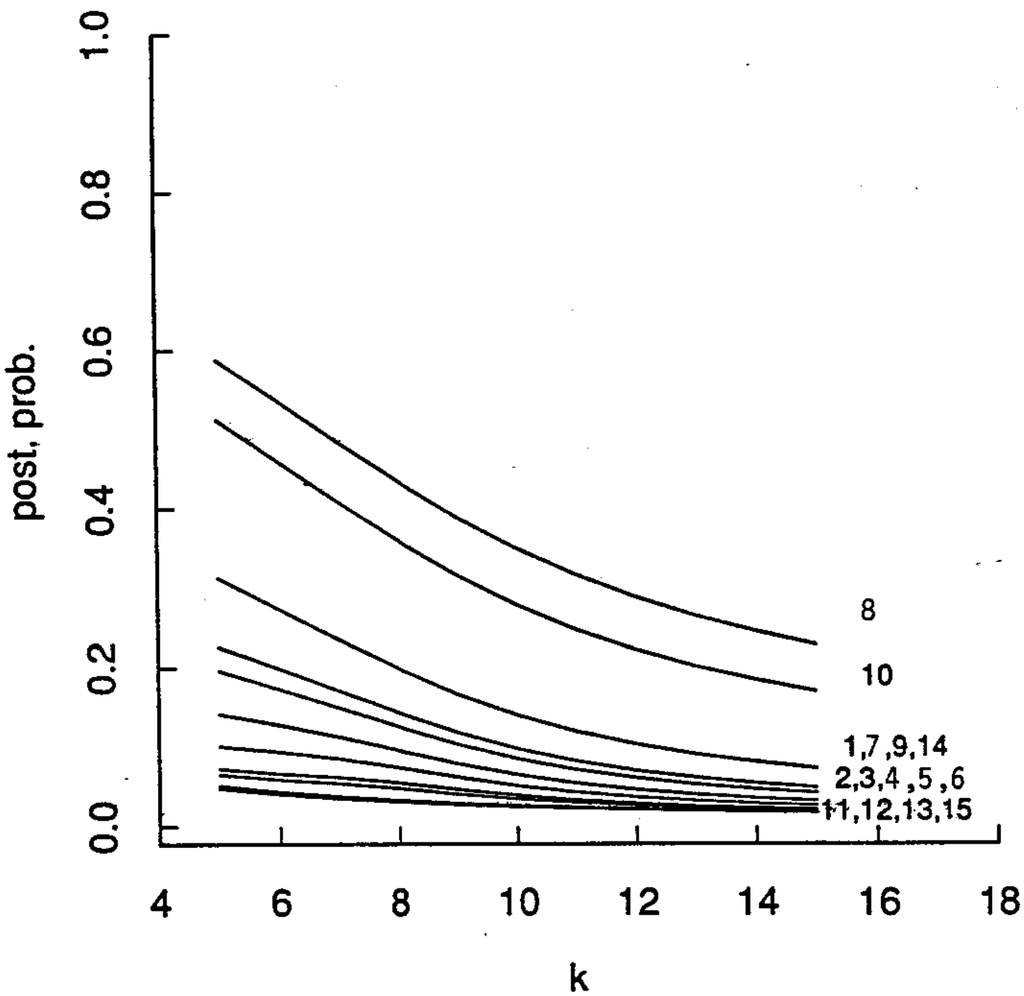

Figure 2d. Continuous plot of posterior probabilities $\{p_i\}$ versus k, α fixed at 0.2, Example 2. Curves are labeled on the right by their column numbers.

Table 2. Posterior probabilities and derivatives with respect to α and k, Examples 1 and 2, $\alpha = 0.2$, $k = 10$.

Example 1

Column	Observed contrast	Posterior prob.	$dp_i/d\alpha$	$50(dp_i/dk)$
1	-0.35	0.0608	0.4163	-0.0358
2	-0.05	0.0248	0.1517	-0.0004
3	2.75	0.9999	0.0025	-0.0002
4	-0.15	0.0286	0.1784	-0.0003
5	-1.90	0.9988	0.0124	0.0038
6	-0.05	0.0248	0.1517	-0.0004
7	0.30	0.0473	0.3156	-0.0556
8	0.60	0.2804	1.4628	-0.0500
9	-0.30	0.0473	0.3156	-0.0556
10	0.45	0.1115	0.7605	-0.1771
11	-0.20	0.0325	0.2062	-0.0002
12	2.30	0.9997	0.0050	0.0003
13	-0.15	0.0286	0.1784	-0.0003
14	-0.10	0.0262	0.1611	-0.0004
15	-0.30	0.0473	0.3156	-0.0556

Example 2

Column	Observed Contrast	Posterior prob.	$dp_i/d\alpha$	$50(dp_i/dk)$
1	-0.096	0.1436	2.0662	-0.4728
2	-0.011	0.0252	0.1702	-0.1145
3	-0.001	0.0244	0.1489	-0.1137
4	0.038	0.0438	0.8258	-0.0816
5	-0.017	0.0268	0.2286	-0.1131
6	0.033	0.0393	0.6927	-0.0863
7	0.075	0.0897	1.5750	-0.1943
8	0.137	0.3466	2.8144	-1.2308
9	-0.082	0.1043	1.7305	-0.2635
10	-0.126	0.2797	2.7020	-1.0652
11	-0.051	0.0561	1.1038	-0.0878
12	-0.013	0.0256	0.1827	-0.1145
13	-0.003	0.0244	0.1500	-0.1138
14	0.062	0.0690	1.3128	-0.1171
15	0.010	0.0250	0.1656	-0.1145

different combinations of these parameters. In the absence of external information about α and k, results which are sensitive to these parameters would usually indicate the need to perform additional runs (see Box and Meyer, (1986b)).

3.2 Posterior Distribution of τ

In an appendix to Box and Meyer (1986b), a brief description of the posterior distribution of an effect τ_i was given. In this section we will expand on this topic.

To review the previous derivation of the posterior distribution of $\underset{\sim}{\tau}_{(r)}$, write

(3.5) $$p(\underset{\sim}{T}|a_{(r)},\underset{\sim}{\tau}_{(r)},\sigma) \propto \sigma^{-(n-1)}\exp\{\frac{-1}{2\sigma^2}[(\underset{\sim}{T}_{(r)}-\underset{\sim}{\tau}_{(r)})'(\underset{\sim}{T}_{(r)}-\underset{\sim}{\tau}_{(r)})+\underset{\sim}{T}'\underset{\sim}{T}-\underset{\sim}{T}'_{(r)}\underset{\sim}{T}_{(r)}]\},$$

(3.6) $$p(\underset{\sim}{\tau}_{(r)}|a_{(r)},\sigma) \propto (k^2-1)^{-r/2}\,\sigma^{-r}\exp\{\frac{-1}{2\sigma^2}(\frac{1}{k^2-1})\,\underset{\sim}{\tau}_{(r)}'\underset{\sim}{\tau}_{(r)}\},$$

(3.7) $$p(\sigma) \propto \frac{1}{\sigma}.$$

The joint conditional posterior distribution of $\underset{\sim}{\tau}_{(r)}$ given $a_{(r)}$ is computed from

(3.8) $$p(\underset{\sim}{\tau}_{(r)}|a_{(r)},\underset{\sim}{T}) \propto \int_0^\infty p(\underset{\sim}{T}|a_{(r)},\underset{\sim}{\tau}_{(r)},\sigma)\;p(\underset{\sim}{\tau}_{(r)}|a_{(r)},\sigma)\;p(\sigma)d\sigma$$

giving

(3.9) $$p(\underset{\sim}{\tau}_{(r)}|a_{(r)},\underset{\sim}{T}) \propto \Big[(\underset{\sim}{T}_{(r)}-\underset{\sim}{\tau}_{(r)})'(\underset{\sim}{T}_{(r)}-\underset{\sim}{\tau}_{(r)}) + \underset{\sim}{T}'\underset{\sim}{T}-\underset{\sim}{T}'_{(r)}\underset{\sim}{T}_{(r)}+\frac{1}{k^2-1}\underset{\sim}{\tau}'_{(r)}\underset{\sim}{\tau}_{(r)}\Big].$$

Rearranging gives (Box and Tiao, (1973))

$$(3.10) \qquad p(\underset{\sim}{\tau}_{(r)}|a_{(r)},\underset{\sim}{T}) \propto \left[1 + \frac{(\underset{\sim}{\tau}_{(r)} - \varphi\underset{\sim}{T}_{(r)})'(\underset{\sim}{\tau}_{(r)} - \varphi\underset{\sim}{T}_{(r)})}{\varphi(\underset{\sim}{T}'\underset{\sim}{T} - \varphi\underset{\sim}{T}'_{(r)}\underset{\sim}{T}_{(r)})}\right]^{-(n-1+r)/2}$$

which implies the posterior distribution of $\underset{\sim}{\tau}_{(r)}$, given $a_{(r)}$, is multivariate t with $n - 1$ degrees of freedom, mean vector $\varphi\underset{\sim}{T}_{(r)}$, and dispersion matrix $\varphi(\underset{\sim}{T}'\underset{\sim}{T} - \varphi\underset{\sim}{T}'_{(r)}\underset{\sim}{T}_{(r)})\underset{\sim}{I}/(n - 1)$. (Recall $\varphi = 1 - 1/k^2$.) In particular, if $s^2_{(r)} = \varphi(\underset{\sim}{T}'\underset{\sim}{T} - \varphi\underset{\sim}{T}'_{(r)}\underset{\sim}{T}_{(r)})/(n - 1)$, then under $a_{(r)}$ each of

$$(3.11) \qquad t = \frac{\tau_i - \varphi T_i}{s_{(r)}}$$

is distributed t_{n-1} for $i \in (r)$. The complete posterior distribution of τ_i is given by summing over all events $a_{(r)}$,

$$(3.12) \qquad p(\tau_i|\underset{\sim}{T}) = (1 - p_i)I_{[\tau_i=0]} + \sum_{(r):i \text{ active}} p(\tau_i|\underset{\sim}{T},a_{(r)})p(a_{(r)}|\underset{\sim}{T}) ,$$

a weighted sum of 2^{n-2} t densities together with mass $1 - p_i$ at zero.

Bayesian intervals for the supposed active τ_i would be provided by the conditional posterior distribution of τ_i given it is active,

$$(3.13) \qquad p(\tau_i|\underset{\sim}{T},\tau_i \text{active}) = \frac{1}{p_i} \sum_{(r):\text{active}} p(\tau_i|\underset{\sim}{T},a_{(r)})p(a_{(r)}|\underset{\sim}{T}) ,$$

the second term of (3.12) normalized to integrate to unity. In general, calculation of exact Bayesian intervals would entail evaluation of 2^{n-2} t densities at every function evaluation of a numerical integration routine. For practical application a more convenient approximation is called for. It will be shown that in many cases the conditional posterior distribution of an expected contrast τ_i, given it is active, can be well-approximated by a single t distribution with $n - 1$ degrees of freedom, mean φT_i, and scale factor

$$(3.14) \qquad \hat{s}^2_i = \frac{1}{p_i} \sum_{(r):\text{active}} s^2_{(r)}p(a_{(r)}|\underset{\sim}{T}) .$$

For illustration, the "exact" conditional posterior density of τ_3 in Example 1 was computed by evaluating the weighted sum of t densities only over those $a_{(r)}$ with posterior probability larger than 0.0001, with $\alpha = 0.2$, $k = 10$. This accounted for over 99% of the total probability. The approximate density was computed as a single t density with scale factor $\hat{s}^2$ defined above. The exact density is plotted as a solid curve in Figure 3a, and the approximate density is plotted as a dashed curve. For this example approximation by a single t density is very good.

This same procedure was followed for Example 2 and contrast column 8, with $\alpha = 0.3$ and $k = 5$ chosen to give a high value of $P_8 = .85$. The exact and approximate densities are shown in Figure 3b. The approximation for this example is much less accurate.

The weighted sum of t densities can be written

$$(3.15) \qquad p(\tau_i | \underset{\sim}{T}, \tau_i \text{active}) = \sum_{(r):i \text{ active}} t(\tau_i | s^2_{(r)}) w_{(r)} ,$$

where the weight $w_{(r)} = p(a_{(r)} | \underset{\sim}{T})/p_i$, and $t(\tau | s^2_{(r)})$ is the t density with scale parameter $s^2_{(r)}$. The approximate density is just

$$(3.16) \qquad p(\tau_i | \underset{\sim}{T}, \tau_i \text{active}) \approx t(\tau_i | \hat{s}^2_i) .$$

The curvature of $t(\tau | s^2)$ with respect to s^2, and the variation of $s^2_{(r)}$ over (r) determine the accuracy of the approximation.

The approximate density is the first term in a Taylor series expansion of the true density, as a function of s^2, about the point $\hat{s}^2_i$. Writing down the first three terms of this expansion, we have

$$(3.17) \qquad p(\tau_i | \underset{\sim}{T}, \tau_i \text{active}) \approx t(\tau_i | \hat{s}^2_i) + \sum_{(r):i \text{ active}} w_{(r)} (s^2_{(r)} - \hat{s}^2_i) t'(\tau_i | \hat{s}^2_i)$$

$$+ \sum_{(r):i \text{ active}} w_{(r)} (s^2_{(r)} - \hat{s}^2_i)^2 \frac{t''(\tau_i | \hat{s}^2_i)}{2} ,$$

where t' and t'' are the first and second derivatives of $t(\tau | s^2)$ with respect to s^2. The second term in (3.17) is identically zero, by the

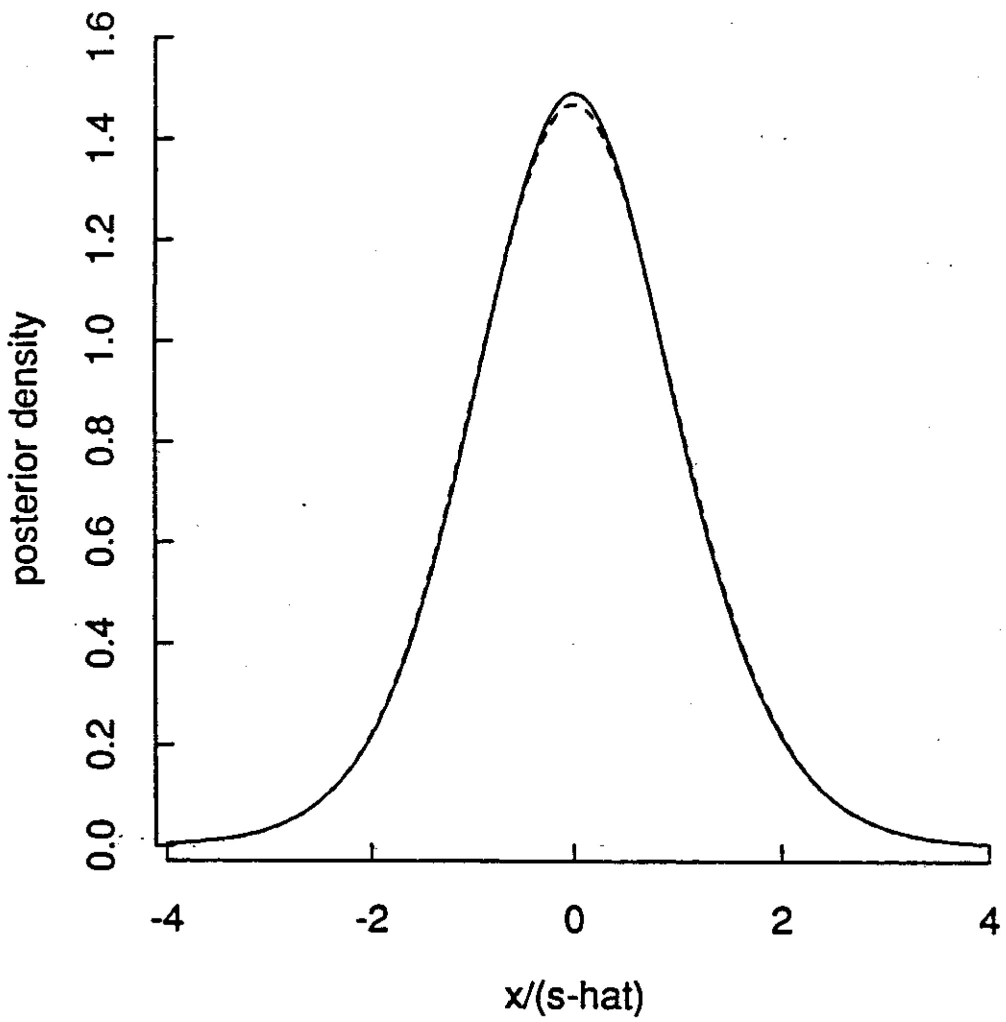

Figure 3a. Exact and approximate posterior densities for largest expected contrast, Example 1, $\alpha = 0.2$, $k = 10$. The exact (solid curve) is obtained by direct calculation and the approximate (dashed curve) is a single t density.

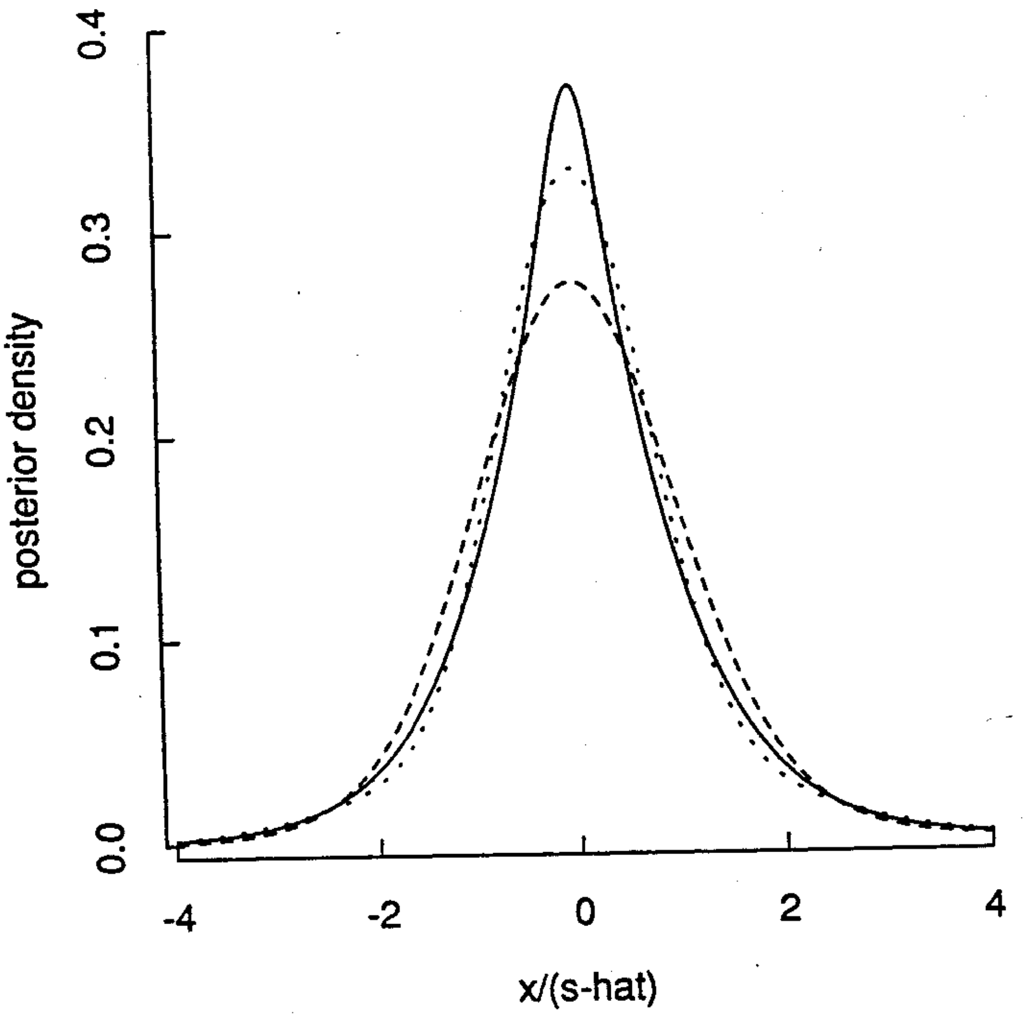

Figure 3b. Exact and approximate posterior densities for largest expected contrast, Example 2, $\alpha = 0.3$, $k = 5$. The exact (solid curve) is obtained by direct calculation, the approximate (dashed curve) is a single t density, and the corrected approximate (dotted curve) is a t density plus a quadratic term from the Taylor's series expansion.

definition of $\hat{s}_i^2$. Changing variables to $\tau_i/\hat{s}_i$, the third term can be rewritten to give

(3.18) $$p(\tau_i/\hat{s}_i|\underset{\sim}{T},\tau_i \text{ active}) = t(\tau_i/\hat{s}_i|1) + CV_i \cdot \frac{1}{2} \cdot t''(\tau_i/\hat{s}_i|1)$$

where the statistic

(3.19) $$CV_i = \frac{\sum_{(r):i \text{ active}} w_{(r)}(s_{(r)}^2 - \hat{s}_i^2)^2}{(\hat{s}_i^2)^2},$$

$t(\tau|1)$ and $t''(\tau|1)$ are the functions t and t'' each with scale parameter set equal to one. The quadratic term is now written as the product of the statistic CV_i which measures the relative variation of $s_{(r)}^2$ in the weighted sum, and the standardized second derivative $t''(\tau_i/\hat{s}|1)$ which measures the nonlinearity of the t density with respect to s^2. Note that there will be a different value of CV_i for each of the expected contrasts τ_i.

The closeness of the t approximation may now be checked conveniently according to the size of CV_i, with larger values indicating a less accurate approximation. For Example 1 with $\alpha = 0.2$ and $k = 10$, $CV_3 = .053$, and the closeness of the curves in Figure 3a indicates this is a low value of CV. For Example 2 with $\alpha = 0.3$ and $k = 5$, $CV_8 = .55$, and a value of this size indicates a less accurate approximation as shown in Figure 3b.

Whereas a small value of CV indicates that quadratic and subsequent terms in the Taylor series expansion are negligible, including the quadratic term in the approximate density may not provide an adequate correction when CV is large, because of non-negligible higher order terms. Thus the chief value of the summary statistic CV is to indicate when it is safe to use a t interval as a Bayesian interval for a true effect. For values of CV greater than 0.5 the t approximation may give a poor estimate of the true coverage probability of a Bayesian interval. However, as large values of CV are caused by different values of $s^2_{(r)}$ having significant posterior probability, they correspond to situations such as Example 2, where the identity of active contrasts is not well-determined by the experimental data.

The relevant statistics to be computed for the t approximation are s_i^2 and CV_i, and these can be computed by a one-dimensional numerical integration in σ just as p_i is computed.

The first step is to derive the conditional posterior distribution of τ_i, given σ and given that τ_i is active,

$$(3.20)\qquad p(\tau_i|\sigma,\underset{\sim}{T},\tau_i \text{ active}) = \frac{p(\sigma,\tau_i|\underset{\sim}{T},\tau_i \text{ active})}{p(\sigma|\underset{\sim}{T},\tau_i \text{ active})} .$$

Both numerator and denominator of this expression are obtained by integrating the appropriate elements of $\underset{\sim}{\tau}$ out of

$$(3.21)\qquad p(\underset{\sim}{\tau},\sigma|\underset{\sim}{T},\tau_i \text{ active}) \propto \sigma^{-n} \frac{1}{(2\pi(k^2-1))^{1/2}\sigma} \exp\{\frac{-1}{2\sigma^2}[(T_i-\tau_i)^2 + \frac{\tau_i^2}{k^2-1}]\} \times \prod_{j\neq i} [(1-\alpha)\exp\{\frac{-T_j^2}{2\sigma^2}\} + \frac{\alpha}{(2\pi(k^2-1))^{1/2}\sigma}\exp\{\frac{-1}{2\sigma^2}(T_j-\tau_j)^2 + \frac{\tau_j^2}{k^2-1}\}] .$$

After performing the integration we have

$$(3.22)\qquad p(\tau_i|\sigma,\underset{\sim}{T},\tau_i \text{ active}) = (2\pi\varphi)^{-1/2}\sigma^{-1}\exp\{\frac{-(\tau_i-\varphi T_i)^2}{2\varphi\sigma^2}\} ,$$

a normal distribution with mean φT_i and variance $\varphi\sigma^2$. (Recall $\varphi = 1 - 1/k^2$.) In addition, the conditional posterior of σ, given τ_i is active, can be written

$$(3.23) \qquad p(\sigma|\underset{\sim}{T},\tau_i \text{ active}) \propto p(\sigma|\underset{\sim}{T})p_{i|\sigma} \ .$$

The quantities of interest, s_i^2 and CV_i, are functions of the second and fourth conditional posterior moments of τ_i, given it is active. Thus they can be obtained as the corresponding second and fourth moments of the conditional posterior distribution (3.22) of τ_i given it is active and given σ, integrated against the conditional posterior distribution (3.23) of σ given τ_i, is active. Doing this, the following expressions are obtained:

$$(3.24) \qquad \hat{s}_i^2 = \frac{n-3}{n-1} \int_0^\infty \varphi\sigma^2 p(\sigma|T,\tau_i \text{ active})d\sigma$$

$$(3.25) \qquad CV_i = \frac{\frac{(n-3)(n-5)}{(n-1)^2}\int_0^\infty \varphi^2\sigma^4 p(\sigma|\underset{\sim}{T},\tau_i \text{ active})d\sigma}{(\hat{s}_i^2)^2} - 1 \ .$$

3.3 Replication and Blocking

The model described here may be applied to any factorial experiment, unreplicated or otherwise. Although it provides a method of analysis for the case when there are no true replicate runs, as a general method for analyzing fractional factorials the model can be applied successfully when there are replicate runs. For example, consider the special case of an n-run orthogonal design, with m independent observations at each point of the design. In general it is assumed that the experiment is run in m blocks of n runs, with each block consisting of one replication of the design, each block having a different mean, with no interaction between blocks and factors. The analysis can be reduced to the case where each block mean is assumed the same, to be applied when the replicates are not randomized in blocks. The situation where the block size is smaller than n is described later.

Let $\underset{\sim}{T}_j$ be the vector of contrasts for the jth replicate. The sampling distribution of $\underset{\sim}{T} = (\underset{\sim}{T}_1,\ldots,\underset{\sim}{T}_m)$ is

$$p(\underset{\sim}{T}|\underset{\sim}{\tau},\sigma) \propto \sigma^{-mn} \prod_{i=0}^{n-1} \exp\{\frac{-\sum_{j=1}^{m}(T_{ij}-\tau_i)^2}{2\sigma^2}\} . \tag{3.26}$$

Utilizing the same prior distributions as given in Section 2, the joint posterior distribution of $\{\underset{\sim}{\tau},\sigma\}$ is

$$\begin{aligned} p(\underset{\sim}{\tau},\sigma|\underset{\sim}{T}) \propto \sigma^{-mn-1} \exp\{\frac{-\sum_{j=1}^{m}(T_{0j}-\tau_{0j})^2}{2\sigma^2}\} \\ \times \prod_{i=1}^{n-1} [\exp\{\frac{-\sum_{j=1}^{m}(T_{ij}-\tau_i)^2}{2\sigma^2}\} \frac{\alpha}{((2\pi)(k^2-1))^{1/2}\sigma} \exp\{\frac{-\tau_i^2}{2(k^2-1)\sigma^2}\} \\ + (1-\alpha)\exp\{\frac{-1}{2\sigma^2}\sum_{j=1}^{m} T_{ij}^2\}] . \end{aligned} \tag{3.27}$$

The quantities

$$\sum_{j=1}^{m}(T_{ij}-\tau_i)^2, \ \sum_{j=1}^{m} T_{ij}^2$$

can be decomposed to give

$$\sum_{j=1}^{m}(T_{ij}-\tau_i)^2 = m((\overline{T}_i-\tau_i)^2+S_i) \tag{3.28}$$

and

$$\sum_{j=1}^{m} T_{ij}^2 = m((\overline{T}_i)^2+S_i) \tag{3.29}$$

with

(3.30)
$$S_i = \frac{\sum_{j=1}^{m} (T_{ij} - \bar{T}_i)^2}{m}, \quad \bar{T}_i = \frac{1}{m} \sum_{j=1}^{m} T_{ij} .$$

Thus the posterior density of $\{\underset{\sim}{\tau},\sigma\}$ can be written

(3.31)
$$p(\underset{\sim}{\tau},\sigma|\underset{\sim}{T}) \propto \sigma^{-(mn-n+1)} \exp\{\frac{-m \sum_{i=1}^{n-1} S_i}{2\sigma^2}\}$$

$$\times \sigma^{-n} \exp\{\frac{-\sum_{j=1}^{m} (T_{0j} - \tau_{0j})^2}{2\sigma^2}\} \prod_{i=1}^{n-1} [(1 - \alpha)\exp\{\frac{-m\bar{T}_i^2}{\sigma^2}\}$$

$$+ \frac{\alpha}{((2\pi)(k^2 - 1))^{1/2}\sigma} \cdot \exp\{\frac{-1}{2\sigma^2} (m(\bar{T}_i - \tau_i)^2 + \frac{\tau_i^2}{k^2 - 1})\}] .$$

This is of the same form as that derived for the unreplicated case (2.6), with $\bar{T}_i$ replacing T_i, σ^2/m replacing σ^2, and the factor σ^{-1} representing the prior density of σ replaced by

$$\sigma^{-(mn-n+1)} \exp\{\frac{-m \sum_{i=1}^{n-1} S_i}{2\sigma^2}\} \exp\{\frac{-\sum_{j=1}^{m} (T_{0j} - \tau_{0j})^2}{2\sigma^2}\} ,$$

which is of the same form as an inverted χ density (see Box and Tiao, 1973, p. 87). The two distinct cases considered here are:

1. For unequal, unknown block effects, the "prior" estimate of σ^2/m is

(3.32)
$$s^2 = \frac{\sum_{i=1}^{n-1} S_i}{(m - 1)(n - 1)}$$

with $(m - 1)(n - 1)$ degrees of freedom.

2. For equal block means (equivalently no block effects, but one overall mean $\tau_{0j} = \tau_0$ for all j), the "prior" estimate of σ^2/m is

(3.33)
$$s^2 = \frac{\sum_{i=1}^{n-1} S_i + \sum_{j=1}^{m} (T_{0j} - \tau_0)^2}{(m - 1)n}$$

with $(m - 1)n$ degrees of freedom.

Thus the Bayesian analysis applied to a replicated experiment is equivalent to pretending the $n - 1$ average contrasts were obtained from an unreplicated experiment, but with an informative prior distribution for σ based on the variance of observed contrasts between replicates. This computational simplification is made possible by the orthogonality among contrasts and replicates obtained by repeating each point the same number of times.

In situations where the block size is smaller than n, effects of supposedly lesser importance (high order interactions) are associated with block differences (see, e.g., Box, Hunter and Hunter, 1978, p. 336). To deal with contrasts associated with block differences, we assign a noninformative prior to the magnitudes of these effects. The result is that contrasts associated with block differences do not enter into the calculation of posterior probabilities and related statistics for the contrasts of interest, and they are integrated out just as the grand mean was in the previous analysis.

Suppose then that the design is replicated m times, with b blocks within each replicate and the same columns associated with blocks in each replicate. Assuming no interaction between blocks and factors, there are $n - b$ contrasts for which posterior probabilities will be computed. If $m > 1$, there will be $(m - 1)(n - b)$ additional degrees of freedom for estimating variance. Following the same steps as in the previous section, the posterior distribution of σ and the contrasts of interest $\underset{\sim}{\tau}$ is

$$(3.34) \qquad p(\underset{\sim}{\tau},\sigma|\underset{\sim}{T}) = \sigma^{-m(n-b)-1}\exp\left\{\frac{-m\sum_{i=1}^{n-b} S_i}{2\sigma^2}\right\}$$

$$\times \prod_{i=1}^{n-b}\left[\exp\left\{\frac{-m(\bar{T}_i - \tau_i)^2}{2\sigma^2}\right\}\frac{\alpha}{(2\pi(k^2 - 1))^{1/2}\sigma}\exp\left\{\frac{-\tau_i^2}{2(k^2 - 1)\sigma^2}\right\} + (1 - \alpha)\exp\left\{\frac{-m\bar{T}_i^2}{2\sigma^2}\right\}\right] .$$

Again, this is of the same form (2.6) as for the unreplicated design, with the noninformative prior for σ replaced by the informative inverted χ distribution. The expression for $p_{i|\sigma}$ is still given by (2.8) and the only change in computing the posterior probabilities $\{p_i\}$ and other statistics of interest is in the posterior density of σ. This is given by integrating $\underset{\sim}{T}$ out of (3.34),

$$(3.35) \qquad p(\sigma|\underset{\sim}{T}) \propto \sigma^{-m(n-b)-1}\exp\{\frac{-m\sum_{i=1}^{n-b} S_i}{2\sigma^2}\}$$

$$\times \prod_{i=1}^{n-b} [\alpha \cdot \frac{1}{k} \cdot \exp\{\frac{-m\bar{T}_i^2}{2k^2\sigma^2}\} + (1-\alpha)\exp\{\frac{-m\bar{T}_i^2}{2\sigma^2}\}] .$$

To illustrate, the data in Table 3 are from a 32-run 2^4 factorial design run in four blocks of eight runs, published by Barnett and Mead (1956). The four-factor interaction CABP was confounded with block differences within each repeat of the design. After allowing for block effects, there are 14 degrees of freedom for estimating σ^2, the variance of a contrast T_i calculated from a block of 16 observations. This estimate is $\hat{\sigma}^2 = 925$. The Bayesian posterior probabilities of the 14 relevant contrasts were computed with $\alpha = 0.2$ and $k = 10$ and are presented in Table 4a, taking into account the prior estimate of σ^2. For comparison the posterior probabilities and related statistics were computed pretending the values of the observed contrasts were obtained from an unreplicated experiment. These values are presented in Table 4b.

The five largest contrasts, corresponding to effects A, B, P, BA, and PB and declared significant at the .01 level by Barnett and Mead using analysis of variance, all have posterior probabilities close to one. One

Table 3. Design matrix, observations, and observed contrasts for Example 3, a twice-replicated 2^4 full factorial experiment run in four blocks of 8 runs, from Barnett and Mead (1956). The CABP contrast is confounded with block differences.

	Factors				Response	
run	C	A	B	P	y_1	y_2
1	-	-	-	-	881	834
2	+	-	-	-	650	494
3	-	+	-	-	191	257
4	+	+	-	-	183	193
5	-	-	+	-	289	178
6	+	-	+	-	188	163
7	-	+	+	-	225	370
8	+	+	+	-	135	156
9	-	-	-	+	1180	1193
10	+	-	-	+	1039	1146
11	-	+	-	+	466	890
12	+	+	-	+	781	775
13	-	-	+	+	298	273
14	+	-	+	+	238	254
15	-	+	+	+	420	429
16	+	+	+	+	350	389

Column (effect)	Block 1 contrast	Block 2 contrast	Column (effect)	Block 1 contrast	Block 2 contrast
0 (mean)	469.6	499.6	8 (P)	253.8	338.0
1 (C)	-48.3	-106.8	9 (CP)	59.3	51.5
2 (A)	-251.5	-134.5	10 (AP)	67.0	38.8
3 (CA)	85.0	-1.5	11 (CAP)	26.5	-20.8
4 (B)	-403.5	-446.3	12 (BP)	-136.5	-218.5
5 (CB)	-32.0	34.8	13 (CBP)	-44.0	-9.0
6 (AB)	280.8	253.5	14 (ABP)	20.8	-12.3
7 (CAB)	-84.8	-53.5	15 (CABP)	-31.8	65.3

could reasonably conclude that these are measuring real effects. The next two largest effects, C and BAC, declared significant at the .05 level by

Table 4a. Posterior probabilities, standard errors (conditional on being active), CV values, and derivatives for Example 3, with $\alpha = 0.2$ and $k = 10$ and a prior estimate of σ^2 of 925 with 14 degrees of freedom obtained from replicates.

Effect	Contrast	Post. prob.	Standard Error|active	CV	dp/dα	50dp/dk
none active		0.000				
C	-77.5	0.261	31.7	0.01	1.37	-0.29
A	-193.0	0.998	34.3	0.02	0.02	0.00
AC	41.8	0.051	33.3	0.02	0.32	-0.19
B	-424.9	1.000	34.4	0.02	0.00	0.00
BC	1.4	0.024	34.4	0.02	0.15	-0.12
BA	267.1	1.000	34.4	0.02	0.00	0.00
BAC	-69.1	0.174	31.9	0.02	1.03	-0.30
P	295.9	1.000	34.4	0.02	0.00	0.00
PC	55.4	0.089	32.5	0.02	0.57	-0.26
PA	52.9	0.079	32.7	0.02	0.51	-0.25
PAC	2.9	0.024	34.4	0.02	0.15	-0.12
PB	-177.5	0.995	34.3	0.01	0.04	0.01
PBC	-26.5	0.033	33.9	0.02	0.20	-0.15
PBA	4.3	0.025	34.4	0.02	0.15	-0.12

Barnett and Mead (no correction for selection), have posterior probabilities of .261 and .174 respectively, and deserve further consideration. In practice, of course, conclusions about such intermediate-sized effects will depend upon the objectives of the experiment.

Table 4b. Posterior probabilities, standard errors (conditional on being active), CV values, and derivatives for Example 3, with $\alpha = 0.2$ and $k = 10$, pretending the design was not replicated.

Effect	Contrast	Post. prob	Se|active	CV	dp/dα	50dp/dk
none active		0.050				
C	-77.5	0.137	45.9	3.99	1.62	-0.18
A	-193.0	0.711	44.5	1.47	4.59	-1.19
AC	41.8	0.039	66.7	2.58	0.35	-0.16
B	-424.9	0.916	63.7	1.48	2.06	0.05
BC	1.4	0.024	78.4	1.86	0.15	-0.12
BA	267.1	0.796	50.2	1.41	4.01	-1.32
BAC	-69.1	0.098	49.8	3.86	1.16	-0.18
P	295.9	0.822	52.7	1.42	3.69	-1.28
PC	55.4	0.058	58.2	3.23	0.62	-0.17
PA	52.9	0.053	59.8	3.10	0.56	0.02
PAC	2.9	0.024	78.3	1.86	0.15	-0.12
PB	-177.5	0.683	43.4	1.53	4.64	0.12
PBC	-26.5	0.029	73.8	2.12	0.21	-0.14
PBA	4.3	0.024	78.3	1.87	0.15	-0.12

Comparing the results to those obtained by pretending the contrasts were calculated from an unreplicated experiment, the posterior probabilities are in fairly close agreement. However, the values for the diagnostic statistics $\partial p/\partial\alpha$, $\partial p/\partial k$ and CV are all much greater for the "unreplicated" analysis. This agrees with intuition. The derivatives with respect to α and k

measure dependence on the choice of these prior parameters, and dependence on the prior would be expected to decrease as additional replicates were added. The statistic CV can be interpreted as measuring the sharpness of the posterior distribution of σ, with larger values indicating less certainty about σ. Thus we would expect smaller CV values when there are repeat runs.

Conclusions

Sensitivity of the Bayesian analysis to the choice of prior parameters α and k is a key consideration with possibly important implications for any particular experiment. Specifically, when the posterior probabilities are sensitive to the choice of prior distribution, this has indicated a lack of information in the data and a need to collect additional data. The partial derivatives of the posterior probabilities with respect to α and k can be computed conveniently and serve as diagnostics to alert the data analyst in these situations.

Conclusions about a certain experiment will often depend not only on the identity of active factors but also on the size of their effects. Confidence intervals or Bayesian intervals are useful in these situations. The posterior standard deviation of a supposed active effect can be computed within the framework presented here, and takes into account the uncertainty about which of the remaining effects are also active. A t interval offers a good approximation to the exact Bayesian interval once the standard deviation is computed, and the goodness of the approximation can be checked by a statistic CV which is a function of the quadratic coefficient of a Taylor series expansion of the posterior density of an effect.

Although intended primarily for the analysis of unreplicated experiments, the method has simple and appealing properties for the analysis of replicated factorials. The analysis in this case is equivalent to that for the unreplicated design, but with a "prior" estimate of σ^2 provided by the sum of squares within replicates. Blocked designs can also be handled easily by integrating out the nuisance parameters (block differences).

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