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A Bayesian Method for Testing TTBT Compliance with Unknown Intercept and Slope

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Abstract

In this report we examine the Bayesian method for testing for compliance to a given threshold studied by Nicholson, Mensing and Gray. It is noted that although this test and accompanying confidence intervals are valid for a single event, it is incorrect to apply it or the confidence intervals to repeated events at the same site unless the number of calibration events is large. Since in any foreseeable future the number of calibration events is likely to be small, this report studies the applicability of the Bayesian test in this case. The results suggest that in many instances the Bayesian method examined here should be used on repeated events with caution if the number of calibration events is less than three.

1 Introduction

Over the last few years much of the interest in yield estimation and threshold test ban treaty monitoring has shifted to the problem of properly monitoring yields that are somewhat smaller than the current test ban limit of 150 Kt. As a result of this interest in smaller yields it has become more important to include the effects of unknown slope (in the standard magnitude/yield relation) on estimated yields, associated confidence intervals, and related hypothesis tests.

The most popular approach for addressing this problem thus far has been through the Baysian methodology. See W. L. Nicholson, R. W. Mensing and H. L. Gray, or R. H. Shumway and Z. A. Der for example. In each of these papers the authors make use of prior distributions on the parameter spaces to obtain estimates of yield, confidence intervals for yield, threshold type test of hypotheses, and associated F-numbers which allow for errors in estimating geological bias and slope as well as several other unknown parameters. Although such results are exactly what was needed in one sense they present a problem in another. That is, although the confidence intervals and hypothesis tests are valid when related to a single event from all possible parameter configurations they do not represent such intervals or hypothesis tests when applied repeatly to a fixed test site (This will be explained in detail in section 4). This problem was noted by Fisk, Gray, McCartor and Wilson (1991) for the case where the slope is known.

In this report we examine the current Baysian approach to yield estimation from several practical aspects. That is we consider:

- 1. The power of the tests for several different parameter configurations and yield training sets.
- 2. The maximum benefit of previous no yield data regarding its contribution to increasing the power or decreasing the F-number.
- 3. The actual error rate or confidence interval (CI) that results when these Baysian tests or CI's are applied to repeated tests at the same site.

Item 3 is of special interest if the number of calibration events is small and the particular test site is an anomaly, i.e. a site whose parameters differ substantial

from their corresponding Bayesian means. We shall refer to our investigation of item 3 as a robustness study.

2 Notation and Background

Let Y_j denote the jth yield at a given test site and let m_{ij} denote the ith magnitude associated with the jth yield,

$$m_{ij} = A_i + B_i W_{0j} + e_{ij} \tag{1}$$

 $i=1,2,\dots,p$ and $j=1,2,\dots,n$, where $W_{0j}=\log Y_j-\log Y_0=W_j-W_0$, with W_0 given and the e_{ij} represent random errors. Further let $\mathbf{A}=(A_1,\dots,A_p)'$, $\mathbf{B}=(B_1,\dots,B_p)'$, and $\mathbf{e}_j=(e_{1j},e_{2j},\dots,e_{pj})'$ where the prime denotes transpose, and the \mathbf{e}_j are normal random vectors with mean $(0,0,\dots,0)'$ and known variance $\Sigma_{\mathbf{e}}$. We can now write (1) in the matrix form

$$\mathbf{m}_j = \mathbf{A} + \mathbf{B}W_{0j} + \mathbf{e}_j. \tag{2}$$

In the model defined by Equation (1) **A** and **B** are vectors of parameters that depend on the test site and the particular magnitude being considered. For example m_{1j} may refer to the jth m_b value while m_{2j} might be the jth m_{L_g} value. Ideally **A** and **B** in (2) would be known. This is in general not the case.

However there may be sufficient information regarding A and B to restrict their possible values. That is, it is arguable that one can reasonably impose a probability distribution on A and B a priori. This is in fact the reasoning that leads to a Bayesian approach to the problem. Specifically we suppose that $\beta = (A', B')'$ has a prior normal distribution with known mean μ_{β} and covariance Σ_{β} . In the future we will denote this by $\beta \sim N(\mu_{\beta}, \Sigma_{\beta})$. Therefore in Equation (2) we no longer treat A and B as fixed parameters but as random variables or, if you like, "parameters" which take on their possible values with some probability.

Now suppose n calibration events are available, i.e. n events at a given site for which the yields W_j are known (or at least known sufficiently well that we can neglect the errors in the observed W_j). Then we can determine a compliance test and its associated F-number which properly integrates the information in the

prior distribution with the data from the calibration events. This is the subject of the next section.

3 A Bayesian Test of Compliance

In order to determine a test for compliance which makes use of prior information regarding β and the calibration events, we need to determine the probability density function (pdf) for $\mathbf{m} = \mathbf{m}_{n+1}$ given $\mathbf{m}_1, \mathbf{m}_2, \dots, \mathbf{m}_n$. We will denote this pdf by $f(\mathbf{m}|\overrightarrow{\mathbf{m}}_n)$, where $\overrightarrow{\mathbf{m}}_n = (\mathbf{m}_1, \mathbf{m}_2, \dots, \mathbf{m}_n)'$. Given n events for which the yields are known we wish to develop a compliance test for an (n+1)st event for which the yield is unknown.

Note that the model in (2) can be written in the form

$$\mathbf{m}_j = \mathbf{D}_j \boldsymbol{\beta} + \mathbf{e}_j, \ j = 1, 2, \cdots, n, \tag{3}$$

where

$$\mathbf{D}_{j} = \begin{pmatrix} 1 & 0 & \cdots & 0 & W_{0j} & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 & 0 & W_{0j} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & W_{0j} \end{pmatrix} = (1, W_{0j}) \otimes \mathbf{I}_{p}$$

and \otimes denotes the kronecker product.

Case 1: β known

The problem is a simple one when β is known since in that event \mathbf{m} is independent of the previous $\mathbf{m}_1, \mathbf{m}_2, \dots, \mathbf{m}_n$, i.e. $\Sigma_{\beta} = 0$. The hypothesis H_0 , to be tested is

$$H_0: W \leq W_T$$
 against (4) $H_1: W > W_T,$

where $W = W_{n+1}$. If we shorten the notation $W_{0,n+1}$ to W_c , i.e. take $W_{0,n+1} = W_c$ we can write the hypothesis test in Equation (4) in the form

$$H_0: W_c \leq W_{cT}$$

$$H_1: W_c > W_{cT},$$

where $W_{cT} = W_T - W_0$. In this case $f(\mathbf{m}|\overrightarrow{\mathbf{m}}_n) = f(\mathbf{m})$. Now let

$$m_r = \sum_{i=1}^p r_i m_i, \tag{5}$$

where the r_i are known weights with $0 \le r_i \le 1$ and $\sum_{i=1}^p r_i = 1$. It is well known that if $\mathbf{e}_j \sim N(0, \Sigma_{\mathbf{e}})$, then $\mathbf{m} \sim N(\mathbf{D}\boldsymbol{\beta}, \Sigma_{\mathbf{e}})$ where $\mathbf{D} = (1, W_c) \otimes \mathbf{I}_p$, and it then follows at once that $m_r \sim N(\mathbf{r}'\mathbf{D}\boldsymbol{\beta}, \mathbf{r}'\Sigma_{\mathbf{e}}\mathbf{r})$, where $\mathbf{r} = (r_1, r_2, \dots, r_p)'$. Therefore, under H_0 , we take $W_c = W_{cT}$ so that a test of the hypothesis in Equation (4) at the 100α percent significance level is given by the following rule

Reject
$$H_0$$
 if $m_r > T_{1\alpha}$, (6)

where

$$T_{1\alpha} = \mathbf{r}' \mathbf{D}_T \boldsymbol{\beta} + z_{\alpha} \sqrt{\mathbf{r}' \boldsymbol{\Sigma}_{\mathbf{e}} \mathbf{r}},$$

$$\mathbf{D}_T = (1, W_{cT}) \otimes \mathbf{I}_p,$$
(7)

and z_{α} is the $100(1-\alpha)$ th percentile point of N(0,1) distribution. We shall refer to the test defined by the rule given by Equation (6) as Test 1.

Case 2: β unknown

Of course β is not known and therefore Test 1 cannot be used in practice. It does however furnish us a base line for comparison purposes. What can be reasonably assumed, as we have already mentioned, is that $\beta \sim N(\mu_{\beta}, \Sigma_{\beta})$, where μ_{β} and Σ_{β} are known. In this case m and \overrightarrow{m}_n are not independent and therefore the problem is a bit more difficult. It can however be solved by making use of the following theorem, the proof of which we include in the Appendix.

Theorem 1. Let $\mathbf{m} = \mathbf{m}_{n+1}$ be a p-dimensional magnitude related to $W_{0,n+1} = W_c$ by the model of Equation (3). For $k = 1, 2, \dots, n+1$, let $\bar{\mathbf{m}}_{(k)} = \sum_{j=1}^k \mathbf{m}_j/k$, $\bar{\mathbf{m}}_{W(k)} = \sum_{j=1}^k W_{0j}\mathbf{m}_j/k$, and $\bar{W}_{0k} = \sum_{j=1}^k W_{0j}/k$. Suppose β has the prior density $N(\mu_{\beta}, \Sigma_{\beta})$. Then the probability density of \mathbf{m} given \mathbf{m}_n ,

 $f(\mathbf{m}|\overrightarrow{\mathbf{m}}_n)$, is $N(\mu, \Sigma)$, where

$$\Sigma = \Sigma_{\mathbf{e}} \left[\Sigma_{\mathbf{e}} - \mathbf{H} \right]^{-1} \Sigma_{\mathbf{e}}, \tag{8}$$

$$\mu = \Sigma \left\{ (1, W_c) \otimes \Sigma_{\mathbf{e}}^{-1} \right\} \Sigma_{\beta} \left[\Sigma_{\beta} + \left\{ \mathbf{E}_{n+1} \otimes \left(\Sigma_{\mathbf{e}} / (n+1) \right) \right\} \right]^{-1} \cdot \left\{ \mathbf{E}_{n+1} \otimes \left(\Sigma_{\mathbf{e}} / (n+1) \right) \right\} \left[\Sigma_{\beta}^{-1} \mu_{\beta} + n \left(\mathbf{I}_2 \otimes \Sigma_{\mathbf{e}}^{-1} \right) \left(\frac{\bar{\mathbf{m}}_{(n)}}{\bar{\mathbf{m}}_{W(n)}} \right) \right], \tag{9}$$

and

$$\mathbf{H} = \left\{ (1, W_c) \otimes \mathbf{I}_p \right\} \mathbf{\Sigma}_{\beta} \left[\mathbf{\Sigma}_{\beta} + \left\{ \mathbf{E}_{n+1} \otimes \left(\mathbf{\Sigma}_e / (n+1) \right) \right\} \right]^{-1} \\ \cdot \left\{ \mathbf{E}_{n+1} \otimes \left(\mathbf{\Sigma}_e / (n+1) \right) \right\} \left\{ \begin{pmatrix} 1 \\ W_c \end{pmatrix} \otimes \mathbf{I}_p \right\},$$

$$\mathbf{E}_{n+1} = \begin{pmatrix} 1 & \bar{W}_{0,n+1} \\ \bar{W}_{0,n+1} & \sum_{j=1}^{n+1} W_{0j}^2 / (n+1) \end{pmatrix}^{-1}.$$

$$(10)$$

Given Theorem 1, the problem is once again trivial and we can again write down a $100\alpha\%$ significance level test. If m_r is defined by Equation (5), then it follows from Theorem 1 that the pdf of m_r given \overrightarrow{m}_n is $N(\mathbf{r}'\boldsymbol{\mu}, \mathbf{r}'\boldsymbol{\Sigma}\mathbf{r})$, where $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ are given by (8) and (9) respectively. The desired test is then

Reject
$$H_0$$
 if $m_r > T_{2\alpha}$,

where

$$T_{2\alpha} = \mathbf{r}' \boldsymbol{\mu} + z_{\alpha} \sqrt{\mathbf{r}' \Sigma \mathbf{r}},\tag{11}$$

 μ and Σ are defined in Theorem 1 with $W_c = W_{cT}$, and z_{α} is the $100(1 - \alpha)$ percentile point of N(0,1). We shall refer to the test of Equation (11) as Test 2.

From Theorem 1 one can also obtain a confidence interval for W. For a general treatment of the confidence interval problem with a Bayesian prior see R. H. Shumway and Z. A. Der.

4 A Constrained Bayesian Test

In a recent report Nicholson, Mensing and Gray (1991) show how previous magnitude data can be used to define a Bayesian prior for β even though the associated yields are not available. We shall refer to such data as "no yield" data as before, and we also assume that n calibration events are available. In this section we consider the question, "What is the maximum information that can be gained by this approach?" In order to accomplish this we will consider the problem of the previous section but we let the number of no-yield events go to infinity. That is, we consider the case where the "no yield" data set is sufficiently large that the parameters that are estimable from that data can be estimated without error, i.e. they are known. By developing a test for this case and comparing its power to Test 2 we are able to determine the maximum improvement in power (or reduction in F-number) obtainable in the approach of Case 2.

Specifically we note that the parameters

$$c_{i-1} = B_i/B_1, i = 2, 3, \dots, p$$

and (12)
 $\mu_{i-1} = A_i - c_{i-1}A_1,$

do not depend on yield and hence consistent estimates for c_{i-1} and μ_{i-1} can be obtained from the "no yield" data. Thus in this case we take c_{i-1} and μ_{i-1} as known, $i = 2, \dots, p$. Moreover under these constraints the model of Equation (3) becomes

$$\mathbf{m}_j = \boldsymbol{\mu}_L + \mathbf{D}_{Lj}\boldsymbol{\beta}_1 + \mathbf{e}_j, \tag{13}$$

where $\beta_1 = (A_1, B_1)', \ \mu_L = (0, \mu_1, \mu_2, \cdots, \mu_{p-1})'$ and

$$\mathbf{D}_{Lj} = \begin{pmatrix} 1 & c_1 & c_2 & \cdots & c_{p-1} \\ W_{0j} & c_1 W_{0j} & c_2 W_{0j} & \cdots & c_{p-1} W_{0j} \end{pmatrix}'.$$

Thus the original 2p dimensional parameter space for β is reduced to the 2 dimensional one due to the constraints in Equation (12).

To determine a test for the model of Equation (13) we need the following theorem, the proof of which is included in the Appendix.

Theorem 2. Let $\mathbf{m} = \mathbf{m}_{n+1}$ be a p-dimensional magnitude related to $W_{0,n+1} = W_c$ by the model of Equation (13). Suppose $\beta_1 = (A_1, B_1)'$ has the prior pdf $N(\mu_1, \Sigma_1)$. Then the pdf of \mathbf{m} given $\overrightarrow{\mathbf{m}}_n$ is $N(\mu_c, \Sigma_c)$, where

$$\Sigma_c = \left[\mathbf{I}_p - \mathbf{D}_{L,n+1} \mathbf{Q}_{n+1}^{-1} \mathbf{D}_{L,n+1}' \mathbf{\Sigma}_{\mathbf{e}}^{-1}\right]^{-1} \Sigma_{\mathbf{e}},$$

$$\mu_c = \mu_L + \Sigma_c \Sigma_{\mathbf{e}}^{-1} \mathbf{D}_{L,n+1} \mathbf{Q}_{n+1}^{-1} \mathbf{R}_n,$$

and

$$\mathbf{Q}_{n+1} = \mathbf{\Sigma}_{1}^{-1} + \sum_{j=1}^{n+1} (\mathbf{D}'_{Lj} \mathbf{\Sigma}_{e}^{-1} \mathbf{D}_{Lj}),$$

$$\mathbf{R}_{n} = \mathbf{\Sigma}_{1}^{-1} \boldsymbol{\mu}_{1} + \sum_{j=1}^{n} \mathbf{D}'_{Lj} \mathbf{\Sigma}_{e}^{-1} (\mathbf{m}_{j} - \boldsymbol{\mu}_{L}),$$

$$\mathbf{D}_{L,n+1} = \begin{pmatrix} 1 & c_{1} & c_{2} & \cdots & c_{p-1} \\ W_{c} & c_{1} W_{c} & c_{2} W_{c} & \cdots & c_{p-1} W_{c} \end{pmatrix}'.$$

From Theorem 2 it follows that $m_r \sim N(\mathbf{r}'\boldsymbol{\mu}_c, \mathbf{r}'\boldsymbol{\Sigma}_c\mathbf{r})$ and hence a $100(\alpha)\%$ significance test of the hypothesis in Equation (4) is given by the following rule:

Reject
$$H_0$$
 if $m_r > T_{3\alpha}$,

where

$$T_{3\alpha} = \mathbf{r}' \mu_c + z_\alpha \sqrt{\mathbf{r}' \Sigma_c \mathbf{r}}, \tag{14}$$

and z_{α} is the $100(1-\alpha)$ percentile point of a N(0,1). We shall refer to the test of Equation (14) as Test 3.

5 Power Curve Comparisons

In order to assess the impact of imposing the prior information, we compare the power of the following tests: Test 1: a test of hypothesis based on the assumption that the population parameters are known.

Test 2: a test of hypothesis based on the unconstrained Bayesian approach and the assumption that the parameters are unknown.

Test 3: a test of hypothesis based on the constrained Bayesian approach and the assumption that the population parameters are unknown.

The power at W is given by

Power(W) =
$$P(\mathbf{m}_r > T_{\alpha} | \overrightarrow{\mathbf{m}}_n, W)$$
.

Also the F-number of the test is given by

$$F = 10^{W_F - W_T}.$$

where W_F is the value of the log yield at which the power is 0.5.

Since we specified the critical values of Test 1, Test 2, and Test 3 in (7), (11), and (14), respectively, it is easy to show that the power of Tests 1, 2, and 3 are

Power(W)₁ = 1 -
$$\Phi\left(z_{\alpha} + \frac{\mathbf{r}'(\mathbf{D}_{T} - \mathbf{D})\boldsymbol{\beta}}{\sqrt{\mathbf{r}'\Sigma_{\mathbf{e}}\mathbf{r}}}\right)$$
, (15)

Power(W)₂ = 1 -
$$\Phi\left(\frac{\mathbf{r}'(\mu - \mu_W) + z_{\alpha}\sqrt{\mathbf{r}'\Sigma_{\mathbf{r}}}}{\sqrt{\mathbf{r}'\Sigma_{W}\mathbf{r}}}\right)$$
, (16)

Power(W)₃ = 1 -
$$\Phi\left(\frac{\mathbf{r}'(\mu_c - \mu_{cW}) + z_{\alpha}\sqrt{\mathbf{r}'\Sigma_c\mathbf{r}}}{\sqrt{\mathbf{r}'\Sigma_{cW}\mathbf{r}}}\right)$$
, (17)

where $\mathbf{D} = (1, W) \otimes \mathbf{I}_p$, Φ is the cumulative distribution function of N(0, 1), and $\{\mu_W, \Sigma_W\}$, $\{\mu_{cW}, \Sigma_{cW}\}$ are defined as in Theorem 1, and Theorem 2, respectively, with W given.

From (16) and (17) it is clear that the power of Test 2 and Test 3 depends on the value of $\overrightarrow{\mathbf{m}}_n$. Therefore in order to compare with Test 1 we generate two equivalent data sets for Test 2 and Test 3 with fixed values of $\{\Sigma_{\mathbf{e}}, \mu_{\beta}, \Sigma_{\beta}, c_1, \mu_1, n\}$ when p = 2. With the known parameter and the generated data sets, we computed the power of Test 1, Test 2, and Test 3 on the 100 equally spaced grid values between log 150 and log 300 for W from (15), (16), and (17), respectively

and $W_0 = \log 125$. We ran this simulation 20 times to get the mean of the powers for Test 2 and Test 3. Power $(W)_1$, mean Power $(W)_2$, and mean Power $(W)_3$ are plotted on Figure 1 through Figure 8 for various values of $\{\Sigma_e, \mu_{\beta}, \Sigma_{\beta}, c_1, \mu_1, n\}$.

Now we summarize some findings from the simulation. As we can see in Figure 1 through Figure 3, mean $Power(W)_2$ and mean $Power(W)_3$ rapidly converge to $Power(W)_1$ as n gets large. Similarly average F_2 and average F_3 converge to F_1 as n grows, where F_1 , F_2 and F_3 are the F-numbers of Test 1, Test 2, and Test 3, respectively.

The relatively better performance of Test 3 over Test 2 is observed regardless of the values of c_1 in Figure 1 and Figure 4. However, Figure 5 and Figure 6 show that the overperformance of Test 3 against Test 2 diminishes as the standard deviations of A_2 and B_2 ($\sigma_{A_2}, \sigma_{B_2}$) decrease to those of A_1 and B_1 , respectively. Figure 7 and Figure 8 show the same phenomenon as σ_{e_2} becomes small enough to be similar to σ_{e_1} . Thus it would appear that if the values used here for $\mu_{\beta}, \Sigma_{\beta}$ and Σ_{e} are representative, additional no yield data would be of little value.

6 Robustness

In the previous sections we have developed a test of the hypothesis of compliance of the (n+1)st event given n calibration events when β is unknown. We referred to this as Test 2. In making use of this test it is important to understand the nature of the false alarm rate or significance level α . Possibly the best way to interpret α is to think through a simulation for estimating α . In order to simulate the process one would first generate β from $N(\mu_{\beta}, \Sigma_{\beta})$ and then, given β and W_i , $i = 1, \dots, n$, generate e_1, e_2, \dots, e_n to obtain \overrightarrow{m}_n . Now letting $W_{n+1} = \log 150$ and generating e_{n+1} to obtain m_{n+1} , one would apply the test and note the decision. This simulates the senario of obtaining n calibration events and one additional event of unknown yield. This entire process would be repeated a large number of times and the proportion of incorrect decisions would approach α . Table 1 below describes the method. The β_i denote the values of β generated on simulation # i. Let $m_{r,n+1}(i) = r'm_{i,n+1}$, where $m_{i,n+1}$ is the

(n+1)st magnitude vector generated in the *i*th simulation, $i=1,2,\cdots,l$.

Table 1. Simulation procedure for estimating the false alarm rate

	Simulation # 1	Simulation # 2	•••	Simulation # l
Given	$\beta_1, W_1, \cdots, W_n$	$\boldsymbol{\beta}_2, W_1, \cdots, W_n$	• • •	$\boldsymbol{\beta}_l, W_1, \cdots, W_n$
${\bf Generate}$	$\mathbf{m}_{11}, \cdots, \mathbf{m}_{1n}$	$\mathbf{m}_{21},\cdots,\mathbf{m}_{2n}$	• • •	$\mathbf{m}_{l1},\cdots,\mathbf{m}_{ln}$
${\bf Generate}$	$\mathbf{m}_{1,n+1}, W = \log 150$	$\mathbf{m}_{2,n+1}, W = \log 150$	• • •	$\mathbf{m}_{l,n+1}, W = \log 150$
Decision	Reject if	Reject if	• • •	Reject if
	$m_{r,n+1}(1) > T_{2\alpha}(1)$	$m_{r,n+1}(2) > T_{2\alpha}(2)$		$m_{r,n+1}(l) > T_{2\alpha}(l)$

Now, if we define a random variable X such that X = 1 if $m_{r,n+1}(j) > T_{2\alpha}(j)$, and otherwise X = 0, it follows that

$$\alpha = \lim_{l \to \infty} \sum_{j=1}^{l} X_j / l = \lim_{l \to \infty} \bar{X}_l$$
 a.s.

We should note, however, that in practice the application of these tests will be to events $m_{n+1}, m_{n+2}, \cdots, m_{n+s}$ at the same site. That is, what is needed is essentially a test so that the empirical false alarm rate or significance level approaches α as s gets large rather than as l gets large. We shall refer to the sample false alarm rate as $s \to \infty$ as the "actual significance level" or "actual false alarm rate" and denote it by $\alpha(\overrightarrow{m}_n|n,\beta)$. Thus

$$\alpha(\overrightarrow{\mathbf{m}}_{n}|n,\boldsymbol{\beta}) = P(m_{n+s} > T_{2\alpha}|\overrightarrow{\mathbf{m}}_{n}, W_{n+s} = \log 150, \boldsymbol{\beta})$$

$$= \lim_{k \to \infty} (\# \text{ of } m_{n+k} > T_{2\alpha})/k.$$
(18)

It can be shown that

$$\lim_{n\to\infty}\alpha(\overrightarrow{\mathbf{m}}_n|n,\boldsymbol{\beta})=\alpha.$$

Thus when n is large, $\alpha(\overrightarrow{m}_n|n,\beta) \approx \alpha$ regardless of the observed value of β . However in most instances n will be small and therefore the question which arrises is, "How robust is α to small values of n and unusual values of β , i.e. values of β far removed from μ_{β} ?" That is, "How close is α to $\alpha(\overrightarrow{m}_n|n,\beta)$,

the actual false alarm rate, when n is small and β is substantially different from μ_{β} ?"

In addition to the "actual false alarm rate" we need to obtain the probability of rejecting H_0 as $s \to \infty$. We shall refer to this as the "actual power" or the "actual probability of detection", and denote it by $P(W|n,\beta)$. Thus

$$P(W|n, \boldsymbol{\beta}) = P(m_{n+s} > T_{2\alpha}|\overrightarrow{\mathbf{m}}_n, \boldsymbol{\beta}, W_{n+s} = W)$$

$$= \lim_{k \to \infty} (\# \text{ of } m_{n+k} > T_{2\alpha})/k.$$
(19)

Then it also can be shown that

$$\lim_{n\to\infty} P(W|n,\boldsymbol{\beta}) = \text{Power}(W).$$

From (18) and (19) it is clear that $\alpha(\overrightarrow{\mathbf{m}}_n|n,\boldsymbol{\beta})$ and $P(W|n,\boldsymbol{\beta})$ depend on $\overrightarrow{\mathbf{m}}_n$. Thus for every sample of $\overrightarrow{\mathbf{m}}_n$ these quantities will be different. We can however estimate $E[\alpha(\overrightarrow{\mathbf{m}}_n|n,\boldsymbol{\beta})]$ and $E[P(W|n,\boldsymbol{\beta})]$ for various values of $\boldsymbol{\beta}$ and n. This is the topic of the remaining portion of this section.

In order to investigate the robustness of the actual false alarm rate, $\alpha(\overrightarrow{\mathbf{m}}_{n}|n,\boldsymbol{\beta})$, a small simulation was performed for a variety of values of n and $\boldsymbol{\beta}$. Specifically, taking p=2, $\boldsymbol{\mu}_{\boldsymbol{\beta}}=(\mu_{A_1},\mu_{A_2},\mu_{B_1},\mu_{B_2})'=(4,4,1,1)'$, $\sigma_{A_1}=\sigma_{A_2}=\sigma_{B_1}=\sigma_{B_2}=0.05$, $\rho_{\mathbf{A}}=\rho_{\mathbf{B}}=0.5$, $\rho_{\mathbf{AB}}=0$, $\sigma_{e_1}=\sigma_{e_2}=0.05$, $\rho_{\mathbf{e}}=0.5$, $W=\log 150$ and $W_0=\log 125$, we considered the cases

$$\boldsymbol{\beta} = \boldsymbol{\mu_{\beta}} + C \cdot (\sigma_{A_1}, \sigma_{A_2}, 0, 0)',$$

where $C = 0, \pm 1, \pm 2$, for n = 1, 2, 3, 5, 10 and 100.

For each case a value of \mathbf{m}_{n+1} was obtained 10,000 times (or equivalently \mathbf{m}_{n+i} , $i = 1, \dots, 10,000$ was obtained) and $\alpha(\overrightarrow{\mathbf{m}}_n|n, \boldsymbol{\beta})$ was estimated by

$$\hat{\alpha}(\overrightarrow{\mathbf{m}}_n|n,\boldsymbol{\beta}) = \frac{\text{\# of rejections}}{10,000}.$$
 (20)

As already noted $\alpha(\overrightarrow{\mathbf{m}}_n|n,\boldsymbol{\beta})$ depends on $\overrightarrow{\mathbf{m}}_n$ and clearly the same is true about $\hat{\alpha}(\overrightarrow{\mathbf{m}}_n|n,\boldsymbol{\beta})$. Therefore a reasonable measure of the robustness of Test 2 when n is small is the $E[\alpha(\overrightarrow{\mathbf{m}}_n|n,\boldsymbol{\beta})] = \mu_{\alpha}$. To obtain an estimate of μ_{α} , for each case we generated 20 repetitions of $\hat{\alpha}(\overrightarrow{\mathbf{m}}_n|n,\boldsymbol{\beta})$, *i.e.*

$$\hat{\mu}_{\alpha} = \frac{1}{20} \sum_{i=1}^{20} \hat{\alpha}_{i}(\overrightarrow{\mathbf{m}}_{n}|n, \boldsymbol{\beta}). \tag{21}$$

The results of these simulations are given in Table 2 for $\alpha=0.025$. It is worth noting the relatively large standard deviation of $\hat{\alpha}(\overrightarrow{\mathbf{m}}_n|n,\boldsymbol{\beta})$. In view of the values of $\hat{\mu}_{\alpha}$ one can conclude that the distribution of $\hat{\alpha}(\overrightarrow{\mathbf{m}}_n|n,\boldsymbol{\beta})$ is quite skewed to the right or at least contains some extreme values on the right side. That is, values of $\hat{\alpha}(\overrightarrow{\mathbf{m}}_n|n,\boldsymbol{\beta})$ much larger than $\hat{\mu}_{\alpha}$ are more frequent than values of $\hat{\alpha}(\overrightarrow{\mathbf{m}}_n|n,\boldsymbol{\beta})$ less than $\hat{\mu}_{\alpha}$, or substantially larger values of $\hat{\alpha}(\overrightarrow{\mathbf{m}}_n|n,\boldsymbol{\beta})$ than $\hat{\mu}_{\alpha}$ may not be unusual. Since $\hat{\alpha}(\overrightarrow{\mathbf{m}}_n|n,\boldsymbol{\beta})$ is obtained from 10,000 repetitions, it follows that $\hat{\alpha}(\overrightarrow{\mathbf{m}}_n|n,\boldsymbol{\beta})\approx \alpha(\overrightarrow{\mathbf{m}}_n|n,\boldsymbol{\beta})$. So similar remarks can be made regarding $\alpha(\overrightarrow{\mathbf{m}}_n|n,\boldsymbol{\beta})$. The result of this is that Table 2 presents these results in a conservative way since most people would interpret the mean as a typical value of the false alarm rate. What we are cautioning here is that, in fact false alarm rates substantially larger than the mean values shown in Table 2 will be much more common than in a symmetric distribution. We probably should have included the median in Table 2, but that was not calculated.

It should be noted that if C < 0, the Bayesian estimator of yield will underestimate yield and hence the true false alarm rate will be too small while if C > 0 the estimator will overestimate yield and hence the false alarm rate will be too large. From inspection of Table 2, it appears that if we have only 1 or 2 calibration events, this effect can be large, and hence in this case the Bayesian significance level or CI may be seriously in error. On the other hand if $n \ge 5$ the method might be considered adequate, even though for C < 0 the false alarm rate may still be sufficiently too small that it could very adversely effect the power, *i.e.* the chances of detecting a violation.

Power Considerations

Figures 1 - 8 compare the power of Test 1, Test 2, and Test 3 for various parameter configurations. As in the case of the false alarm rate, if these parameter values are representative, little is to be gained from additional no yield data. Also, from the comparison of the F-numbers it does not appear that a great deal is to be gained by taking n > 2. Unfortunately these rather pleasant results do not uniformly extend to the actual power.

Figure 9 through Figure 36 compare the "actual" power of Test 2 to the power of Test 2, *i.e.* they compare $P(W|n,\beta)$ to P(W). The figures also compare the F-number for Test 2 to the "actual" F-number. For $n \leq 2$ it is clear that both the power and the F-number are seriously effected if $C = \pm 2$ and the same is true for $C = \pm 1$ if n = 1. It should be pointed out that the small F-numbers associated with C < 0 are a result of very large false alarm rates and should not be viewed as improved tests.

Concluding Remarks

In this report we have investigated the robustness of the Bayesian method (referred to as Test 2) for testing compliance of an observed yield to a threshold. Although the simulations reported here were not exhaustive, they were adequate to demonstrate that the Bayesian method for testing compliance is probably not satisfactory if there are only one or two calibration events. Moreover it is highly desirable to have five or more calibration events to guarantee good agreenent with the stated significance level. Similar remarks could be made regarding the corresponding confidence intervals.

The consequence of these findings is that if it is unlikely that several calibration events will be available, Test 2 and confidence intervals associated with Test 2, the Bayesian tests and CI discussed by Nicholson, Mensing and Gray, and those introduced by Shumway and Der should be used with care. In fact if the number of calibration events is less than 3 it would probably be wise to consider a constrained likelihood method as an alternative to the Bayesian method, or, if possible, the Bayesian method should be extended to include the case of several events following the calibration events.

Table 2. Estimate of Actual False Alarm Rate $E[\alpha(n, \beta)], \alpha = 0.025$

	C = -2	C = -1	C = 0	C = 1	C=2
			n=0	-	
$\hat{\mu}_{m{lpha}}$	0.0000	0.0000	0.0023	0.0488	0.3165
st. dev. $\hat{\mu}_{\alpha}$	0.0000	0.0000	0.0001	0.0006	0.0011
st. dev. $\hat{\alpha}(\overrightarrow{\mathbf{m}}_{n} n,\boldsymbol{\beta})$	0.0000	0.0000	0.0004	0.0025	0.0050
			n = 1		
$\hat{\mu}_{m{lpha}}$	0.0006	0.0034	0.0149	0.0532	0.1418*
st. dev. $\hat{\mu}_{\alpha}$	0.0003	0.0013	0.0044	0.0112	0.0205
st. dev. $\hat{\alpha}(\overrightarrow{\mathbf{m}}_n n,\boldsymbol{\beta})$	0.0012	0.0058	0.0197	0.0499	0.0919
(**************************************			n = 2		
$\hat{\mu}_{m{lpha}}$	0.0034	0.0089	0.0225	0.0498	0.0985
st. dev. $\hat{\mu}_{\alpha}$	0.0014	0.0030	0.0061	0.0107	0.0173
st. dev. $\hat{\alpha}(\overrightarrow{\mathbf{m}}_{n} n,\boldsymbol{\beta})$	0.0062	0.0132	0.0273	0.0479	0.0774
, .,,			n = 3		
$\hat{\mu}_{m{lpha}}$	0.0046	0.0099	0.0193	0.0364	0.0643
st. dev. $\hat{\mu}_{\alpha}$	0.0018	0.0033	0.0055	0.0087	0.0132
st. dev. $\hat{\alpha}(\overrightarrow{\mathbf{m}}_n n,\boldsymbol{\beta})$	0.0079	0.0146	0.0246	0.0389	0.0592
			n = 5		
$\hat{\mu}_{lpha}$	0.0076	0.0121	0.0192	0.0283	0.0425
st. dev. $\hat{\mu}_{\alpha}$	0.0019	0.0029	0.0042	0.0058	0.0081
st. dev. $\hat{\alpha}(\overrightarrow{\mathbf{m}}_n n,\boldsymbol{\beta})$	0.0084	0.0128	0.0190	0.0259	0.0363
			n = 10		
$\hat{\mu}_{m{lpha}}$	0.0119	0.0155	0.0201	0.0255	0.0316
st. dev. $\hat{\mu}_{\alpha}$	0.0017	0.0025	0.0030	0.0034	0.0040
st. dev. $\hat{\alpha}(\overrightarrow{\mathbf{m}}_n n,\pmb{\beta})$	0.0075	0.0110	0.0132	0.0152	0.0179
			n = 100		
$\hat{\mu}_{m{lpha}}$	0.0229	0.0230	0.0234	0.0238	0.0240
st. dev. $\hat{\mu}_{\alpha}$	0.0015	0.0013	0.0016	0.0014	0.0015
st. dev. $\hat{\alpha}(\overrightarrow{\mathbf{m}}_n n,\boldsymbol{\beta})$	0.0065	0.0058	0.0072	0.0063	0.0065

* note: For symetric confidence intervals a $100(1-2\alpha)\%$ two sided confidence interval corresponds to a one sided α -level significance test. For example, for Test 1 of size 0.025, the corresponding two sided confidence interval is a 95% C.I. This suggests that if the "actual" significance level is 0.14, the actual C.I. could be a 72% C.I. That is, if the site geological bias is 2σ greater than the expected bias, μ_A , then even though the Bayesian significance level is 0.025 and the Bayesian C.I. is 0.95, the actual significance level is estimated here as 0.14 and one would assume that the actual two sided C.I. is around 72%.

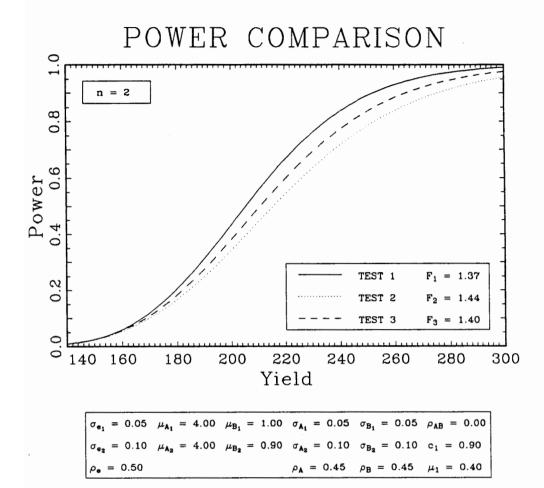


Figure 1

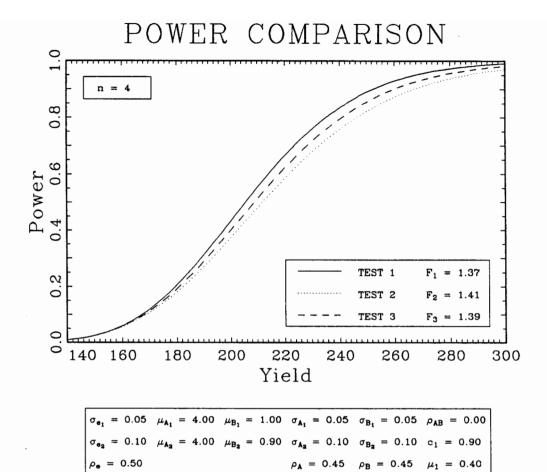


Figure 2

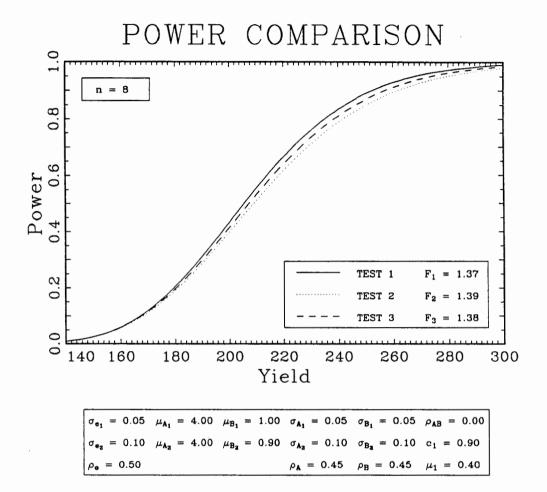
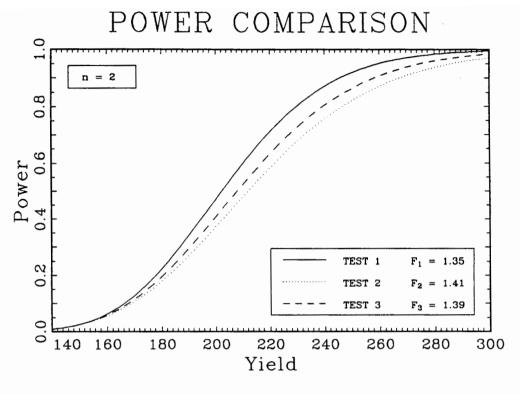


Figure 3



$$\sigma_{\mathbf{e}_1} = 0.05 \quad \mu_{\mathbf{A}_1} = 4.00 \quad \mu_{\mathbf{B}_1} = 1.00 \quad \sigma_{\mathbf{A}_1} = 0.05 \quad \sigma_{\mathbf{B}_1} = 0.05 \quad \rho_{\mathbf{A}\mathbf{B}} = 0.00$$

$$\sigma_{\mathbf{e}_2} = 0.10 \quad \mu_{\mathbf{A}_2} = 4.00 \quad \mu_{\mathbf{B}_2} = 1.00 \quad \sigma_{\mathbf{A}_2} = 0.10 \quad \sigma_{\mathbf{B}_2} = 0.10 \quad c_1 = 1.00$$

$$\rho_{\mathbf{e}} = 0.50 \quad \rho_{\mathbf{B}} = 0.50 \quad \mu_1 = 0.00$$

Figure 4

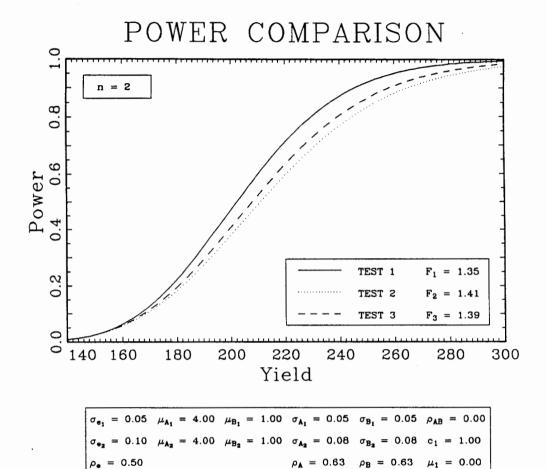


Figure 5

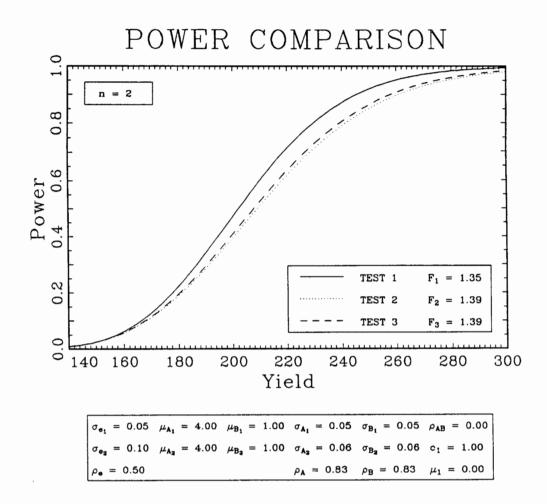


Figure 6

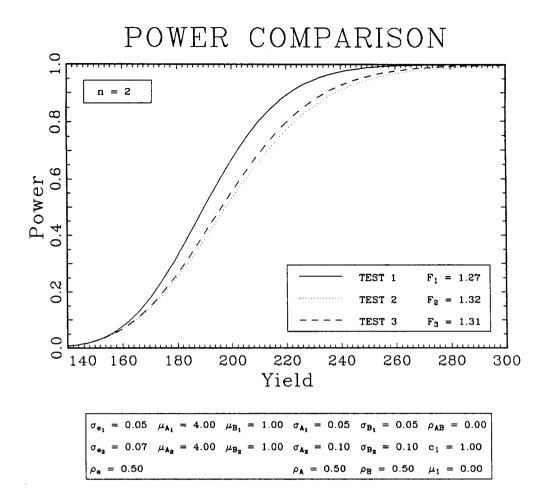


Figure 7

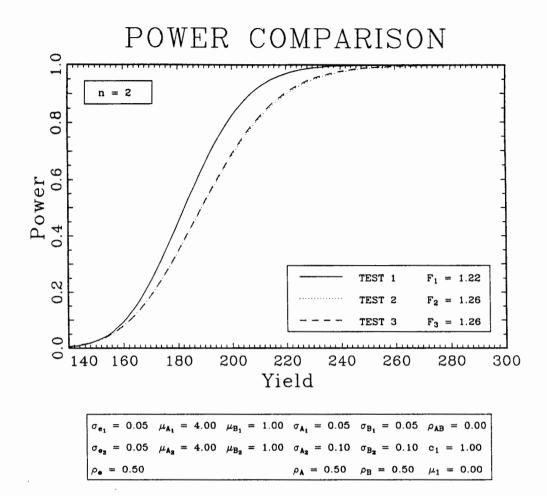


Figure 8

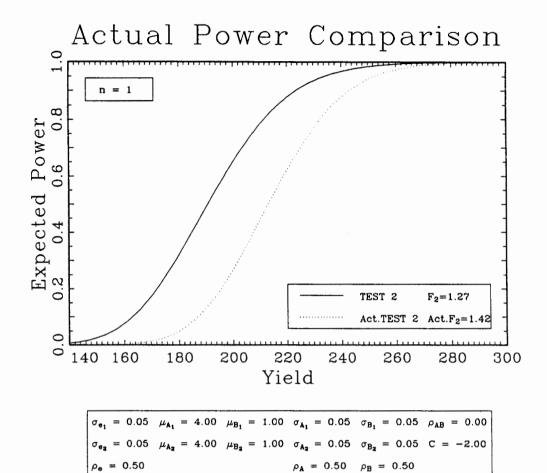


Figure 9

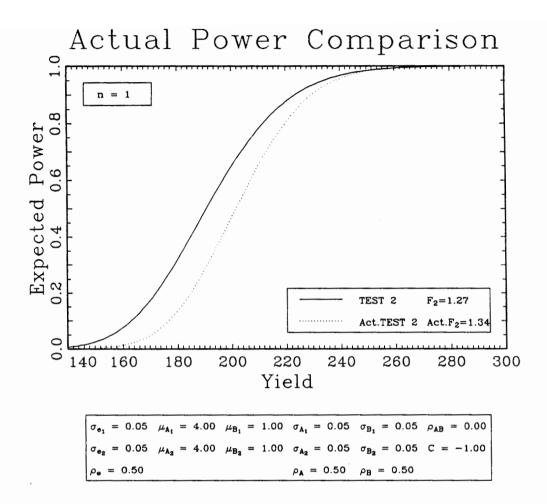


Figure 10

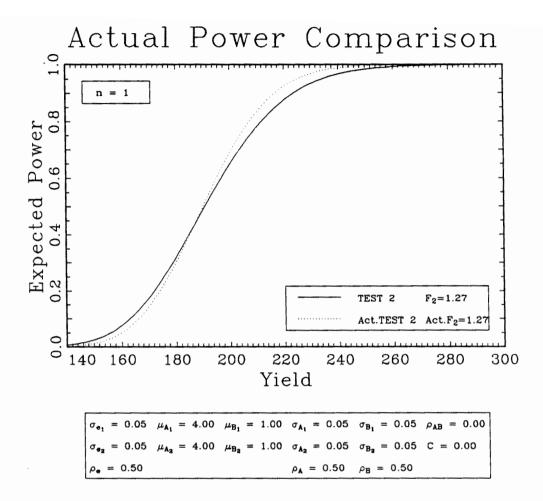


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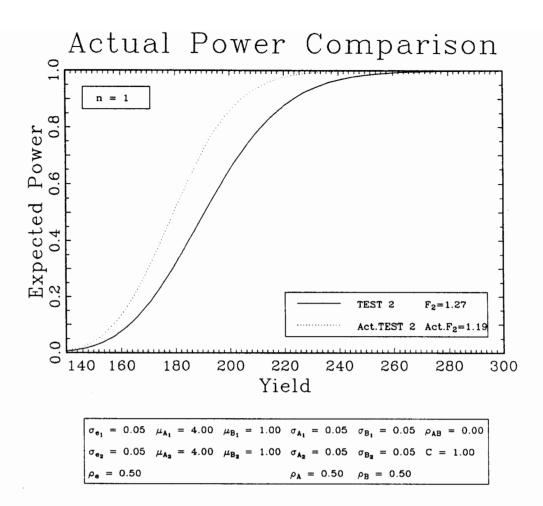


Figure 12

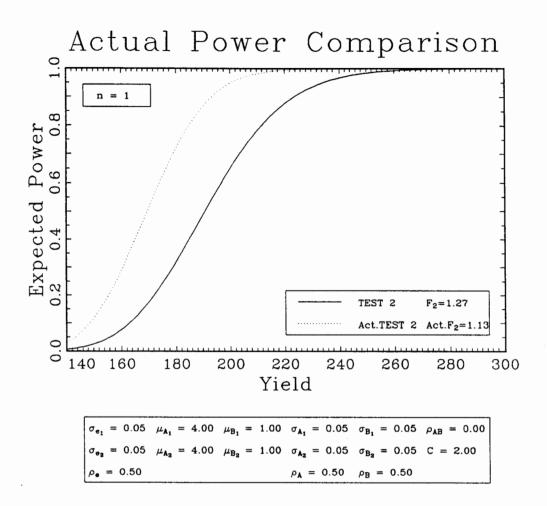


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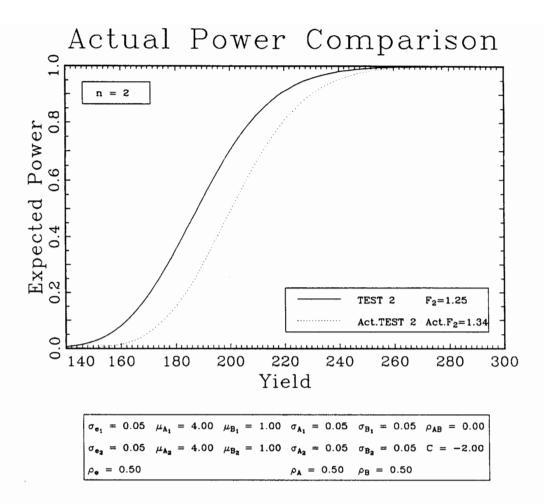


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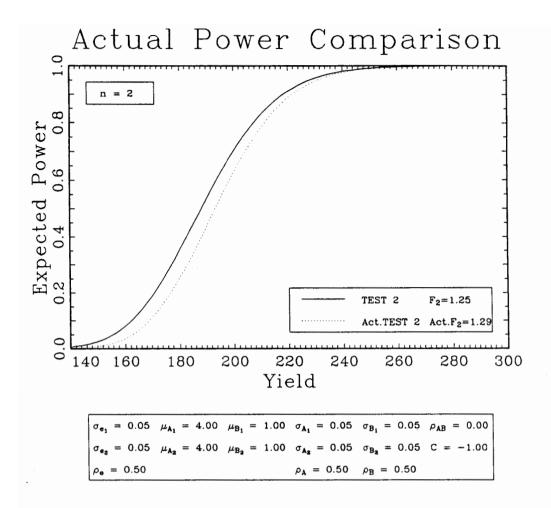
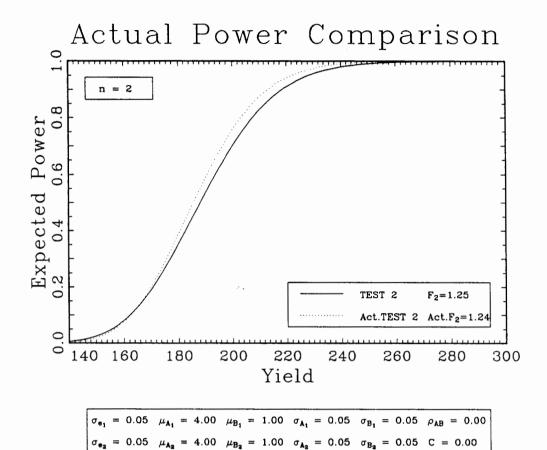


Figure 15



 $\rho_{e} = 0.50$

Figure 16

 $\rho_{A} = 0.50 \quad \rho_{B} = 0.50$

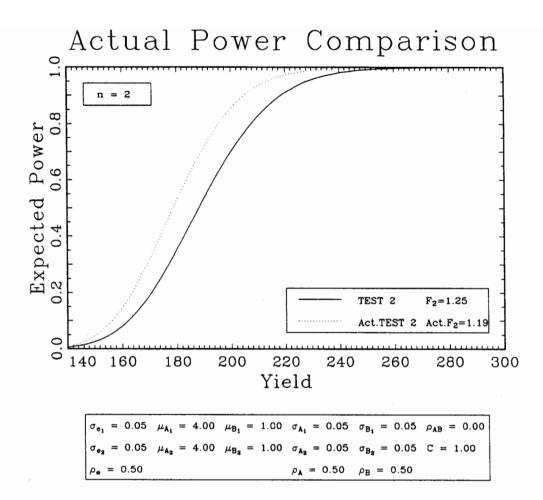


Figure 17

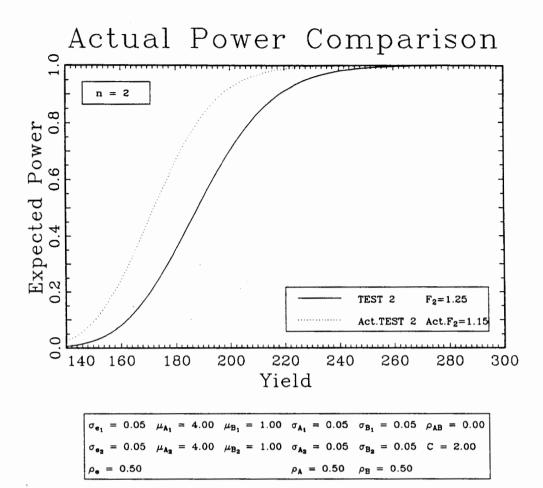


Figure 18

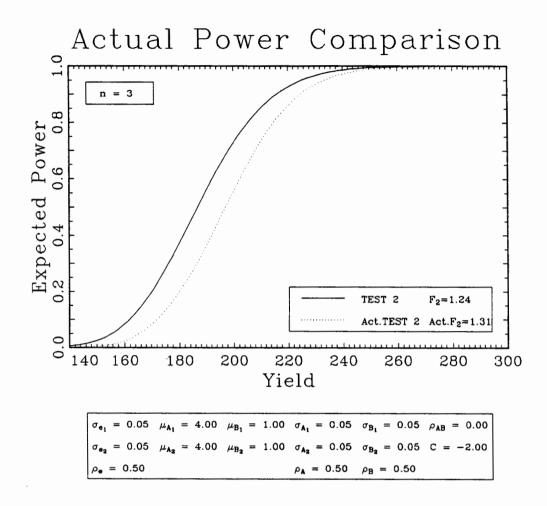


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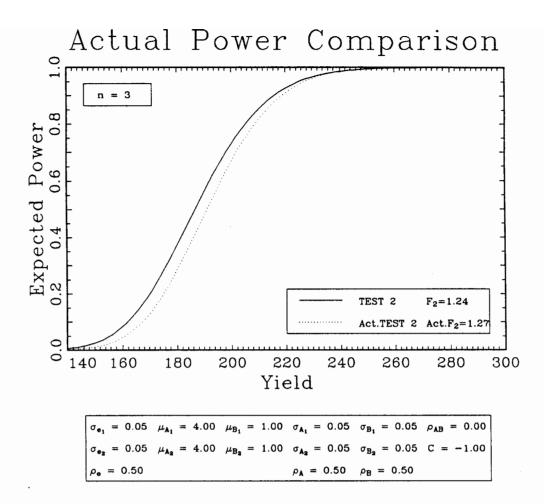


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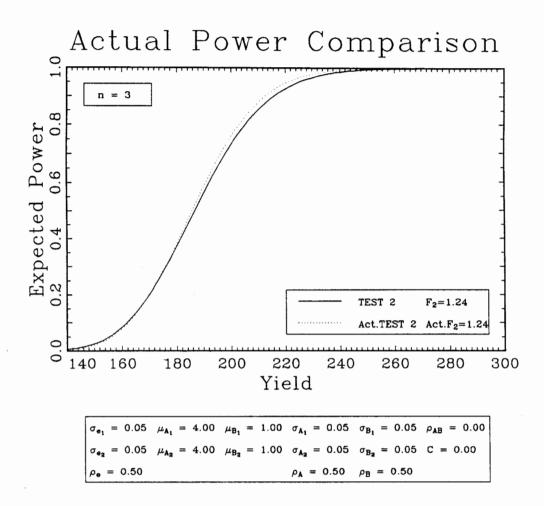
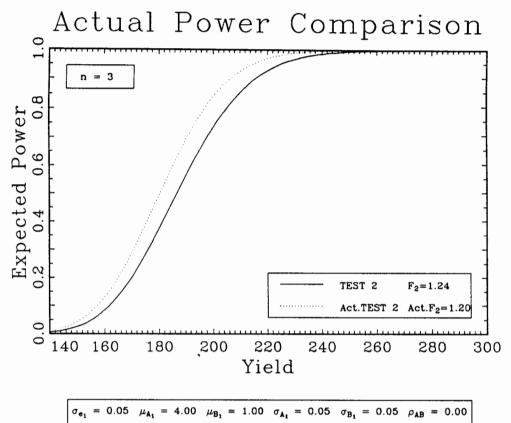


Figure 21



 $\sigma_{e_2} = 0.05$ $\mu_{A_2} = 4.00$ $\mu_{B_2} = 1.00$ $\sigma_{A_2} = 0.05$ $\sigma_{B_2} = 0.05$ C = 1.00 $\rho_{e} = 0.50$ $\rho_{B} = 0.50$

Figure 22

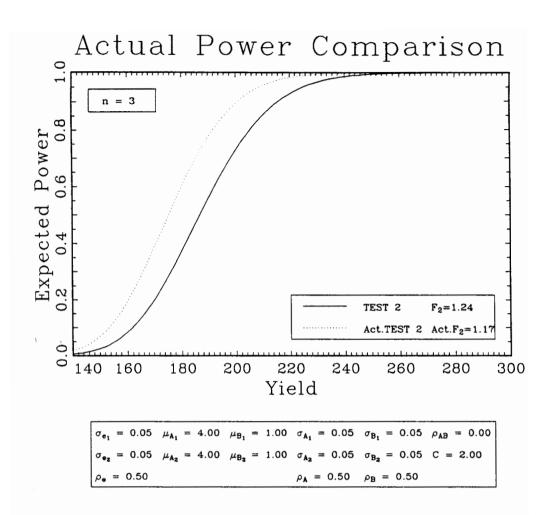


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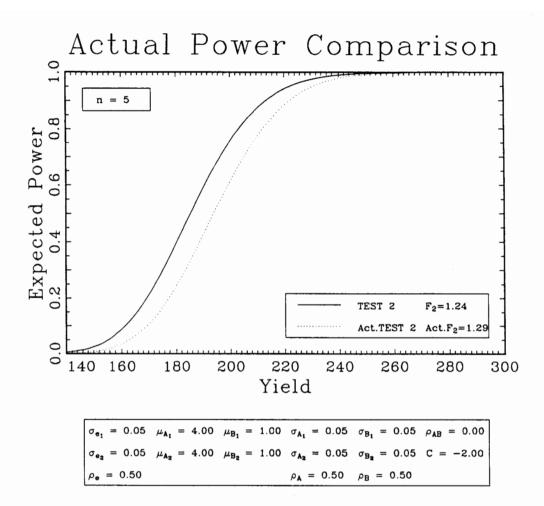


Figure 24

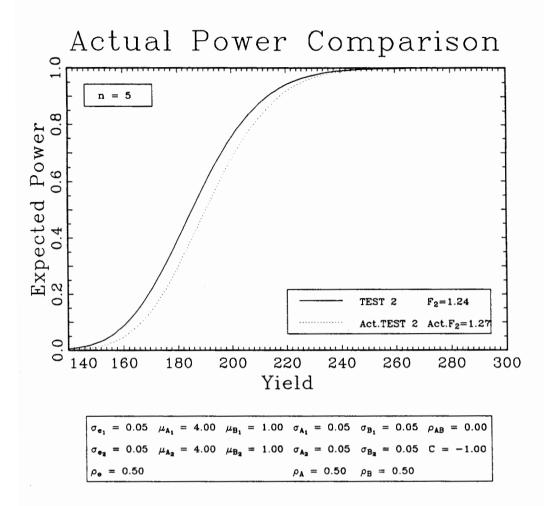


Figure 25

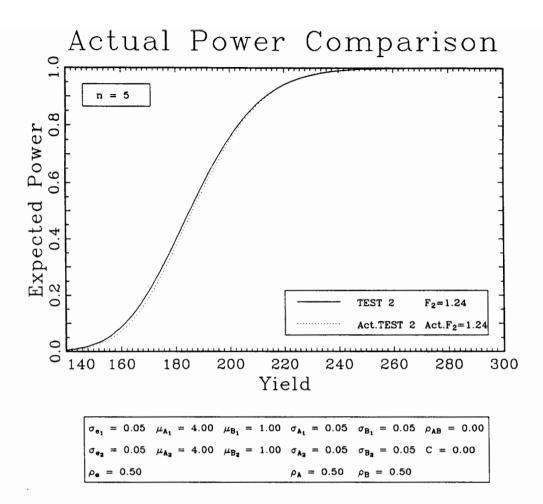
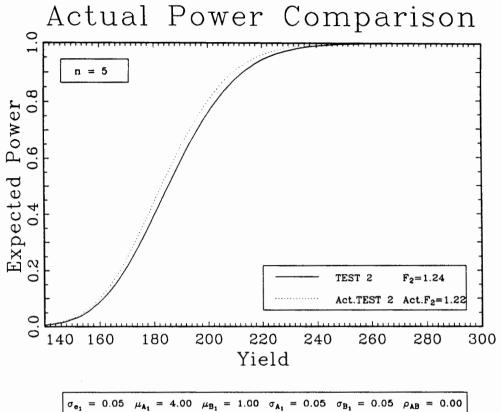


Figure 26



 $\sigma_{e_1} = 0.05 \quad \mu_{A_1} = 4.00 \quad \mu_{B_1} = 1.00 \quad \sigma_{A_1} = 0.05 \quad \sigma_{B_1} = 0.05 \quad \rho_{AB} = 0.00$ $\sigma_{e_2} = 0.05 \quad \mu_{A_2} = 4.00 \quad \mu_{B_2} = 1.00 \quad \sigma_{A_2} = 0.05 \quad \sigma_{B_2} = 0.05 \quad C = 1.00$ $\rho_{e} = 0.50 \quad \rho_{A} = 0.50 \quad \rho_{B} = 0.50$

Figure 27

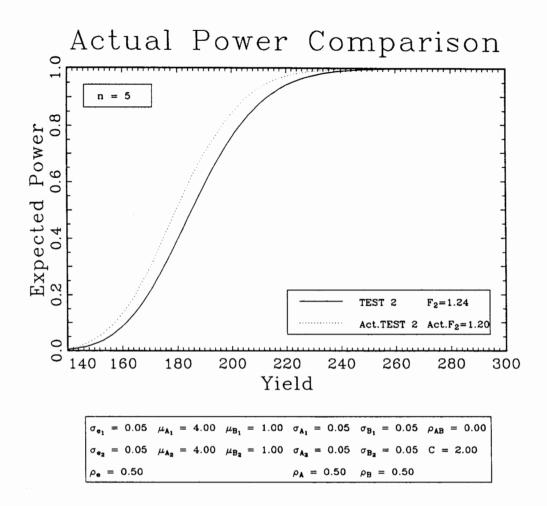


Figure 28

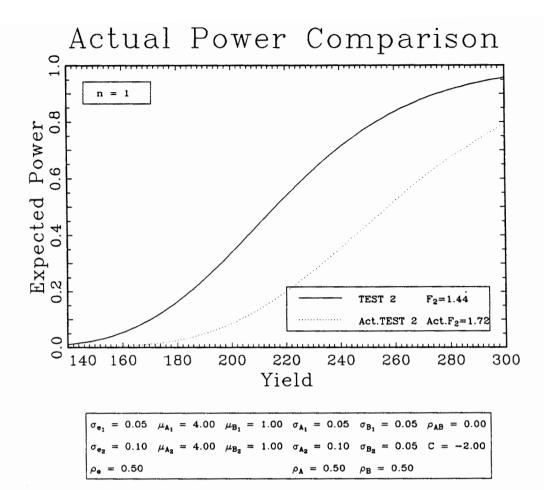


Figure 29

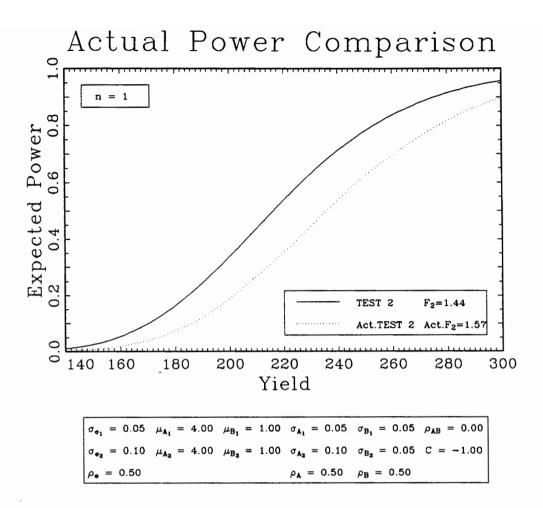


Figure 30

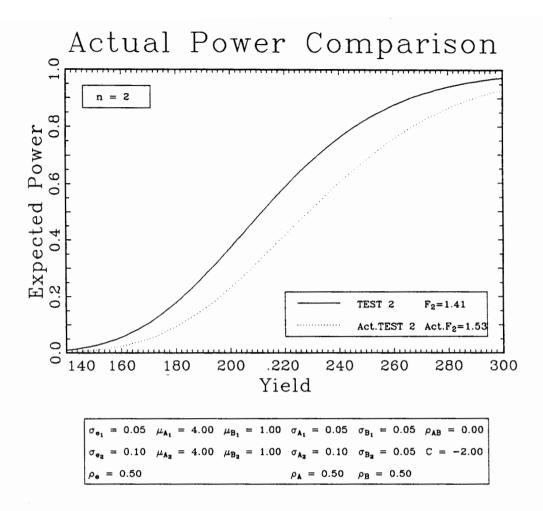


Figure 31

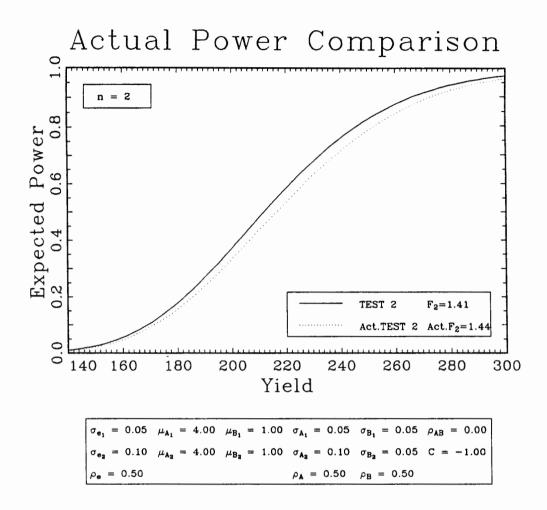


Figure 32

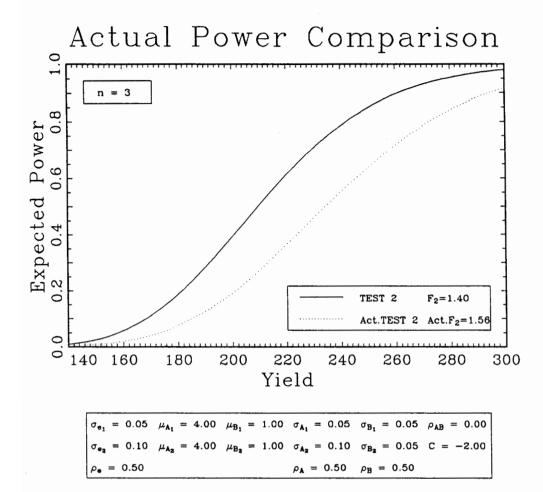


Figure 33

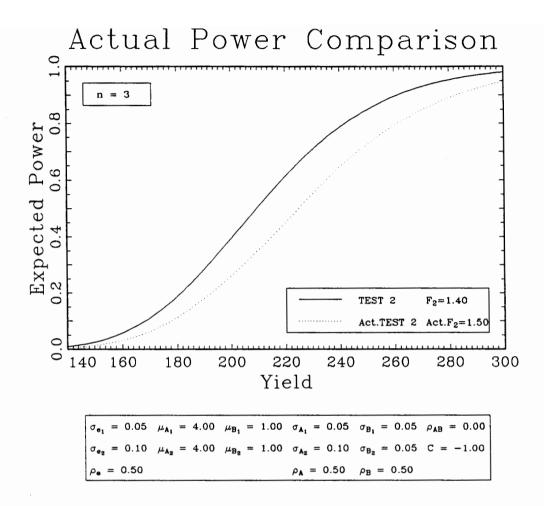


Figure 34

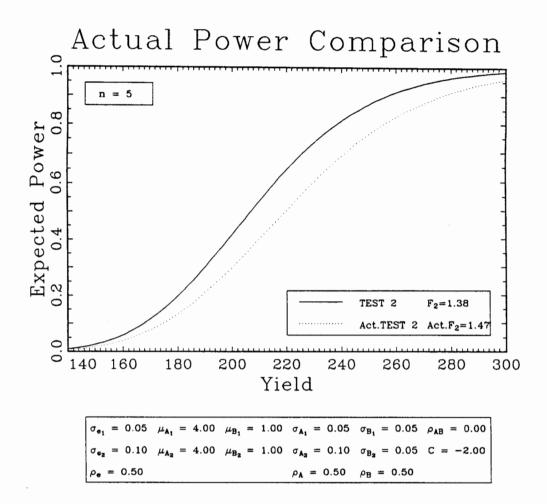


Figure 35

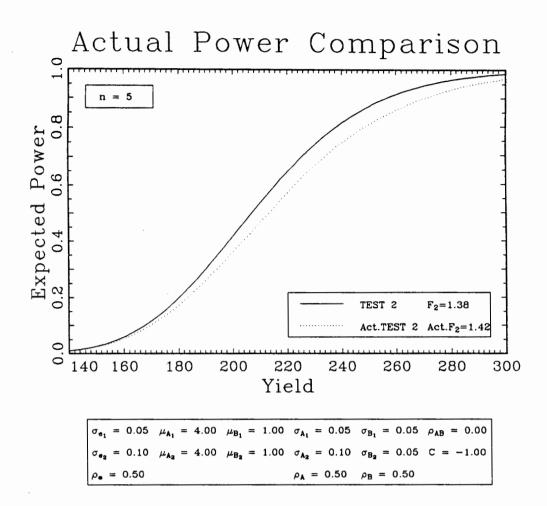


Figure 36

APPENDIX: PROOFS

Proof of Theorem 1

For the new observation \mathbf{m} related to W_c , the conditional pdf of \mathbf{m} given $\overrightarrow{\mathbf{m}}_n$, $f(\mathbf{m}|\overrightarrow{\mathbf{m}}_n)$ is as follows:

$$f(\mathbf{m}|\overrightarrow{\mathbf{m}}_{n}) = \int f_{1}(\mathbf{m}, \boldsymbol{\beta}|\overrightarrow{\mathbf{m}}_{n})d\boldsymbol{\beta}$$

$$= \int f_{2}(\mathbf{m}|\boldsymbol{\beta}, \overrightarrow{\mathbf{m}}_{n})f_{3}(\boldsymbol{\beta}|\overrightarrow{\mathbf{m}}_{n})d\boldsymbol{\beta}$$

$$= \int f_{2}(\mathbf{m}|\boldsymbol{\beta})f_{3}(\boldsymbol{\beta}|\overrightarrow{\mathbf{m}}_{n})d\boldsymbol{\beta}, \tag{A1}$$

where f_1, f_2 , and f_3 are the probability densities. The last equation is obtained due to the independence between \mathbf{m} and \mathbf{m}_n when $\boldsymbol{\beta}$ is given. The conditional distribution of $\boldsymbol{\beta}$ given \mathbf{m}_n may be computed using Bayes' law as follows:

$$f_3(\boldsymbol{\beta}|\overrightarrow{\mathbf{m}}_n) = \frac{h(\boldsymbol{\beta})L(\overrightarrow{\mathbf{m}}_n|\boldsymbol{\beta})}{\int h(\boldsymbol{\beta})L(\overrightarrow{\mathbf{m}}_n|\boldsymbol{\beta})d\boldsymbol{\beta}},\tag{A2}$$

where h is the prior density of the parameter vector $\boldsymbol{\beta}$ and L is the likelihood function for the data $\overrightarrow{\mathbf{m}}_n$, given values of $\boldsymbol{\beta}$. If we assume \mathbf{e}_j are independent multivariate normal, then

$$L(\overrightarrow{\mathbf{m}}_n|\boldsymbol{\beta}) = \prod_{j=1}^n \psi(\mathbf{m}_j|\boldsymbol{\beta}),$$

where

$$\psi(\mathbf{m}_j|\boldsymbol{\beta}) = (2\pi)^{-p}|\boldsymbol{\Sigma}_{\mathbf{e}}|^{-1/2}exp\Big\{-\frac{1}{2}(\mathbf{m}_j - \mathbf{D}_j\boldsymbol{\beta})'\boldsymbol{\Sigma}_{\mathbf{e}}^{-1}(\mathbf{m}_j - \mathbf{D}_j\boldsymbol{\beta})\Big\}.$$

Note

$$f_2(\mathbf{m}|\boldsymbol{\beta})L(\overrightarrow{\mathbf{m}}_n|\boldsymbol{\beta}) = L(\overrightarrow{\mathbf{m}}_{n+1}|\boldsymbol{\beta}, \mathbf{m}_{n+1} = \mathbf{m}, W_{n+1} = W_c)$$

since e_j are independent. Thus referring to (A1) and (A2) leads to

$$f(\mathbf{m}|\overrightarrow{\mathbf{m}}_n) = \frac{\int h(\boldsymbol{\beta})L(\overrightarrow{\mathbf{m}}_{n+1}|\boldsymbol{\beta}, \mathbf{m}_{n+1} = \mathbf{m}, W_{n+1} = W_c)d\boldsymbol{\beta}}{\int h(\boldsymbol{\beta})L(\overrightarrow{\mathbf{m}}_n|\boldsymbol{\beta})d\boldsymbol{\beta}}.$$

Thus if $h(\beta)$ is available, f is completely determined.

Note

$$h(\boldsymbol{\beta})L(\overrightarrow{\mathbf{m}}_{n}|\boldsymbol{\beta}) \propto exp\Big[-\frac{1}{2}\{(\boldsymbol{\beta}-\boldsymbol{\mu}_{\boldsymbol{\beta}})'\boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1}(\boldsymbol{\beta}-\boldsymbol{\mu}_{\boldsymbol{\beta}}) + \sum_{j=1}^{n}(\mathbf{m}_{j}-\mathbf{D}_{j}\boldsymbol{\beta})'\boldsymbol{\Sigma}_{\mathbf{e}}^{-1}(\mathbf{m}_{j}-\mathbf{D}_{j}\boldsymbol{\beta})\}\Big]. \tag{A3}$$

The exponential of (A3) is -1/2 times

$$\beta' \left[\Sigma_{\beta}^{-1} + \sum_{j=1}^{n} \mathbf{D}_{j}' \Sigma_{\mathbf{e}}^{-1} \mathbf{D}_{j}\right] \beta - 2 \left[\mu_{\beta}' \Sigma_{\beta}^{-1} + \sum_{j=1}^{n} \mathbf{m}_{j}' \Sigma_{\mathbf{e}}^{-1} \mathbf{D}_{j}\right] \beta + \mu_{\beta}' \Sigma_{\beta}^{-1} \mu_{\beta}$$

$$+ \sum_{j=1}^{n} \mathbf{m}_{j}' \Sigma_{\mathbf{e}}^{-1} \mathbf{m}_{j}. \tag{A4}$$

Let $\bar{W}_{0n} = \sum_{j=1}^{n} W_{0j}/n$. Since $\mathbf{D}_j = (1, W_{0j}) \otimes \mathbf{I}_p$,

$$\begin{split} \sum_{j=1}^{n} \mathbf{D}_{j}' \boldsymbol{\Sigma}_{\mathbf{e}}^{-1} \mathbf{D}_{j} &= \sum_{j=1}^{n} \left((1, W_{0j})' \otimes \mathbf{I}_{p} \right) \boldsymbol{\Sigma}_{\mathbf{e}}^{-1} \left((1, W_{0j}) \otimes \mathbf{I}_{p} \right) \\ &= \sum_{j=1}^{n} \left\{ \begin{pmatrix} 1 & W_{0j} \\ W_{0j} & W_{0j}^{2} \end{pmatrix} \otimes \boldsymbol{\Sigma}_{\mathbf{e}}^{-1} \right\} \\ &= \left\{ \sum_{j=1}^{n} \begin{pmatrix} 1 & W_{0j} \\ W_{0j} & W_{0j}^{2} \end{pmatrix} \right\} \otimes \boldsymbol{\Sigma}_{\mathbf{e}}^{-1} \\ &= \begin{pmatrix} 1 & \bar{W}_{0n} \\ \bar{W}_{0n} & \sum_{j=1}^{n} W_{0j}^{2} / n \end{pmatrix} \otimes \left(\boldsymbol{\Sigma}_{\mathbf{e}} / n \right)^{-1} \\ &= \left\{ \begin{pmatrix} 1 & \bar{W}_{0n} \\ \bar{W}_{0n} & \sum_{j=1}^{n} W_{0j}^{2} / n \end{pmatrix}^{-1} \otimes \left(\boldsymbol{\Sigma}_{\mathbf{e}} / n \right) \right\}^{-1} \\ &= \left\{ \mathbf{E}_{n} \otimes \left(\boldsymbol{\Sigma}_{\mathbf{e}} / n \right) \right\}^{-1}, \end{split}$$

where

$$\mathbf{E}_{n} = \begin{pmatrix} 1 & \bar{W}_{0n} \\ \bar{W}_{0n} & \sum_{j=1}^{n} W_{0j}^{2}/n \end{pmatrix}^{-1}.$$

Let $\bar{\mathbf{m}}_{(n)} = \sum_{j=1}^n \mathbf{m}_j/n$ and $\bar{\mathbf{m}}_{W(n)} = \sum_{j=1}^n W_{0j} \mathbf{m}_j/n$. Then it is easy to verify that

$$\sum_{j=1}^{n} \mathbf{m}_{j}^{\prime} \Sigma_{\mathbf{e}}^{-1} \mathbf{D}_{j} = \left(\bar{\mathbf{m}}_{(n)}^{\prime}, \bar{\mathbf{m}}_{W(n)}^{\prime} \right) \left(\mathbf{I}_{2} \otimes \left(\Sigma_{\mathbf{e}} / n \right)^{-1} \right).$$

We can rewrite (A4) as follows:

$$\beta' \left[\Sigma_{\beta}^{-1} + \left\{ \mathbf{E}_{n} \otimes \left(\Sigma_{\mathbf{e}}/n \right) \right\}^{-1} \right] \beta - 2 \left[\mu_{\beta}' \Sigma_{\beta}^{-1} + \left(\bar{\mathbf{m}}_{(n)}', \bar{\mathbf{m}}_{W(n)}' \right) \right] \\ \cdot \left(\mathbf{I}_{2} \otimes \left(\Sigma_{\mathbf{e}}/n \right)^{-1} \right) \right] \beta + \mu_{\beta}' \Sigma_{\beta}^{-1} \mu_{\beta} + \sum_{j=1}^{n} \mathbf{m}_{j}' \Sigma_{\mathbf{e}}^{-1} \mathbf{m}_{j}$$

$$= \left(\beta - \mathbf{Z}_{n} \right)' \left[\Sigma_{\beta}^{-1} + \left\{ \mathbf{E}_{n} \otimes \left(\Sigma_{\mathbf{e}}/n \right) \right\}^{-1} \right] \left(\beta - \mathbf{Z}_{n} \right)$$

$$- \mathbf{Z}_{n}' \left[\Sigma_{\beta}^{-1} + \left\{ \mathbf{E}_{n} \otimes \left(\Sigma_{\mathbf{e}}/n \right) \right\}^{-1} \right] \mathbf{Z}_{n} + \mu_{\beta}' \Sigma_{\beta}^{-1} \mu_{\beta} + \sum_{j=1}^{n} \mathbf{m}_{j}' \Sigma_{\mathbf{e}}^{-1} \mathbf{m}_{j},$$

where

$$\mathbf{Z}_{n} = \left[\boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1} + \left\{\mathbf{E}_{n} \otimes \left(\boldsymbol{\Sigma}_{\mathbf{e}}/n\right)\right\}^{-1}\right]^{-1} \left[\boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1} \boldsymbol{\mu}_{\boldsymbol{\beta}} + \left\{\mathbf{I}_{2} \otimes \left(\boldsymbol{\Sigma}_{\mathbf{e}}/n\right)^{-1}\right\} \begin{pmatrix} \bar{\mathbf{m}}_{(n)} \\ \bar{\mathbf{m}}_{W(n)} \end{pmatrix}\right].$$

Since $-(1/2)(\boldsymbol{\beta} - \mathbf{Z}_n)'[\boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1} + \{\mathbf{E}_n \otimes (\boldsymbol{\Sigma}_{\mathbf{e}}/n)\}^{-1}](\boldsymbol{\beta} - \mathbf{Z}_n)$ is the exponential of the multivariate normal density with mean \mathbf{Z}_n and variance $[\boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1} + \{\mathbf{E}_n \otimes (\boldsymbol{\Sigma}_{\mathbf{e}}/n)\}^{-1}]^{-1}$, and $\int exp[-(1/2)(\boldsymbol{\beta} - \mathbf{Z}_n)'[\boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1} + \{\mathbf{E}_n \otimes (\boldsymbol{\Sigma}_{\mathbf{e}}/n)\}^{-1}](\boldsymbol{\beta} - \mathbf{Z}_n)]d\boldsymbol{\beta}$ is a constant, it can be shown that

$$\int h(\boldsymbol{\beta}) L(\overrightarrow{\mathbf{m}}_{n}|\boldsymbol{\beta}) d\boldsymbol{\beta} \propto exp \Big[-(1/2) \Big\{ -\mathbf{Z}_{n}' \Big[\boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1} + \Big\{ \mathbf{E}_{n} \otimes \left(\boldsymbol{\Sigma}_{\mathbf{e}}/n \right) \Big\}^{-1} \Big] \mathbf{Z}_{n} + \boldsymbol{\mu}_{\boldsymbol{\beta}}' \boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1} \boldsymbol{\mu}_{\boldsymbol{\beta}} + \sum_{j=1}^{n} \mathbf{m}_{j}' \boldsymbol{\Sigma}_{\mathbf{e}}^{-1} \mathbf{m}_{j} \Big\} \Big].$$

For the new observation m, let $f(m|\vec{m}_n)$ be the conditional density of m given \vec{m}_n in the unconstrained case. Then

$$f(\mathbf{m}|\overrightarrow{\mathbf{m}}_{n}) = \frac{\int h(\boldsymbol{\beta})L(\overrightarrow{\mathbf{m}}_{n+1}|\boldsymbol{\beta}, \mathbf{m}_{n+1} = \mathbf{m}, W_{0,n+1} = W_{c})d\boldsymbol{\beta}}{\int h(\boldsymbol{\beta})L(\overrightarrow{\mathbf{m}}_{n}|\boldsymbol{\beta})d\boldsymbol{\beta}}$$

$$\propto exp\Big[-(1/2)\Big\{-\mathbf{Z}'_{n+1}\Big[\boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1} + \Big\{\mathbf{E}_{n+1} \otimes \Big(\boldsymbol{\Sigma}_{\mathbf{e}}/(n+1)\Big)\Big\}^{-1}\Big]\mathbf{Z}_{n+1} + \mathbf{Z}'_{n}\Big[\boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1} + \Big\{\mathbf{E}_{n} \otimes \Big(\boldsymbol{\Sigma}_{\mathbf{e}}/n\Big)\Big\}^{-1}\Big]\mathbf{Z}_{n} + \mathbf{m}'\boldsymbol{\Sigma}_{\mathbf{e}}^{-1}\mathbf{m}\Big\}\Big], \quad (A5)$$

where

$$\begin{split} \mathbf{Z}_{n+1} &= \mathbf{R}_{n+1}^{-1} \left[\Sigma_{\beta}^{-1} \mu_{\beta} + \left\{ \mathbf{I}_{2} \otimes \left(\Sigma_{\mathbf{e}} / (n+1) \right)^{-1} \right\} \begin{pmatrix} \bar{\mathbf{m}}_{(n+1)} \\ \bar{\mathbf{m}}_{W(n+1)} \end{pmatrix} \right], \\ \mathbf{R}_{n+1} &= \Sigma_{\beta}^{-1} + \left\{ \mathbf{E}_{n+1} \otimes \left(\Sigma_{\mathbf{e}} / (n+1) \right) \right\}^{-1}, \\ \mathbf{E}_{n+1} &= \begin{pmatrix} 1 & \bar{W}_{0,n+1} \\ \bar{W}_{0,n+1} & \sum_{j=1}^{n+1} W_{0j}^{2} / (n+1) \end{pmatrix}^{-1}, \\ \bar{\mathbf{m}}_{(n+1)} &= \sum_{j=1}^{n+1} \mathbf{m}_{j} / (n+1), \\ \bar{\mathbf{m}}_{W(n+1)} &= \sum_{j=1}^{n+1} W_{0j} \mathbf{m}_{j} / (n+1), \\ \bar{W}_{0,n+1} &= \sum_{j=1}^{n+1} W_{0j} / (n+1), \end{split}$$

with $\mathbf{m}_{n+1} = \mathbf{m}$ and $W_{0,n+1} = W_c$.

Note

$$\begin{split} \bar{\mathbf{m}}_{(n+1)} &= \left(n/(n+1)\right) \bar{\mathbf{m}}_{(n)} + \left(1/(n+1)\right) \mathbf{m} \\ \bar{\mathbf{m}}_{W(n+1)} &= \left(n/(n+1)\right) \bar{\mathbf{m}}_{W(n)} + \left(W_c/(n+1)\right) \mathbf{m}. \end{split}$$

Then

$$\begin{pmatrix} \bar{\mathbf{m}}_{(n+1)} \\ \bar{\mathbf{m}}_{W(n+1)} \end{pmatrix} = \left(n/(n+1) \right) \begin{pmatrix} \bar{\mathbf{m}}_{(n)} \\ \bar{\mathbf{m}}_{W(n)} \end{pmatrix} + \left(1/(n+1) \right) \begin{pmatrix} 1 \\ W_c \end{pmatrix} \otimes \mathbf{m}.$$

Therefore the exponential of (A5) is -1/2 times

$$-\mathbf{M}_{n+1}'\mathbf{R}_{n+1}\mathbf{M}_{n+1} + \mathbf{Z}_{n}'\left[\boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1} + \left\{\mathbf{E}_{n} \otimes \left(\boldsymbol{\Sigma}_{\mathbf{e}}/n\right)\right\}^{-1}\right]\mathbf{Z}_{n} - \boldsymbol{\mu}'\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu} + \left(\mathbf{m} - \boldsymbol{\mu}\right)'\boldsymbol{\Sigma}^{-1}\left(\mathbf{m} - \boldsymbol{\mu}\right), \tag{A6}$$

where

$$\begin{split} \mathbf{M}_{n+1} &= \mathbf{R}_{n+1}^{-1} \left[\mathbf{\Sigma}_{\pmb{\beta}}^{-1} \pmb{\mu}_{\pmb{\beta}} + \left(n/(n+1) \right) \left\{ \mathbf{I}_{2} \otimes \left(\mathbf{\Sigma}_{\mathbf{e}}/(n+1) \right)^{-1} \right\} \begin{pmatrix} \bar{\mathbf{m}}_{(n)} \\ \bar{\mathbf{m}}_{W(n)} \end{pmatrix} \right], \\ \mathbf{\Sigma} &= \mathbf{\Sigma}_{\mathbf{e}} \Big[\mathbf{\Sigma}_{\mathbf{e}} - \mathbf{H} \Big]^{-1} \mathbf{\Sigma}_{\mathbf{e}}, \\ \boldsymbol{\mu} &= \mathbf{\Sigma} \Big\{ (1, W_{c}) \otimes \mathbf{\Sigma}_{\mathbf{e}}^{-1} \Big\} \mathbf{\Sigma}_{\pmb{\beta}} \Big[\mathbf{\Sigma}_{\pmb{\beta}} + \Big\{ \mathbf{E}_{n+1} \otimes \left(\mathbf{\Sigma}_{\mathbf{e}}/(n+1) \right) \Big\} \Big]^{-1} \\ & \cdot \Big\{ \mathbf{E}_{n+1} \otimes \left(\mathbf{\Sigma}_{\mathbf{e}}/(n+1) \right) \Big\} \left[\mathbf{\Sigma}_{\pmb{\beta}}^{-1} \pmb{\mu}_{\pmb{\beta}} + n \Big(\mathbf{I}_{2} \otimes \mathbf{\Sigma}_{\mathbf{e}}^{-1} \Big) \begin{pmatrix} \bar{\mathbf{m}}_{(n)} \\ \bar{\mathbf{m}}_{W(n)} \end{pmatrix} \right], \end{split}$$

with

$$\mathbf{H} = \left\{ (1, W_c) \otimes \mathbf{I}_p \right\} \mathbf{\Sigma}_{\boldsymbol{\beta}} \left[\mathbf{\Sigma}_{\boldsymbol{\beta}} + \left\{ \mathbf{E}_{n+1} \otimes \left(\mathbf{\Sigma}_{\mathbf{e}} / (n+1) \right) \right\} \right]^{-1} \cdot \left\{ \mathbf{E}_{n+1} \otimes \left(\mathbf{\Sigma}_{\mathbf{e}} / (n+1) \right) \right\} \left\{ \begin{pmatrix} 1 \\ W_c \end{pmatrix} \otimes \mathbf{I}_p \right\}.$$

Since the first three terms in (A6) are not function of m, which are constants, the theorem holds.

Proof of Theorem 2

Note the distribution of \mathbf{m}_j given $\boldsymbol{\beta}_1$ is the multivariate normal with mean $\mu_L + \mathbf{D}_{Lj}\boldsymbol{\beta}_1$ and variance Σ_e .

$$h(\boldsymbol{\beta}_1)L(\overrightarrow{\mathbf{m}}_n|\boldsymbol{\beta}_1) \propto exp\Big[-(1/2)\Big\{(\boldsymbol{\beta}_1 - \boldsymbol{\mu}_1)'\boldsymbol{\Sigma}_1^{-1}(\boldsymbol{\beta}_1 - \boldsymbol{\mu}_1) + \sum_{j=1}^{n} (\mathbf{m}_j - \boldsymbol{\mu}_L - \mathbf{D}_{Lj}\boldsymbol{\beta}_1)'\boldsymbol{\Sigma}_{\mathbf{e}}^{-1}(\mathbf{m}_j - \boldsymbol{\mu}_L - \mathbf{D}_{Lj}\boldsymbol{\beta}_1)\Big\}\Big]. (A7)$$

The exponential of (A7) is -1/2 times

$$(\beta_{1} - \mathbf{Z}_{n})' \Big[\Sigma_{1}^{-1} + \sum_{j=1}^{n} \Big(\mathbf{D}'_{Lj} \Sigma_{\mathbf{e}}^{-1} \mathbf{D}_{Lj} \Big) \Big] (\beta_{1} - \mathbf{Z}_{n}) - \mathbf{Z}'_{n} \Big[\Sigma_{1}^{-1} + \sum_{j=1}^{n} \Big(\mathbf{D}'_{Lj} \Sigma_{\mathbf{e}}^{-1} \mathbf{D}_{Lj} \Big) \Big] \\ \cdot \mathbf{Z}_{n} + \mu'_{1} \Sigma_{1}^{-1} \mu_{1} + \sum_{j=1}^{n} (\mathbf{m}_{j} - \mu_{L})' \Sigma_{\mathbf{e}}^{-1} (\mathbf{m}_{j} - \mu_{L}),$$

where

$$\mathbf{Z}_{n} = \left[\mathbf{\Sigma}_{1}^{-1} + \sum_{j=1}^{n} \left(\mathbf{D}'_{Lj} \mathbf{\Sigma}_{e}^{-1} \mathbf{D}_{Lj} \right) \right]^{-1} \left[\mathbf{\Sigma}_{1}^{-1} \boldsymbol{\mu}_{1} + \sum_{j=1}^{n} \mathbf{D}'_{Lj} \mathbf{\Sigma}_{e}^{-1} (\mathbf{m}_{j} - \boldsymbol{\mu}_{L}) \right].$$

Hence

$$\begin{split} &\int h(\boldsymbol{\beta}_1)L(\overrightarrow{\mathbf{m}}_n|\boldsymbol{\beta}_1)d\boldsymbol{\beta}_1 \\ &\propto exp\Big[-(1/2)\Big\{-\mathbf{Z}_n'\Big[\boldsymbol{\Sigma}_1^{-1} + \sum_{j=1}^n\Big(\mathbf{D}_{Lj}'\boldsymbol{\Sigma}_\mathbf{e}^{-1}\mathbf{D}_{Lj}\Big)\Big]\mathbf{Z}_n \\ &+ \mu_1'\boldsymbol{\Sigma}_1^{-1}\mu_1 + \sum_{j=1}^n(\mathbf{m}_j - \mu_L)'\boldsymbol{\Sigma}_\mathbf{e}^{-1}(\mathbf{m}_j - \mu_L)\Big\}\Big]. \end{split}$$

For the new observation m, let $f_c(\mathbf{m}|\overrightarrow{\mathbf{m}}_n)$ be the conditional density of m given $\overrightarrow{\mathbf{m}}_n$ in the constrained case. Then

$$f_{c}(\mathbf{m}|\overrightarrow{\mathbf{m}}_{n}) = \frac{\int h(\boldsymbol{\beta}_{1})L(\overrightarrow{\mathbf{m}}_{n+1}|\boldsymbol{\beta}_{1}, \mathbf{m}_{n+1} = \mathbf{m}, W_{0,n+1} = W_{c})d\boldsymbol{\beta}_{1}}{\int h(\boldsymbol{\beta}_{1})L(\overrightarrow{\mathbf{m}}_{n}|\boldsymbol{\beta}_{1})d\boldsymbol{\beta}_{1}}$$

$$\propto exp\left[-(1/2)\left\{-\mathbf{Z}_{n+1}'\left[\boldsymbol{\Sigma}_{1}^{-1} + \sum_{j=1}^{n+1}\left(\mathbf{D}_{Lj}'\boldsymbol{\Sigma}_{e}^{-1}\mathbf{D}_{Lj}\right)\right]\mathbf{Z}_{n+1}\right] + \mathbf{Z}_{n}'\left[\boldsymbol{\Sigma}_{1}^{-1} + \sum_{j=1}^{n}\left(\mathbf{D}_{Lj}'\boldsymbol{\Sigma}_{e}^{-1}\mathbf{D}_{Lj}\right)\right]\mathbf{Z}_{n} + (\mathbf{m} - \boldsymbol{\mu}_{L})'\boldsymbol{\Sigma}_{e}^{-1}(\mathbf{m} - \boldsymbol{\mu}_{L})\right],$$
(A8)

where \mathbf{Z}_{n+1} is defined as \mathbf{Z}_n with $\mathbf{m}_{n+1} = \mathbf{m}$, and

$$\mathbf{D}_{L,n+1} = \begin{pmatrix} 1 & c_1 & c_2 & \cdots & c_{p-1} \\ W_c & c_1 W_c & c_2 W_c & \cdots & c_{p-1} W_c \end{pmatrix}'.$$

For $k = 1, 2, \dots, n+1$, let $\mathbf{R}_k = \Sigma_1^{-1} \mu_1 + \sum_{j=1}^k \mathbf{D}'_{Lj} \Sigma_{\mathbf{e}}^{-1} (\mathbf{m}_j - \mu_L)$, and let $\mathbf{Q}_k = \Sigma_1^{-1} + \sum_{j=1}^k (\mathbf{D}'_{Lj} \Sigma_{\mathbf{e}}^{-1} \mathbf{D}_{Lj})$. Then with $\mathbf{Z}_{n+1} = \mathbf{R}_n + \mathbf{D}'_{L,n+1} \Sigma_{\mathbf{e}}^{-1} (\mathbf{m} - \mu_L)$, it is easy to show that (A8) is

$$exp\Big[-(1/2)\Big\{-\mathbf{R}'_{n}\mathbf{Q}_{n+1}^{-1}\mathbf{R}_{n}+\mathbf{Z}'_{n}\mathbf{Q}_{n}\mathbf{Z}_{n}+(\mathbf{m}-\boldsymbol{\mu}_{L})'\Big[\boldsymbol{\Sigma}_{\mathbf{e}}^{-1}-\boldsymbol{\Sigma}_{\mathbf{e}}^{-1}\mathbf{D}_{L,n+1}\mathbf{Q}_{n+1}^{-1}\\\cdot\mathbf{D}'_{L,n+1}\boldsymbol{\Sigma}_{\mathbf{e}}^{-1}\Big](\mathbf{m}-\boldsymbol{\mu}_{L})-2\mathbf{R}'_{n}\mathbf{Q}_{n+1}^{-1}\mathbf{D}'_{L,n+1}\boldsymbol{\Sigma}_{\mathbf{e}}^{-1}(\mathbf{m}-\boldsymbol{\mu}_{L})\Big\}\Big]\\\propto exp\Big[-(1/2)\Big\{(\mathbf{m}-\boldsymbol{\mu}_{c})'\boldsymbol{\Sigma}_{c}^{-1}(\mathbf{m}-\boldsymbol{\mu}_{c})\Big\}\Big],$$

where

$$\Sigma_c = \left[\mathbf{I}_p - \mathbf{D}_{L,n+1} \mathbf{Q}_{n+1}^{-1} \mathbf{D}_{L,n+1}' \Sigma_{\mathbf{e}}^{-1}\right]^{-1} \Sigma_{\mathbf{e}},$$

$$\mu_c = \mu_L + \Sigma_c \Sigma_{\mathbf{e}}^{-1} \mathbf{D}_{L,n+1} \mathbf{Q}_{n+1}^{-1} \mathbf{R}_n.$$

The last result is obtained because Q_n , Q_{n+1} , R_n , and Z_n are not function of m.

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