Statistical Analysis and Validation Procedures under the Common Random Number Correlation Induction Strategy for Multipopulation Simulation Experiments

by

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(ABSTRACT)

This thesis provides statistical analysis methods and a validation procedure for conducting this statistical analysis, under the common random number (CRN) correlation-induction strategy. The proposed statistical analysis provides estimates for the unknown parameters that are needed for validating the model. While conducting this statistical analysis, we make some key assumptions. Validation comprises of a three-stage statistical procedure. The first stage tests for the multivariate normality , the second stage tests the structure of the covariance matrix between responses, and the third stage tests for the adequacy of the proposed model.

The statistical analysis and validation procedures are illustrated with an example of a hospital simulation study.

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CHAPTER I INTRODUCTION

In this thesis we consider a correlation induction strategy for performing simulation experiments to reduce the variance of the estimator of the response of interest. The aim of this thesis is two-fold : (a) present methods for conducting statistical analysis under the prescribed correlation induction strategy, and (b) develop a procedure for validating these statistical analysis methods.

Chapter 1 of Pritsker (1987) defines computer simulation as being " the process of designing a mathematical-logical model of a real system and experimenting with this model on a computer. " A *system* is a collection of items from a circumscribed sector of reality that is the object of study or interest. *Models* are descriptions of systems. Throughout this thesis we will consider computer simulation models of *stochastic* systems only. Such systems are characterized by having both probabilistic and time-evolutionary behaviour. Often, real-world problems pertaining such systems are too complex to be solved analytically. In such cases, the system is modeled using simulation in order to provide relevant estimates of system performance.

Rather than describing the aggregate behaviour of a stochastic system, a *simulation model* describes the operation of the system in terms of the *individual events* of the individual components of the system. The system is divided into elements whose behaviour can be predicted, at least probabilistically. The

inter-relationships between the elements also are built into the model. After constructing the model, it is then activated (by generating input data) to simulate the actual operation of the system over time and record its aggregate behaviour. By repeating this simulation for various alternative design configurations and comparing their performances, much can be learned about the behaviour of the system with comparatively little cost. This process of repetitive simulation for for various alternative design configurations is referred to as a statistical experiment or *sampling experiment.* Simulation is alternatively defined (see Hillier and Lieberman, 1987) as the technique of performing sampling experiments on the model of the system. These sampling experiments be can alternatively termed as *simulation experiments.* Others have defined computer simulation in similar terms. Naylor(1971) defines simulation as a numerical technique for conducting experiments with certain types of mathematical models that describe the behaviour of a complex system on a digital computer over extended periods of time. The principal difference between a simulation experiment and a "real world" experiment is that, with simulation, the experiment is conducted with a model of the real world instead of the actual system itself.

A statistical discrete event simulation is a time series experiment. Proper statistical techniques must be applied to simulation output data if the results are to be useful. Since many large-scale simulations require great amounts of computer time and storage, proper statistical analyses can become extremely costly. This is because we need more replications of the simulation to be performed to attain better point estimates and confidence intervals around these estimates. Sometimes the cost of making even a modest statistical analysis can be so high that the precision of the results, perhaps measured by confidence-interval width, will be unacceptably poor.

The simulation analyst should therefore try to increase the efficiency of the simulation. In this document, we focus on statistical efficiency, as measured by the variances of the output random variables from a simulation. If we can somehow reduce the variance of the estimator of an output random variable of interest (such as average delay in queue, or average cost per month in an inventory system) without disturbing its mean (or the expected value), we can obtain greater precision, e.g., smaller confidence intervals, for the same amount of simulating or, alternatively, achieve a prespecified precision with less simulating. Sometimes such a *variance reduction technique* (VRT), properly applied, can make the difference between a prohibitively expensive simulation experiment and a useful one.

This thesis is organized as follows. In Chapter 2 the literature is reviewed. Chapter 3 develops statistical analysis methods under the common random number strategy and also presents validation procedures for the same. The application of these analysis methods and validation procedures is illustrated by means of a numerical example in Chapter 4. Chapter 5 provides a brief conclusion, and future avenues which should be explored as an extension to this work.

CHAPTER II LITERATURE REVIEW

In this chapter we review the literature relevant to the development of this thesis, introduce notation, and define important concepts used throughout this thesis. This chapter is divided into five topical sections : (a) simulation experiments, (b) correlation induction strategies for simulation experiments, (c) statistical analysis of correlation induction strategies, (d) validation of these analysis methods, and (e) a general distribution theory for a class of likelihood criteria. In each section, we give a concise overview of the specific topic. In Section 2.1 we provide the statistical framework necessary to formally define a simulation experiment. In Section 2.2 we focus our attention on two very important correlation induction strategies: (a) common random numbers and (b) the Schruben-Margolin correlation induction strategy. In Section 2.3 we review the statistical analysis procedures devised by Nozari, Arnold, and Pegden (1987) for conducting statistical analysis under the Schruben-Margolin strategy. In Section 2.4 we present the validation procedure offered by Tew and Wilson (1990) for the Nozari, Arnold, and Pegden statistical analysis, and in Section 2.5 we discuss the general distribution theory for a class of likelihood ratio criteria developed by Box (1949) which are critical to the development of our validation procedure.

Throughout this thesis we use $\mathbf{1}_r$ to denote an r-dimensional column vector whose elements are all 1, and $\mathbf{I}_r$ to denote a $(r \times r)$ identity matrix. On occasion, in the de-

velopment of our statistical methodologies, we will make use of the following matrix operation. For any $(t \times s)$ matrix $\mathbf{A}$ and $(m \times n)$ matrix $\mathbf{B} = (b_{ij})$, the Kronecker product of $\mathbf{A}$ and $\mathbf{B}$ is defined as the $(mt \times ns)$ matrix

$$\mathbf{A} \otimes \mathbf{B} = \begin{bmatrix} \mathbf{A}b_{11} & \mathbf{A}b_{12} & \cdots & \mathbf{A}b_{1n} \\ \mathbf{A}b_{21} & \mathbf{A}b_{22} & \cdots & \mathbf{A}b_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ \mathbf{A}b_{m1} & \mathbf{A}b_{m2} & \cdots & \mathbf{A}b_{mn} \end{bmatrix}$$

2.1 Simulation Experiment

Two purposes of simulation analysis could be : (1) The comparison of experimental results under alternative operating conditions (factor settings), and (2) The detection and estimation of the functional relationship that exists between the quantitative input factors and the experimental results. A brief exposition of these topics is provided next.

We define *response* to mean the output of a simulation experiment, and *factors* as the non random inputs. We assume that the simulation analyst controls the values of the factors without error, and that there are d such factors comprising the experiment. The value of factor i is called its factor level, which is denoted by ϕ_i, $i = 1, 2, ..., d$. A particular design point in an experiment is identified by the specific levels of the d experimental factors, denoted by $\varphi = (\phi_1, \phi_2, ..., \phi_d)'$. We assume that there is a linear relationship between the response and the selected setting of φ, that is,

$$y = \mu(\varphi) + \varepsilon, \tag{2.1}$$

where μ, the metamodel of the response variable is linear in the unknown parameters that relate the response to the factor settings, φ, and ε represents the error in μ's to determine y. Often, at each design point the simulation experiment is performed several times in order to acquire a good estimate of the error term variation. However, in simulation much work has been done on acquiring estimates of the error term variation with exactly *one* run performed at each design point (see Section 5 of Schruben and Margolin, 1978). Unlike all other forms of statistical experimentations, simulation experiments offer the researcher a high level of control over the variation in the output response. This control is attained by judicious choice of the random number streams used to drive the random components of the simulation model. In particular, the simulation analyst can induce correlation between the responses sampled during the study (see p. 506 of Schruben and Margolin, 1978). The idea is to choose variates for succesive replications in a clever way.

We now define the random number streams used to drive the simulation model. A simulation model is usually driven by streams of random numbers. These streams are sequences of real numbers scaled to the interval [0,1] and constructed to appear random in nature. We assume that m random number streams are used to drive the simulation model and we let $\mathbf{R}_i$, $i = 1, 2, ..., m$ be the set of m such random number streams such that $\mathbf{R}_i$ is used at the ith design point. The jth component of ith experiment is then

$$y_{ij}(\mathbf{R}_i) = \mu(\varphi_i) + \varepsilon_{ij}(\mathbf{R}_i), \quad \text{for } i = 1, 2, ..., m \text{ and } j = 1, 2, ..., r, \tag{2.2}$$

where y_{ij} is the response at the ith design point and the jth replicate, φ_i is the setting of the d factors at the ith design point, and ε_{ij} is the error at the ith design point and jth replicate. Typically μ is unknown and one of the objectives of the simulation

analysis is to estimate this function. The estimation process usually involves two steps : (a) hypothesize a functional approximation of μ and (b) estimate any unknown parameters in the hypothesized approximation (see p. 210 of Neter, Wasserman, and Kutner, 1989).

For example, under the assumption that μ is first-order and linear in the unknown parameters, equation (2.2) can be written as

$$y_{ij}(\mathbf{R}_i) = \beta_0 + \sum_{k=1}^{p-1} \beta_k x_k(\varphi_i) + \varepsilon_{ij}(\mathbf{R}_i), \quad \text{for } i = 1, 2, ..., m \text{ and } j = 1, 2, ..., r; \tag{2.3}$$

where $\boldsymbol{\beta} = (\beta_0, \beta_1, ..., \beta_{p-1})'$ is the $(p \times 1)$ vector of unknown metamodel coefficients; x_k $(k = 1,2, ...,p - 1)$ represent known functions of these settings and y_{ij}, φ_i, and ε_{ij} are as defined above.

Equation (2.3) can be written in matrix notation as :

$$\mathbf{y}_j = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}_j, \quad \text{for } j = 1, 2, ..., r, \tag{2.4}$$

where $\mathbf{y} = (y_{1j}, y_{2j}, ..., y_{mj})'$, is the vector of responses at the jth replication, $\mathbf{X}$ is the $(m \times p)$ design matrix whose first column is all ones and whose $(i, j + 1)$th element is $x_j(\varphi_i)$, $(i = 1, 2, ..., m$ and $j = 1, 2, ..., p - 1)$, $\boldsymbol{\beta}$ is defined above, and $\boldsymbol{\varepsilon}_j = (\varepsilon_{1j}, \varepsilon_{2j}, ..., \varepsilon_{mj})'$ is the vector of random errors.

We also assume that $\boldsymbol{\varepsilon}_j$ $(j = 1, 2, ..., r)$ has the following multivariate normal distribution :

$$\boldsymbol{\varepsilon}_j \sim \mathbf{N}_m(\mathbf{0}_m, \boldsymbol{\Sigma}), \quad \text{for } j = 1, 2, ..., r, \tag{2.5}$$

where $\mathbf{0}_m$ is a $(m \times 1)$ vector of zeros and $\boldsymbol{\Sigma}$ is a $(m \times m)$ covariance matrix, such that the distribution of $\boldsymbol{\varepsilon}$ is nondegenerate. (Typically, in classical linear models $\boldsymbol{\Sigma} = \sigma^2\mathbf{I}_m$, that is, the error terms are uncorrelated across design points.)

From (2.4) and (2.5) we get that

$$\mathbf{y}_j \sim \mathbf{N}_m(\mathbf{X}\boldsymbol{\beta}, \boldsymbol{\Sigma}), \quad \text{for } j = 1, 2, ..., r. \tag{2.6}$$

Under these assumptions, and for $m > p$ (see p. 210 of Neter and Wasserman, and Kutner, 1989), the least-squares estimate of $\boldsymbol{\beta}$,

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\bar{\mathbf{y}}, \tag{2.7}$$

has the following distribution :

$$\hat{\boldsymbol{\beta}} \sim \mathbf{N}_p(\boldsymbol{\beta}, (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\Sigma}\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}), \tag{2.8}$$

where $\bar{\mathbf{y}} = \sum_{j=1}^{r}\mathbf{y}_j$, Thus, knowing the distribution of $\hat{\boldsymbol{\beta}}$, the least-squares estimator of $\boldsymbol{\beta}$, we can obtain $100(1-\alpha)\%$ confidence intervals for $\boldsymbol{\beta}$ (see p. 114 of Myers and Milton, 1991). Also, hypotheses tests can be performed on $\boldsymbol{\beta}$ (see p. 116 of Myers and Milton, 1991), and we could check for any linear dependence in β_i's.

2.2 Correlation Induction Strategies For Simulation Experiments

Variance reduction techniques (VRT) reduce the variance of the estimator by replacing the original sampling procedure by a new procedure that yields the same expected value but with a smaller variance. Often, attention is restricted to the

estimation of the mean value or the expected value. Hence VRTs can be regarded as methods that reduce the variance of the estimate of the mean response. This response can be the waiting time of a customer in the steady state, the total profit of a firm over the planning period, etc. Some of the different VRTs used are stratified sampling, control variates, importance sampling, antithetic variates, common random numbers, and joint application of antithetic variates and common random numbers (see pp. 110-200 of Kleijnen, 1974). (A detailed treatment on VRTs can be found in Chapter 11 of Law and Kelton, 1991, chapters 2 and 8 of Bratley, Fox, and Schrage, 1983, and Chapter 3 of Kleijnen, 1974.) In the remainder of this thesis we will direct our attention to the techniques of common random numbers and joint application of the antithetic variates and common random numbers.

Simulation offers unusual opportunities for deliberately and advantageously inducing correlation, positive or negative, among observations. When comparing policies, using random number streams common to all of these policies offers a fairer comparison than would statistically independent streams since one source of variability has been removed by testing all policies under the same conditions (see p. 42 of Bratley, Fox, and Schrage, 1983). In a simulation experiment, usually more than one random number stream is employed at one setting of the factors. This, in practice, tends to amplify the magnitudes of the purposefully induced correlations between the observations at different factor settings (see p. 507 of Schruben, 1979).

When the same set of random number streams is used at two design points, the two output responses tend to exhibit positive correlation (see p. 614 of Law and Kelton, 1991, p. 46 of Bratley, Fox and Schrage, 1983, or, p. 200 of Kliejnen, 1974). If the same stream of random numbers were used in two different simulations (common random

number strategy), one producing an univariate output y_1 and the other an univariate output y_2, then we expect $\text{cov}(y_1, y_2) = \sigma^2\rho_+ > 0$. The variance of $(y_1 - y_2)$ is given by

$$var(y_1 - y_2) = var(y_1) + var(y_2) - 2cov(y_1, y_2).$$

Consequently, the statistic $y_1 - y_2$ has a smaller variance than would occur with independent streams because this leads to $\text{cov}(y_1, y_2) = 0$. Thus, the common random number allows in detection of smaller differences between y_1 and y_2 than do independent streams.

By contrast, the antithetic variates strategy induces negative correlations between responses (see p. 628 of Law and Kelton, 1991, p. 54 of Bratley, Fox, and Schrage, 1983, or, p. 186 of Kleijnen, 1974). This technique is implemented by generating one response from random number seed **R**, and the other response from its antithetic random number seed $(\mathbf{1} - \mathbf{R})$. If y_1 and y_2 are the corresponding univariate outputs, then we expect $\text{cov}(y_1, y_2) = \sigma^2\rho_- < 0$ so that $\frac{(y_1 + y_2)}{2}$ has a smaller variance than occurs when independent streams are used.

If independent streams are used, then there is no correlation between the responses. (see p. 614 of Law and Kelton, 1991, or, p. 507 of Schruben and Margolin, 1978). This is due to the fact that the output response variables obtained are independent of each other.

Schruben and Margolin (1978) recommended a correlation induction strategy for a special class of multipopulation experiments. This strategy partitions the design matrix **X** (see equation (2.4)) into two blocks. A set of common random number streams is applied to the first block, and a set of random number streams antithetic to the one in the first block is applied to the second block. Their strategy, under certain re-

strictions effectively combines common random numbers and antithetic variates' strategies in the same experiment to reduce the variance of the response.

Next, we consider the concept of blocking. A block is a portion of the experimental material that is expected to be more homogeneous than the aggregate. By confining treatment comparisons within such blocks, greater precision can often be obtained (see p. 102 of Box, Hunter, and Hunter, 1978. Blocking is also discussed in Chapter 6 of Cochran and Cox, 1966).

The idea of blocking applied to a simulation experiment is as follows. We consider the sets of random number streams as producing random controllable block effects that should be incorporated into the model (see p. 512 of Schruben and Margolin, 1978).

Let $\mathbf{R}$ (possibly with an index) denote a set of random number streams, and let $\overline{\mathbf{R}}$ denote its antithetic set, i.e. $\overline{\mathbf{R}} = \mathbf{1} - \mathbf{R}$. If v random block effects are denoted by the components of

$$\gamma = (\gamma_1, \gamma_2, \ldots, \gamma_v)',$$

and the $(m \times s)$ block incidence matrix ω is defined as $\omega = [\omega_{ih}]$ where,

$$\omega_{ik} = \begin{cases} 1 & \text{if observation } i \text{ is in block } k, \\ 0 & \text{otherwise} \end{cases}$$

then the generalization of equation (2.3) to incorporate block effects is

$$\mathbf{y} = \mathbf{X}\beta + \omega\gamma + \varepsilon. \tag{2.9}$$

We now define *orthogonal blocking*.

Definition : An m-point experimental design whose corresponding **X** matrix is partitioned as $\mathbf{X} = (\mathbf{1}_m | \mathbf{T})$ with $\mathbf{T}'\mathbf{1}_m = \mathbf{0}_{p-1}$, admits orthogonal blocking into s blocks if there exists an $(m \times s)$ block incidence matrix ω , defined above, such that $\mathbf{1}'_m\omega$ is a vector of positive integers and

$$\mathbf{T}'\omega = \mathbf{0}.$$

where $\mathbf{0}$ is a $((p-1) \times s)$ matrix of zeros.

This definition is clearly model-dependent and implies that a design admitting orthogonal blocking into s blocks also admits orthogonal blocking into s' blocks, for $s > s'$ (see p. 513 of Schruben and Margolin, 1978). Under the assumption that **X** can be partitioned as stated above,

$$(\mathbf{X}'\mathbf{X})^{-1} = \begin{bmatrix} m^{-1} & \mathbf{0} \\ \mathbf{0} & (\mathbf{T}'\mathbf{T})^{-1} \end{bmatrix}. \tag{2.10}$$

For an experimental design that admits orthogonal blocking, Schruben and Margolin (1978) formulated the Assignment Rule for prescribing how to assign random number streams across design points. This rule is stated below.

Assignment Rule : For the linear model in (2.3) with p parameters, if the m-point experimental design admits orthogonal blocking into two blocks of sizes m_1 and m_2, preferably chosen to be as nearly equal in size as possible, then for all m_1 design

points in the first block, use a set of pseudorandom numbers **R**, chosen randomly, and for all m_2 design points in the second block, use $\overline{\mathbf{R}}$.

They also showed that if an experimental design admits orthogonal blocking and the earlier assumptions about induced dependence hold, then the Assignment Rule always yields Ordinary Least Squares (OLS) estimators with a smaller value of the Dispersion matrix (D-value) than will (a) the assignment of one common set of random number streams to all design points, or (b) the assignment of a different set of random number streams to each design point, provided

$$\{1 + (m-1)\rho_+ - 2m^{-1}m_1m_2(\rho_+ + \rho_-)\}(1-\rho_+)^p < 1$$

in the latter case.

They further showed that maximum benefit is obtained from the Assignment Rule if the two block sizes are equal; i.e. if $m_1 = m_2 = m/2$.

If g sets of seeds are used in a simulation experiment, then define, $\mathbf{R}_{j+g} = \overline{\mathbf{R}}_j$, $(j = 1, 2, ..., g)$. Let $k(i)$ denote the index of the set of random number streams chosen for the ith experimental point, i.e. $\mathbf{R}_{(k(i))}$ is chosen. They proposed a model for the experimental error on the randomly chosen set of random number streams which is given by,

$$\boldsymbol{\varepsilon} = \mathbf{b} + \boldsymbol{\varepsilon}^*,$$

where, $\mathbf{b} = \{b(\mathbf{R}_{(k(1))}), b(\mathbf{R}_{(k(2))}), ..., b(\mathbf{R}_{(k(m))})\}$ is the $(m \times 1)$ column vector of random block effects across the whole design.

That is, the error is decomposed into two random components, the block effect **b**, and pure error, ε^*.

For the analysis of their assignment rule, Schruben and Margolin (1978) made the following eight assumptions :

1. When two observations are made with the same randomly selected streams, a positive correlation of unknown magnitude, ρ_+, is induced between the mean responses.
2. When two observations are made with the same selected sets of seeds, but with antithetic streams, a negative correlation, ρ_-, is induced between the mean responses.
3. When two observations are made with different randomly selected streams, the output responses have zero correlation, i.e., $\text{corr}(y_1, y_2) = 0$.
4. The positive correlation induced by using $\mathbf{R}_j$, $(j = 1, 2, ..., g)$ at two design points is a constant ρ_+, which does not depend on the specific sets of seeds or the specific pair of design points. Similarly, the negative correlation induced by using $\mathbf{R}_j$ and $\overline{\mathbf{R}}_j$ at two design points is a constant $-\rho_-$ with $\rho_+ \geq -\rho_-$. (Note that $\rho_- > 0$).
5. ε^* and **b** are uncorrelated, i.e., $\text{corr}(\varepsilon^*, \mathbf{b}) = \mathbf{0}_{(m \times m)}$.
6. The components of ε^* are uncorrelated.
7. $E[\varepsilon^*] = E[\mathbf{b}] = \mathbf{0}_m$.
8. The component $b(\mathbf{R}_{(k(i))})$, $(i = 1, 2, ..., m)$, depends on the ith design point only through the set of random number streams used here.

Assumptions 1-8 imply (see p. 513 of Schruben-Margolin, 1978)

1. $$cov(b(R_{(k(i))}), b(R_{(k(j))})) = \begin{cases} \rho_+ \text{ if } k(i) = k(j), \\ -\rho_- \text{ if } |k(i) - k(j)| = g, \\ 0 \quad \text{otherwise.} \end{cases}$$

2. $$cov(\varepsilon^*) = (1 - \rho_+)\mathbf{I}_m.$$

which indicates that the variance of the error is reduced by an amount ρ_+.

Using the above assumptions we can obtain the Schruben-Margolin covariance structure. Now, $\mathbf{X}$ is assumed to be orthogonally blockable into two blocks. Let $\mathbf{X}_1$ denote the rows corresponding to the first block, and let $\mathbf{X}_2$ denote the rows of the second block. Without loss of generality suppose that observations in each replication are arranged so that $\mathbf{X} = (\mathbf{X}'_1\, \mathbf{X}'_2)'$. Then, the assumptions of Schruben and Margolin yield $\Xi = \Sigma \otimes \mathbf{I}_r$, where Σ is given by,

$$\Sigma = \sigma^2 \begin{bmatrix} 1 & \rho_+ & & & \rho_+ & -\rho_- & -\rho_- & & & -\rho_- \\ \rho_+ & 1 & & & \rho_+ & -\rho_- & -\rho_- & & & -\rho_- \\ \vdots & \vdots & & & \vdots & \vdots & \vdots & & & \vdots \\ \rho_+ & \rho_+ & & & 1 & -\rho_- & -\rho_- & & & -\rho_- \\ -\rho_- & -\rho_- & & & -\rho_- & 1 & \rho_+ & & & \rho_+ \\ -\rho_- & -\rho_- & & & -\rho_- & \rho_+ & 1 & & & \rho_+ \\ \vdots & \vdots & & & \vdots & \vdots & \vdots & & & \vdots \\ -\rho_- & -\rho_- & & & -\rho_- & \rho_+ & \rho_+ & & & 1 \end{bmatrix}. \tag{2.11}$$

Under these assumptions, all feasible correlation matrices can be permuted into block diagonal form (see p. 513 of Schruben and Margolin, 1978). For $h = 1, 2, ..., 2g$, define the indicators

$$\omega_{ik} = \begin{cases} 1 & \text{if } \mathbf{R}_h \text{ is used for experimental point } i, \\ 0 & \text{otherwise} \end{cases}$$

and define the $(m \times 2g)$ matrix $\mathbf{W} = [\omega_{ih}]$, where g is the number of sets of seeds used. Similarly, define

$$\mathbf{B} = \{\mathbf{b}(\mathbf{R}_1), \mathbf{b}(\mathbf{R}_2), ..., \mathbf{b}(\mathbf{R}_{2g})\}'.$$

Then the general linear model can be rewritten as :

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{W}\mathbf{B} + \boldsymbol{\varepsilon}^*. \tag{2.12}$$

The selection of m sets of random number streams for a simulation experiment is now equivalent to specifying $\mathbf{W}$ consistently.

The Schruben-Margolin correlation induction strategy is an important and interesting example of the use of a statistical approach in a stochastic simulation. But this strategy is limited to an experimental design that admits orthogonal blocking into two blocks. In general, this conditions may be neither satisfied nor desired (see p. 126 of Myers, 1976).

Under the eight assumptions listed earlier, for a wide class of problems, Schruben and Margolin give a simulation experiment strategy that satisfies the D-optimality criterion, that is, under the assignment rule, the determinant of the covariance matrix of β_i's, $i = 0, 1, ..., p$, the unknown parameters in (2.4) for the ordinary least squares and the weighted least squares is minimized. Also, under the assignment rule, the trace of this covariance matrix is minimized, which is the A-optimality criterion.

2.3 Statistical Analysis under the Schruben-Margolin Strategy

Nozari, Arnold, and Pegden (1987) presented methods for conducting statistical analysis for use with the above mentioned Schruben-Margolin correlation induction strategy in the context of univariate responses.

Nozari, Arnold, and Pegden (1987) assume that the vector of responses across all design points and replicates has the following multivariate normal distribution.

$$\mathbf{y} = \begin{bmatrix} \mathbf{y}_1 \\ \vdots \\ \mathbf{y}_r \end{bmatrix} \sim N_{mr}\left[\begin{bmatrix} \mathbf{X} \\ \vdots \\ \mathbf{X} \end{bmatrix}\beta, \Xi\right], \tag{2.13}$$

where, $\mathbf{X} = (\mathbf{1}_m | \mathbf{T})$ is an $(m \times p)$ known design matrix of rank $p \leq m$, $\beta = (\beta_0, \beta_1)'$ is an unknown p-dimensional vector, Ξ is the $(mr \times mr)$ covariance matrix, and r is the number of times the design is replicated.

Nozari, Arnold and Pegden (1987) presented four procedures for conducting statistical analysis in conjunction with the Schruben-Margolin strategy. These procedures provide the following :

- optimal (unifomly minimum variance unbiased) estimate of $\boldsymbol{\beta}$,
- a confidence interval for β_0,
- a confidence interval for $\boldsymbol{\beta}_1$, and
- a joint confidence interval for β_0 and $\boldsymbol{\beta}_1$.

In a statistical framework, we use point estimates, hypothesis tests, and confidence intervals to answer questions regarding the adequacy of the proposed model, or, whether there exist a subset of variables that adequately explain the observed variation in response, or, whether there is a particular variable in the model useful in helping to predict a response (see p. 144 of Milton and Myers, 1991).

We now investigate the four procedures presented by Nozari, Arnold, and Pegden.

Let $\hat{\boldsymbol{\beta}}$ and $\hat{\sigma}^2$ be the usual unbiased estimators for this model :

$$\hat{\boldsymbol{\beta}} = (\hat{\beta}_0, \hat{\boldsymbol{\beta}}_1)' = (\mathbf{G}'\mathbf{G})^{-1}\mathbf{G}'\mathbf{y}, \tag{2.14}$$

$$\hat{\sigma}^2 = \|\mathbf{y} - \mathbf{G}\hat{\boldsymbol{\beta}}\|^2, \tag{2.15}$$

where,

$$\mathbf{G} = \begin{bmatrix} \mathbf{X} \\ \vdots \\ \mathbf{X} \end{bmatrix};$$

then we have

Result 1 : $\hat{\boldsymbol{\beta}}$ is the UMVU estimator of $\boldsymbol{\beta}$

Let y_{ijl} denote the lth observation in the jth block of the ith replication for $i = 1, 2, \ldots, r$, $j = 1, 2$, and $l = 1, 2, \ldots, m$. Define

$$\bar{y}_{ij.} = \sum_{l=1}^{m} \frac{y_{ijl}}{m}, \quad \bar{y}_{i..} = \sum_{j=1}^{2} \frac{y_{ij.}}{2}, \quad \bar{y}_{...} = \sum_{i=1}^{r} \frac{y_{i..}}{r}, \tag{2.16}$$

and

$$\hat{\tau}^2 = 2m \sum_{i=1}^{r} \frac{(\bar{y}_{i..} - \bar{y}_{...})^2}{(r-1)} \tag{2.17}$$

then we have

Result 2 : $\dfrac{[(2mr)^{(1/2)}(\hat{\beta}_0 - \beta_0)]}{\hat{\tau}_1} \sim t_{r-1}$. This result can be used in the obvious way to construct $100(1-\alpha)\%$ confidence intervals for β_0. That is,

$\beta_0 \in \hat{\beta}_0 \pm \dfrac{\hat{\tau}}{(2mr)^{1/2}} t^{\alpha/2}_{r-1}$.

Let f be the usual test statistic for testing $H_0 : \mathbf{H}\boldsymbol{\beta}_1 = \mathbf{0}_h$ vs $H_1 : \mathbf{H}\boldsymbol{\beta}_1 \neq \mathbf{0}_h$, where $\mathbf{H}$ is a known $(h \times (p-1))$ matrix of rank $h < p$, when $\boldsymbol{\Xi} = \sigma^2 \mathbf{I}_n$. That is,

$$f = \frac{(r(\mathbf{H}\hat{\boldsymbol{\beta}}_1)'(\mathbf{H}(\mathbf{T}'\mathbf{T})^{-1}\mathbf{H}')^{-1}(\mathbf{H}\hat{\boldsymbol{\beta}}_1))}{h\hat{\sigma}^2} \tag{2.18}$$

Let HW_l denote the half-width of the $100(1-\alpha)\%$ simultaneous confidence intervals for the set of $\mathbf{l}'\mathbf{H}\boldsymbol{\beta}_1$, for all $\mathbf{l} \in R^k$, when $\boldsymbol{\Xi} = \sigma^2 I_n$. That is

$$HW_l = \hat{\sigma}\left[\frac{h}{r}\left(F^{\alpha}_{h,n-p}\mathbf{l}'\mathbf{H}(\mathbf{T}'\mathbf{T})^{-1}\mathbf{H}'\mathbf{l}\right)\right]^{1/2}.$$

Define

$$\hat{\tau}_3^2 = \frac{(n-p)\hat{\sigma}^2 - m\sum_{i=1}^{r}\sum_{j=1}^{2}(\bar{y}_{ij.} - \bar{y}_{...})^2}{(n-p-2r+1)}; \tag{2.19}$$

then we have

Result 3 : The optimal test for testing $H_0 : \mathbf{H}\boldsymbol{\beta}_1 = \mathbf{0}_h$ vs $H_1 : \mathbf{H}\boldsymbol{\beta}_1 \neq \mathbf{0}_h$, where $\mathbf{H}$ is a known $(h \times (p-1))$ matrix of rank $h < p$, rejects H_0 if

$$f^* = \frac{f\hat{\sigma}^2}{\hat{\tau}_3^2} > F^{\alpha}_{h,n-p-2r+1}. \tag{2.20}$$

The $100(1-\alpha)\%$ simultaneous confidence interval for the set of $\mathbf{l}'\mathbf{H}\boldsymbol{\beta}_1$ for all $\mathbf{l} \in R^k$ when $\boldsymbol{\Xi} = \boldsymbol{\Sigma} \otimes \mathbf{I}$, is

$$\mathbf{l}'\mathbf{H}\boldsymbol{\beta}_1 \in \mathbf{l}'\mathbf{H}\boldsymbol{\beta} \pm \frac{\hat{\tau}_3^2 F^{\alpha}_{h,n-p-2r+1}}{\hat{\sigma}^2 F^{\alpha}_{h,n-p}}^{1/2} HW_l. \tag{2.21}$$

One might be interested in inferences that involve both β_0 and $\boldsymbol{\beta}_1$ simultaneously. Let $\bar{\mathbf{y}}$ be the m-dimensional vector of sample means, and $\mathbf{S}$ be the $(m \times m)$ sample covariance matrix of $\mathbf{y}_i$'s,

$$\bar{\mathbf{y}} = \frac{1}{r}\sum_{i=1}^{r}\mathbf{y}_i, \qquad \mathbf{S} = \left(\frac{1}{(r-1)}\right)\sum_{i=1}^{r}(\mathbf{y}_i - \bar{\mathbf{y}})(\mathbf{y}_i - \bar{\mathbf{y}})'; \tag{2.22}$$

then we have

Result 4 : A size α procedure for testing $H_0 : \mathbf{K}\boldsymbol{\beta} = \mathbf{0}_k$ vs $H_1 : \mathbf{K}\boldsymbol{\beta} \neq \mathbf{0}_k$, where $\mathbf{K}$ is a $(k \times p)$ known matrix of rank $k \leq p$, is to reject H_0 if

$$\left[\frac{r(r-k)}{k(r-k)} \hat{\boldsymbol{\beta}}'\mathbf{K}'(\mathbf{K}\hat{\Delta}\mathbf{K}')^{-1}\mathbf{K}\hat{\boldsymbol{\beta}} \right] > F^{\alpha}_{k,r-k},$$

where $\hat{\Delta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{S}\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}$. A set of $100(1-\alpha)\%$ simultaneous confidence intervals is given by

$$\mathbf{l}'\mathbf{K}\boldsymbol{\beta} \in \mathbf{l}'\mathbf{K}\boldsymbol{\beta} \pm \left[\frac{k(r-1)}{r(r-1)} F^{\alpha}_{k,r-k} \mathbf{l}'\mathbf{K}\hat{\Delta}\mathbf{K}'\mathbf{l} \right]^{1/2} \tag{2.23}$$

for all $\mathbf{l} \in R^k$.

The proofs of these results are given on pages 135 through 137 in Nozari, Arnold, and Pegden (1987).

In order to derive results for drawing inferences about β_0 and $\boldsymbol{\beta}_1$ separately, it is useful to transform the model to one with with independent observations. In other words the aim is to get a block diagonal structure for the covariance matrix. This is done using an $(n \times n)$ orthogonal transformation $\boldsymbol{\Gamma}^{[SM]}$, where

$$\boldsymbol{\Gamma}^{[SM]} = \begin{bmatrix} ((2m)^{(-1/2)}\mathbf{1}'_m \quad (2m)^{(-1/2)}\mathbf{1}'_m)\otimes\mathbf{I}_r \\ ((2m)^{(-1/2)}\mathbf{1}'_m \quad -(2m)^{(-1/2)}\mathbf{1}'_m)\otimes\mathbf{I}_r \\ \mathbf{C}'_m \otimes_m \mathbf{I}_{2r} \end{bmatrix}, \tag{2.24}$$

where $\mathbf{C}_m$ is a $(m \times (m-1))$ matrix such that $(m^{(-1/2)}\mathbf{1}_m\mathbf{C}_m)$ is orthogonal. Define

$$\mathbf{y}^* = \begin{bmatrix} \mathbf{y}_1^* \\ \mathbf{y}_2^* \\ \mathbf{y}_3^* \end{bmatrix} = \mathbf{\Gamma}^{[SM]}\mathbf{y}, \quad \mathbf{T}^* = \begin{bmatrix} \mathbf{C}'_m\mathbf{T}_1 \\ \mathbf{C}'_m\mathbf{T}_2 \\ \vdots \\ \mathbf{C}'_m\mathbf{T}_2 \end{bmatrix}, \tag{2.25}$$

$$\mathbf{G}^* = \mathbf{\Gamma}^{[SM]}\mathbf{G}, \quad \mathbf{\Xi}^{[SM]*} = \mathbf{\Gamma}^{[SM]}\mathbf{\Xi}^{[SM]}\mathbf{\Gamma}^{[SM]}, \tag{2.26}$$

where $\mathbf{y}_1^*$ and $\mathbf{y}_2^*$ are $(r \times 1)$. Let $\mathbf{y}_{ij}$ denote the $(m \times 1)$ vector of observations in the jth block of the ith replication for $i = 1, 2, ..., r$ and $j = 1, 2$, then,

$$\mathbf{y}_1^* = \begin{bmatrix} (2m)^{(-1/2)}(\mathbf{1}'_m\mathbf{y}_{11} + \mathbf{1}'_m\mathbf{y}_{12}) \\ \vdots \\ (2m)^{(-1/2)}(\mathbf{1}'_m\mathbf{y}_{r1} + \mathbf{1}'_m\mathbf{y}_{r2}) \end{bmatrix}, \tag{2.27}$$

$$\mathbf{y}_2^* = \begin{bmatrix} (2m)^{(-1/2)}(\mathbf{1}'_m\mathbf{y}_{11} - \mathbf{1}'_m\mathbf{y}_{12}) \\ \vdots \\ (2m)^{(-1/2)}(\mathbf{1}'_m\mathbf{y}_{r1} - \mathbf{1}'_m\mathbf{y}_{r2}) \end{bmatrix}, \tag{2.28}$$

and

$$\mathbf{y}_3^* = \begin{bmatrix} \mathbf{C}'_m\mathbf{y}_{11} \\ \mathbf{C}'_m\mathbf{y}_{12} \\ \vdots \\ \mathbf{C}'_m\mathbf{y}_{r2} \end{bmatrix}. \tag{2.29}$$

Thus, we have $\mathbf{y} \sim N_{mr}(\mathbf{G}^*\boldsymbol{\beta}, \mathbf{\Xi}^{[SM]*})$, with

$$\mathbf{G}^* = \begin{bmatrix} (2m)^{(1/2)}\mathbf{I}_r & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{T}^* \end{bmatrix}, \tag{2.30}$$

and

$$\Xi^* = \begin{bmatrix} \tau_1^2 \mathbf{I}_r & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \tau_2^2 \mathbf{I}_r & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \tau_3^2 \mathbf{I}_{(2r(m-1))} \end{bmatrix}, \tag{2.31}$$

where $\tau_1^2 = \sigma^2(1 + (m-1)\rho_+ - m\rho_-)$, $\tau_2^2 = \sigma^2(1 + (m-1)\rho_+ + m\rho_-)$ and $\tau_3^2 = \sigma^2(1 - \rho_+)$. Nozari, Arnold and Pegden (1987) further developed the following theorems which are a consequence of the above transformation.

Theorem 1 : $\mathbf{y}_1^*$, $\mathbf{y}_2^*$, and $\mathbf{y}_3^*$ are independent.

Theorem 2 : $\mathbf{y}_1^* \sim N_r((2m)^{(1/2)}\mathbf{1}_r\beta_0, \tau_1^2\mathbf{I}_r)$.

Theorem 3 : $\mathbf{y}_2^* \sim N_r(0, \tau_2^2\mathbf{I}_r)$.

Theorem 4 : $\mathbf{y}_3^* \sim N_{2r(m-1)}(\mathbf{T}^*\boldsymbol{\beta}_1, \tau_3^2\mathbf{I}_{2r(m-1)})$.

Thus, using the transformation $\mathbf{\Gamma}^{[SM]}$ on the response vector $\mathbf{y}$, the transformed vector of responses, $\mathbf{y}^*$ is obtained, which has its covariance matrix in a desirable block diagonal form. Also, this transformation is invertible and does not involve any unknown parameters, so that any procedure based on $\mathbf{y}^*$ is also optimal among procedures based on $\mathbf{y} = \mathbf{\Gamma}^{[SM]'}\mathbf{y}^*$. Clearly, from (2.17) and Theorems 1-4, we see that the model involving $\mathbf{y}^*$ is really three separate ordinary linear models, one involving $(\mathbf{y}_1^*, \beta_0, \tau_1^2)$, one involving $(\mathbf{y}_2^*, \tau_2^2)$, and one involving $(\mathbf{y}_3^*, \boldsymbol{\beta}_1, \tau_3^2)$.

Nozari, Arnold, and Pegden (1987), as a part of their conclusions state that the assumption of constant correlation magnitudes is doubtful. (However, see the results of Tew and Wilson (1990) provided in the next section). They assert that the as-

sumption that the magnitudes of the positive induced correlations are greater than the magnitudes of the negative induced correlations seems reasonable.

2.4 Validation Of Simulation Analysis Methods

Tew and Wilson (1990) have presented a procedure for validating the simulation analysis methods for the Schruben-Margolin correlation induction strategy. There are certain assumptions made while conducting the statistical analysis, such as the multivariate normality of the response vector **y** as given by (2.13), the Schruben-Margolin covariance structure in (2.11), and the adequacy of the proposed linear model in (2.4). This validation procedure determines the extent to which the underlying assumptions are satisfied and identifies modifications of the experimental protocol that might be required to correct significant violations of these assumptions. The procedure is divided into three stages. Each stage of the validation procedure tests a key assumption about the behaviour of the response across all points in the experimental design. We now outline the validation procedure.

The Validation Procedure: The three-stage procedure for comprehensive diagnostic testing follows :

1. Test for Multivariate Normality :

   H_0 : $\mathbf{y}_i \sim N_m(\mu, \Sigma^{[SM]})$, where $\Sigma^{[SM]}$ is positive definite but otherwise μ and $\Sigma^{[SM]}$ are unspecified,

   versus,

   H_1 : $\mathbf{y}_i$ has any non-singular m -dimensional distribution.

2. Test for the induced covariance structure :

H_0: cov $(\mathbf{y}_i) = \Sigma_\delta^{[SM]}$ with σ^2, ρ_+, and ρ_- as in (2.13) so that $\Sigma_\delta^{[SM]}$ is positive definite, $\rho_+ > 0$; otherwise σ^2, ρ_+, and σ_- are unspecified,

versus,

H_1 : cov($\mathbf{y}_i$) is positive definite.

3. Test for Lack-of-Fit in the Linear Model :
$H_0 : E[\mathbf{y}_i] = \mathbf{X}\boldsymbol{\beta}$, versus, $H_1 : E[\mathbf{y}_i] \neq \mathbf{X}\boldsymbol{\beta}$.

The first stage of the validation procedure uses a multivariate extension of the Shapiro-Wilk statistic to test the assumption of joint normality for the set of simulation responses taken across all points in the experiment. The second stage uses a modified likelihood ratio statistic to test for the type of " generalized repeated measures " covariance structure that is assumed to result from applying the Schruben-Margolin strategy. Finally, the third stage uses a lack-of-fit test specialized for the Schruben-Margolin covariance structure.

The results obtained by Tew and Wilson show that the diagnostic tools developed for validation of the Schruben-Margolin assumptions enhance the capability of the practitioner to analyze effectively simulation experiments performed with the Schruben-Margolin strategy.

2.5 Distribution Theory For Likelihood Criteria

For the validation of certain key assumptions made while conducting statistical analysis, such as the multivariate normality of the response vector **y** as given by (2.12), the Schruben-Margolin covariance structure in (2.13), and that of the adequacy of the

proposed linear model in (2.4), we need to perform some statistical tests similar to the ones offered by Tew and Wilson (1990). Generalized tests were developed by Box(1949), and we apply these to develop our validation procedure.

As observed by Box (1949), the likelihood ratio method of Neyman and Pearson (1928) has been used frequently to derive criteria for testing a large number of hypotheses. The problem lies not so much in deriving the criterion, but finding the exact distributions of the likelihood ratio when the hypotheses are true, and determining the best critical region to adopt (see p. 317 of Box, 1949).

Let N denote the total sample size and L_1 denote the likelihood ratio statistic. Then, the statistic $M = -N \ln(L_1)$ would be asymptotically (for L_1) distributed as χ^2 with N degrees of freedom (see p. 317 of Box, 1949).

Box used the generalized expression for moments of the likelihood ratio statistic to obtain a distribution for the logarithmic statistic M, a χ^2 approximation, and an asymptotic χ^2 series. This was done to match the moments of the distribution of the likelihood ratio statistic to the moments of a chi-squared distribution. He investigated this method for two general criteria :

1. The test for constancy of variance and covariance of m sets of p- variate samples. This includes, as an important special case when $p = 1$, the test for constancy of variance in the samples.
2. Wilk's test (see p.318 of Box, 1949) for the independence of m sets of residuals, the lth set having p_l variates. When $m = 2$ this corresponds to the test of significance used in multivariate regression, and analysis of variance and covariance,

and when $m = 2$ and p_1 or p_2 is unity, it gives the corresponding univariate tests. In the latter case, of course, the exact distributions are known.

Box refers to these criteria as generalized tests for homoscedasticity and independence, respectively. Box assumes normality or multinormality for the original observations.

Suppose s_{ijl} is the usual unbiased estimate of the variance or covariance Σ between the ith and jth variable in the lth sample based on sums of squares and products having v_l degrees of freedom, and suppose there are m such samples and s_{ij} is the average variance or covariance $\frac{(\sum_{l=1}^{k} v_l s_{ilj})}{N}$, where $N = \sum_{l=1}^{k} v_l$. Box (1949, p. 320) then takes the criterion to test for homoscedasticity as the generalized form of Bartlett's criterion to be

$$M = N \ln |s_{ij}| - \sum_{l=1}^{k} \ln |s_{ijl}| = -N \ln(L'_1) \tag{2.32}$$

where

$$L'_1 = \prod_{l=1}^{k} \left[\frac{|s_{ijl}|}{|s_{ij}|} \right]^{\left(\frac{v_l}{N}\right)} \tag{2.33}$$

Box (1949, p. 321) obtained the moments of L'_1 when the null hypothesis, that of the constancy of variance and covariance of m sets of p-variate samples, is true. If c_{ijl} are the sums of squares and products based on v_l degrees of freedom corresponding

to the s_{ijl}, we have $c_{ijl} = \nu_l s_{ijl}$, $c_{ij} = \sum_l c_{ijl}$. The joint probability density of the c_{ijl} for the lth sample is given by the Wishart distribution :

$$p(c_{11l}, c_{12l}, \ldots, c_{ppl}) = K(\nu_l)|c_{ijl}|^{\frac{1}{2}(\nu_l - p - 1)} \exp\{\frac{-1}{2}\sum_{ij}(\Sigma^{-1}c_{ijl})\}, \quad (2.34)$$

$$\{K(\nu_l)\}^{-1} = 2^{\frac{1}{2}(\nu_l p)}\pi^{\frac{1}{4}p(p-1)}\prod_{j=0}^{p-1}\Gamma(\frac{(\nu_l - j)}{2})|\Sigma|^{\frac{1}{2}\nu_l}, \quad (2.35)$$

Taking the gth moment of $|c_{ij}|$ Box calculated the moments of M and then obtained an expression for the characteristic function of ρM, where $\rho \leq 1$ is a constant of our choice. The expression for the characteristic function of ρM is given by

$$\phi(t) = \prod_{l=1}^{m}(\frac{m\mu}{\mu_l})^{-itp\mu_l}\prod_{j=0}^{p-1}\frac{\Gamma[\frac{1}{2}\{m\mu + k\beta - j\}]}{\Gamma[\frac{1}{2}\{m\mu(1-2it) + m\beta - j\}]} \prod_{l=1}^{m}\frac{\Gamma[\frac{1}{2}\{\mu_l(1-2it) + \beta_l - j\}]}{\Gamma[\frac{1}{2}\{\mu_l + \beta_l - j\}]} \quad (2.36)$$

where

$$\mu_l = \rho\nu_l, \ \mu = \rho\nu, \ \nu = \mu + \beta, \ \nu_l = \mu_l + \beta_l, \quad (2.37)$$

Taking logarithms of (2.36), leads to the cumulant generating function in the form

$$\psi(t) = g(t) - g(0), \quad (2.38)$$

where

$$g(t) = -\sum_{l=1}^{m} it\mu_l p \ln\left(\frac{(m\mu)}{(\mu_l)}\right) + \sum_{j=0}^{p-1}\sum_{l=1}^{m} \ln \Gamma\left[\frac{1}{2}\{\mu_l(1-2it)+\beta_l-j\}\right] - \ln \Gamma\left[\frac{1}{2}\{m\mu(1-2it)+m\beta-j\}\right], \tag{2.39}$$

and $g(0)$ is a constant independent of t obtained by putting $t=0$ in the above expression.

Further, Box showed that the cumulant generating function can be written in the form

$$\psi(t) = \frac{-1}{2} f \ln(1-2it) + \sum_{r=1}^{n}\left\{\frac{\alpha_r}{\mu_r}(1-2it)^{-r} - 1\right\} + R_{n+1}(\mu, t) - R_{n+1}(\mu,0), \tag{2.40}$$

where $f = \frac{1}{2}(m-1)p(p-1)$, $R_{n+1}(\cdot)$ is the remainder term in the generalized Stirling's theorem, and α_r is given by

$$\alpha_r = \frac{(-1)^r m}{(r(r+1)(r+2))} \sum_{s=0}^{r+1}\left[\binom{r+2}{s+1} 2^s D_s \beta^{r+1-s}\right], \tag{2.41}$$

where

$$D_s = \Delta_s \gamma_s, \tag{2.42}$$

$$\Delta_s \simeq B_{s+1}\left\{-\frac{(B+p)}{2}\right\} - B_{s+1}\left\{\frac{-B}{2}\right\}, \tag{2.43}$$

$$\gamma_s = \frac{1}{m}\sum_{l=1}^{m}\left(\frac{v}{v_l}\right)^{s-1} - \frac{1}{m^s}, \tag{2.44}$$

and $B_r(x)$ is the Bernoulli polynomial (see Milne-Thomson, 1933). Using the properties of the Bernoulli polynomials, for different values of r and s, we can obtain the values of Δ_s and α_r.

For $\rho = 1$, Box (1949, equation (46)) showed that the cumulant generating function can be written as

$$\psi(t) = \sum_{j=1}^{\infty} \frac{(it)^j}{j!} 2^{j-1}(j-1)!f\{1 + \sum_{r=1}^{\infty} \binom{j+r-1}{r} 2r \frac{\alpha_r}{v^r f}\}. \tag{2.45}$$

The jth cumulant of M is then given by

$$\kappa_j = 2^{j-1}(j-1)!f\{1 + jA_1 + j\frac{(j+1)}{2}A_2 + ...\}, \tag{2.46}$$

$$A_r = \frac{2r\alpha'_r}{v^r f}, \tag{2.47}$$

and, in particular, for the generalized test for homoscedasticity,

$$A_1 = \frac{(2p_2 + 3p - 1)}{(6(m-1)(p+1))} \sum_{l=1}^{k} (\frac{1}{v_l} - \frac{1}{N}) \tag{2.48}$$

$$A_2 = \frac{(p-1)(p-2)}{6(m-1)} \sum_{l=1}^{k} (\frac{1}{v_l^2} - \frac{1}{N^2}). \tag{2.49}$$

Now $2^{j-1}(j-1)!f$ is the jth cumulant of the χ^2 distribution with f degrees of freedom. Thus, to order v^{-1}, (2.39) is identical with the jth cumulant of $C\chi^2$, where C is either $1 + A_1$ or $(1 - A_1)^{-1}$. The idea here is to match the moments of the distribution of the

likelihood ratio statistic to the moments of a chi-squared distribution in order to accelerate the rate of convergence. Thus, for $j = 1$, we match the first moments, for $j = 2$, we match upto the second moments, and so on.

For the univariate case it is clear that

$$C = 1 + A_1 = 1 + \frac{1}{3(m-1)} \sum_{l=1}^{m} \left(\frac{1}{v_l} - \frac{1}{N} \right). \tag{2.50}$$

Box (1949, p. 329) also showed that for the multivariate statistic, $p > 1$ and we take M/C to be approximately χ^2 with $f = \frac{1}{2}(m-1)p(p+1)$ degrees of freedom and

$$\frac{1}{C} = (1 - A_1) = 1 - \frac{(2p^2 + 3p - 1)}{6(p+1)(m-1)} \sum_{l=1}^{m} \left(\frac{1}{v_l} - \frac{1}{N} \right); \tag{2.51}$$

if the degrees of freedom are equal this becomes

$$\frac{1}{C} = 1 - \frac{(2p^2 + 3p - 1)(m+1)}{6(p+1)mv} \tag{2.52}$$

Morrison (1976, p. 258) applied Box's technique to address the problem considered by Wilks(1935) for the generalized test for independence. Let $\mathbf{S}_i$ be the unbiased estimate of $\mathbf{\Sigma}_i$ based on v_i degrees of freedom, where $v_i = N_i - 1$. Note that we are assuming m p-dimensional multinormal populations that are being tested for independence, and $\mathbf{\Sigma}_i$, $(i = 1, .., m)$ are their respective covariance matrices. Now, if the ith of the m sets contains p_i variates, so that the covariance matrix can be partitioned into submatrices $\mathbf{\Sigma}_{ij}$ of dimensions $(p_i \times p_j)$, the hypothesis is

$$H_0 : \mathbf{\Sigma}_{ij} = 0$$

for all $i \neq j$. Within the ith set the covariance matrix $\boldsymbol{\Sigma}_{ii}$ need only be positive definite. To test the independence of these m populations, the Wilk's test statistic is the determinantal ratio (see p. 258 of Morrison, 1976)

$$V = \frac{|\mathbf{S}|}{|\mathbf{S}_{11}| \ldots |\mathbf{S}_{mm}|}, \tag{2.53}$$

where

$$\mathbf{S} = \frac{1}{\sum_i v_i} \sum_{i=1}^{m} v_i \mathbf{S}_i, \tag{2.54}$$

and $\mathbf{S}_i$ is partitioned into submatrices $\mathbf{S}_{11}, \mathbf{S}_{22}, \ldots, \mathbf{S}_{mm}$.

Although the exact distribution of V is complicated, Wilks and other researchers have obtained good approximations to it in terms of tabulated functions. In particular, Box (1949) has shown that M/C is distributed as χ^2 with f degrees of freedom, where

$$\frac{1}{C} = 1 - \frac{1}{12fv}(2\boldsymbol{\Omega}_3 + 3\boldsymbol{\Omega}_2), \quad \text{and } f = \frac{1}{2}\boldsymbol{\Omega}_2 \tag{2.55}$$

where $\boldsymbol{\Omega}_s = (\sum_i p_i)^s - \sum_i (p_i)^s$. Box also considered the test of independence for testing m groups, each group having only one variate. The likelihood ratio criterion as obtained by Wilks then becomes the determinant of the sample correlation matrix. He showed that the Bartlett's factor is

$$\frac{1}{C} = 1 - \frac{2m+5}{6v}, \quad \text{and } f = \frac{1}{2}m(m-1). \tag{2.56}$$

MC^{-1} will then be asymptotically distributed as χ^2 with $1/2m(m-1)$ degrees of freedom.

Thus, knowing the moments of the likelihood statistic, Box obtained an expression for the distribution of the statistic M, a χ^2 approximation and an asymptotic χ^2 series. The key idea is to match the moments of the distribution of the likelihood ratio statistic with those of a chi-squared distribution. In particular, we will match the first moments. We apply the generalized tests for homoscedasticity and independence developed by Box (1949) in the validation procedure which is discussed in the next Chapter.

Concluding Remarks

In this Chapter we have reviewed the Schruben-Margolin correlation-induction strategy which jointly employs the common random numbers and antithetic variates for variance reduction. More importantly, we have reviewed the statistical analysis of Nozari, Arnold, and Pegden (1987) and its validation under the Schruben-Margolin correlation-induction strategy. We have also discussed methods to conduct the statistical tests used in the validation procedure. In the next Chapter we provide a similar statistical analysis and validation procedure for the common random number correlation-induction strategy.

CHAPTER III Statistical Analysis and Validation Procedure for the CRN Strategy

In this chapter we present methods for conducting statistical analysis under the common random number (CRN) strategy for multipopulation simulation experiments and offer a three-stage validation procedure.

3.1 Common Random Numbers

The basic idea of the CRN strategy is to compare alternative systems under similar experimental conditions to improve confidence that observed differences in performance are due to the differences in the system design rather than to differences in the experiment itself (see p. 61 of Law and Kelton, 1991). To see the rationale for CRN more clearly, consider two alternative systems in which y_{1i} and y_{2i} are the output responses for the first and second systems, respectively, on the ith independent replication. We want to estimate $\delta = E[y_{1i}] - E[y_{2i}]$. If we perform r independent replications of each system and let $z_i = y_{1i} - y_{2i}$ $(i = 1, 2, ..., r)$, then $E[z_i] = \delta$ and $\bar{z} = \sum_{i=1}^{r} \frac{z_i}{r}$ is an unbiased estimator of δ. Since the z_i's are independent random variables,

$$\text{var}[\bar{z}] = \frac{\text{var}(z_i)}{r} = \frac{(\text{var}(y_{1i}) + \text{var}(y_{2i}) - 2\text{cov}(y_{1i}, y_{2i}))}{r}.$$

If we could carry out the simulation so that y_{1i} and y_{2i} are positively correlated, then cov $(y_{1i}, y_{2i}) > 0$, so that the variance of the estimator $\bar{z}(r)$ would be reduced. CRN is a technique through which we try to induce positive correlation so as to effect such a reduction in var $(\bar{z})$.

Under the CRN technique, the same set of random number streams $\mathbf{R}_i$ $(i = 1, 2, ..., m)$ is applied to all m design points in the ith replication. We define $\mathbf{y}$, to be a mr-dimensional vector of observations which has the multivariate normal distribution as stated in (2.12).

In addition, when the same set of random number streams is used at two design points, we assume a positive correlation, ρ_+, is induced between the two responses. Further, ρ_+ is a constant, and does not depend on the specific set of seeds or the specific pair of design points, i.e. corr $(y_i, y_j) = \rho_+$ (for all i, j, and $i \neq j$). Under these assumptions, the covariance matrix between observations for the common random number strategy, $\Xi^{(CRN)}$, is given by

$$\Xi^{(CRN)} = \Sigma^{(CRN)} \otimes \mathbf{I}_r,$$

where

$$\Sigma^{(CRN)} = \sigma^2 \begin{bmatrix} 1 & \rho_+ & \cdot & \cdot & \cdot & \rho_+ \\ \rho_+ & 1 & \cdot & \cdot & \cdot & \rho_+ \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \rho_+ & \rho_+ & & & & 1 \end{bmatrix} \tag{3.2}$$

Note that the covariance structure of $\Sigma^{[CRN]}$ does not have the diagonal form, and hence, simple linear model theory cannot be applied directly to this model. However,

if we could transform this covariance structure to a diagonal form, then we could use the theory of simple linear models to estimate the unknown parameters, form confidence intervals, and also perform the usual statistical tests on these parameters with the transformed responses. Once we know how these transformed responses can be used to perform these tasks, we can rewrite the procedures in terms of the original (untransformed) responses by taking the inverse transformation on the transformed responses; this can be done, of course, only if the transformation is invertible (for obvious reasons we limit our discussion to such transformations).

Unfortunately, there is no general proof that CRN produces the desired variance reduction. When it does work, we will still not know beforehand how great a reduction in variance we might experience. The efficacy of CRN depends on the random variate generation algorithms used and also on the particular models being compared. Further, its use presupposes the analyst's belief that the different models will respond "similarly" to large or small values of the random variates driving the models. For example, we would expect that smaller interarrival times for several designs of a queueing facility would result in longer delays and queues for each system (see p. 615 of Law and Kelton, 1991).

There are, however, some classes of models for which variance reduction using the CRN technique is guaranteed. Heidelberger and Iglehart (1979) showed this for certain types of regenerative simulations, and Bratley, Fox, and Schrage (1978, Chapter 2) derive results indicating conditions under which CRN will work. Our own extensive computational experience has also showed that substantial variance reductions are realizable for a wide variety of simulation models.

Two advantages of the CRN strategy are that it is easy to employ and that it can be applied to *any* multiple-run simulation experiment. This latter property makes this strategy extremely useful for fitting second-order and higher metamodels in simulation experiments. Experimental designs for fitting a second-order response surface must involve at least three levels of each variable so that the coefficients in the model can be estimated (see p. 126 of Myers, 1976). The Schruben-Margolin correlation-induction strategy requires that the design be blockable into *two* blocks. This requirement is untenable for *many* second-order designs of interest (see p. 126 of Myers, 1976), thus restricting the applicability of the Schruben-Margolin correlation-induction strategy significantly. On the other hand, the CRN strategy, which yields the *same* variance reduction for all parameter estimates, except β_0, as the Schruben-Margolin strategy requires no such blocking restriction on the design. Thus, the CRN strategy is a competitive alternative to the Schruben-Margolin correlation-induction strategy for many metamodel estimation situations in simulation experiments.

3.2 The Statistical Analysis

In this section we outline four basic methods for conducting statistical analysis for use with the common random number strategy for multipopulation experiments. The results are parallel to those presented by Nozari, Arnold and Pegden (1987) and are proved in Appendices I through IV. The results yield the following :

- optimal (UMVU) estimate of β,
- a confidence interval for β_0,
- confidence intervals for β_1, and
- joint confidence intervals for β_0 and β_1.

Let m be the number of design points of a simulation experiment. Now consider the linear model

$$\mathbf{y} = \mathbf{G}\boldsymbol{\beta} + \boldsymbol{\varepsilon} \tag{3.3}$$

where $\mathbf{y}$ is as defined in (3.1), $\boldsymbol{\varepsilon}$ is the error term, and

$$\mathbf{G} = \begin{bmatrix} \mathbf{X} \\ \vdots \\ \mathbf{X} \end{bmatrix},$$

is a $(mr \times p)$ design matrix. Here r is the number of replications and p is the number of model parameters.

Suppose we average both sides of (3.3) over the number of replications, and denote the left hand side average of $\mathbf{y}$'s by $\bar{\mathbf{y}}$, and the average of $\boldsymbol{\varepsilon}$'s by $\bar{\boldsymbol{\varepsilon}}$, then we get

$$\bar{\mathbf{y}} = \mathbf{X}\boldsymbol{\beta} + \bar{\boldsymbol{\varepsilon}}$$

Solving the above as an unconstrained minimization problem to minimize $\|\bar{\boldsymbol{\varepsilon}}\|^2$ gives the least squares estimator for $\boldsymbol{\beta}$ which is also the UMVU estimator since $\boldsymbol{\varepsilon}$ is assumed to have a normal distribution. This solution is found to be

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\bar{\mathbf{y}}.$$

This is the same estimator of $\boldsymbol{\beta}$ as in the general linear model, that is, in a linear model which has uncorrelated responses. In the CRN case we in fact have correlated responses, but still the UMVU estimator of $\boldsymbol{\beta}$ has the same form.

By applying an orthogonal transformation to the correlated responses, we can transform the problem to one with independent responses (as seen in Section 2.3 and also will be seen later in this section). In doing so, the basic problem is unchanged and therefore the properties of the estimators are not destroyed. Hence, $\hat{\boldsymbol{\beta}}$ has the same form whether the responses are correlated or not.

Let $\hat{\boldsymbol{\beta}}$ and $\hat{\sigma}_1^2$ be the usual unbiased estimators for this model, that is :

$$\hat{\boldsymbol{\beta}} = (\hat{\beta}_0 , \hat{\beta}_1)' = (\mathbf{G}'\mathbf{G})^{-1}\mathbf{G}'\mathbf{y}, \tag{3.3}$$

and

$$\hat{\sigma}_1^2 = \frac{(\|\mathbf{y} - \mathbf{G}\hat{\boldsymbol{\beta}}\|^2)}{n - p} . \tag{3.4}$$

Note that $\hat{\sigma}_1^2$, the unbiased estimator of σ^2 is model dependent. Then we have :

Result 1 : $\hat{\boldsymbol{\beta}}$ is the optimal estimator of $\boldsymbol{\beta}$.

Let y_{ij} denote the jth observation of the ith replication ($i = 1, 2, ..., r$, and $j = 1, 2, ..., q$). Define $\bar{y}_{i.}$ as the mean of the observations across each replication, and $\bar{y}_{..}$ the overall mean of the observations. Then,

$$\bar{y}_{i.} = \sum_{j=1}^{m} \frac{y_{ij}}{m} , \qquad \bar{y}_{..} = \sum_{i=1}^{r} \frac{\bar{y}_{i.}}{r} , \tag{3.5}$$

Also define $\hat{\lambda}_1^2$ is the variance between replicates. Then,

$$\hat{\lambda}_1^2 = m\sum_{i=1}^{r}\frac{(\bar{y}_{i.}-\bar{y}_{..})^2}{r} \tag{3.6}$$

Then we have

Result 2 :

$$\frac{[(mr)^{1/2}(\hat{\beta}_0-\beta_0)]}{\hat{\lambda}_1} \sim t_{r-1}.$$

This result can be used in the obvious way to construct $100(1-\alpha)\%$ confidence intervals for β_0.

Let f be the usual test statistic for testing $H_0: \mathbf{H}\boldsymbol{\beta}_1 = \mathbf{0}_h$ vs $H_1: \mathbf{H}\boldsymbol{\beta}_1 \neq \mathbf{0}_h$, where $\mathbf{H}$ is a known $(h \times (p-1))$ matrix of rank $h < p$, when $\Xi = \sigma^2\mathbf{I}_n$. That is,

$$f = \frac{r(\mathbf{H}\hat{\boldsymbol{\beta}}_1)'(\mathbf{H}(\mathbf{T}'\mathbf{T})^{-1}\mathbf{H}')^{-1}(\mathbf{H}\hat{\boldsymbol{\beta}}_1)}{h\hat{\sigma}_1^2}$$

Let HW_l denote the half-width of the $100(1-\alpha)\%$ simultaneous confidence intervals for the set of $\mathbf{l}'\mathbf{H}\boldsymbol{\beta}_1$, for all $\mathbf{l} \in R^k$, when $\Xi = \sigma^2\mathbf{I}_n$ That is

$$HW_l = \hat{\sigma}_1\left[h\frac{F_{h,n-p}^{\alpha}\mathbf{l}'\mathbf{H}(\mathbf{T}'\mathbf{T})^{-1}\mathbf{H}'\mathbf{l}}{r}\right]^{1/2}. \tag{3.7}$$

Define

$$\hat{\lambda}_2^2 = \frac{(mr-m)\hat{\sigma}_2^2 - m\sum_{i=1}^{r}(\bar{y}_{i.}-\bar{y}_{..})^2}{r(m-1)}; \tag{3.8}$$

where $\hat{\lambda}_2^2$ is the pure error of the fitted model, and $\hat{\sigma}^2$ is given by

$$\hat{\sigma}_2^2 = [m(r-1)]^{-1} \sum_{i=1}^{r} \sum_{j=1}^{m} (y_{ij} - \bar{\mathbf{y}}_{.j})^2. \tag{3.9}$$

Note that $\hat{\sigma}_2^2$ is another estimator of σ^2, and is model independent. Then we have

Result 3 : The optimal test for testing $H_0 : \mathbf{H}\beta_1 = \mathbf{0}_h$ vs $H_1 : \mathbf{H}\beta_1 \neq \mathbf{0}_h$, where $\mathbf{H}$ is a known $(h \times (p-1))$ matrix of rank $h < p$, rejects H_0 if

$$f^* = \frac{f\hat{sig}_{.1}^2}{\hat{\lambda}_2^2} > F_{h,n-p-r}^{\alpha}. \tag{3.10}$$

The $100(1-\alpha)\%$ simultaneous confidence interval for the set of $\mathbf{l}'\mathbf{H}\beta_1$ for all $\mathbf{l} \in R^k$ when $\Xi = \Sigma \otimes \mathbf{I}_r$ is

$$\mathbf{l}'\mathbf{H}\beta_1 \in \mathbf{l}'\mathbf{H}\hat{\beta}_1 \pm \frac{(\hat{\lambda}_2^2)F_{h,n-p-r}^{\alpha}}{(\hat{\sigma}_1^2 F_{h,n-p}^{\alpha})^{(1/2)}} HW_l. \tag{3.11}$$

Next we consider inferences that involve both β_0 and β_1 simultaneously. Let $\bar{\mathbf{y}}$ be the m-dimensional vector of sample means, and $\mathbf{S}$ be the $(m \times m)$ sample covariance matrix of the $\mathbf{y}_i$'s, that is,

$$\bar{\mathbf{y}} = \frac{1}{r} \sum_{i=1}^{r} \mathbf{y}_i, \qquad \mathbf{S} = \frac{1}{r-1} \sum_{i=1}^{r} (\mathbf{y}_i - \bar{\mathbf{y}})(\mathbf{y}_i - \bar{\mathbf{y}})'; \tag{3.12}$$

then we have

Result 4 : A size α procedure for testing $H_0 : \mathbf{K}\boldsymbol{\beta} = \mathbf{0}_k$ vs $H_1 : \mathbf{K}\boldsymbol{\beta} \neq \mathbf{0}_k$, where $\mathbf{K}$ is a $(k \times p)$ known matrix of rank $k \leq p$, is to reject H_0 if

$$\frac{r(r-k)}{k(r-1)} \hat{\boldsymbol{\beta}}'\mathbf{K}'(\mathbf{K}\hat{\Delta}\mathbf{K}')^{-1}\mathbf{K}\hat{\boldsymbol{\beta}} > F^{\alpha}_{k,r-k}, \tag{3.13}$$

where $\hat{\Delta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{S}\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}$. A set of $100(1-\alpha)\%$ simultaneous confidence intervals is given by

$$\mathbf{l}'\mathbf{K}\boldsymbol{\beta} \in \mathbf{l}'\mathbf{K}\boldsymbol{\beta} \pm \left[k \frac{(r-1)}{r(r-k)} F^{\alpha}_{k,r-k} \mathbf{l}'\mathbf{K}\hat{\Delta}\mathbf{K}'\mathbf{l} \right]^{1/2} \tag{3.14}$$

for all $\mathbf{l} \in R^k$.

In order to derive results for drawing inferences about $\boldsymbol{\beta}_0$ and $\boldsymbol{\beta}_1$ separately, it is useful to transform the model to one with independent observations. The derivation of these results are analogous to the ones presented in Section 4 of Nozari, Arnold and Pegden (1987) and as discussed in Section 2.3. In other words, the aim is to get a block diagonal structure for the covariance matrix between the responses. This is done by by applying an $(mr \times mr)$ orthogonal transformation $\boldsymbol{\Gamma}^{(CRN)}$, where

$$\boldsymbol{\Gamma}^{(CRN)} = \begin{bmatrix} (m^{-1/2}\mathbf{1}'_m) \otimes \mathbf{I}_r \\ \mathbf{C}'_m \otimes \mathbf{I}_r \end{bmatrix}, \tag{3.15}$$

where $\mathbf{C}_m$ is a $(m \times (m-1))$ matrix such that $(m^{-1/2}\mathbf{1}_m\mathbf{C}_m)$ is orthogonal. Note that for the Schruben-Margolin covariance structure, the transformation matrix $\boldsymbol{\Gamma}^{(SM)}$ was given by Nozari, Arnold, and Pegden (1987) on p.134 as,

$$\Gamma^{(SM)} = \begin{bmatrix} ((2m)^{-1/2}\mathbf{1}'_m & (2m)^{-1/2}\mathbf{1}'_m)\otimes \mathbf{I}_r \\ ((2m)^{-1/2}\mathbf{1}'_m & -(2m)^{-1/2}\mathbf{1}'_m)\otimes \mathbf{I}_r \\ \mathbf{C}'_m\otimes \mathbf{I}_{2r} & \end{bmatrix}, \tag{3.16}$$

Define

$$\mathbf{y}^* = \begin{bmatrix} \mathbf{y}_1^* \\ \mathbf{y}_2^* \end{bmatrix} = \Gamma^{(CRN)}\mathbf{y}, \quad \mathbf{T}^* = \begin{bmatrix} \mathbf{C}'_m\mathbf{T} \\ \mathbf{C}'_m\mathbf{T} \\ \vdots \\ \mathbf{C}'_m\mathbf{T} \end{bmatrix}, \tag{3.17}$$

$$\mathbf{G}^* = \Gamma^{(CRN)}\mathbf{G}, = \begin{bmatrix} m^{(1/2)}\mathbf{I}_r & \mathbf{0} \\ \mathbf{0} & \mathbf{T}^* \end{bmatrix}, \text{ and,} \tag{3.18}$$

and

$$\Xi^{(CRN)*} = \Gamma^{(CRN)}\Xi^{(CRN)}\Gamma^{(CRN)'} = \begin{bmatrix} \lambda_1^2\mathbf{I}_r & \mathbf{0} \\ \mathbf{0} & \lambda_2^2\mathbf{I}_{(r(m-1))} \end{bmatrix}, \tag{3.19}$$

where $\mathbf{y}_1^*$ is $(r \times 1)$, and $\mathbf{y}_2^*$ is $((m-1)r \times 1)$, $\lambda_1^2 = \sigma^2(1+(m-1)\rho_+)$, and $\lambda_2^2 = \sigma^2(1-\rho_+)$. Note that for the Schruben-Margolin covariance structure we had $\tau_1^2 = \sigma^2(1+(m-1)\rho_+ - m\rho_-)$, $\tau_2^2 = \sigma^2(1+(m-1)\rho_+ + m\rho_-)$ and $\tau_3^2 = \sigma^2(1-\rho_+)$.

For the Schruben-Margolin strategy, the transformed vector of observations, $\mathbf{y}^*$, had three components. The second component, $\mathbf{y}_2^*$, was the difference between the observations on a given replication across the two blocks. For the CRN case, no such blocking is required, so this second component does not exist. Hence, for the CRN case, we have only two components of $\mathbf{y}^*$.

Also, λ_1^2 is equal to τ_1^2 in the Schruben-Margolin case, but for the term, ρ_- This is due to the fact that there are no negative correlations induced in the CRN strategy. $\mathbf{y}_2^*$, in the CRN case, and $\mathbf{y}_3^*$, in the Schruben-Margolin case are identical in that both have the vector of observations across the m design points $\mathbf{y}_i$, where i is the number of replications, being pre-multiplied by the same matrix $\mathbf{C}_m$. Hence we expect $\mathbf{y}_2^*$, in the CRN case, and $\mathbf{y}_3^*$, in the Schruben-Margolin case to behave in an identical manner. Their variances λ_2^2, and τ_3^2, respectively, are also the same.

By the definition of $\mathbf{y}_i$ given in equation (3.1), we have,

$$\mathbf{y}_1^* = \left[m^{-1/2} \mathbf{1}_r \sum_{i=1}^{m} \mathbf{y}_i \right] \tag{3.20}$$

and

$$\mathbf{y}_2^* = \begin{bmatrix} \mathbf{C}'_m \mathbf{y}_1 \\ \mathbf{C}'_m \mathbf{y}_2 \\ \vdots \\ \mathbf{C}'_m \mathbf{y}_r \end{bmatrix}. \tag{3.21}$$

Thus, we have

$$\mathbf{y} \sim N_{mr}(\mathbf{G}^* \boldsymbol{\beta}, \boldsymbol{\Xi}^*) \tag{3.22}$$

We notice that the term τ_2^2 is 0 for the CRN case.

We see that by applying the transformation $\boldsymbol{\Gamma}^{(CRN)}$ to the response vector $\mathbf{y}$, the transformed vector of responses, $\mathbf{y}^*$, is obtained. The covariance matrix of $\mathbf{y}^*$ is block diagonal. Also, this transformation is invertible and does not involve any unknown

parameters, so that any optimal procedure based on $\mathbf{y}^*$ is also optimal among procedures based on $\mathbf{y} = \mathbf{\Gamma}^{(CRN)'}\mathbf{y}^*$. Inspection of (3.19) clearly indicates that the model involving $\mathbf{y}^*$ is really two separate ordinary linear models, one involving $(\mathbf{y}_1^*, \boldsymbol{\beta}_0, \lambda_1^2)$, and one involving $(\mathbf{y}_2^*, \boldsymbol{\beta}_1, \lambda_2^2)$.

As a consequence of the above transformation, we can establish the following properties.

- $\mathbf{y}_1^*$ and $\mathbf{y}_2^*$ are independent.
- $\mathbf{y}_1^* \sim N_r(m^{1/2}\mathbf{1}_r\beta_0, \lambda_1^2\mathbf{I}_r)$.
- $\mathbf{y}_2^* \sim N_{r(m-1)}(\mathbf{T}^*\boldsymbol{\beta}_1, \lambda_2^2\mathbf{I}_{r(m-1)})$.

We have thus developed statistical analysis methods under the CRN strategy for multipopulation simulation experiments. That is, we have provided optimal estimation of $\boldsymbol{\beta}$, individual confidence intervals for β_0 and $\boldsymbol{\beta}_1$, as well as joint confidence intervals for β_0 and $\boldsymbol{\beta}_1$. Further, we have provided optimal tests of hypotheses to test for the linear combinations in β_i's, $i = 1, ,2, ..., p$.

While stating the above results, and also proving them, we have made certain basic assumptions, such as the multivariate normality of $\mathbf{y}$, the CRN covariance structure as given by equation (3.2), and also that of the appropriateness of the proposed linear model given by (3.3). We therefore need to develop a procedure to formally test these assumptions in order to legitimately employ the above stated results. In the next section we develop these required tests.

3.3 The Validation Procedure

In the previous section we presented methods for conducting statistical analysis under the CRN strategy. We now develop a three-stage procedure for validating the use of the analysis. This validation procedure parallels that given by Tew and Wilson (1990). It is mainly intended for use in a relatively small *pilot study* prior to the execution of a full-scale simulation experiment to determine the extent to which the underlying assumptions are satisfied and to identify modifications of the experimental protocol that might be required to correct significant violations of these assumptions.

Each stage of the procedure checks a key assumption across all points in the design. The test in each stage depends upon validation of hypothesized properties of the previous stages, and hence, these diagnostic checks on the experimental design and analysis must be performed in order. At each stage of the validation procedure, a highly significant test statistic will generally indicate the need for some corrective action by the user. The following three diagnostic checks need to be performed.

Test for Multivariate Normality :

$$\begin{aligned} &H_0 : \mathbf{y}_i \sim N_m(\boldsymbol{\mu}, \boldsymbol{\Sigma}^{(CRN)}), \text{ where } \boldsymbol{\Sigma}^{(CRN)} \text{ is positive definite but} \\ &\qquad \text{otherwise } \boldsymbol{\mu} \text{ and } \boldsymbol{\Sigma}^{(CRN)} \text{ are unspecified,} \\ &\text{versus} \\ &H_1 : \mathbf{y}_i \text{ has any non-singular } m\text{-dimensional distribution.} \end{aligned} \tag{3.23}$$

Test for the induced covariance structure :

$$\begin{aligned} &H_0 : \text{cov}(\mathbf{y}_i) = \boldsymbol{\Sigma}^{(CRN)} \text{ with } \sigma^2, \ \rho_+, \text{ as in (3.2)} \\ &\qquad \text{so that } \boldsymbol{\Sigma}^{(CRN)} \text{ is positive definite, } \rho_+ > 0; \\ &\qquad \text{otherwise } \sigma^2, \ \rho_+, \text{ are unspecified,} \\ &\text{versus} \\ &H_1 : \text{cov}(\mathbf{y}_i) \text{ is positive definite.} \end{aligned} \tag{3.24}$$

Test for Lack-Of-Fit in the Linear Model :

$$H_0 : E[\mathbf{y}_i] = \mathbf{X}\boldsymbol{\beta}, \quad \text{versus} \quad H_1 : E[\mathbf{y}_i] \neq \mathbf{X}\boldsymbol{\beta}. \tag{3.25}$$

Performing these tests would validate our key assumptions which are as follows :

1. The response variance is constant across all design points so that

$$\sigma_i^2 = \text{var}[y_i(\mathbf{R}_i)] = \sigma^2 \text{ for } i = 1, 2, \ldots, m,$$

   where m is the number of design points.

2. There is a constant nonnegative correlation between all pair of responses y_i and y_j $i \neq j$. That is,

$$\text{corr}(y_i, y_j) = \rho_+ \text{ for } i \neq j, \quad 1 < i, j < q, \quad \text{where } 0 < \rho_+ < 1.$$

3. $(\mathbf{y}_i : i = 1, 2, \ldots, r)$ IID $\sim N_m(\mathbf{X}\boldsymbol{\beta}, \boldsymbol{\Sigma}^{(CRN)})$.

We use the test offered by Tew and Wilson (1990) as a diagnostic for testing the multivariate normality of the response vector $\{\mathbf{y}_i\}$. This test is a general test for a random observation sample of size r. The only restriction is that the sample size should be in the range $\max\{2m, 16\} \leq 32$. We select the values of r and m such that this restriction is satisfied.

If we reject the null hypothesis of (3.24), then the lack-of-fit test performed would be the same as that developed by Tew and Wilson (1990). Otherwise we use the lack-of-fit test presented in Section 3.5.

If the null hypotheses in (3.23) and (3.25) are validated, but we fail to accept the null hypothesis in (3.24), we need alternative methods for follow-up analysis of the metamodel. Of particular interest is the construction of a meaningful confidence re-

gion for the full vector β of metamodel parameters. For this test also we use the same test developed by Tew and Wilson (1990).

Test for the CRN covariance structure is discussed in Section 3.4, and a lack-of-fit test assuming the CRN covariance structure is discussed in Section 3.5.

3.4 Test For The CRN Covariance Structure

This stage of diagnostic testing is based on a modified likelihood ratio test of the composite null hypothesis for the second diagnostic check mentioned earlier in (3.16). Some cautions about this test are required. First, these tests maybe sensitive to the assumption that the responses $\{\mathbf{y}_i;\ (i = 1, , 2, ..., r)\}$ have a multivariate normal distribution. Second, although the simulation analysis method may not be very sensitive to the normality assumption, these analysis methods are unjustified when the experimenter has clear evidence of departures from the covariance structure as given by (3.2).

This test is performed as follows. The conventional likelihood ratio test statistic for the composite null hypothesis H_0 in (3.23) has the form

$$L = \left[\frac{\det(r^{-1}\mathbf{A})}{\hat{\lambda}_1(\hat{\lambda}_2^{m-1})} \right]^{r/2}, \tag{3.26}$$

where

$$\mathbf{A} = \sum_{i=1}^{r} (\mathbf{y}_i - \bar{\mathbf{y}})(\mathbf{y}_i - \bar{\mathbf{y}})' . \tag{3.27}$$

If the responses $\{\mathbf{y}_i;\ (i = 1, 2, ..., r)\}$ are multinormal with the prescribed covariance structure given in (3.2) then the test statistic $M \equiv -2\ln(L)$ asymptotically has a chi-squared distribution with $1/2m(m+1) - 2$ degrees of freedom as $r \to \infty$. However, the rate of convergence to this limiting distribution can be slow. To achieve adequate convergence to this limiting distribution of M with moderate values of r, we have developed the modified likelihood ratio statistic

$$\mathbb{N} = -2\psi_0 \ln(L), \tag{3.28}$$

where

$$\psi_0 = \frac{\frac{m(m+1)}{2} - 3}{\frac{m^2 - 3m + 2}{2\psi_1} + \frac{2m-1}{\psi_2} + \frac{m-2}{\psi_3}}, \tag{3.29}$$

with

$$\psi_1 = 1 - \frac{2m+3}{6r}, \tag{3.30}$$

$$\psi_2 = 1 - \frac{3m^2 - 1}{6r(m-1)}, \tag{3.31}$$

$$\psi_3 = 1 + \frac{m}{3r(m-1)}, \tag{3.32}$$

The adjustment factor ψ_0 has been chosen such that $r > m$ and the null hypothesis of the tests for multivariate normality of $\{\mathbf{y}_i;\ (i = 1, 2, ..., r)\}$ as in (3.23) and for the CRN covariance structure as in (3.24) hold. Then, to the terms of order $(r-1)^{-2}$, the expected value of $\mathbb{N}$ is identical to the expected value of $\chi^2[1/2m(m+1) - 2]$, a chi-squared variate with $1/2m(m+1) - 2$ degrees of freedom. In other words, the ad-

justment factor ψ_0 has been chosen so that for multivariate normal responses having the covariance structure given by (3.2).

That is,

$$\begin{aligned} E[\mathbb{N}] - E\{\chi^2[\frac{1}{2}m(m+1)-2]\} &= E[\mathbb{N}] - \frac{1}{2}m(m+1) - 2 \\ &= O[(r-1)^{-3}] \text{ as } r \to \infty, \end{aligned} \tag{3.33}$$

and

$$\mathbb{N} \xrightarrow{D} \chi^2[\frac{1}{2}m(m+1)-2] \text{ as } r \to \infty. \tag{3.34}$$

(3.34) is proved in Appendix V. Performing the test on the CRN covariance structure is equivalent to performing the following three independent tests on $\mathbf{y}_{i1}^*$, and $\mathbf{y}_{i2}^*$

H_0 : Components of $\mathbf{y}_{i2}^*$ are mutually independent,
versus
H_1 : Components of $\mathbf{y}_{i2}^*$ are not independent. (3.35)

H_0 : The variates y_{i1}^* and $\mathbf{y}_{i2}^*$ are mutually independent,
versus
H_1 : The variates y_{i1}^* and $\mathbf{y}_{i2}^*$ are not independent. (3.36)

H_0 : Components of $\mathbf{y}_{i2}^*$ have equal variances,
versus
H_1 : Components of $\mathbf{y}_{i2}^*$ have unequal variances. (3.37)

Let $\mathbf{S}_i$ to be the unbiased estimate of the covariance matrix $\Sigma^{(CRN)}$ of component i, having v_i degrees of freedom, and the matrix $\mathbf{S}$ given by equation (2.54). Let $\mathbf{S}^* = \Gamma^{(CRN)}\mathbf{S}\Gamma^{(CRN)'}$ and let s_{ii}^*, $i = 1, 2, ..., m$ denote the diagonal elements of $\mathbf{S}^*$.

Note that $\mathbf{S}^*$ is a diagonal matrix, the first diagonal element being s_{11}, and the second being the $((m-1)\times(m-1))$ matrix $\mathbf{S}_2^*$. Then, the likelihood ratios respectively corresponding to the null hypothesis in (3.35), (3.36) and (3.37) are

$$L_1 = \left[\frac{\det(\mathbf{S}_2^*)}{\prod_{g=2}^{m} s_{gg}^*} \right]^{r/2}, \tag{3.38}$$

$$L_2 = \left[\frac{\det(\mathbf{S}^*)}{s_{11}^* \det(\mathbf{S}_2^*)} \right]^{r/2}, \tag{3.39}$$

$$L_3 = \left[\frac{\prod_{g=2}^{m} s_{gg}^*}{[(m-1)^{-1}\sum_{g=2}^{m} s_{gg}^*]^{m-1}} \right]^{r/2}; \tag{3.40}$$

(see p. 37 of Tew and Wilson, 1990). Define M_i, for $i = 1, 2, 3$ as

$$M_i = -2\ln(L_i), \tag{3.41}$$

Then, the null hypotheses in (3.35), (3.36) and (3.37) imply

$$M_1 \xrightarrow{D} \chi^2[\tfrac{1}{2}(m^2 - 3m + 2)] \text{ as } r \to \infty, \tag{3.42}$$

$$M_2 \xrightarrow{D} \chi^2[2m - 1] \text{ as } r \to \infty, \tag{3.43}$$

and

$$M_3 \xrightarrow{D} \chi^2[m-2] \text{ as } r \to \infty \tag{3.44}$$

based on the same type of argument as presented in equation (3.28). Combining (3.26), (3.38), (3.39) and (3.40), we see that

$$M = M_1 + M_2 + M_3. \tag{3.45}$$

From equations (2.55), (2.54) and (2.50), we see that, respectively,

$$\psi_1 \equiv 1 - \frac{2m+3}{6r} \Rightarrow E[\psi_1 M_1] = \frac{1}{2}(m^2 - 3m + 2) + O[(r-1)^{-3}], \tag{3.46}$$

$$\psi_2 \equiv 1 - \frac{3m^2 - 1}{6r(m-1)} \Rightarrow E[\psi_2 M_2] = \frac{1}{2}(2m-1) + O[(r-1)^{-3}], \tag{3.47}$$

and

$$\psi_3 \equiv 1 + \frac{m}{3r(m-1)} \Rightarrow E[\psi_3 M_3] = \frac{1}{2}(m-2) + O[(r-1)^{-3}]. \tag{3.48}$$

Note that in each of the cases corresponding to equations (3.46) through (3.48), the appropriate version of Box's scale factor ρ or Bartlett's factor $1/C$ is equal to $\frac{r\psi_l}{(r-1)}$ for $l = 1, 2, 3$. Combining (3.46), (3.47) and (3.48), we obtain

$$\psi_0 = \frac{\frac{m(m+1)}{2} - 3}{\frac{m^2 - 3m + 2}{2\psi_1} + \frac{2m-1}{\psi_2} + \frac{m-2}{\psi_3}} \tag{3.49}$$

$$\Rightarrow E[\psi_0 M] = \frac{1}{2} m(m+1) - 2 + O[(r-1)^{-3}].$$

From (3.46) through (3.49) we get

$$\lim_{r\to\infty} \psi_l = 1 \quad \text{for } l = 0, 1, 2, 3; \tag{3.50}$$

and thus (3.34) follows from (3.28) and (3.50), and Slutsky's Theorem (Theorem 1.5.4 of Serfling, 1980).

3.5 Lack-Of -Fit Test

The last stage of the validation procedure is a test for lack-of-fit in the model given by (2.4). At this point in the procedure, there are two possible situations to consider : (a) we have established multivariate normality as well as the covariance structure given by (3.2). (b) we have established multivariate normality without the covariance structure given by (3.2). These two situations are discussed separately.

3.5.1 Lack Of Fit Test With the CRN Covariance Structure

We had defined the ($mr \times mr$) orthogonal matrix in (3.15) as

$$\Gamma^{(CRN)} = \begin{bmatrix} (m^{(-1/2)}\mathbf{1}'_m)\otimes \mathbf{I}_r \\ \mathbf{C}'_m \otimes \mathbf{I}_r \end{bmatrix},$$

so that under the null hypotheses for the three validation tests as given by equations (3.23), (3.24) and (3.25), equations (3.1) and (3.25) are satisfied.

Testing the hypothesis for the lack-of-fit test in (3.25) is equivalent to performing the following test :

$$H_0 : \mathrm{E}[\mathbf{y}^*_{i2}] = \mathbf{T}^*\boldsymbol{\beta}_1 \quad \text{versus} \quad H_1 : \mathrm{E}[\mathbf{y}^*_{i2}] \neq \mathbf{T}^*\boldsymbol{\beta}_1. \tag{3.51}$$

To test (3.51), we begin by computing

$$S_E \equiv \sum_{i=1}^{r} \|\mathbf{y}_i - \mathbf{X}\beta\|^2 , \tag{3.52}$$

where $\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\bar{\mathbf{y}}$ is the least squares estimate of β and $\bar{\mathbf{y}}$ is the sample mean of the original m-dimensional response vectors. Thus S_E is the residual sum of squares for the full regression model given by (2.4). With respect to the reduced regression model $E[\mathbf{y}_{i2}^*] = \mathbf{T}^*\beta_1$ for the $(m-1)$-dimensional transformed responses $\{\mathbf{y}_{i2}^*\}$, we compute the corresponding error sum of squares S_E^* with v_E^* degrees of freedom as well as pure error sum of squares S_{PE}^* with v_{PE}^* degrees of freedom, where all these quantities are expressed in terms of the original data :

$$S_E^* = S_E - m\sum_{i=1}^{r}(\bar{y}_{i.} - \bar{y}_{..})^2 \text{ with } v_E^* = mr - p + 1 \tag{3.53}$$

and

$$S_{PE}^* = r(m-2)\hat{\lambda}_2^2 \text{ with } v_{PE}^* = m(r-1).$$

We reject H_0 in (3.45) if

$$\frac{(S_E^* - S_{PE}^*)/(v_E^* - v_{PE}^*)}{S_{PE}^*/v_{PE}^*} > F_{1-\delta}(v_E^* - v_{PE}^*, v_{PE}^*) , \tag{3.54}$$

where $F_{1-\delta}(v_E^* - v_{PE}^*, v_{PE}^*)$ is the quantile of order $1-\delta$ for the F distribution with $v_E^* - v_{PE}^*$ and v_{PE}^* degrees of freedom. Equation (3.54) is a standard lack-of-fit test applied to the transformed responses $\{\mathbf{y}_{i2}^*\}$.

Concluding Remarks

This thesis was motivated by a desire to aid the simulation analyst with the commonly required statistical tools for use with the CRN correlation strategy, and also provide a validation procedure for the assumptions made while using these tools. In the next Chapter we illustrate the application of the above procedures with a numerical example.

One of our contributions to the existing literature was the development of the statistical analysis for the common random number strategy for multipopulation simulation experiments. The other contribution was the development of the test for the induced covariance structure and the lack-of-fit test for the model assumed for the CRN strategy. We use the same test for checking the multi-normality of the responses $\{\mathbf{y}_i\}$ as used by Tew and Wilson (1990).

Chapter IV Application Of Analysis Methods and Validation Procedure

To illustrate the simulation analysis and validation methods presented in Chapter 3, we apply these procedures to the hospital simulation study previously discussed by Schruben and Margolin (1978), Hussey, Myers, and Houck (1987a), and by Tew and Wilson (1990). The pilot study was originally intended to provide a preliminary indication of how many beds should be respectively assigned to the intensive care unit (ICU), the coronary care unit (CCU), and the intermediate care unit of a new hospital facility.

The new hospital facility operates as follows. Patient arrivals at the facility constitute a Poisson process with a mean arrival rate of 3.3 patients per day. Seventy-five percent of the arriving patients attempt to enter the ICU and stay there for a period of time that is lognormally distributed with mean $\mu = 3.4$ days and a standard deviation $\sigma = 3.5$ days. The remaining twenty-five percent of arriving patients try to enter the CCU and stay there for a period of time that is lognormally distributed with mean $\mu = 3.8$ days and a standard deviation of $\sigma = 1.6$ days. Twenty-seven percent of the patients leaving the ICU will depart the facility, and the remaining seventy-three percent of ICU patients attempt to enter the intermediate care unit. For ICU patients, sojourn time in the intermediate care unit is lognormally distributed with mean

μ = 15 days and standard deviation of σ = 7 days. Twenty percent of the patients leaving the CCU will depart the hospital facility, and the remaining eighty percent of CCU patients try to enter the intermediate care unit. For CCU patients, sojourn time in the intermediate care unit is lognormally distributed with mean μ = 17 days and standard deviation σ = 3 days. The overall flow of patients through this facility is depicted in Figure 1 along with the path probabilities for each of the four possible paths that the patients may attempt to follow.

The purpose of the pilot study was to estimate and validate the relationship between the overall balking rate of patients in the hospital and the following controllable factors : (a) the number of ICU beds (x_1); (b) the number of CCU beds (x_2); and (c) the number of intermediate care beds (x_3). In this context, the balking rate is the long-run average number of times per month that a patient is denied admission to a specialized care unit because that unit is operating at capacity. To investigate the dependence of the balking rate on the specified factors and to validate the simulation metamodel representing the dependence, we use the metamodel

$$y_g = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_1 x_2 + \beta_5 x_1 x_3 + \beta_6 x_2 x_3 + \varepsilon_g. \qquad (4.1)$$

where $g = 1, 2, ..., 8$; y_g is the sample average balking rate at the gth design point; β_0 is the long-run balking rate averaged across all design points; β_h is the hth component of the vector of partial differences of the long-run balking rate with respect to the number of ICU, CCU, and intermediate care beds; x_i is the ith coded design variable at one of the design points; and, ε_g is the experimental error at the gth design point.

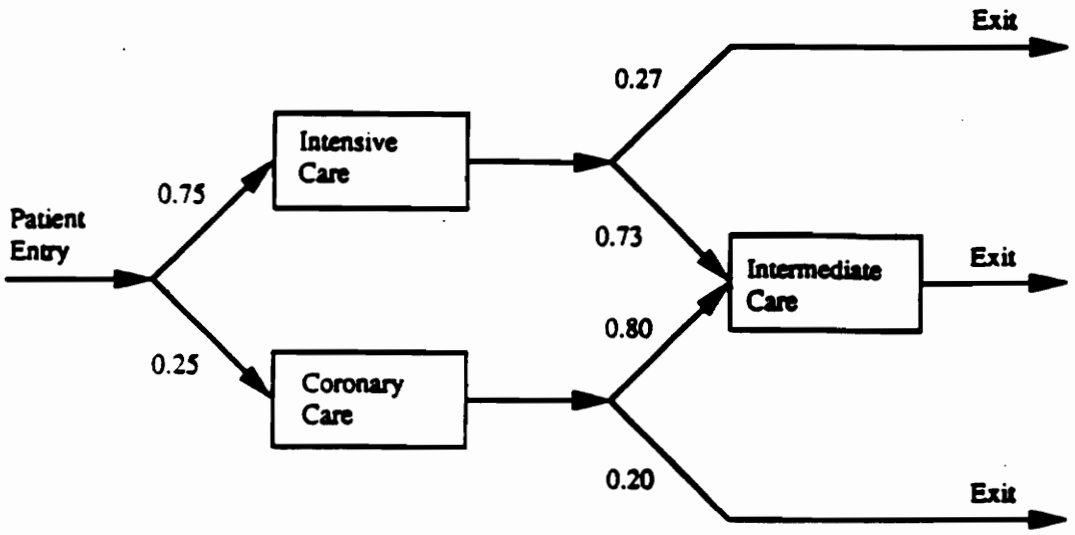

Figure 1. Hospital Simulation Study Model

The hospital simulation model was implemented in the SLAM II simulation language (Pritsker, 1986), and is given in Appendix VI. On the gth run of the simulation ($g = 1, 2, ..., 8$), sample statistics were cleared at the end of a 10-month start-up period; then the average monthly balking rate y_g was accumulated over 50 months of simulated hospital operation. To ensure the desired sign pattern for the induced correlations among the responses $\{y_g\}$, we structured the hospital simulation so as to maintain the following property across all eight runs representing alternative system configurations : y_g has the same type of *monotonic* dependence on the lth random number sampled within a run when all the other random numbers are fixed ($l = 1, ...$).

Table 1 gives the design points used for the Hospital Simulation Model. Table 2 shows the random number streams that are used drive the different stochastic components in the system. Table 3 gives the observations recorded from the simulation experiment. Twenty independent replications were made across eight design points. Thus, we have, $r = 20$, $m = 8$, $n = 160$, and $p = 7$.

Table 1. Design Points used for Hospital Simulation Model

Design Point Number	ICU beds	CCU beds	Int. Care beds
1	13	4	15
2	13	4	17
3	13	6	15
4	13	6	17
5	15	4	15
6	15	4	17
7	15	6	15
8	15	6	17

Table 2. Random Number Assignment for Hospital Simulation Model

Stream Number	Stochastic Process Sampled
1	Arrival process of patients to hospital
2	Path selection upon entering the hospital
3	Intensive care stay of patients
4	Coronary care stay of patients
5	Path selection for intensive care patients
6	Path selection for coronary care patients
7	Intermediate care stay for intensive care patients
8	Intermediate care stay for coronary care patients

Table 3. Balking Rates at the Hospital ICU, CCU and Int. Care Units for 20 replications at 8 design points

Repl. No.	Design Point 1	2	3	4	5	6	7	8	$\bar{y}_{i.}$
1	47.57	45.05	46.82	43.30	47.07	43.62	46.40	42.77	45.20
2	46.80	43.15	46.42	42.72	46.57	43.00	46.37	42.72	44.72
3	45.85	42.22	45.17	41.57	45.57	42.15	44.65	41.17	43.54
4	49.90	46.40	45.17	45.42	49.35	46.62	48.22	44.67	47.32
5	49.07	45.67	48.10	44.55	48.47	45.02	47.70	44.07	46.58
6	49.82	46.07	48.92	45.30	49.12	45.50	45.40	44.65	47.23
7	47.15	43.47	45.92	42.20	46.40	42.92	45.40	41.85	44.41
8	48.71	45.10	47.85	44.37	47.92	44.40	47.02	43.45	46.10
9	46.97	43.30	46.42	42.97	46.42	46.62	45.95	42.20	44.60
10	46.77	43.17	46.05	42.47	46.32	42.82	45.52	41.97	44.31
11	46.45	42.77	45.80	42.30	46.12	42.45	45.47	41.90	44.15
12	47.27	43.82	46.62	42.97	46.80	43.27	46.15	42.47	44.92
13	47.65	43.95	47.20	43.57	47.22	43.60	46.70	43.02	45.36
14	50.37	46.72	49.65	45.87	49.85	46.25	49.02	43.35	47.88
15	50.75	47.12	50.02	46.27	50.17	46.40	49.50	45.87	48.26
16	46.87	43.40	46.12	42.70	46.50	42.95	45.87	42.27	44.60
17	49.30	45.67	48.60	44.87	48.67	45.02	47.90	44.22	46.78
18	47.72	43.80	46.97	43.20	47.22	43.47	46.50	42.70	45.20
19	46.77	43.12	46.07	42.55	45.80	42.27	45.25	41.70	44.19
20	45.95	42.62	45.15	41.65	45.32	41.87	44.57	41.05	43.52
$\bar{y}_{.j}$	47.88	44.28	47.14	43.54	47.34	43.76	46.63	43.01	$\bar{y}_{..} = 45.45$

The design matrix **X** is as follows

$$\mathbf{X} = \begin{bmatrix} +1 & -1 & -1 & -1 & +1 & +1 & +1 \\ +1 & -1 & -1 & +1 & +1 & -1 & -1 \\ +1 & -1 & +1 & -1 & -1 & +1 & -1 \\ +1 & -1 & +1 & +1 & -1 & -1 & +1 \\ +1 & +1 & -1 & -1 & -1 & -1 & +1 \\ +1 & +1 & -1 & +1 & -1 & +1 & -1 \\ +1 & +1 & +1 & -1 & +1 & -1 & -1 \\ +1 & +1 & +1 & +1 & +1 & +1 & +1 \end{bmatrix},$$

The sample covariance matrix of the responses, $\mathbf{S}^{(CRN)}$ was computed to be

$$\mathbf{S}^{(CRN)} = \begin{bmatrix} 2.2619 & 2.2403 & 2.1879 & 2.1133 & 2.1828 & 2.1057 & 2.0931 & 2.0384 \\ 2.2403 & 2.2368 & 2.1628 & 2.0948 & 2.1616 & 2.0933 & 2.0674 & 2.0197 \\ 2.1879 & 2.1628 & 2.1480 & 2.0736 & 2.1275 & 2.0446 & 2.0652 & 2.0070 \\ 2.1133 & 2.0948 & 2.0736 & 2.0117 & 2.0514 & 1.9718 & 1.9903 & 1.9365 \\ 2.1828 & 2.1616 & 2.1275 & 2.0514 & 2.1361 & 2.0584 & 2.0563 & 2.0031 \\ 2.1057 & 2.0933 & 2.0446 & 1.9718 & 2.0584 & 1.9944 & 1.9745 & 1.9270 \\ 2.0931 & 2.0674 & 2.0652 & 1.9903 & 2.0563 & 1.9745 & 2.0171 & 1.9566 \\ 2.0384 & 2.0197 & 2.0070 & 1.9365 & 2.0031 & 1.9270 & 1.9566 & 1.9046 \end{bmatrix}, \quad (4.2)$$

and the sample correlation matrix of the responses, was computed to be

$$\text{corr}(\mathbf{y}) = \begin{bmatrix} 1.0000 & 0.9960 & 0.9926 & 0.9907 & 0.9930 & 0.9914 & 0.9799 & 0.9821 \\ 0.9960 & 1.0000 & 0.9867 & 0.9875 & 0.9889 & 0.9911 & 0.9733 & 0.9785 \\ 0.9926 & 0.9867 & 1.0000 & 0.9975 & 0.9932 & 0.9878 & 0.9921 & 0.9923 \\ 0.9907 & 0.9875 & 0.9975 & 1.0000 & 0.9896 & 0.9844 & 0.9881 & 0.9893 \\ 0.9930 & 0.9889 & 0.9932 & 0.9896 & 1.0000 & 0.9973 & 0.9907 & 0.9931 \\ 0.9914 & 0.9911 & 0.9878 & 0.9844 & 0.9973 & 1.0000 & 0.9844 & 0.9887 \\ 0.9799 & 0.9733 & 0.9921 & 0.9881 & 0.9907 & 0.9844 & 1.0000 & 0.9983 \\ 0.9821 & 0.9785 & 0.9923 & 0.9893 & 0.9931 & 0.9887 & 0.9983 & 1.0000 \end{bmatrix}. \quad (4.3)$$

Then, according to Result 1, the optimal estimator of $\boldsymbol{\beta}$ is computed as

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\bar{\mathbf{y}} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_2 \\ \hat{\beta}_3 \\ \hat{\beta}_4 \\ \hat{\beta}_5 \\ \hat{\beta}_6 \end{bmatrix} = \begin{bmatrix} 45.4822 \\ -0.2536 \\ -0.3861 \\ -1.8117 \\ 0.0017 \\ 0.0061 \\ -0.0070 \end{bmatrix}$$

From equation (3.6), we obtain $\hat{\lambda}_1 = 15.6739$. According to Result 2, a $100(1-\alpha)\%$ confidence interval for β_0 can be computed from

$$\beta_0 \in \hat{\beta}_0 \pm \frac{\hat{\lambda}_1}{\sqrt{(mr)}} t_{r-1}^{\alpha/2}.$$

For this example, the 95% confidence interval for β_0 is

$$\beta_0 \in 45.4822 \pm 0.8657$$

Now suppose we want to test the hypothesis

$H_0 : \beta_1 = \beta_2 = \ldots \beta_6 = 0$
versus
H_1 : not all $\beta_i = 0$; $i = 1, \ldots, 6$.

We use Result 3, with the **H** matrix as $\mathbf{I}_6$; hence $h = 6$. σ^2 and f can be obtained by applying the ordinary linear model, i.e., observations are independent. We then obtain the values of $\hat{\lambda}_2^{\S} = 0.0230$ and $f^* = 4052.1$ using equations (3.8) and (3.10) respectively. f^* is compared to $F_{6,133}^{\S}$ which, for $\alpha = 0.05$, is 2.15. Hence we reject the null hypothesis.

Looking at $\hat{\boldsymbol{\beta}}$, the optimal estimator of $\boldsymbol{\beta}$, we observe that the interaction terms have very low coefficient values. We thus test for $\beta_4 = \beta_5 = \beta_6 = 0$. In other words, we test the hypothesis

$H_0 : \beta_4 = \beta_5 = \beta_6 = 0$
versus
H_1 : not all $\beta_i = 0$; $i = 4, 5, 6$.

We use Result 3, with the **H** matrix as shown below

$$\mathbf{H} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

We calculated $\mathbf{f}^*$ to be 0.211, which was compared to $F_{3,133}^{\S}$, which for $\alpha = 0.05$ is 2.67. The test, as expected accepts H_0, and hence, the interaction effects are negligible.

Next we consider constructing simultaneous confidence intervals for elements of β_1, using the Bonferroni approach. We use Result 3 by using three different **H**'s : (1,0,0), (0,1,0), and (0,0,1). Let $l = 1$. From equation (3.11), we note that setting $l = 1$, and with **H** as specified, yield confidence intervals for β_i's,

$$\beta_i \in \hat{\beta}_i \pm \hat{\lambda}_2 \left[\frac{1}{r} F^{\alpha}_{1,n-p-r} [(\mathbf{T}'\mathbf{T})^{-1}]_{ii} \right]^{1/2}.$$

where $i = 1, 2, 3$, $[(\mathbf{T}'\mathbf{T})^{-1}]_{ii}$ is the ith diagonal element of $[(\mathbf{T}'\mathbf{T})^{-1}]$. In Bonferroni type intervals, α at each interval is set so that the lower bound of the overall coverage, $1 - 3\alpha$, is at the desired level. For at least 95% overall coverage we let $\alpha \simeq .015$. For this example, the centers of the intervals are the estimates of the parameters reported earlier, and the half-widths of the 95% Bonferroni type intervals are equal to 0.003. Thus, we have,

$$\begin{aligned} -0.2566 &\leq \beta_1 \leq -0.2506, \\ -0.3891 &\leq \beta_2 \leq -0.3831, \\ -1.8147 &\leq \beta_3 \leq -1.8087. \end{aligned}$$

We have thus demonstrated the statistical analysis of the simulation experiment under the common random number strategy. We now proceed with the validation procedure. The sample variances at the 8 design points are 2.2619, 2.2368, 2.1480, 2.0117, 2.1361, 1.9944, 2.0171, 1.9046. We perform the test for multivariate normality on the responses using the same procedure suggested by Tew and Wilson (1990). We compute the Shapiro-Wilk test-statistic W^* to be 0.6306 and compare it with the estimated lower critical value $\hat{\omega}^*_{\alpha}(m,r)$ of the multivariate Shapiro-Wilk Test for $m = 8$, $\alpha = 0.05$ and $r = 20$. Interpolating the table given by Tew and Wilson, we find $\hat{\omega}^*_{0.05}(8,20) = 0.5983$. Thus we see that $W^* > \hat{\omega}^*_{0.05}(8,20)$, and hence we accept the multivariate normal assumption of the responses.

To check for the CRN covariance structure as given by equation (3.2), we evaluate equations (3.6), (3.8), and (3.9). This yields $\hat{\sigma}^2 = 2.0836$, $\hat{\lambda}_1 = 15.6739$ $\hat{\lambda}_2 = 0.0230$. Consequently, the modified likelihood ratio statistic in equation (3.28) is $\mathbb{N} = 9.8278$; and the corresponding 99% critical value for the chi-squared distribution with 34 degrees of freedom is $\chi^2_{0.99}(34) = 56.01$. Thus we conclude that the hypothesis in (3.24) is reasonable for the hospital simulation.

For the Lack-Of-Fit test with the CRN covariance structure, we tested the null hypothesis in equation (3.51). The left hand side of equation (3.54) is computed to be 0.0921 which is compared to $F_{1-0.005}(1,133) = 3.9$. Thus we conclude that the postulated model in equation (4.1) provides an adequate description of the relationship between the response and the factors of interest.

In the development of the statistical analysis for the hospital simulation study, we had assumed the multivariate normality of the response vector, the CRN covariance structure as given in (3.2), and also the adequacy of the proposed model in (4.1). These three assumptions were validated in the subsequent validation procedure. The interaction terms β_4, β_5, and β_6 were shown to have negligible effect on the behaviour of the model, and hence can be discarded. Thus, with the theoretical development in Chapter 3, and with this illustration of the hospital simulation study, we now have a tool to conduct statistical analysis, and a validation procedure, for simulation experiments conducted under the common random number strategy.

Chapter V Summary and Conclusions

This chapter summarizes the contributions of this research and reviews the conclusions regarding the statistical analysis on the estimation of the parameters of interest for a multipopulation model in a simulation experiment performed under the common random number strategy, as well as the validation procedure for the necessary assumptions made while conducting this statistical analysis.

As mentioned in the introduction, this research focussed on two goals : (a) Developing a statistical analysis procedure for multipopulation simulation experiments performed under the CRN strategy, and (b) Developing a validation procedure for testing the necessary assumptions made while conducting this statistical analysis. Both procedures were developed in Chapter 3 and were illustrated by means of an example in Chapter 4. A brief review and summary of this research is given in Section 5.1. Future research is discussed in Section 5.2.

5.1 Overview and Summary of Research

Common random number strategy is one of the simplest variance reduction technique that can be applied to almost all classes of simulation experiments. In contrast, the Schruben-Margolin strategy needs the design matrix to be blockable into two orthogonal blocks. For second and higher order designs this technique is not applicable. For the Schruben-Margolin strategy a statistical analysis and validation proce-

dure was developed earlier. Thus, we found a need to do the same for the common random number strategy.

Chapter 3 developed statistical analysis and validation procedures under the common random number strategy for multipopulation simulation experiments. First, this statistical analysis procedure allows for optimal estimation of the unknown parameters of a general linear model. It also gives confidence intervals about these optimal estimates, and also the joint confidence intervals. There are certain assumptions made while conducting this statistical analysis, like the multivariate normality of the vector of responses, the special covariance structure for the covariance matrix between the responses, and also the adequacy of the proposed linear model. These assumptions, if violated, would jeopardize the results obtained by the statistical analysis. Thus, the importance of the validation procedure is the realization of the fallacy of statistical analysis, if performed with violations of any of the above mentioned assumptions.

These methods were applied to the hospital simulation in Chapter 4 which illustrates the use of these methods under the common random number strategy across an eight-point simulation experiment. The results give the estimates of the unknown parameters as well as the desired confidence intervals on these parameters. Performing the validation tests for this example show that the assumptions made while conducting the statistical analysis are true, and hence we can have more confidence in the appropriateness of the results obtained from the applied statistical analysis procedure.

5.2 *Future Research*

The directions for future research stemming from the material studied in this thesis pertain to simulation experiments in which there is more than one response of interest in a single experiment.

In our thesis, we considered only one response of interest in *a* simulation experiment. But in practice, there can be many situations where, in a single experiment, there can be multiple responses of interest. For example, in the hospital simulation model, some other responses of interest could have been the sojourn time of the patients in the hospital, or, the number of patients who do not need the intermediate care facility. For such a situation, the statistical analysis and validation procedures would need to be at least modified, if not re-developed. Such a situation may involve a multivariate statistical analysis, that is, the responses of interest may be correlated. This would be an interesting avenue for further research.

A second avenue for research could be developing statistical validation procedures for simulation experiments, conducted, not under the common random number strategy, but under combined correlation induction strategies. For example, antithetic and control variates could be used together to achieve variance reduction (see C. Kwon, 1990).

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1.0 APPENDIX I

Result 1 in Chapter 3 of this thesis is proved here. This result yields an optimal estimate of β. By optimal estimate, we mean the minimum variance, unbiased estimate.

Since $\mathbf{y}^*$ is comprised of two separate ordinary linear models, one involving $(\mathbf{y}_1^*, \beta_0, \lambda_1^2)$, and the other involving $(\mathbf{y}_2^*, \beta_1, \lambda_2^2)$, the optimal estimators for β_0 and β_1 are just the obvious ones based on $\mathbf{y}_1^*$ and $\mathbf{y}_2^*$ (see Graybill, 1976, pp. 173-175), namely

$$\hat{\beta}_0^* = (m)^{(-1/2)} r^{-1} \mathbf{1}'_r \mathbf{y}_1^* \sim N_1(\beta_0, \lambda_1^2 (mr)^{-1}), \qquad (A1.1)$$

and,

$$\hat{\boldsymbol{\beta}}_1^* = (\mathbf{T}^{*'}\mathbf{T}^*)^{-1}\mathbf{T}^{*'}\mathbf{y}_2^* \sim N_{(p-1)}(\boldsymbol{\beta}_1, \lambda_2^2 (\mathbf{T}^{*'}\mathbf{T}^*)^{-1}) \qquad (A1.2)$$

We now show that these estimators are the same as the ordinary least squares estimators, $\hat{\beta}_0$ and $\hat{\boldsymbol{\beta}}_1$. Since $\boldsymbol{\Gamma}^{(CRN)}$ is orthogonal,

$$\hat{\boldsymbol{\beta}} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\boldsymbol{\beta}}_1 \end{bmatrix} = (\mathbf{G}'\mathbf{G})^{-1}\mathbf{G}'\mathbf{y} = (\mathbf{G}^{*'}\mathbf{G}^*)^{-1}\mathbf{G}^{*'}\mathbf{y}^* = \begin{bmatrix} \hat{\beta}_0^* \\ \hat{\boldsymbol{\beta}}_1^* \end{bmatrix}. \qquad (A1.3)$$

2.0 APPENDIX II

Result 2 in Chapter 3 of this thesis is proved here. This result yields the confidence interval for β_0.

Let $\hat{\lambda}_1^2$ be the usual unbiased estimator of λ_1^2 (see p. 173 of Graybill, 1976). on $\mathbf{y}_1^*$, i.e.,

$$\hat{\lambda}_1^2 = \frac{\|\mathbf{y}_1^* - (m)^{(1/2)}\mathbf{1}_r\hat{\beta}_0\|^2}{r-1}. \qquad (A2.1)$$

Then, by standard results for the linear model (see Graybill, 1976), we see that

$$\frac{(mr)^{(1/2)}(\hat{\beta}_0 - \beta_0)}{\hat{\lambda}_1} \sim t_{(r-1)}. \qquad (A2.2)$$

We can use this fact in an obvious way to find size α tests and a $100(1-\alpha)\%$ confidence interval for β_0. The tests associated with this t-statistic are likelihood ratio tests, UMP unbiased and UMP invariant for the problems based on $\mathbf{y}_1^*$ and have these properties for the original problem. We now find a formula for $\hat{\lambda}_1^2$ in terms of the original observations. From the definition of $\mathbf{y}_1^*$, we see that it ith component is $(m)^{(1/2)}\bar{y}_{i.}$. Therefore $\hat{\beta}_0 = \bar{y}_{..}$, and

$$\lambda_1^2 = \frac{m\sum_{i=1}^{r}(\bar{y}_{i.} - \bar{y}_{..})^2}{r-1}. \qquad (A2.3)$$

3.0 APPENDIX III

Result 3 in Chapter 3 of this thesis is proved here. This result yields a confidence interval for $\boldsymbol{\beta}_1$

Consider testing H_0: $\mathbf{H}\boldsymbol{\beta}_1 = \mathbf{0}_h$ vs. H_1: $\mathbf{H}\boldsymbol{\beta}_1 \neq \mathbf{0}_h$, where $\mathbf{H}$ is a $(h \times (p-1))$ matrix of rank $h < p$. Let $\hat{\lambda}_2^2$ be the usual unbiased estimator to λ_2^2 based on $\mathbf{y}_2^*$ (see p. 175 of Graybill, 1976),

$$\hat{\lambda}_2^2 = \frac{(\|\mathbf{y}_2^* - \mathbf{T}^*\hat{\boldsymbol{\beta}}_1\|^2)}{(r(m-1)-p)}. \qquad (A3.1)$$

Then the optimal test for the problem, based on $\mathbf{y}_2^*$ (see p. 190 of Graybill, 1976), is to reject the null hypothesis if

$$\mathbf{f}^* = \frac{(\mathbf{H}\hat{\boldsymbol{\beta}}_1)'\mathbf{H}(\mathbf{T}^{*\prime}\mathbf{T}^*)^{-1}(\mathbf{H}\hat{\boldsymbol{\beta}}_1)}{(h\hat{\lambda}_2^2)} > F^{\alpha}_{(r(m-1)-p)}. \qquad (A3.2)$$

When $\boldsymbol{\Xi}^{(CRN)} = \sigma^2\mathbf{I}_n$, the optimal test for H_0: $\mathbf{H}\boldsymbol{\beta}_1 = \mathbf{0}_h$ vs. H_1: $\mathbf{H}\boldsymbol{\beta}_1 \neq \mathbf{0}_h$ rejects H_0 if

$$f = \frac{(r(\mathbf{H}\hat{\boldsymbol{\beta}}_1)'\mathbf{H}(\mathbf{T}'\mathbf{T})^{-1}(\mathbf{H}\hat{\boldsymbol{\beta}}_1))}{(h\hat{\sigma}^2)} > F^{\alpha}_{(h,\, n-p)}, \qquad (A3.3)$$

where $\hat{\sigma}^2$, is as given in (3.4), that is,

$$\hat{\sigma}^2 = \frac{(\|\mathbf{y} - \mathbf{G}\hat{\boldsymbol{\beta}}\|^2)}{(n-p)}.$$

Since $\mathbf{H}(\mathbf{T}^{*\prime}\mathbf{T}^*)^{-1}\mathbf{H}' = (1/r)\mathbf{H}(\mathbf{T}'\mathbf{T})^{-1}\mathbf{H}'$, we have

$$(n-p)\hat{\sigma}^2 = \|\mathbf{y} - \mathbf{G}\hat{\boldsymbol{\beta}}\|^2 = \|\mathbf{y}_1^* - (m)^{(1/2)}\mathbf{1}_r\hat{\beta}_0\|^2 + \|\mathbf{y}_2^* - \mathbf{T}^*\hat{\boldsymbol{\beta}}_1\|^2. \quad (A3.4)$$

Therefore, we get,

$$(n-p)\hat{\sigma}^2 = m\sum_{i=1}^{r}(\bar{y}_{i.} - \bar{y}_{..})^2 + \|\mathbf{y}_2^* - \mathbf{T}^*\hat{\boldsymbol{\beta}}_1\|^2. \quad (A3.5)$$

Thus, by equations (A3.1) and (A3.5), we have

$$\hat{\lambda}_2^2 = \frac{(n-p)\sigma^2 - m\sum_{i=1}^{r}(\bar{y}_{i.} - \bar{y}_{..})^2}{(n-p-r)}. \quad (A3.6)$$

Now, consider the simultaneous confidence intervals for $\mathbf{1}'\mathbf{H}\boldsymbol{\beta}_1$ for all $\mathbf{1} \in R^k$. Based on $\mathbf{y}_2^*$, the Scheffe $100(1-\alpha)\%$ simultaneous confidence intervals for $\mathbf{1}'\mathbf{H}\boldsymbol{\beta}_1$ are given by (see p. 198 of Graybill, 1976, Theorem 6.5.2) ,

$$\mathbf{1}'\mathbf{H}\boldsymbol{\beta}_1 \in \mathbf{1}'\mathbf{H}\hat{\boldsymbol{\beta}}_1 \pm \hat{\lambda}_2\left[hF^{\alpha}_{(h,(m-1)r-p)}\mathbf{1}'\mathbf{H}(\mathbf{T}^{*\prime}\mathbf{T}^*)^{-1}\mathbf{H}'\mathbf{1}\right]^{1/2} \text{ for all } \mathbf{1} \in R^h. \quad (A3.7)$$

When $\boldsymbol{\Xi} = \sigma^2\mathbf{I}_n$, the Scheffe $100(1-\alpha)\%$ simultaneous confidence intervals are

$$\mathbf{1}'\mathbf{H}\boldsymbol{\beta}_1 \in \mathbf{1}'\mathbf{H}\hat{\boldsymbol{\beta}}_1 \pm \hat{\sigma}\left[(h/r)F^{\alpha}_{(h,\,n-p)}\mathbf{1}'\mathbf{H}(\mathbf{T}'\mathbf{T})^{-1}\mathbf{H}'\mathbf{1}\right]^{1/2}. \quad (A3.8)$$

Therefore, if we let HW_l denote the half width of the Scheffe $100(1-\alpha)\%$ simultaneous confidence intervals for $\mathbf{1}'\mathbf{H}\boldsymbol{\beta}_1$ in the ordinary linear model, the $100(1-\alpha)\%$ simultaneous confidence intervals for $\Xi^{(CRN)} = \Sigma^{(CRN)} \otimes \mathbf{I}_r$ are

$$\mathbf{1}'\mathbf{H}\boldsymbol{\beta}_1 \in \mathbf{1}'\mathbf{H}\hat{\boldsymbol{\beta}}_1 \pm \left[\frac{(\hat{\lambda}_2^2 F^{\alpha}_{(h,\, n-p-r)})}{(\hat{\sigma}^2 F^{\alpha}_{(h,\, n-p)})} \right]^{1/2} HW_l. \qquad (A3.9)$$

4.0 APPENDIX IV

Result 4 in Chapter 3 of this thesis is proved here. This result yields a joint confidence interval for β_0 and β_1.

We derive the formulas for drawing inferences that involve both β_0 and β_1. By resorting to multivariate analysis, we can give exact but non-optimal procedures. Let

$$\bar{\mathbf{y}} = \frac{1}{r}\sum_{i=1}^{r}\mathbf{y}_i, \tag{A4.1}$$

and

$$\mathbf{S} = \frac{1}{r-1}\sum_{i=1}^{r}(\mathbf{y}_i - \bar{\mathbf{y}})(\mathbf{y}_i - \bar{\mathbf{y}})'. \tag{A4.2}$$

where $\bar{\mathbf{y}}$ and $\mathbf{S}$ are independent (see pp. 328-329 of Arnold, 1981, Theorem 18.2). Also, the estimator of $\boldsymbol{\beta}$ can be written as

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\bar{\mathbf{y}} \sim N_p(\boldsymbol{\beta}, \frac{1}{r}\Delta), \tag{A4.3}$$

where $\Delta = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\Sigma\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}$. Because of the independence of $\bar{\mathbf{y}}$ and $\mathbf{S}$, $\hat{\boldsymbol{\beta}}$ and $\hat{\Delta}$ are independent. Also by Theorem 17.6 of Arnold (1981), $\hat{\Delta}$ has a Wishart distribution, i.e.

$$\hat{\Delta} \sim W_p(r-1, 1/(r-1)\Delta). \tag{A4.4}$$

For a $(k \times p)$ known matrix of rank $k \leq p$, we observe that $\mathbf{K}\hat{\boldsymbol{\beta}}$ and $\mathbf{K}\hat{\Delta}\mathbf{K}'$ are independent and

$$\mathbf{K}\hat{\boldsymbol{\beta}} \sim N_k(\mathbf{K}\boldsymbol{\beta}, 1/r\mathbf{K}\Delta\mathbf{K}'), \tag{A4.5}$$

$$\mathbf{K}\hat{\Delta}\mathbf{K}' \sim W_k(r-1, \frac{1}{r-1}\mathbf{K}\Delta\mathbf{K}'). \tag{A4.6}$$

Therefore, by Hotelling's T^2 distribution (see p. 320 of Arnold, 1981, Theorem 17.11), we have

$$t^2 = \frac{(r(r-k))}{(k(r-1))}(\mathbf{K}\hat{\boldsymbol{\beta}})'(\mathbf{K}\hat{\Delta}\mathbf{K}')^{-1}\mathbf{K}\hat{\boldsymbol{\beta}} \sim F^{\alpha}_{(k,r-k)}((\mathbf{K}\boldsymbol{\beta})'(\mathbf{K}\Delta\mathbf{K}')^{-1}(\mathbf{K}\boldsymbol{\beta})r). \tag{A4.7}$$

Hence, a size α procedure for testing H_0: $\mathbf{K}\boldsymbol{\beta} = \mathbf{0}_k$ vs. $\mathbf{K}\boldsymbol{\beta} \neq \mathbf{0}_k$ is to reject the null hypothesis if $t^2 > F^{\alpha}_{k,r-k}$.

Note that under the null hypothesis the non-centrality parameter is zero. The associated $100(1-\alpha)\%$ Scheffe-type simultaneous confidence intervals are

$$\mathbf{1}'\mathbf{K}\boldsymbol{\beta} \in \mathbf{1}'\mathbf{K}\hat{\boldsymbol{\beta}} \pm \left[\frac{k(r-1)}{r(r-k)}F^{\alpha}_{(k,r-k)}\mathbf{1}'\mathbf{K}\hat{\Delta}\mathbf{K}'\mathbf{1}\right]^{\frac{1}{2}} \text{ for all } \mathbf{1} \in R^k. \tag{A4.8}$$

Since it is required that $r - k > 0$, which should hold for all $k \leq p$, we must have $r > p$. That is, the number of replications must be greater than the number of parameters.

5.0 APPENDIX V

Relation (3.34) in Chapter 3 is proved here.

First we define Θ, the parameter space corresponding to the alternative hypothesis H_1 of equation (3.24). Let σ_{gk} denote the (g,k) element of the covariance matrix $\Sigma^{(CRN)}$ for the original response $\mathbf{y}_i$, and let θ denote the $[1/2m(m+1)] \times 1$ vector of parameters obtained by respectively stacking into a single column those entries in each column of $\Sigma^{(CRN)}$ that lie on or below the diagonal

$$\theta = \text{vech}(\Sigma^{(CRN)}) = (\sigma_{11}, \sigma_{12}, \ldots, \sigma_{m1}, \sigma_{22}, \sigma_{23}, \ldots, \sigma_{m2}, \sigma_{33}, \ldots, \sigma_{mm})'.$$

It follows that Θ is the open subset of $[1/2m(m+1)]$-dimensional Euclidean space given by

$$\Theta = \{\theta = vech(\Sigma^{(CRN)}) : \Sigma^{(CRN)} \text{ is symmetric and positive definite}\}. \quad (A5.1)$$

Next we define the subspace $\Theta_0 \subset \Theta$ corresponding to the null hypothesis H_0 of display (3.24). Let $\zeta \equiv (\zeta_1, \zeta_2)' \equiv (\sigma^2, \rho_+)'$ denote the vector of parameters describing the induced covariance structure of the response $\mathbf{y}_i$ under this hypothesis. In this situation, there are at most two distinct eigenvalues $\{\lambda_1, \lambda_2\}$ of $\text{cov}(\mathbf{y}_i)$; and when these

eigenvalues are expressed in terms of the components of ζ, we see that the null hypothesis H_0 in (3.24) holds if and only if

$$\text{cov}(\mathbf{y}_i^*) = \begin{bmatrix} \lambda_1 & \mathbf{0} \\ \mathbf{0} & \lambda_2 \mathbf{I}_{m-1} \end{bmatrix}, \tag{A5.2}$$

where

$$\lambda_1 \equiv \zeta_1[1 + (q-1)\zeta_2) > 0$$

$$\lambda_2 \equiv \zeta_1(1 - \zeta_2) > 0$$

$$\zeta_1 > 0$$

$$0 < \zeta_2 < 1.$$

These above conditions are equivalent to requiring ζ to belong to the open subset of 2-dimensional Euclidean space given by

$$\mathbf{Z} \equiv \{\zeta = (\zeta_1, \zeta_2)' : \zeta_1 > 0,\ 0 < \zeta_2 < 1\}. \tag{A5.3}$$

We now define the topological transformation $\tau{:}\zeta \in \mathbf{Z} \rightarrow \tau(\zeta) \in \boldsymbol{\Theta}_o$ by the relation

$$\tau(\zeta) \equiv vech\left[\zeta_1\left[\frac{1}{2}\zeta_1 \mathbf{G}\right] + (1 - \zeta_2)\mathbf{I}_m\right] = \text{vech}(\boldsymbol{\Sigma}^{(CRN)}),$$

where $\mathbf{G} \equiv \mathbf{1}_m \mathbf{1}_m'$, and $\boldsymbol{\Sigma}^*$ is obtained from equation (3.2) when all its elements are expressed in terms of the components of ζ. Thus $\boldsymbol{\Theta}_o$ is the image of *Zeta.* under the mapping τ.

To establish the desired asymptotic property of the likelihood ratio L in (3.26), we observe that the mapping τ possesses continuous first-order partial derivatives; and it is straightforward to verify that the $[1/2m(m+1)] \times 3$ Jacobian matrix

$$\mathbf{J}_{\tau}(\zeta) \equiv \| \frac{\delta \tau_i}{\delta \zeta_j} \| \text{ has rank 2 for every } \zeta \in \mathbf{Z}. \qquad (A5.4)$$

Combining (A5.3), and (A5.4), we apply Theorem 4.4.4 of Serfling (1980, p. 58) to conclude that the conventional likelihood ratio L in (3.26) has the asymptotic property

$$\mathbb{N} \equiv -2 \ln(L) \xrightarrow{D} \chi^2[\frac{1}{2} m(m+1) - 2] \text{ as } r \to \infty. \qquad (A5.5)$$

6.0 Appendix VI

SLAM II Code for Hospital Simulation Model

```
      PROGRAM MAIN
      COMMON/SCOM1/ATRIB(100),DD(100),DDL(100),DTNOW,II,MFA,
     *MSTOP,NCLNR,NCRDR,NPRNT,NNRUN,NNSET,NTAPE,SS(100),
     *SSL(100),TNEXT,TNOW,XX(100)
      COMMON/UCOM1/FX(3),XVAL(3),NCUST(3)
      COMMON QSET(5000)
      DIMENSION NSET(5000)
      EQUIVALENCE (NSET(1),QSET(1))
      NNSET = 5000
      NCRDR = 5
      NPRNT = 6
      NTAPE = 7
      WRITE(88,111)
  111 FORMAT(2X,'IS DESIGN POINT 1',/,/)
      CALL SLAM
      STOP
      END

      SUBROUTINE EVENT(I)
      INCLUDE (SLMSCOM1)
      GO TO (1),I
    1 WRITE(88,2) XX(1)
    2 FORMAT(2X,F9.4)
      RETURN
      END

GEN,SSJ,THESIS 1991,3/21/1991,20,NO,NO,,NO,NO;
LIMITS,3,8,100;
NETWORK;
;     THIS IS THE SLAM II NETWORK CODE FOR THE PATIENT PATHS
;     IN HOSPITAL UNIT SIMULATION GIVEN BY SCHRUBEN AND MARGOLIN(1978)
```

```
;    AND ALSO BY HUSSEY, MYERS, AND HOUCK (1987)
;    CREAT THE ARRIVING PATIENTS TO THE SYSTEM
     CREATE,EXPON(.303,8),0.0,,,1;
     ACT,0.;
;    ASSIGN ALL OF THE SEVICE TIMES TO THE ENTITY AS WELL AS THE
;    PATH PROBABILITIES
     ASSIGN,ATRIB(1) = UNFRM(0.0,1.0,2),
          ATRIB(2) = RLOGN(3.4,3.5,3),
          ATRIB(3) = RLOGN(3.8,1.6,4),
          ATRIB(4) = UNFRM(0.0,1.0,5),
          ATRIB(5) = UNFRM(0.0,1.0,6);
     ACT,0.;
     ASSIGN,ATRIB(6) = RLOGN(15.0,7.0,7),
          ATRIB(7) = RLOGN(17.0,3.0,1),
          ATRIB(8) = 0.0;
     ACT,0.;
;
;    GO TO EITHER INTENSIVE CARE UNIT OR CORONARY UNIT
;

     GOON,1;
     ACT,0.0,ATRIB(1) .LE. .75,ICU;
     ACT,0.0,,CCU;

;
;    INTENSIVE CARE UNIT
;
ICU  QUEUE(1),0,0,BALK(FAIL);
     ACT(13)/1,ATRIB(2);
     GOON,1;
     ACT,0.0,ATRIB(4) .LE. .27,TERM;
     ACT,0.0;
     ASSIGN,ATRIB(8) = ATRIB(6);
     ACT,0.0,,INTRC;
;
;    CORONARY CARE UNIT
;
CCU  QUEUE(2),0,0,BALK(FAIL);
     ACT(4)/2,ATRIB(3);
     GOON,1;
     ACT,0.0,ATRIB(5) .LE. .20,TERM;
     ACT,0.0;
     ASSIGN,ATRIB(8) = ATRIB(7);
     ACT,0.0,,,INTRC;
;    INTERMEDIATE CARE UNIT
INTRC QUEUE(3),0,0,BALK(FAIL);
     ACT(15)/3,ATRIB(8),,TERM;
;
;    TERMINATE PATIENTS WHO DID NOT BALK
;
TERM TERMINATE;
```

```
;    COUNT THE NUMBER OF PATIENTS WHO FAILED TO GAIN ADMISSION
;    IF NOT WITHIN THE FIRST 10 MONTHS OF OPERATION
;
FAIL  GOON,1;
      ACT,0.0,TNOW .LE. 300,TERM;
      ACT,0.0;
      ASSIGN, XX(1) = XX(1)+1.0;
      ACT,0.0;
      TERMINATE;
;     WRITE THE DESIRED OUTPUT AT THE END OF THE SIMULATION RUN
      CREATE,,1500,,1,1;
      ACT,0.0;
      ASSIGN,XX(1) = XX(1)/40.;
      ACT,0.0;
      EVENT,1,1;
      TERMINATE;
      ENDNETWORK;
SEEDS,14669(1),19827(2),10915(3),17639(4),18261(5),
      19819(6),11671(7),12295(8);
INIT,0,1500;
SIMULATE;
FIN;
```

VITA

Shirish Joshi was born on August 27, 1965, in Bombay, India. He received a B.S. in Electrical Engineering from Bombay University in June 1986. He worked as a computer hardware engineer with IDM Ltd., Bombay for one year. He received a M.S. in Mathematical Sciences from Virginia Commonwealth University, Richmond, Virginia in August, 1989.