ABSTRACT

GREGORY, WALTON CARLYLE. Design Procedures and Use of Prior Information in the Estimation of Parameters of the Non-Linear Model $\eta = \alpha - \beta\gamma^{X}$. (Under the direction of RICHARD L. ANDERSON.)

For this model, sometimes referred to as the Mitscherlich law, the problems of design and parameter estimation are considered from two points of view.

Case (1): It is assumed that no prior information is available on the parameters. A design recommended by Box and Lucas (1959) is compared with an equal-spacing design and a geometric-spacing design. To specify the Box-Lucas design, a value for γ must be assumed. The Box-Lucas design, whose performance is dependent upon the true and assumed γ's, is better than the equal-spacing design. The geometric-spacing design compares favorably with Box-Lucas, and would seem to be preferred unless the experimenter is confident that the assumed γ value is close to the true γ.

Case (2): It is assumed that the non-linear parameter γ has a beta distribution, which is known by the experimenter. The prior information is used in estimation of the parameters. The Box-Lucas and geometric-spacing designs are compared for this situation. The use of the prior information significantly improved the estimator for γ. In this case, the Box-Lucas design is better than the geometric-spacing design for estimating α and β.

BIOGRAPHY

The author was born May 10, 1941, in Cookeville, Tennessee. He was reared in Raleigh, North Carolina. In 1959, he graduated from Needham Broughton High School, Raleigh, North Carolina.

He received the Bachelor of Science degree with a major in experimental statistics from North Carolina State University in 1963. In June, 1963, he entered the graduate school at North Carolina State University to study experimental statistics. In June, 1965, he received the Master of Experimental Statistics degree. In June, 1966, after beginning the doctoral program in experimental statistics at North Carolina State University, he was employed by the Procter & Gamble Company as a consultant in statistics. In December, 1966, he returned to school at North Carolina State University on a leave of absence from the Procter & Gamble Company. In July, 1968, he returned to work. In December, 1969, he completed the research requirement for his doctorate in experimental statistics.

The author is single.

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1. INTRODUCTION

This thesis is concerned with design comparison and the effects of prior information on parameter estimation for the non-linear model

$$Y_i = \alpha - \beta\gamma^{X_i} + \varepsilon_i,\ i = 1, 2, \ldots, n; \tag{1.1}$$

where $0 < \gamma < 1$, $\alpha > \beta > 0$.

This model was first used in the fitting of data from fertilizer experiments. For this application, the response, Y, is the yield of some crop, and the independent variable, X, is the quantity of fertilizer applied. The value $\alpha - \beta$ is the expected yield when no fertilizer is added to the soil. α is the expected yield when a very large amount of fertilizer is added, with the stipulation that this amount of fertilizer is not large enough to adversely affect yield.

Other physical phenomena, of interest to engineers, may be described by this model. The engineer uses the laws of conservation of mass, energy, and momentum to derive the differential equation describing his process. He then solves the differential equation and estimates the parameters in the integrated form. For processes described by the differential equation

$$\frac{dY}{dX} = \Theta(\alpha - Y) \tag{1.2}$$

where $Y(0) = \alpha - \beta$, the integrated form is

$$Y = \alpha - \beta e^{-\Theta X} \tag{1.3}$$

Substituting $\gamma = e^{-\Theta}$ in (1.3) yields the model under consideration.

Three examples, each illustrating conservation of mass, energy, or momentum, respectively, are:

(1) Convective transfer of mass from a solid to a liquid stream,

(2) Heating of a solid in which conduction is essentially instantaneous relative to convection, and

(3) Movement of a projectile through some medium where the force retarding the object is directly proportional to the object's velocity.

In case (1) the response, Y, is the concentration of some substance, in the liquid, which is dissolving from the surface of the solid. The independent variable, X, is time. $\alpha - \beta$ is the concentration in the liquid at time zero. α is the maximum concentration attainable.

In case (2) the response, Y, is the temperature of a solid immersed in a quantity of liquid large enough that the temperature of the liquid is not materially affected by the temperature of the solid. The independent variable, X, is time. $\alpha - \beta$ is the temperature of the solid at time zero. α is the temperature of the liquid.

In case (3) the response, Y, is the velocity of an object moving through some medium. The independent variable, X, is time. $\alpha - \beta$ is the velocity at time zero. α is the terminal velocity of the object.

In this thesis it is assumed that the model represents the underlying physical mechanism, and the experimenter wishes to determine precisely the parameter values α, β, and γ.

Two basic approaches to the problems of design and estimation are taken.

In chapter 3, a design recommended by Box & Lucas (1959) is compared with an equal-spacing design and a geometric-spacing design. Knowledge of γ is required to specify the Box-Lucas design properly. The consequences of specifying γ incorrectly are considered.

In chapter 4, it is assumed that the experimenter can define a class of problems of which his present problem is a member. In addition, it is assumed that the γ's associated with the class of problems follow a beta distribution. The experimenter either knows or thinks he knows the form of this distribution from past experience. It is felt that if an experimenter has prior information on γ and uses it in designing his experiment, he should also use this information in estimating the parameters. The Box-Lucas and geometric-spacing designs are compared for a limited number of assumed and actual prior distributions on γ.

The criteria used in evaluating different strategies include the estimated mean square errors of $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\gamma}$, and the corresponding large sample variances.

Since the model under consideration is non-linear in γ, the small sample properties can not be determined analytically. Different experimental situations are each simulated many times, using IBM 360/65 and 360/75 computers.

2. REVIEW OF LITERATURE

This section is divided into two parts. The first is concerned with experimental design for a non-linear model. Some of the previous research makes use of prior distributions on the parameters. Both sequential and non-sequential procedures are developed. The second part is concerned with estimation where possibly incorrect prior information has been incorporated.

2.1 Experimental Design

Box & Lucas (1959) consider the problem of design specification for the non-linear model

$$y_i = f(\underline{X}_i,\underline{\Theta}) + \varepsilon_i,\ i = 1, 2, \ldots, n \qquad (2.1)$$

where $E(y_i) = \eta_i = f(\underline{X}_i,\underline{\Theta})$, and

$$E(y_i - \eta_i)(y_j - \eta_j) = \begin{cases} \sigma^2, & i = j \\ 0, & i \neq j \end{cases} .$$

In (2.1), $f(\underline{X}_i,\underline{\Theta})$ is non-linear in $\underline{\Theta}$.

The variance-covariance matrix of the least squares estimate of $\underline{\Theta}$ is approximated by $(F'F)^{-1}\sigma^2$, where $F_{nXp} = \{f_{ij}\}$, and

$$f_{ij} = \left[\frac{\partial f(\underline{X}_i,\underline{\Theta})}{\partial\Theta_j}\right]\Bigg|_{\underline{\Theta}=\underline{\Theta}_0} \qquad (2.2)$$

where $\underline{\Theta}_0$ is the true value of $\underline{\Theta}$. This method of determining the asymptotic variance-covariance matrix is equivalent to inverting F'F where the elements of F'F are found by taking the negative expectation of all second order partials of the log likelihood function with respect to the parameters.

The Box-Lucas criterion is to choose the design D that minimizes the determinant, $|(F'F)^{-1}|$. The number of distinct design points is required to equal the number of parameters to be estimated. Increased precision is attained by replicating the entire experiment as many times as desired. The problem that arises with this procedure is that the non-linear parameters must be known to correctly specify the design D. Therefore, a preliminary guess of the non-linear parameter values must be made to determine D.

This criterion has also been chosen by other authors working with sequential and Bayesian procedures for design selection in the non-linear case.

Box & Hunter (1965) derive a method for the sequential design of experiments based on Bayes' Theorem. Their model assumptions include those of Box & Lucas (1959). Experiments are planned one at a time, i.e., given n observations the (n+1)th experiment is planned. The prior on the parameters is assumed locally uniform, i.e., essentially constant in the range where the likelihood function of the data has appreciable value. The data are assumed normally distributed and the posterior distribution at stage n is used as the prior for stage n+1. Box & Hunter (1965) choose as their criterion, the maximization of the posterior density. This choice results in minimization of the same determinant as in Box & Lucas (1959).

Box & Hunter (1964) use a non-sequential, non-Bayesian approach. For this work the non-linear model is linearized with respect to both the parameters and the independent variables. The moment matrix for an n-run design is determined according to some desirable criterion (uncorrelated estimates, minimization of the average variance, etc.). Then settings of the independent variables are determined so as to satisfy the moment requirements.

Draper & Hunter (1966) assume a multinormal prior for the parameters in the non-linear model. Their procedure determines the settings for n experimental runs given the prior information and N experimental runs in hand. The criterion used is maximization of the posterior density.

2.2 Estimation of Parameters

In the unpublished Ph.D. thesis by E. L. Battiste (1967) the non-Bayesian application of prior information to parameter estimation is considered. Battiste investigated the effect of the use of incorrect prior information on parameter estimation in a linear regression model with two independent variables. It is determined that improvement (using a mean square error criterion) in the estimates is obtained when the prior information is incorrect, provided the bias in the prior mean is small relative to the prior standard deviation and the prior variance is not underestimated.

R. L. Anderson (1969) considers the use of prior information with the simplest linear model

$$y_i = \mu + \varepsilon_i, \; i = 1, 2, \ldots, n. \tag{2.3}$$

For this case, Anderson derives (using the average mean square error criterion) a formula for the optimal weighting of prior information in terms of the true prior variance and the squared bias. It has not been possible to generalize this result analytically to models of greater complexity.

3. COMPARISON OF DESIGNS WHEN ASSUMED VALUES OF γ ARE USED IN DESIGN SPECIFICATION

In this chapter the Box-Lucas design is compared with two other designs.

In section 3.1 the Box-Lucas design is compared with a design in which non-replicated experiments are run with X at equally spaced intervals. The estimated mean square errors for $\hat{\alpha}$, $\hat{\beta}$, $\hat{\gamma}$ are the primary criteria for comparing designs and truncation strategies. The results of the work in section 3.1, though not conclusive with respect to design recommendation, indicated a direction in which to move for further work discussed in section 3.2.

In section 3.2 the Box-Lucas design is compared with a design in which non-replicated experiments are run with X at geometrically spaced intervals. In addition to the estimated mean square errors of $\hat{\alpha}$, $\hat{\beta}$, $\hat{\gamma}$, data sets yielding a $\hat{\gamma}$ very near either to zero or one are deleted but the number of each is counted. Since such data sets do not exhibit the exponential form under consideration, they are not included in the simulation summary results.

The Box-Lucas design is specified as replications of a basic design with three levels of X: X_1, X_2, X_3, where

$$X_2 = -\frac{1}{\ln\gamma} + \frac{X_1\gamma^{X_1} - X_3\gamma^{X_3}}{\gamma^{X_1} - \gamma^{X_3}} \qquad (3.1)$$

and $X_1 < X_2 < X_3$. X_1 and X_3 are the minimum and maximum design points which may be used by the experimenter. X_2 is determined so as to minimize the determinant of the large sample variance-covariance matrix of $\hat{\alpha}$, $\hat{\beta}$, $\hat{\gamma}$. From (3.1) it is seen that in addition to X_1 and X_3, γ is required for proper design specification.

3.1 Box-Lucas Designs Versus Equal-Spacing Designs When Maximum X Based on Assumed Value of γ

For the work in this section, the minimum value of the independent variable X is zero. The maximum X is that value which the experimenter thinks will lead to 95% of the maximum increase in the expected response. Figure 3.1 indicates the experimenter wants his maximum X at X_m.

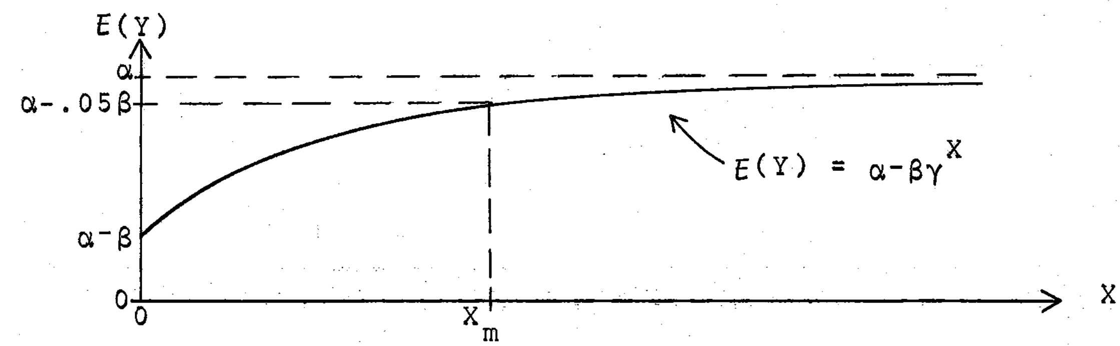

Figure 3.1 Determination of maximum X

Guessing the maximum X value (95% point) is equivalent to guessing γ. This result follows since

$$\alpha - .05\beta = \alpha - \beta\gamma^{X_m}$$

implies

$$\gamma = (.05)^{\frac{1}{X_m}} \tag{3.2}$$

As stated earlier, γ must be specified for determination of the middle point of the Box-Lucas design. Guessing the 95% point might be a good way for an experimenter to guess γ.

In some experimental situations, the cost of experimentation per data point increases with increasing X. The procedure given here for determining the maximum X, though reasonable in the above situation, is not the recommendation of Box & Lucas (1959). Therefore, the simulation work of this section does not compare the equal-spacing design with the exact Box-Lucas design. However, the work of section 3.2 is precise with regard to this point.

The performance of the Box-Lucas design depends on the accuracy of the guess ($\tilde{\gamma}$) of the true gamma (γ_0). The equal-spacing design was considered as a conservative alternative to the Box-Lucas design. It was thought that the correct middle design point as specified by Box-Lucas would more likely be attained by the equal-spacing design when γ was guessed incorrectly.

In other words, even though knowing equal-spacing would not perform as well as Box-Lucas when the true γ was guessed correctly (i.e. $\tilde{\gamma} = \gamma_0$), it was hoped that equal-spacing would be superior to Box-Lucas when $\tilde{\gamma}$ deviated considerably from γ_0. It was also hoped that equal-spacing would not be too inferior to Box-Lucas when $\tilde{\gamma}$ was fairly close to γ_0. Thus a design was desired that would eliminate severe penalties associated with poor guesses of the true γ.

One thousand data sets were generated for each design and each of several parameter situations. The sample size was six with $\alpha=10$, $\sigma=.1$, and all combinations of $\beta=1,3$ and $(\gamma_0,\tilde{\gamma})$ = (.10, .05), (.10, .50), (.90, .50), (.90, .95), (.99, .50), (.99, .95), (.10, .10), (.50, .50), (.90, .90), (.99, .99). The combination $(\gamma_0,\tilde{\gamma})$ = (.50, .95) was simulated with $\beta=1$ to illustrate the difficulties incurred through a gross overguess of γ.

In order to eliminate the variability caused by different sets of random numbers, the same generating seed was used for each parameter-design situation.

Although the number of observations per data set is low, σ^2 is such that when the Box-Lucas design is used with γ guessed correctly, useful estimates of α, β, and γ are obtainable.

Table 3.1 gives the values of X for the Box-Lucas and equal-spacing designs for each $\tilde{\gamma}$ considered.

Table 3.1 Values of X's for Box-Lucas and equal-spacing designs

$\tilde{\gamma}$	Box-Lucas	equal-spacing
.05	0.0000	0.0000
	0.0000	0.2000
	0.2812	0.4000
	0.2812	0.6000
	1.0000	0.8000
	1.0000	1.0000
.10	0.0000	0.0000
	0.0000	0.2602
	0.3658	0.5204
	0.3658	0.7806
	1.3010	1.0408
	1.3010	1.3010
.50	0.0000	0.0000
	0.0000	0.8644
	1.2152	1.7288
	1.2152	2.5932
	4.3219	3.4575
	4.3219	4.3219
.90	0.0000	0.0000
	0.0000	5.6866
	7.9947	11.3733
	7.9947	17.0599
	28.4332	22.7465
	28.4332	28.4332
.95	0.0000	0.0000
	0.0000	11.6808
	16.4218	23.3616
	16.4218	35.0424
	58.4040	46.7232
	58.4040	58.4040
.99	0.0000	0.0000
	0.0000	59.6146
	83.8111	119.2291
	83.8111	178.8437
	298.0729	238.4583
	298.0729	298.0729

The output of the computer program which generated and analyzed the data sets included estimated mean square errors for $\hat{\alpha}$, $\hat{\beta}$, $\hat{\gamma}$, the small sample variance-covariance matrix, and the large sample variance-covariance matrix. These summary results were obtained for desired truncation levels of $\hat{\gamma}$.

When required for clarity, estimates based on Box-Lucas will have the subscript b, those based on equal-spacing will use the subscript e, and subsequently, those based on geometric-spacing will use the subscript g.

Table 3.2 Summary of estimated mean square errors and large sample variances of $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\gamma}$ and biases of $\hat{\gamma}$ based on 1000 experiments of six samples each for each of selected sets of parameter values[(a)]

$\beta = 1$, $(\gamma_0, \tilde{\gamma}) = (.10, .05)$

Design Type	Truncation Point	Number of Truncations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$
B	1.00	≤ 4	*	*	.023284	.040030
E	1.00	≤10	*	*	.034459	.054835
B	.98	4	8.196579	8.160165	.023142	.039950
E	.98	10	22.987525	22.880912	.034124	.054646
B	.95	4	1.510844	1.489983	.022934	.039830
E	.95	12	4.059825	4.004503	.033541	.054310
B	.90	5	.588031	.572414	.022599	.039627
E	.90	12	1.153885	1.118689	.032551	.053710
			Large Sample Variance			
B			.023003	.023566	.008461	
E			.035318	.034103	.011768	

(a) B = Box-Lucas design; E = equal-spacing design; $\hat{\gamma}$ truncated at 0 and upper values as stated. An * indicates that the mean square error was too large for the computer program format, being limited in size by how close the algorithm let $\hat{\gamma}$ approach unity.

Table 3.2 (continued)

$\beta = 1, (\gamma_0, \tilde{\gamma}) = (.10, .50)$

Design Type	Truncation Point	Number of Truncations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$
B	1.00	0	.004622	.008897	.009565	.005052
E	1.00	0	.003315	.012410	.007502	.009831
B	.98	0	.004622	.008897	.009565	.005052
E	.98	0	.003315	.012410	.007502	.009831
B	.95	0	.004622	.008897	.009565	.005052
E	.95	0	.003315	.012410	.007502	.009831
B	.90	0	.004622	.008897	.009565	.005052
E	.90	0	.003315	.012410	.007502	.009831
			Large Sample Variance			
B			.005027	.010026	.017292	
E			.002969	.012856	.009420	

$\beta = 1, (\gamma_0, \tilde{\gamma}) = (.90, .50)$

Design Type	Truncation Point	Number of Truncations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$
B	1.00	≤420	*	*	.071206	-.111008
E	1.00	≤421	*	*	.095328	-.132452
B	.98	420	5.618605	5.622295	.069722	-.119256
E	.98	421	6.074143	6.090456	.093843	-.140708
B	.95	440	.589788	.589254	.068056	-.132097
E	.95	451	.674136	.675221	.092152	-.153748
B	.90	477	.192502	.188473	.066926	-.154982
E	.90	485	.217066	.208903	.090990	-.177224
			Large Sample Variance			
B			15.331821	15.055718	.222099	
E			15.807922	15.423323	.220323	

Table 3.2 (continued)

$\beta = 1$, $(\gamma_0, \tilde{\gamma}) = (.90, .95)$

Design Type	Truncation Point	Number of Truncations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$
B	1.00	0	.006043	.010140	.027504	-.040391
E	1.00	0	.005221	.013250	.005916	-.012120
B	.98	0	.006043	.010140	.027504	-.040391
E	.98	0	.005221	.013250	.005916	-.012120
B	.95	4	.006000	.010117	.027502	-.040409
E	.95	17	.004964	.013161	.005906	-.012212
B	.90	475	.004229	.008907	.027267	-.049370
E	.90	491	.003025	.012600	.005626	-.021977
			Large Sample Variance			
B			.005404	.010348	.000878	
E			.004173	.013448	.000928	

$\beta = 1$, $(\gamma_0, \tilde{\gamma}) = (.99, .50)^{(b)}$

Design Type	Truncation Point	Number of Truncations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$
B	1.00	≤395	*	*	.419964	-.465919
E	1.00	≤346	*	*	.405233	-.472513
B	.98	395	1.240054	1.281958	.419965	-.473783
E	.98	346	1.428497	1.495029	.405234	-.479411
B	.95	403	.873339	.890209	.420567	-.485812
E	.95	355	.897794	.922120	.405761	-.489923
B	.90	415	.874133	.882285	.423234	-.506298
E	.90	371	.878586	.887913	.408126	-.508065
			Large Sample Variance			
B			**	**	22.353654	
E			**	**	19.449032	

(b) The values denoted by ** are too large for the computer program output format.

Table 3.2 (continued)

$\beta = 1,\ (\gamma_0, \tilde{\gamma}) = (.99,\ .95)$

Design Type	Truncation Point	Number of Truncations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$
B	1.00	≤605	*	*	.002329	-.011399
E	1.00	≤589	*	*	.025189	-.037718
B	.98	605	.194088	.184486	.002346	-.021029
E	.98	589	.219614	.203664	.025205	-.047125
B	.95	897	.339757	.311706	.003543	-.044064
E	.95	833	.372015	.329813	.026328	-.068860
B	.90	988	.433248	.410558	.009817	-.092079
E	.90	949	.455455	.412237	.032280	-.114312
			Large Sample Variance			
B			5.321516	5.167085	.000971	
E			5.782243	5.560405	.001001	

$\beta = 1,\ (\gamma_0, \tilde{\gamma}) = (.10,\ .10)$

Design Type	Truncation Point	Number of Truncations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$
B	1.00	0	.028346	.029015	.008817	.018986
E	1.00	0	.291420	.282237	.015629	.030492
B	.98	0	.028346	.029015	.008817	.018986
E	.98	0	.291420	.282237	.015629	.030492
B	.95	0	.028346	.029015	.008817	.018986
E	.95	0	.291420	.282237	.015629	.030492
B	.90	0	.028346	.029015	.008817	.018986
E	.90	1	.184521	.177690	.015548	.030443
			Large Sample Variance			
B			.011609	.014821	.005404	
E			.016114	.020257	.007721	

Table 3.2 (continued)

$\beta = 1,\ (\gamma_0, \tilde{\gamma}) = (.50,\ .50)$

Design Type	Truncation Point	Number of Truncations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$
B	1.00	0	.028350	.029019	.013551	-.003191
E	1.00	≤1	.291182	.282001	.018739	.000362
B	.98	0	.028350	.029019	.013551	-.003191
E	.98	1	.235255	.227103	.018734	.000358
B	.95	0	.028350	.029019	.013551	-.003191
E	.95	4	.119471	.114740	.018670	.000289
B	.90	1	.025560	.026301	.013533	-.003214
E	.90	6	.055764	.053532	.018440	.000016
			Large Sample Variance			
B			.011609	.014821	.012243	
E			.016114	.020257	.017493	

$\beta = 1,\ (\gamma_0, \tilde{\gamma}) = (.90,\ .90)$

Design Type	Truncation Point	Number of Truncations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$
B	1.00	≤2	.028362	.029030	.001185	-.004328
E	1.00	≤6	.290093	.280930	.001549	-.004487
B	.98	2	.023798	.024600	.001184	-.004337
E	.98	6	.047063	.045326	.001535	-.004568
B	.95	39	.015625	.017620	.001139	-.004722
E	.95	68	.022071	.024602	.001435	-.005404
B	.90	479	.006824	.011401	.000806	-.015173
E	.90	476	.006741	.014923	.001005	-.017465
			Large Sample Variance			
B			.011609	.014821	.000916	
E			.016114	.020257	.001309	

Table 3.2 (continued)

$\beta = 1,\ (\gamma_0, \tilde{\gamma}) = (.99, .99)$

Design Type	Truncation Point	Number of Truncations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$
B	1.00	≤986	.028489	.029157	.000014	-.000519
E	1.00	≤978	.320088	.310440	.000018	-.000555
B	.98	986	.024361	.023621	.000102	-.010060
E	.98	978	.022858	.021526	.000102	-.010062
B	.95	1000	.056062	.059400	.001600	-.040000
E	.95	1000	.049689	.052385	.001600	-.040000
B	.90	1000	.059033	.063449	.008100	-.090000
E	.90	1000	.054213	.062192	.008100	-.090000
			Large Sample Variance			
B			.011609	.014821	.000010	
E			.016114	.020257	.000014	

$\beta = 3,\ (\gamma_0, \tilde{\gamma}) = (.10, .05)$

Design Type	Truncation Point	Number of Truncations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$
B	1.00	0	.026840	.026324	.001036	.002631
E	1.00	0	.042371	.038814	.001496	.004430
B	.98	0	.026840	.026324	.001036	.002631
E	.98	0	.042371	.038814	.001496	.004430
B	.95	0	.026840	.026324	.001036	.002631
E	.95	0	.042371	.038814	.001496	.004430
B	.90	0	.026840	.026324	.001036	.002631
E	.90	0	.042371	.038814	.001496	.004430
			Large Sample Variance			
B			.023003	.023566	.000940	
E			.035318	.034103	.001308	

Table 3.2 (continued)

$\beta = 3,\ (\gamma_0, \tilde{\gamma}) = (.10,\ .50)$

Design Type	Trun-cation Point	Number of Trun-cations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$
B	1.00	0	.005409	.009639	.002027	-.004345
E	1.00	0	.003187	.012439	.000958	.000278
B	.98	0	.005409	.009639	.002027	-.004345
E	.98	0	.003187	.012439	.000958	.000278
B	.95	0	.005409	.009639	.002027	-.004345
E	.95	0	.003187	.012439	.000958	.000278
B	.90	0	.005409	.009639	.002027	-.004345
E	.90	0	.003187	.012439	.000958	.000278
			Large Sample Variance			
B			.005027	.010026	.001921	
E			.002969	.012856	.001047	

$\beta = 3,\ (\gamma_0, \tilde{\gamma}) = (.90,\ .50)$

Design Type	Trun-cation Point	Number of Trun-cations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$
B	1.00	≤309	*	*	.013003	-.021837
E	1.00	≤298	*	*	.013812	-.023620
B	.98	309	34.165065	34.022464	.011967	-.027613
E	.98	298	35.133281	34.947886	.012805	-.029227
B	.95	364	3.365000	3.318143	.010669	-.037656
E	.95	364	3.556794	3.492771	.011506	-.039294
B	.90	477	.834808	.808384	.009666	-.058648
E	.90	487	.904759	.863862	.010492	-.060677
			Large Sample Variance			
B			15.331821	15.055718	.024678	
E			15.807922	15.423323	.024480	

Table 3.2 (continued)

$\beta = 3,\ (\gamma_0, \tilde{\gamma}) = (.90,\ .95)$

Design Type	Truncation Point	Number of Truncations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$
B	1.00	0	.006017	.010130	.000117	-.001469
E	1.00	0	.004519	.012989	.000103	-.000854
B	.98	0	.006017	.010130	.000117	-.001469
E	.98	0	.004519	.012989	.000103	-.000854
B	.95	0	.006017	.010130	.000117	-.001469
E	.95	0	.004519	.012989	.000103	-.000854
B	.90	475	.004519	.009134	.000080	-.004928
E	.90	491	.003271	.012716	.000064	-.004457
			Large Sample Variance			
B			.005404	.010348	.000098	
E			.004173	.013448	.000103	

$\beta = 3,\ (\gamma_0, \tilde{\gamma}) = (.99,\ .50)^{(c)}$

Design Type	Truncation Point	Number of Truncations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$
B	1.00	≤430	*	*	.315699	-.377701
E	1.00	≤393	*	*	.332360	-.402098
B	.98	430	5.788642	5.769987	.315700	-.386190
E	.98	393	6.006942	5.973214	.332361	-.409933
B	.95	438	6.919073	6.875116	.316354	-.399257
E	.95	404	6.952910	6.875524	.332962	-.421916
B	.90	459	7.593086	7.538737	.319267	-.421592
E	.90	420	7.620991	7.526282	.335648	-.442524
			Large Sample Variance			
B			**	**	2.483739	
E			**	**	2.161004	

(c) The values denoted by ** are too large for the computer program output format.

Table 3.2 (continued)

$\beta = 3, (\gamma_0, \tilde{\gamma}) = (.99, .95)$

Design Type	Truncation Point	Number of Truncations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}(\hat{\gamma})}$
B	1.00	≤827	*	*	.000081	-.001210
E	1.00	≤806	*	*	.000086	-.001360
B	.98	827	1.288176	1.217582	.000127	-.010899
E	.98	806	1.391934	1.287885	.000131	-.011044
B	.95	1000	3.006157	2.711841	.001600	-.040000
E	.95	1000	3.266115	2.842275	.001600	-.040000
B	.90	1000	3.892963	3.644442	.008100	-.090000
E	.90	1000	4.093395	3.640284	.008100	-.090000
			Large Sample Variance			
B			5.321516	5.167085	.000108	
E			5.782243	5.560405	.000111	

$\beta = 3, (\gamma_0, \tilde{\gamma}) = (.10, .10)$

Design Type	Truncation Point	Number of Truncations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}(\hat{\gamma})}$
B	1.00	0	.013039	.015331	.000630	.001073
E	1.00	0	.018063	.020667	.000909	.002344
B	.98	0	.013039	.015331	.000630	.001073
E	.98	0	.018063	.020667	.000909	.002344
B	.95	0	.013039	.015331	.000630	.001073
E	.95	0	.018063	.020667	.000909	.002344
B	.90	0	.013039	.015331	.000630	.001073
E	.90	0	.018063	.020667	.000909	.002344
			Large Sample Variance			
B			.011609	.014821	.000600	
E			.016114	.020257	.000858	

Table 3.2 (continued)

$\beta = 3,\ (\gamma_0, \tilde{\gamma}) = (.50,\ .50)$

Design Type	Truncation Point	Number of Truncations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$
B	1.00	0	.013039	.015331	.001400	-.001626
E	1.00	0	.018065	.020668	.001927	-.000964
B	.98	0	.013039	.015331	.001400	-.001626
E	.98	0	.018065	.020668	.001927	-.000964
B	.95	0	.013039	.015331	.001400	-.001626
E	.95	0	.018065	.020668	.001927	-.000964
B	.90	0	.013039	.015331	.001400	-.001626
E	.90	0	.018065	.020668	.001927	-.000964
			Large Sample Variance			
B			.011609	.014821	.001360	
E			.016114	.020257	.001944	

$\beta = 3,\ (\gamma_0, \tilde{\gamma}) = (.90,\ .90)$

Design Type	Truncation Point	Number of Truncations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$
B	1.00	0	.013039	.015331	.000107	-.000774
E	1.00	0	.018064	.020669	.000146	-.000713
B	.98	0	.013039	.015331	.000107	-.000774
E	.98	0	.018064	.020669	.000146	-.000713
B	.95	0	.013039	.015331	.000107	-.000774
E	.95	0	.018064	.020669	.000146	-.000713
B	.90	479	.007890	.012183	.000062	-.004500
E	.90	476	.008623	.016045	.000081	-.005185
			Large Sample Variance			
B			.011609	.014821	.000102	
E			.016114	.020257	.000145	

Table 3.2 (continued)

$\beta = 3$, $(\gamma_0, \tilde{\gamma}) = (.99, .99)$

Design Type	Truncation Point	Number of Truncations	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$
B	1.00	<1000	.013049	.015334	.000001	-.000087
E	1.00	<1000	.018060	.020674	.000002	-.000082
B	.98	1000	.197289	.148515	.000100	-.010000
E	.98	1000	.189964	.098221	.000100	-.010000
B	.95	1000	.490981	.484961	.001600	-.040000
E	.95	1000	.437736	.390818	.001600	-.040000
B	.90	1000	.518225	.522543	.008100	-.090000
E	.90	1000	.479011	.482166	.008100	-.090000
			Large Sample Variance			
B			.011609	.014821	.000001	
E			.016114	.020257	.000002	

3.1.1 Small Sample Properties of Estimators

Typically the estimate of γ is adversely affected by bad design. For the cases considered, Table 3.2 indicates that the Box-Lucas design always yields a lower estimated mean square error of $\hat{\gamma}_b$ when γ is guessed correctly than when it is not. For the equal-spacing design, only the range of experimentation is dependent upon $\tilde{\gamma}$. Guessing γ correctly does not necessarily minimize the estimated mean square error of $\hat{\gamma}_e$. For example in Table 3.2 with $\beta = 1$ and $(\gamma_0, \tilde{\gamma}) = (.10, .10)$, the equal-spacing design yielded .01563 for the estimated mean square error of $\hat{\gamma}_e$. The corresponding value for $(\gamma_0, \tilde{\gamma}) = (.10, .50)$ was .00750. Thus overguessing γ improved the performance of $\hat{\gamma}_e$ in this case. However, for $\beta = 1$ and $(\gamma_0, \tilde{\gamma}) = (.90, .90)$ the estimated mean square error of $\hat{\gamma}_e$ was .001549. The corresponding value for $(\gamma_0,\tilde{\gamma}) = (.90, .95)$ was .005916. Overguessing γ hurt the performance of $\hat{\gamma}_e$ in this case. Apparently, guessing γ too large (i.e. increasing the experimental range) is helpful provided enough design points remain in the bending region of the true response.

The estimated mean square error of $\hat{\gamma}$ is a decreasing function of β in the simulation results. This relationship was expected since it holds for the large sample variance of $\hat{\gamma}$.

In some cases incorrect guesses of γ caused data sets to be generated which yielded $\hat{\gamma}$'s near either zero or unity. Such data sets usually do not exhibit the exponential form under consideration. Underguessing γ often results in the generation of data sets with $\hat{\gamma}$ near unity and overguessing often results in a $\hat{\gamma}$ near zero.

Figure 3.2 shows for the Box-Lucas design that the mean of the two observations for the middle design point must fall in the range $(\ell(X_2),\bar{y}_3)$ if the data is to exhibit the proper exponential form. In Figure 3.2, $\ell(X_2) = \bar{y}_1 + \frac{\bar{y}_3-\bar{y}_1}{X_3} X_2$ and $\bar{y}_i$ is the mean of the observations at X_i.

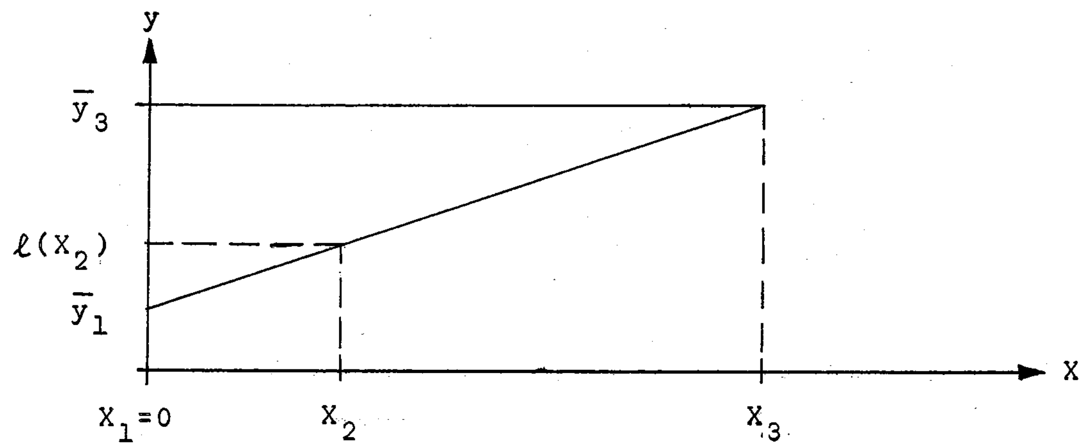

Figure 3.2 Range of $\bar{y}_2$ yielding proper exponential form

If $\bar{y}_2 < \ell(X_2)$, the data indicate increasing returns to scale instead of the decreasing returns for the true model. If $\bar{y}_2 > \bar{y}_3$, the data indicate decreasing total returns, which violates the requirement of monotonic increase in the true model.

The location of X_2 can have a large effect on the probability of $\bar{y}_2 \; \varepsilon(\ell(X_2), \bar{y}_3)$ for a particular γ.

The number of data sets in each of the parameter design situations yielding a $\hat{\gamma}$ greater than .98, .95, or .90 may be found in Table 3.2. For most of the data sets with $\hat{\gamma} > .98$, $\hat{\gamma}$ is as close to unity as the computing algorithm allows. This problem occurs with both designs and does so whenever a straight line would fit the data better than the assumed exponential model. For the Box-Lucas design, this problem occurs whenever $\bar{y}_2 \leq \ell(X_2)$. The problem is prevalent for the $(\gamma_0, \tilde{\gamma})$ combinations (.90, .50), (.99, .50), (.99, .95).

For those cases of $\tilde{\gamma} > \gamma_0$ which resulted in the generation of data sets yielding $\hat{\gamma}$'s near zero, all X's except X=0 were larger than the X's in the maximum bending region of the expected response. In these cases a straight line with a zero or negative slope would fit the data for the non-zero design points better than the assumed exponential model. Thus the computing algorithm generates a $\hat{\gamma}$ as close to zero as possible, yielding a predicted response that is essentially flat in the range of the non-zero design points. For γ large this problem causes the small sample variance of $\hat{\gamma}$ to be much greater than the large sample variance of $\hat{\gamma}$. A count of the number of such cases was not made for the simulation work in this section. However, those cases in Table 3.2 having large negative biases for $\hat{\gamma}$ are cases with many $\hat{\gamma}$'s near zero.

For both designs and for parameter values $\beta = 1$, $(\gamma_0, \tilde{\gamma}) = (.50, .95)$ and $(.90, .95)$, the first three hundred of the one thousand estimates of γ were recorded. This was also done for the equal-spacing design with $\beta = 1$, $(\gamma_0, \tilde{\gamma}) = (.99, .95)$. Table 3.3 gives the first twenty estimates of obtained for the case $(\gamma_0, \tilde{\gamma}) = (.50, .95)$. For the three $(\gamma_0, \tilde{\gamma})$ combinations, the three hundred estimates of γ were bimodally distributed as follows:

$(\gamma_0, \tilde{\gamma})$	Box-Lucas Design	Equal-Spacing Design
(.50, .95)	137 estimates less than .12, 163 estimates greater than .62.	175 estimates less than .07, 125 estimates greater than .54.
(.90, .95)	11 estimates less than .12, 289 estimates greater than .72.	3 estimates less than .05, 297 estimates greater than .71.
(.99, .95)		7 estimates less than .05, 293 estimates greater than .82.

Table 3.3 Simulated experimental values of $\hat{\gamma}$ for $\beta = 1$, $(\gamma_0, \tilde{\gamma}) = (.50, .95)$

Experiment	Box-Lucas Design	Equal-Spacing Design
1	.7324	.0352
2	.7757	.0360
3	.0850	.7921
4	.8912	.0393
5	.1000	.7926
6	.0939	.0379
7	.7996	.8529
8	.0941	.7885
9	.1030	.8769
10	.0930	.8782
11	.0938	.0328
12	.0982	.8069
13	.0985	.6676
14	.8426	.0395
15	.0883	.0433
16	.8749	.5978
17	.0947	.0353
18	.8245	.8356
19	.8299	.8058
20	.8769	.8156

For $\beta = 1$ and $(\gamma_0, \tilde{\gamma}) = (.50, .95)$, it is almost impossible to get a good estimate of γ. The difficulty involved here is the same as for some of the other parameter-design situations. However, since the problem appears here to a greater extent, it will be examined in some detail. For the

Box-Lucas design, the 1000 estimates of γ were distributed bimodally around .10 and .85 with almost no estimates near the true value of .50. This resulted from the fact that X_2 was greater than the X's in the maximum bending region. In fact, $E(Y_{X_2})$ is almost at the maximum (α).

The design points are $X_1 = 0.0$, $X_2 = 16.4218$, $X_3 = 58.4040$. The corresponding expected responses are approximately $E(Y_{X_1}) = 9$, $E(Y_{X_2}) = 10$, $E(Y_{X_3}) = 10$. Although $E(Y_{X_3}) > E(Y_{X_2})$, the expectations are the same practically speaking. Thus approximately one-half of the generated data sets have $\bar{y}_2 \geq \bar{y}_3$, so that approximately one-half of the estimates of γ are close to zero. The simulation work shows these γ's to be clustering around .10. The error sum of squares curve (as seen by the computer) as a function of $\hat{\gamma}$ is flat for $\hat{\gamma}$ near zero. The maximum $\hat{\gamma}$ in the flat region is chosen as the estimate, thus explaining the clustering near .10 rather than near zero. For the remaining data sets (i.e., when $\bar{y}_2 < \bar{y}_3$) the probability of having a data set yield a $\hat{\gamma}$ near .5 is essentially zero. This result may be seen as follows.

Provided, as in Figure 3.2, $\ell(X_2) < \bar{y}_2 < \bar{y}_3$ the fitted model must pass through the points $(0, \bar{y}_1)$, $(X_2, \bar{y}_2)$, $(X_3, \bar{y}_3)$. Thus parameter estimates may be obtained from

$$\left.\begin{aligned} \bar{y}_1 &= \alpha - \beta + e_1 = 9 + e_1 = \hat{\alpha} - \hat{\beta} \\ \bar{y}_2 &= \alpha - \beta\gamma^{X_2} + e_2 = 10 - \gamma^{X_2} + e_2 = \hat{\alpha} - \hat{\beta}\hat{\gamma}^{X_2} \\ \bar{y}_3 &= \alpha + e_3 = 10 + e_3 = \hat{\alpha} \end{aligned}\right\} \quad (3.3)$$

where $\sigma^2_{e_i} = .005$. The estimates are

$$\hat{\alpha} = 10 + e_3$$

$$\hat{\beta} = 1 + e_3 - e_1$$

$$\hat{\gamma} = \left(\frac{e_3 - e_2 + \gamma^{X_2}}{1 + e_3 - e_1}\right)^{\frac{1}{X_2}} \equiv K^{\frac{1}{X_2}}$$

In order to have $.4 < \hat{\gamma} < .6$, for example, it must be that $K_1 < K < K_2$, where $K_1 = .000000292$, and $K_2 = .000227$. The chance of obtaining a $\hat{\gamma} \varepsilon (.4, .6)$ is small since $P(K_1 < K < K_2)$ is small.

Only two estimates of γ fell in the interval (.4, .6) out of the 1000 estimates obtained for the above situation. The average value for the 1000 estimates was .476.

3.1.2 Truncation of $\hat{\gamma}$

For certain data sets the error sum of squares as a function of $\hat{\gamma}$ approaches its minimum value monotonically as $\hat{\gamma}$ approaches unity. In such cases, the estimates $\hat{\alpha}$ and $\hat{\beta}$ increase (apparently without bound) as $\hat{\gamma}$ approaches unity. As shown in Table 3.2, such cases (denoted by *) led to estimated mean square errors for $\hat{\alpha}$ and $\hat{\beta}$ that were ridiculously large. Table 3.4 illustrates the problem for a particular data set. This data set was created for $\beta = 1$, $(\gamma_0, \tilde{\gamma}) = (.90, .50)$ and the Box-Lucas design.

Table 3.4 Computer iterations for one data set with Box-Lucas design

X	Y
0.0	9.08965 9.00089
1.21525	9.23288 8.88109
4.32193	9.35364 9.22890

Iteration	$\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	Error Sum of Squares	$\hat{\alpha}-\hat{\beta}$
1	9.1821	.1439	.1000	.1246	9.0382
2	9.2087	.1880	.3000	.1122	9.0207
3	9.2498	.2403	.5000	.0978	9.0095
4	9.2811	.2730	.6000	.0916	9.0081
5	9.3309	.3217	.7000	.0865	9.0092
6	9.4298	.4179	.8000	.0826	9.0119
7	9.5293	.5157	.8500	.0810	9.0136
8	9.7296	.7141	.9000	.0797	9.0155
9	10.3335	1.3161	.9500	.0786	9.0174
10	217.8032	208.7838	.9997	.0777	9.0194

The difference $\hat{\alpha}-\hat{\beta}$ is essentially independent of $\hat{\gamma}$, even though $\hat{\alpha}$ and $\hat{\beta}$ are sharply affected individually by $\hat{\gamma}$. In cases such as this one, where the expected response is essentially linear in the range of experimentation, the model is over parametrized. Therefore, as is the case here, good prediction is possible even though individual parameter estimates are unacceptable.

The behavior of $\hat{\alpha}$ and $\hat{\beta}$ for $\hat{\gamma}$ near unity indicated that truncation of $\hat{\gamma}$ at some level below unity would be beneficial. Truncation of $\hat{\gamma}$ at levels of .90, .95, and .98 was tried. Improvement in the estimated mean square errors of $\hat{\alpha}$, $\hat{\beta}$ and, of course, $\hat{\gamma}$ was obtained for all gamma values except $\gamma = .99$. For $\gamma = .99$, the truncation points were all below .99. In this case, truncation led to inflation of $\hat{\sigma}^2$ and severe prediction biases.

3.1.3 Large Sample Properties

Under the assumption of normality of the data, the least squares estimates of α, β, and γ are equivalent to the maximum likelihood estimates. The theory of maximum likelihood estimation is applied to obtain the large sample properties (asymptotic variances and covariances) of $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\gamma}$. The model under consideration requires $0 < \gamma < 1$. Thus these properties are not applicable unless the sample size and/or the design are such that the probability of a data set yielding a $\hat{\gamma}$ near zero or one is very small. In addition, of course, the sample size must attain a certain magnitude before good agreement will exist between large and small sample properties, since $\hat{\alpha}$, $\hat{\beta}$, $\hat{\gamma}$ are not linear functions of the observations.

Table 3.5 gives the large and small sample variance-covariance matrices of $\hat{\alpha}$, $\hat{\beta}$, $\hat{\gamma}$ for $\beta = 1$ and $(\gamma_0, \tilde{\gamma})$ = (.10, .10), (.50, .50), (.90, .90) and the Box-Lucas design. Table 3.6 gives the same information for the equal-spacing design.

Table 3.5 Variances and covariances of the estimators for $\beta = 1$, selected $(\gamma_0, \tilde{\gamma})$ combinations, and the Box-Lucas design

$(\gamma_0, \tilde{\gamma})$	Large Sample			Small Sample		
(.10, .10)	.0116			.0274		
	.0107	.0148		.0255	.0281	
	.0063	.0046	.0054	.0129	.0109	.0085
(.50, .50)	.0116			.0274		
	.0107	.0148		.0255	.0281	
	.0094	.0069	.0122	.0147	.0120	.0136
(.90, .90)	.0116			.0274		
	.0107	.0148		.0255	.0281	
	.0026	.0019	.0009	.0040	.0032	.0012

Table 3.6 Variances and covariances of the estimators for $\beta = 1$, selected $(\gamma_0, \tilde{\gamma})$ combinations, and the equal-spacing design

$(\gamma_0, \tilde{\gamma})$	Large Sample			Small Sample		
(.10, .10)	.0161			.2851		
	.0134	.0203		.2756	.2752	
	.0098	.0062	.0077	.0447	.0397	.0147
(.50, .50)	.0161			.2848		
	.0134	.0203		.2753	.2749	
	.0148	.0093	.0175	.0369	.0311	.0188
(.90, .90)	.0161			.2837		
	.0134	.0203		.2743	.2739	
	.0040	.0026	.0013	.0090	.0074	.0015

As may be seen in Tables 3.5 and 3.6, agreement between large and small sample properties is not good. For $(\gamma_0, \tilde{\gamma}) = (.50, .50)$, even though there is very little chance of a generated data set yielding a $\hat{\gamma}$ near zero or one, agreement is poor. A larger sample size is required before the large sample properties may be used to evaluate designs.

Tables 3.5 and 3.6 also indicate that $\mathrm{Var}(\hat{\alpha})$, $\mathrm{Var}(\hat{\beta})$, and $\mathrm{Cov}(\hat{\alpha},\hat{\beta})$ are essentially the same for all γ as long as $\tilde{\gamma} = \gamma_0$. For the large sample values with the Box-Lucas design, the above is exact. The proof is in section 9.2.

If n samples are taken using the Box-Lucas design with $\tilde{\gamma} = \gamma_0$, and the maximum design point is located so that the associated expected response has achieved 100(1-p)% of the maximum increase in the expected response, then the large sample variances and covariance of $\hat{\alpha}$ and $\hat{\beta}$ are

$$\mathrm{Var}(\hat{\alpha}) = \frac{3\sigma^2(BF - D^2)}{n(3BF - A^2F - BC^2 + 2ACD - 3D^2)} ,$$

$$\mathrm{Var}(\hat{\beta}) = \frac{\sigma^2(9F - 3C^2)}{n(3BF - A^2F - BC^2 + 2ACD - 3D^2)} ,$$

$$\mathrm{Cov}(\hat{\alpha},\hat{\beta}) = \frac{3\sigma^2(AF - CD)}{n(3BF - A^2F - BC^2 + 2ACD - 3D^2)}$$

where,

$$A = 1 + p + e^K , \quad B = 1 + p^2 + e^{2K}$$

$$C = Ke^K + p \ln p , \quad D = Ke^{2K} + p^2 \ln p$$

$$F = K^2e^{2K} + p^2(\ln p)^2 , \quad K = 1 - \frac{p \ln p}{1-p} .$$

Therefore, in this case, where the experimental range depends on $\tilde{\gamma}$, two experiments may have radically different experimental ranges and in each case α and β would be estimated with the same precision.

The same pattern as above appears for the equal-spacing design. However, the result does not hold exactly in that case.

The variance and covariances involving $\hat{\gamma}$ are dependent on β and γ in this case. The formulas are

$$\operatorname{Var}(\hat{\gamma}) = \frac{(\ln\gamma)^2}{n\beta^{*2}} \left(\frac{\sigma^2(9B - 3A^2)}{3BF - A^2F - BC^2 + 2ACD - 3D^2} \right) ,$$

$$\operatorname{Cov}(\hat{\alpha},\hat{\gamma}) = \frac{\ln\gamma}{n\beta^*} \left(\frac{3\sigma^2(BC - AD)}{3BF - A^2F - BC^2 + 2ACD - 3D^2} \right) ,$$

$$\operatorname{Cov}(\hat{\beta},\hat{\gamma}) = \frac{\ln\gamma}{n\beta^*} \left(\frac{\sigma^2(3AC - 9D)}{3BF - A^2F - BC^2 + 2ACD - 3D^2} \right) ,$$

where $\beta^* = \dfrac{\beta}{\gamma}$.

For given β, $\operatorname{Var}(\hat{\gamma})$ is maximized for $\gamma = e^{-1} \simeq .36788$. For given β, $\operatorname{Cov}(\hat{\alpha},\hat{\gamma})$ and $\operatorname{Cov}(\hat{\beta},\hat{\gamma})$ are maximized in absolute value for $\gamma = e^{-1}$.

The above results are derived in section 9.2.

Incorrectly guessing γ may result in near-singularity of the large sample information matrix. This problem may occur in either of two ways:

(1) $\tilde{\gamma} >> \gamma_0$, which may result, practically speaking, in only two distinct expected responses at the design points (at X = 0 and at the maximum), or

(2) $\tilde{\gamma} << \gamma_0$, which may cause the design points to include only an experimental range where the expected response is essentially linear (i.e. not to include even the bending region).

Since the experimental range is a function of $\tilde{\gamma}$, both the Box-Lucas and equal-spacing designs can lead to near-singularity of the large sample information matrix for either of the above two situations.

The large sample information matrix is given by equation (3.4).

$$R = \frac{1}{\sigma^2} \begin{bmatrix} n & -\sum_{i=1}^{n} \gamma^{X_i} & -\beta \sum_{i=1}^{n} X_i \gamma^{X_i - 1} \\ & \sum_{i=1}^{n} \gamma^{2X_i} & \beta \sum_{i=1}^{n} X_i \gamma^{2X_i - 1} \\ \text{symmetric} & & \beta^2 \sum_{i=1}^{n} X_i^2 \gamma^{2X_i - 2} \end{bmatrix} \qquad (3.4)$$

For example, consider the situation for the Box-Lucas design with $n = 6$ and $(\gamma_0, \tilde{\gamma})$ such that $\gamma^{X_i} \approx 0$ except when $X_i = 0$. This case occurs when $\tilde{\gamma} >> \gamma_0$. Thus the information matrix would be

$$R_1 = \frac{2}{\sigma^2}\begin{bmatrix} 3 & -1-\varepsilon & \frac{-\beta X_2\varepsilon}{\gamma} \\ -1-\varepsilon & 1+\varepsilon^2 & \frac{\beta X_2\varepsilon^2}{} \\ \frac{-\beta X_2\varepsilon}{\gamma} & \frac{\beta X_2\varepsilon^2}{\gamma} & \frac{\beta^2 X_2{}^2\varepsilon^2}{\gamma^2} \end{bmatrix}$$

where $\varepsilon = \gamma^{X_2} \simeq 0$. Hence R_1 is almost singular.

Correspondingly, for $(\gamma_0, \tilde{\gamma})$ such that γ^{X_i} is near one for all X_i, the information matrix would almost be

$$R_2 \simeq \frac{2}{\sigma^2}\begin{bmatrix} 3 & -3 & -\beta(X_2+X_3) \\ -3 & 3 & \beta(X_2+X_3) \\ -\beta(X_2+X_3) & \beta(X_2+X_3) & \beta^2(X_2{}^2+X_3{}^2) \end{bmatrix}$$

This result follows since $\lim_{\gamma\to 1} \gamma^X = 1$ for any fixed X.

The determinant of R_2 is also zero indicating almost-singularity for the true information matrix. This case occurs when $\tilde{\gamma} << \gamma_0$.

Table 3.7 gives an illustration of the effects of near-singularity on the large and small sample variance-covariance matrices for both case (1) and case (2) and each design, with $\beta = 1$.

Table 3.7 Variances and covariances of the estimators when the large sample information matrix is nearly singular

Box-Lucas Designs

$(\gamma_0, \tilde{\gamma})$	Large Sample			Small Sample		
(.50, .95)	.0050			.0033		
	.0050	.0100		.0033	.0084	
	13.3653	13.3651	71,452.	.0071	.0078	.1392
(.90, .50)	15.3318			*		
	15.1912	15.0557		*	*	
	1.8422	1.8243	.2221	204.7	204.7	.0589

Equal-Spacing Designs

$(\gamma_0, \tilde{\gamma})$	Large Sample			Small Sample		
(.50, .95)	.0025			.0023		
	.0025	.0125		.0023	.0123	
	.3515	.3511	246.90	.0048	.0037	.1460
(.90, .50)	15.8079			*		
	15.6114	15.4233		*	*	
	1.8620	1.8370	.2203	230.8	230.8	.0779

The asterisks in Table 3.7 are for values that were too large to be handled by the computer program output format. Their actual magnitude is not meaningful as they are quite sensitive to how close the computing algorithm lets $\hat{\gamma}$ get to unity.

3.1.4 Summary and Conclusions

The difference in performance of Box-Lucas and equal-spacing, for a particular parameter situation, is small relative to the effects of incorrectly guessing γ or truncating $\hat{\gamma}$ when $\hat{\gamma}$ exceeds some truncation point near unity.

Using the estimated mean square error of $\hat{\gamma}$ as the criterion, Box-Lucas is generally better than equal-spacing when $\tilde{\gamma} \leq \gamma_0$ and equal-spacing is better when $\tilde{\gamma} > \gamma_0$.

Both designs perform better with β equal to three rather than one. This fact is also indicated by the large sample properties. Only the variance and covariances involving $\hat{\gamma}$ are functions of β. β appears in the denominators of $\mathrm{Cov}(\hat{\alpha},\hat{\gamma})$ and $\mathrm{Cov}(\hat{\beta},\hat{\gamma})$. β^2 appears in the denominator of $\mathrm{Var}(\hat{\gamma})$.

Whenever a data set is generated which yields a $\hat{\gamma}$ near zero or one, the sample data are not exhibiting the exponential form under consideration. Since the form of the model is correct, such an occurrence is attributable to chance. However, the probability of a data set exhibiting non-exponential form is sharply affected by the experimental design used. For a case referred to earlier [β=1, $(\gamma_0,\tilde{\gamma})$ = (.50, .95), Box-Lucas design] roughly one-half of the data sets yielded $\hat{\gamma}$'s near zero. But, using the same parameter-design setup, except for changing $(\gamma_0,\tilde{\gamma})$ to (.50, .50), all of the data sets exhibited the proper exponential form.

In a real world application, if an experimenter obtained a data set yielding a $\hat{\gamma}$ near zero or one, he would not accept such a $\hat{\gamma}$. His data would not be exhibiting the exponential form which he has assumed. For prediction purposes, the experimenter probably would fit a different model. If $\hat{\gamma}$ were near one the experimenter might fit a straight line to the data. If $\hat{\gamma}$ were near zero the experimenter might fit two intersecting straight lines to the data, of the form shown in Figure 3.3.

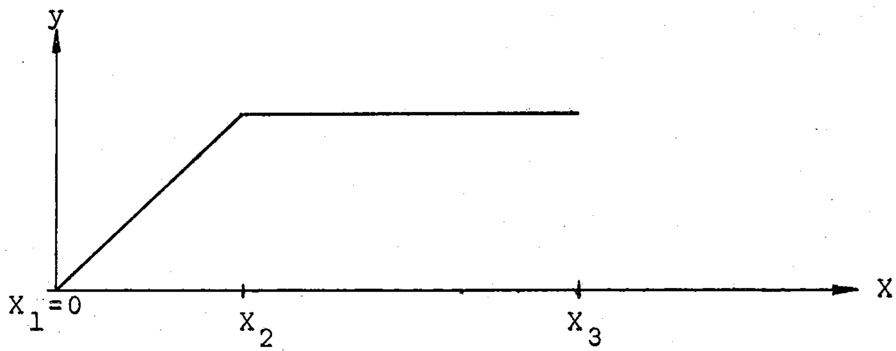

Figure 3.3 General form of model that might be fitted to data having $\hat{\gamma}$ near zero

The simulation studies did not explore the effects of such a strategy.

Typically, non-exponential form may occur when there are, practically speaking, only two unique expectations ($\hat{\gamma}$ may be near zero) or when the expected response is essentially linear in the range of experimentation ($\hat{\gamma}$ may be near one). The Box-Lucas design is particularly vulnerable to the first situation when $\tilde{\gamma}$ is too large, because only one design point is aimed at the bending region of the expected response.

With the equal-spacing design such a problem may still occur if the range of experimentation is large enough.

Of course, given few enough observations and large enough experimental error, the problem could occur with any design. A design is desired that makes the occurrence unlikely no matter how bad $\tilde{\gamma}$ is (i.e. independent of $\tilde{\gamma}$) whenever "problem" data sets would be unlikely using the Box-Lucas design with $\tilde{\gamma}$ equal to γ_0.

Thus the simulation work of this section does not indicate a clear choice between Box-Lucas and equal-spacing since neither design protects the experimenter against a bad $\tilde{\gamma}$.

The problems encountered here suggest a design which always places design points at small, non-zero X values. The geometric-spacing design has this property and is considered in the next section.

3.2 Box-Lucas Designs Versus Geometric-Spacing Designs When Maximum X Independent of Assumed Value of γ

For the work in this section, the minimum value of the independent variable X is still zero. Two values, 16 and 32, are used for the maximum X.

The geometric-spacing design with nine data points is specified as follows:

$$\{0, X_0, 2X_0, 4X_0, 8X_0, 16X_0, 32X_0, 64X_0, 128X_0\},$$

where X_0 is chosen so that $128X_0$ equals the maximum X desired. For the two cases considered here, X_0 takes the values 1/8 and 1/4.

The Box-Lucas design is specified as in section 3.1 except that the maximum design point is not dependent upon $\tilde{\gamma}$.

Some of the data sets generated in section 3.1 did not exhibit the exponential form under consideration. However, these data sets were included in the simulation summary results. Such a strategy does not simulate the behavior of an experimenter as he would not accept parameter estimates from such data sets. Therefore, in this section rules for the exclusion of data sets from the simulation summary results were set up as follows:

(1) For either design any data set yielding a $\hat{\gamma}$ greater than .98 was excluded.

(2) For the Box-Lucas design any data set for which the mean at the third design point was less than or equal to the mean at the middle point was excluded.

(3) For the geometric-spacing design any data set yielding a $\hat{\gamma}$ less than .01 was excluded.

A count was made of the number of data sets in the above categories for each parameter-design situation. Only the remaining data sets were used for the simulation summary results.

Five hundred data sets were generated for each design and each of several sets of parameter values. The sample size was nine with $\alpha = 10$, $\sigma = .1$, and all combinations of $\beta = 1, 3$; maximum design point = 16, 32; and $(\gamma_0, \tilde{\gamma})$ pairs as indicated in Table 3.8 by *.

Table 3.8 Combinations of $\tilde{\gamma}$ and γ_0 used in simulated experiments

$\tilde{\gamma}$ \ γ_0	.10	.30	.50	.70	.90
.05	*				
.10	*	*	*		
.30	*	*	*	*	
.50	*	*	*	*	*
.70		*	*	*	*
.90			*	*	*
.95					*

In addition, the situation $\gamma_0 = .9$, $\beta = 1$, maximum $X = 16$ was simulated where data sets having $\hat{\gamma} > .95$ were excluded. This simulation was performed for comparison with the effect of exclusion at .98 in a case where many $\hat{\gamma}$'s were near one.

Table 3.9 gives the Box-Lucas designs used for the two maximum design points and each $\tilde{\gamma}$ considered. Three samples are taken at each design point.

Table 3.9 shows very little change in the middle design point when X is increased from 16 to 32 for $\tilde{\gamma} \leq .7$. This insensitivity to the maximum X results from the expected responses at 16 and 32 being essentially the same.

The two geometric-spacing designs are

{0.0, 0.125, 0.25, 0.5, 1.0, 2.0, 4.0, 8.0, 16.0}

and

{0.0, 0.25, 0.5, 1.0, 2.0, 4.0, 8.0, 16.0, 32.0}

Table 3.9 Design points for Box-Lucas designs

$\tilde{\gamma}$	Maximum X=16	Maximum X=32
.05	0.0000	0.0000
	0.3338	0.3338
	16.0000	32.0000
.10	0.0000	0.0000
	0.4343	0.4343
	16.0000	32.0000
.30	0.0000	0.0000
	0.8306	0.8306
	16.0000	32.0000
.50	0.0000	0.0000
	1.4425	1.4427
	16.0000	32.0000
.70	0.0000	0.0000
	2.7503	2.8033
	16.0000	32.0000
.90	0.0000	0.0000
	5.8520	8.3534
	16.0000	32.0000
.95	0.0000	0.0000
	6.9178	11.8077
	16.0000	32.0000

For the results of simulation work to be useful, there must be some continuity in the relationship between changes in the parameter situations simulated and the corresponding changes in the properties of the estimators. Otherwise, the results are useful only for the situations included in the simulation study, which severely limits the scope of inference.

For the initial simulation work in this thesis, there appeared to be a definite lack of "continuity". It was discovered that slight changes in parameter values allowed the generation of data sets with $\hat{\gamma}$ very near one which caused estimates of α and β to be unreasonably large. These few very large estimates caused the estimated mean square errors of $\hat{\alpha}$ and $\hat{\beta}$ to increase well beyond reasonable size. This observation led to the truncation rules used in section 3.1.

Before beginning the work of section 3.2 it was discovered that in some cases a large number of $\hat{\gamma}$'s were near zero. The question then arose: By allowing the two types of "problem" data sets to be included in the summary results (even with truncation), is the behavior of a reasonable experimenter really being simulated?

This process of reasoning and experimentation led to the simulation procedure used in section 3.2.

3.2.1 Small Sample Properties of Estimators

As was the case in section 3.1, incorrectly guessing γ may result in poor estimates of γ when the Box-Lucas design is used. Of the 42,000 data sets generated using the Box-Lucas design, 1860 yielded $\hat{\gamma}$'s near zero and 286 yielded $\hat{\gamma}$'s near unity. The corresponding figures for the geometric-spacing design were one and 41, respectively. Table 3.10 gives the frequency distribution of $\hat{\gamma}$ for the 500 data sets generated in each parameter-design situation.

Increasing the experimental range from 16 to 32 had little, if any, effect on $\hat{\alpha}$, $\hat{\beta}$, $\hat{\gamma}$ for $\gamma \leq .5$ when the Box-Lucas design was used. The increase helped $\hat{\alpha}$ and hurt $\hat{\beta}$ in the above situation when the geometric-spacing design was used. For $\gamma \geq .7$, the larger experimental range was generally better for $\hat{\alpha}$, $\hat{\beta}$, $\hat{\gamma}$ and both designs. Until γ is as large as .7, the expected response at 16 is essentially the same as at 32. Apparently, once the expected response has stabilized close to its asymptotic value, increases in the experimental range are not significantly helpful.

Table 3.10 Frequency distribution of $\hat{\gamma}$ (c)

$\beta = 1$, Maximum X = 16

$(\gamma_0, \tilde{\gamma})$	Design Type	0.0–0.0+	0.0+–0.1	0.1–0.2	0.2–0.3	0.3–0.4	0.4–0.5	0.5–0.6	0.6–0.7	0.7–0.8	0.8–0.9	0.9–0.98	0.98–1.0
.10, .05	B		233	248	18	1							
.10, .10	B		233	255	12								
.10, .30	B	21	222	239	18								
.10, .50	B	150	94	154	91	11							
γ_0 = .10	G		251	217	30	2							
.30, .10	B		3	38	195	204	50	9	1				
.30, .30	B		4	39	190	238	27	2					
.30, .50	B	10	13	54	166	217	38	2					
.30, .70	B	150	3	25	66	110	122	24					
γ_0 = .30	G		2	60	181	197	53	7					
.50, .10	B				16	71	160	156	71	19	5	2	
.50, .30	B				4	38	189	226	40	3			
.50, .50	B				7	40	186	246	21				

(c) B = Box-Lucas design; G = geometric-spacing design; for the geometric-spacing design 0.0+ is .01. For the Box-Lucas design $\hat{\gamma}$'s from data sets with the sample mean at the middle design point greater than or equal to the sample mean at the third design point are counted for the interval (0.0, 0.0+).

Table 3.10 (continued)

$\beta = 1$, Maximum X = 16

$(\gamma_0, \tilde{\gamma})$	Design Type	0.0–0.0+	0.0+–0.1	0.1–0.2	0.2–0.3	0.3–0.4	0.4–0.5	0.5–0.6	0.6–0.7	0.7–0.8	0.8–0.9	0.9–0.98	0.98–1.0
.50, .70	B	20	1	5	16	50	150	225	33				
.50, .90	B	199			4	6	36	81	142	32			
γ_0 = .50	G				12	64	169	197	56	2			
.70, .30	B						7	46	194	186	57	7	3
.70, .50	B						3	30	203	245	19		
.70, .70	B						4	24	203	262	7		
.70, .90	B	36				2	15	36	156	241	14		
γ_0 = .70	G					2	4	47	199	220	28		
.90, .50	B								5	47	193	138	117
.90, .70	B									24	216	209	51
.90, .90	B								1	14	223	250	12
.90, .95	B								4	17	212	256	11
γ_0 = .90	G						1		6	23	225	205	40

Table 3.10 (continued)

β = 3, Maximum X = 16

$(\gamma_0, \tilde{\gamma})$	Design Type	0.0–0.0+	0.0+–0.1	0.1–0.2	0.2–0.3	0.3–0.4	0.4–0.5	0.5–0.6	0.6–0.7	0.7–0.8	0.8–0.9	0.9–0.98	0.98–1.0
.10, .05	B		232	268									
.10, .10	B		233	267									
.10, .30	B		243	257									
.10, .50	B	49	195	253	3								
γ_0 = .10	G		251	249									
.30, .10	B				236	264							
.30, .30	B				233	267							
.30, .50	B			3	240	257							
.30, .70	B	47	6	37	154	240	16						
γ_0 = .30	G				243	257							
.50, .10	B					4	243	250	3				
.50, .30	B						231	269					
.50, .50	B						233	267					

Table 3.10 (continued)

β = 3, Maximum X = 16

$(\gamma_0, \tilde{\gamma})$	Design Type	0.0 – 0.0+	0.0+ – 0.1	0.1 – 0.2	0.2 – 0.3	0.3 – 0.4	0.4 – 0.5	0.5 – 0.6	0.6 – 0.7	0.7 – 0.8	0.8 – 0.9	0.9 – 0.98	0.98 – 1.0
.50, .70	B					7	235	258					
.50, .90	B	121		2	2	23	97	209	46				
γ_0 = .50	G					1	244	255					
.70, .30	B								247	253			
.70, .50	B								236	264			
.70, .70	B								231	269			
.70, .90	B							7	238	255			
γ_0 = .70	G								251	249			
.90, .50	B										245	248	7
.90, .70	B										240	260	
.90, .90	B										238	262	
.90, .95	B										233	267	
γ_0 = .90	G										255	245	

Table 3.10 (continued)

β = 1, Maximum X = 32

$(\gamma_0,\tilde{\gamma})$	Design Type	0.0–0.0+	0.0+–0.1	0.1–0.2	0.2–0.3	0.3–0.4	0.4–0.5	0.5–0.6	0.6–0.7	0.7–0.8	0.8–0.9	0.9–0.98	0.98–1.0
.10, .05	B		233	248	18	1							
.10, .10	B		233	255	12								
.10, .30	B	21	222	239	18								
.10, .50	B	150	94	154	91	11							
γ_0 = .10	G	1	258	204	34	3							
.30, .10	B		3	38	195	204	50	9	1				
.30, .30	B		4	39	190	238	27	2					
.30, .50	B	10	13	54	166	217	38	2					
.30, .70	B	154	4	23	64	105	122	28					
γ_0 = .30	G		1	57	194	188	54	6					
.50, .10	B				16	71	160	156	72	18	6	1	
.50, .30	B				4	38	189	226	40	3			
.50, .50	B				7	40	186	246	21				

Table 3.10 (continued)

$\beta = 1$, Maximum X = 32

$(\gamma_0, \tilde{\gamma})$	Design Type	0.0–0.0+	0.0+–0.1	0.1–0.2	0.2–0.3	0.3–0.4	0.4–0.5	0.5–0.6	0.6–0.7	0.7–0.8	0.8–0.9	0.9–0.98	0.98–1.0
.50, .70	B	22		6	16	51	147	223	35				
.50, .90	B	237					12	25	87	131	8		
γ_0 = .50	G				4	65	174	211	43	3			
.70, .30	B						7	44	196	193	53	7	
.70, .50	B						2	30	204	248	16		
.70, .70	B						4	21	208	262	5		
.70, .90	B	123					3	23	96	225	30		
γ_0 = .70	G						5	39	200	243	13		
.90, .50	B									28	213	187	72
.90, .70	B									5	243	239	13
.90, .90	B									3	233	264	
.90, .95	B	2							1	4	230	263	
γ_0 = .90	G								1	8	240	250	1

Table 3.10 (continued)

β = 3, Maximum X = 32

$(\gamma_0, \tilde{\gamma})$	Design Type	0.0 – 0.0+	0.0+ – 0.1	0.1 – 0.2	0.2 – 0.3	0.3 – 0.4	0.4 – 0.5	0.5 – 0.6	0.6 – 0.7	0.7 – 0.8	0.8 – 0.9	0.9 – 0.98	0.98 – 1.0
.10, .05	B		232	268									
.10, .10	B		233	267									
.10, .30	B		243	257									
.10, .50	B	49	195	253	3								
γ_0 = .10	G		259	241									
.30, .10	B				236	264							
.30, .30	B				233	267							
.30, .50	B			3	240	257							
.30, .70	B	53	4	36	152	234	21						
γ_0 = .30	G				252	248							
.50, .10	B					4	243	250	3				
.50, .30	B						231	269					
.50, .50	B						233	267					

Table 3.10 (continued)

$\beta = 3$, Maximum X = 32

$(\gamma_0, \tilde{\gamma})$	Design Type	0.0–0.0+	0.0+–0.1	0.1–0.2	0.2–0.3	0.3–0.4	0.4–0.5	0.5–0.6	0.6–0.7	0.7–0.8	0.8–0.9	0.9–0.98	0.98–1.0
.50, .70	B					7	235	258					
.50, .90	B	217			2	4	26	75	165	11			
γ_0 = .50	G						243	257					
.70, .30	B								247	253			
.70, .50	B								236	264			
.70, .70	B								233	267			
.70, .90	B	19				1	2	22	201	255			
γ_0 = .70	G								244	256			
.90, .50	B										241	259	
.90, .70	B										248	252	
.90, .90	B										236	264	
.90, .95	B										237	263	
γ_0 = .90	G										249	251	

Generally the performances of $\hat{\alpha}$ and $\hat{\beta}$ are unaffected by an increase in β from one to three. This result was expected since the large sample properties of $\hat{\alpha}$ and $\hat{\beta}$ are independent of β. The performance of $\hat{\gamma}$ is always better when β is three. Table 3.11 contains information leading to the above results.

The geometric-spacing design is not as good a design for estimating β. β is the difference between the minimum and maximum expected response. Geometric-spacing places fewer data points at the extremes of the experimental range than Box-Lucas.

Table 3.11 Summary of estimated mean square error and large sample variance of $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\gamma}$ and bias of $\hat{\gamma}$ based on 500 experiments of nine samples each for each of selected sets of parameter values[(d)]

$\beta = 1$, Maximum X = 16

$(\gamma_0, \tilde{\gamma})$	Design Type	Number $\hat{\gamma}$'s Near Zero	Number $\hat{\gamma}$'s Near One	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$	Large Sample Variance $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$
.10, .05	B	0	0	.003227	.006437	.002147	.005866	.003333	.006667	.002091
.10, .10	B	0	0	.003227	.006437	.001927	.004345	.003333	.006667	.002004
.10, .30	B	21	0	.002980	.006299	.002880	.006828	.003333	.006667	.003871
.10, .50	B	150	0	.002898	.006347	.008801	.054443	.003333	.006667	.023726
γ_0 = .10	G	0	0	.002439	.009001	.003218	.008521	.002483	.009320	.003101
.30, .10	B	0	0	.003227	.006437	.006956	.005335	.003333	.006667	.006867
.30, .30	B	0	0	.003227	.006437	.004877	-.000628	.003333	.006667	.004932
.30, .50	B	10	0	.003053	.006343	.007304	-.003827	.003333	.006667	.007949
.30, .70	B	150	0	.002898	.006348	.014781	.069290	.003333	.006667	.057547
γ_0 = .30	G	0	0	.003009	.007780	.007179	.002814	.003234	.007958	.008039
.50, .10	B	0	0	.004469	.007140	.013788	.007298	.003335	.006664	.013036
.50, .30	B	0	0	.003224	.006431	.005882	-.000298	.003335	.006666	.005763
.50, .50	B	0	0	.003232	.006438	.004913	-.004247	.003335	.006668	.004543

(d) B = Box-Lucas design; G = geometric-spacing design. The number of $\hat{\gamma}$'s recorded as near zero or near one may also be found (in Table 3.10) in cells (0.0, 0.0+) and (.98, 1.0), respectively. The corresponding data sets are not included in the small sample properties.

Table 3.11 (continued)

$\beta = 1$, Maximum X = 16

$(\gamma_0, \tilde{\gamma})$	Design Type	Number $\hat{\gamma}$'s Near Zero	Number $\hat{\gamma}$'s Near One	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$	Large Sample Variance $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$
.50, .70	B	20	0	.002986	.006307	.009084	-.008692	.003337	.006670	.008722
.50, .90	B	199	0	.003198	.006568	.019119	.098297	.003349	.006682	.160372
γ_0 = .50	G	0	0	.004177	.007159	.007969	-.005412	.004350	.007534	.007838
.70, .30	B	0	3	.008695	.009468	.007486	.000581	.003548	.006466	.007245
.70, .50	B	0	0	.003672	.006385	.003744	-.001357	.003546	.006650	.003508
.70, .70	B	0	0	.003525	.006567	.002941	-.004489	.003594	.006817	.002513
.70, .90	B	36	0	.003608	.006868	.006450	-.006543	.003854	.007146	.006330
γ_0 = .70	G	0	0	.007891	.008863	.005392	-.008104	.007416	.008919	.004830
.90, .50	B	0	117	.108781	.101080	.005246	-.032325	.149554	.126768	.008779
.90, .70	B	0	51	.124645	.116784	.002517	-.010080	.063066	.053243	.003252
.90, .90	B	0	12	.092115	.087202	.001954	-.004844	.045145	.042881	.001849
.90, .95	B	0	11	.096006	.092774	.002363	-.006335	.048901	.047665	.001962
γ_0 = .90	G	0	40	.182558	.176496	.003666	-.014042	.102432	.092841	.003505

Table 3.11 (continued)

$\beta = 3$, Maximum X = 16

$(\gamma_0, \tilde{\gamma})$	Design Type	Number $\hat{\gamma}$'s Near Zero	Number $\hat{\gamma}$'s Near One	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$	Large Sample Variance $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$
.10, .05	B	0	0	.003227	.006437	.000226	.000408	.003333	.006667	.000232
.10, .10	B	0	0	.003227	.006437	.000215	.000269	.003333	.006667	.000223
.10, .30	B	0	0	.003227	.006437	.000410	-.000107	.003333	.006667	.000430
.10, .50	B	49	0	.002957	.006230	.001642	.005717	.003333	.006667	.002636
γ_0 = .10	G	0	0	.002402	.009002	.000336	.000996	.002483	.009320	.000345
.30, .10	B	0	0	.003227	.006437	.000759	.000086	.003333	.006667	.000763
.30, .30	B	0	0	.003227	.006437	.000541	-.000400	.003333	.006667	.000548
.30, .50	B	0	0	.003227	.006438	.000893	-.001354	.003333	.006667	.000883
.30, .70	B	47	0	.002964	.006246	.004657	.001188	.003333	.006667	.006394
γ_0 = .30	G	0	0	.003010	.007742	.000850	-.000037	.003234	.007958	.000893
.50, .10	B	0	0	.003229	.006433	.001460	.000000	.003335	.006664	.001448
.50, .30	B	0	0	.003229	.006437	.000643	-.000479	.003335	.006666	.000640
.50, .50	B	0	0	.003229	.006438	.000507	-.000757	.003335	.006668	.000505

Table 3.11 (continued)

β = 3, Maximum X = 16

$(\gamma_0, \tilde{\gamma})$	Design Type	Number $\hat{\gamma}$'s Near Zero	Number $\hat{\gamma}$'s Near One	Estimated Mean Square Error			$\widehat{\text{Bias}}(\hat{\gamma})$	Large Sample Variance		
				$\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$		$\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$
.50, .70	B	0	0	.003230	.006440	.001051	-.002514	.003337	.006670	.000969
.50, .90	B	121	0	.002947	.006307	.006201	.022069	.003349	.006682	.017819
γ_0 = .50	G	0	0	.004075	.007121	.000874	-.001345	.004350	.007534	.000871
.70, .30	B	0	0	.003449	.006169	.000819	-.000383	.003548	.006466	.000805
.70, .50	B	0	0	.003419	.006383	.000395	-.000508	.003546	.006650	.000390
.70, .70	B	0	0	.003462	.006556	.000284	-.000685	.003594	.006817	.000279
.70, .90	B	0	0	.003704	.006869	.000847	-.003048	.003854	.007146	.000703
γ_0 = .70	G	0	0	.007043	.008277	.000534	-.001441	.007416	.008919	.000537
.90, .50	B	0	7	.430954	.398793	.000920	-.000428	.149554	.126768	.000975
.90, .70	B	0	0	.096549	.083974	.000369	-.000078	.063066	.053243	.000361
.90, .90	B	0	0	.047825	.044894	.000208	-.000429	.045145	.042881	.000205
.90, .95	B	0	0	.051135	.049289	.000222	-.000546	.048901	.047665	.000218
γ_0 = .90	G	0	0	.144337	.133684	.000382	-.000523	.102432	.092841	.000389

Table 3.11 (continued)

$\beta = 1$, Maximum X = 32

$(\gamma_0, \tilde{\gamma})$	Design Type	Number $\hat{\gamma}$'s Near Zero	Number $\hat{\gamma}$'s Near One	Estimated Mean Square Error			$\widehat{\text{Bias}}(\hat{\gamma})$	Large Sample Variance		
				$\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$		$\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$
.10, .05	B	0	0	.003227	.006437	.002147	.005866	.003333	.006667	.002091
.10, .10	B	0	0	.003227	.006437	.001927	.004345	.003333	.006667	.002004
.10, .30	B	21	0	.002980	.006299	.002880	.006828	.003333	.006667	.003871
.10, .50	B	150	0	.002898	.006347	.008806	.054452	.003333	.006667	.023745
γ_0 = .10	G	1	0	.002037	.010297	.003491	.009341	.001996	.010801	.002990
.30, .10	B	0	0	.003227	.006437	.006956	.005335	.003333	.006667	.006867
.30, .30	B	0	0	.003227	.006437	.004877	-.000628	.003333	.006667	.004932
.30, .50	B	10	0	.003053	.006343	.007307	-.003832	.003333	.006667	.007951
.30, .70	B	154	0	.002904	.006359	.015612	.066012	.003333	.006667	.063068
γ_0 = .30	G	0	0	.002410	.009096	.007123	.002594	.002444	.009428	.007601
.50, .10	B	0	0	.003249	.006423	.013561	.006945	.003333	.006667	.013031
.50, .30	B	0	0	.003227	.006437	.005870	-.000335	.003333	.006667	.005760
.50, .50	B	0	0	.003227	.006437	.004908	-.004269	.003333	.006667	.004541

Table 3.11 (continued)

β = 1, Maximum X = 32

$(\gamma_0, \tilde{\gamma})$	Design Type	Number $\hat{\gamma}$'s Near Zero	Number $\hat{\gamma}$'s Near One	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$	Large Sample Variance $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$
.50, .70	B	22	0	.002981	.006310	.009238	-.008542	.003333	.006667	.009066
.50, .90	B	237	0	.003257	.006679	.041229	.185508	.003333	.006667	2.547011
γ_0 = .50	G	0	0	.002841	.008017	.006708	-.002231	.003035	.008198	.007322
.70, .30	B	0	0	.004971	.007571	.007256	.000580	.003334	.006665	.006933
.70, .50	B	0	0	.003235	.006429	.003518	-.001997	.003335	.006666	.003337
.70, .70	B	0	0	.003231	.006438	.002792	-.004948	.003335	.006667	.002358
.70, .90	B	123	0	.002952	.006328	.005597	.020478	.003339	.006672	.017279
γ_0 = .70	G	0	0	.004092	.007167	.004444	-.006759	.004274	.007531	.004052
.90, .50	B	0	72	.027023	.025522	.002931	-.015255	.010920	.008486	.004061
.90, .70	B	0	13	.017142	.015361	.001297	-.002179	.006783	.007248	.001349
.90, .90	B	0	0	.006906	.008932	.000632	-.002111	.006081	.008584	.000525
.90, .95	B	2	0	.007472	.009964	.001001	-.004029	.006819	.009620	.000647
γ_0 = .90	G	0	1	.024579	.022703	.001262	-.004497	.015823	.015255	.001027

Table 3.11 (continued)

β = 3, Maximum X = 32

$(\gamma_0, \tilde{\gamma})$	Design Type	Number $\hat{\gamma}$'s Near Zero	Number $\hat{\gamma}$'s Near One	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$	Large Sample Variance $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$
.10, .05	B	0	0	.003227	.006437	.000226	.000408	.003333	.006667	.000232
.10, .10	B	0	0	.003227	.006437	.000215	.000269	.003333	.006667	.000223
.10, .30	B	0	0	.003227	.006437	.000410	-.000107	.003333	.006667	.000430
.10, .50	B	49	0	.002957	.006230	.001643	.005715	.003333	.006667	.002638
γ_0 = .10	G	0	0	.002016	.010353	.000351	.001105	.001996	.010801	.000332
.30, .10	B	0	0	.003227	.006437	.000759	.000086	.003333	.006667	.000763
.30, .30	B	0	0	.003227	.006437	.000541	-.000400	.003333	.006667	.000548
.30, .50	B	0	0	.003227	.006437	.000893	-.001355	.003333	.006667	.000883
.30, .70	B	53	0	.002914	.006251	.004699	.002916	.003333	.006667	.007008
γ_0 = .30	G	0	0	.002372	.009096	.000817	.000332	.002444	.009428	.000845
.50, .10	B	0	0	.003227	.006438	.001459	-.000004	.003333	.006667	.001448
.50, .30	B	0	0	.003227	.006437	.000643	-.000480	.003333	.006667	.000640
.50, .50	B	0	0	.003227	.006437	.000507	-.000758	.003333	.006667	.000505

Table 3.11 (continued)

β = 3, Maximum X = 32

$(\gamma_0, \tilde{\gamma})$	Design Type	Number $\hat{\gamma}$'s Near Zero	Number $\hat{\gamma}$'s Near One	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$	Large Sample Variance $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$
.50, .70	B	0	0	.003227	.006437	.001102	-.002671	.003333	.006667	.001007
.50, .90	B	217	0	.003155	.006577	.016556	.102725	.003333	.006667	.283001
γ_0 = .50	G	0	0	.002835	.007993	.000776	-.000483	.003035	.008198	.000814
.70, .30	B	0	0	.003229	.006434	.000782	-.000511	.003334	.006665	.000770
.70, .50	B	0	0	.003228	.006437	.000376	-.000564	.003335	.006666	.000371
.70, .70	B	0	0	.003228	.006438	.000267	-.000726	.003335	.006667	.000262
.70, .90	B	19	0	.002979	.006298	.002599	-.007148	.003339	.006672	.001920
γ_0 = .70	G	0	0	.004001	.007131	.000459	-.001254	.004274	.007531	.000450
.90, .50	B	0	0	.029406	.023822	.000471	.000060	.010920	.008486	.000451
.90, .70	B	0	0	.007224	.007249	.000154	-.000212	.006783	.007248	.000150
.90, .90	B	0	0	.005768	.008109	.000059	-.000316	.006081	.008584	.000058
.90, .95	B	0	0	.006455	.009093	.000075	-.000482	.006819	.009620	.000072
γ_0 = .90	G	0	0	.015681	.014883	.000114	-.000580	.015823	.015255	.000114

For the parameter situation ($\beta = 1$, $\gamma = .9$, maximum $X = 16$) a large number of data sets yielded $\hat{\gamma}$'s greater than .98. This same simulation was performed with data sets yielding $\hat{\gamma}$'s greater than .95 being excluded. Summary results may be found in Table 3.12. For data sets with $\hat{\gamma} \in (.95, .98)$, the estimates of α and β are consistently high. For example, a typical data set yielded $\hat{\alpha} = 10.918$, $\hat{\beta} = 1.902$, $\hat{\gamma} = .959$, where the true values are 10, 1, and .9, respectively, and the standard deviation of an individual observation is .1.

Table 3.12 Summary results as included in Tables 3.10 and 3.11 with data sets having $\hat{\gamma} \epsilon$ (.95, 1.0) being excluded

$\beta = 1$, Maximum X = 16

$(\gamma_0, \tilde{\gamma})$	Design Type	Number $\hat{\gamma}$'s Near Zero	Number $\hat{\gamma}$'s Near One	Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$	$\widehat{\text{Bias}}(\hat{\gamma})$	Large Sample Variance $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$
.90, .50	B	0	153	.026061	.023255	.005373	-.042213	.149554	.126768	.008779
.90, .70	B	0	98	.029877	.027972	.002332	-.018661	.063066	.053243	.003252
.90, .90	B	0	47	.032236	.032749	.001804	-.009993	.045145	.042881	.001849
.90, .95	B	0	46	.034961	.036660	.002247	-.011572	.048901	.047665	.001962
γ_0 = .90	G	0	84	.050792	.048670	.003614	-.022283	.102432	.092841	.003505

Table 3.12 (continued)

$(\gamma_0, \tilde{\gamma})$	Design Type	0.0–0.0+	0.0+–0.1	0.1–0.2	0.2–0.3	0.3–0.4	0.4–0.5	0.5–0.6	0.6–0.7	0.7–0.8	0.8–0.9	0.9–0.95	0.95–1.0
		β = 1, Maximum X = 16 Frequency Distribution of $\hat{\gamma}$											
.90, .50	B								5	47	193	102	153
.90, .70	B									24	216	162	98
.90, .90	B								1	14	223	215	47
.90, .95	B								4	17	212	221	46
γ_0 = .90	G						1		6	23	225	161	84

3.2.2 Large Sample Properties

When γ is guessed well enough (i.e., when there is little or no problem with $\hat{\gamma}$ being near zero or one) or when geometric-spacing is used, agreement between large and small sample properties is good. Table 3.13 gives the large and small sample variance-covariance matrices for $\beta = 1$, maximum $X = 16$, $\tilde{\gamma} = \gamma_0$, and the Box-Lucas design. Table 3.14 gives the same information for the geometric-spacing design.

Agreement between large and small sample properties is such that useful work in design comparison could be done through the use of large sample properties, for $\gamma \leq .7$.

Table 3.13 Selected large and small sample variance-covariance matrices for $\beta = 1$, maximum $X = 16$, and the Box-Lucas design

$(\gamma_0, \tilde{\gamma})$	Large Sample			Small Sample		
(.10, .10)	.0033			.0032		
	.0033	.0067		.0032	.0064	
	.0013	.0006	.0020	.0011	.0003	.0019
(.30, .30)	.0033			.0032		
	.0033	.0067		.0032	.0064	
	.0021	.0009	.0049	.0019	.0006	.0049
(.50, .50)	.0033			.0032		
	.0033	.0067		.0032	.0064	
	.0020	.0008	.0045	.0019	.0007	.0049
(.70, .70)	.0034			.0035		
	.0035	.0068		.0034	.0066	
	.0017	.0008	.0025	.0017	.0008	.0029
(.90, .90)	.0451			.0856		
	.0423	.0429		.0814	.0803	
	.0087	.0078	.0018	.0098	.0090	.0019

Table 3.14 Selected large and small sample variance-covariance matrices for $\beta = 1$, maximum $X = 16$, and the geometric-spacing design

γ_0	Large Sample			Small Sample		
.10	.0025			.0024		
	.0020	.0093		.0021	.0089	
	.0013	-.0014	.0031	.0012	-.0014	.0032
.30	.0032			.0030		
	.0026	.0080		.0025	.0077	
	.0027	-.0013	.0080	.0023	-.0015	.0072
.50	.0044			.0042		
	.0036	.0075		.0033	.0071	
	.0035	.0001	.0078	.0034	-.0002	.0080
.70	.0074			.0078		
	.0064	.0089		.0065	.0087	
	.0042	.0020	.0048	.0045	.0022	.0053
.90	.1024			.1734		
	.0963	.0928		.1685	.1660	
	.0180	.0165	.0035	.0173	.0161	.0035

3.2.3 Summary and Conclusions

As was the case in section 3.1, the Box-Lucas design is better than the alternative design (geometric-spacing) when γ is guessed well and poorer when γ is not guessed well. When γ is guessed badly enough the Box-Lucas design is unsatisfactory. Increasing the sample size to any level within economic reason may not help sufficiently.

The geometric-spacing design is constructed to protect against $\tilde{\gamma} \neq \gamma_0$ and therefore is not as good as Box-Lucas with $\tilde{\gamma} = \gamma_0$ (and occasionally is decidedly inferior to Box-Lucas). On the other hand, it rarely yields unacceptable results in situations where the Box-Lucas design may.

The work in which data sets were excluded for $\hat{\gamma}$ greater than .95 indicates that the experimenter might be better off to set some truncation point in the .90 to .95 range, rather than discarding data sets if he felt that γ was indeed large, but not larger than the truncation point. For $\hat{\gamma}$ large, $\hat{\alpha}$ and $\hat{\beta}$ are quite sensitive to the actual magnitude of $\hat{\gamma}$. The reliability of $\hat{\alpha}$ and $\hat{\beta}$ is damaged less by truncating below γ than by allowing a $\hat{\gamma}$ near one.

Probably the most useful result is the indication that some sort of compromise between Box-Lucas and geometric-spacing would be a defensible design strategy to follow, particularly for larger sample sizes. For example, although an experimenter can not guess γ exactly, there should be many cases in which he could give a range $R \in (0,1)$ that he was quite confident would contain γ. The interior design points would be chosen so as to protect the experimenter for any γ in R. Thus, the more confidence an experimenter had in $\tilde{\gamma}$ the more nearly his design would resemble the Box-Lucas design.

4. SOME RESULTS WHEN γ IS ASSUMED TO HAVE A PRIOR BETA DISTRIBUTION

In this chapter, it is assumed that the experimenter can define a class of problems of which his present problem is a member. In addition, it is assumed that the γ's associated with the class of problems follow a beta distribution. The experimenter either knows or thinks he knows the form of this distribution from past experience.

Different experimental situations were simulated 2000 times each using both the geometric-spacing design and the Box-Lucas design. Data sets of nine observations each were generated and the parameters were estimated by a maximum constrained likelihood technique.

Prior distributions are not used for α and β. In the absence of knowledge of the behavior of α and β for the class of problems under consideration, the Bayesian might use uniform priors for α and β over the region where the likelihood function of the data had appreciable value.

If the parameters α and β are assumed to have locally uniform prior distributions, over sufficiently large intervals, the posterior distribution of α, β, and γ is proportional to $L(\alpha,\beta,\gamma)$, as given in equation (4.1). $L(\alpha,\beta,\gamma)$ is defined to be the constrained likelihood function. Under the assumptions made here, the posterior likelihood function, $L^*(\alpha,\beta,\gamma)$, is given by equation (4.2), where

$$\Phi(\alpha,\beta) = \int_0^1 L(\alpha,\beta,\gamma)\, d\gamma .$$

$$L(\alpha,\beta,\gamma) = \left(\frac{1}{2\pi}\right)^{\frac{n}{2}} \left(\frac{1}{\sigma}\right)^{n} e^{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - \alpha + \beta Z_i)^2}$$

$$\cdot \frac{\gamma^{u-1}(1-\gamma)^{v-1}}{B(u,v)} \quad (4.1)$$

where $Z_i = \gamma^{X_i}$.

$$L^*(\alpha,\beta,\gamma) = \frac{L(\alpha,\beta,\gamma)}{\Phi(\alpha,\beta)} \quad (4.2)$$

The natural logarithm of $L(\alpha,\beta,\gamma)$ is given by equation (4.3).

$$\ln L(\alpha,\beta,\gamma) = \frac{n}{2}\ln\left(\frac{1}{2\pi}\right) + n\ln\left(\frac{1}{\sigma}\right) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i-\alpha+\beta Z_i)^2$$

$$+ (u-1)\ln\gamma + (v-1)\ln(1-\gamma) - \ln B(u,v)$$

$$(4.3)$$

The estimates used in the simulations are the solutions of the system (4.4).

$$\frac{\partial \ln L(\alpha,\beta,\gamma)}{\partial\alpha} = 0$$

$$\frac{\partial \ln L(\alpha,\beta,\gamma)}{\partial\beta} = 0 \quad (4.4)$$

$$\frac{\partial \ln L(\alpha,\beta,\gamma)}{\partial\gamma} = 0$$

The solutions of (4.4) will be called maximum constrained likelihood estimates although the posterior likelihood is given by (4.2). If (4.2) were maximized, the estimates would be the solutions to (4.5).

$$\frac{\partial \ln L^*(\alpha,\beta,\gamma)}{\partial \alpha} = \frac{\partial \ln L(\alpha,\beta,\gamma)}{\partial \alpha} - \frac{\partial \ln \Phi(\alpha,\beta)}{\partial \alpha} = 0$$

$$\frac{\partial \ln L^*(\alpha,\beta,\gamma)}{\partial \beta} = \frac{\partial \ln L(\alpha,\beta,\gamma)}{\partial \beta} - \frac{\partial \ln \Phi(\alpha,\beta)}{\partial \beta} = 0 \qquad (4.5)$$

$$\frac{\partial \ln L^*(\alpha,\beta,\gamma)}{\partial \gamma} = \frac{\partial \ln L(\alpha,\beta,\gamma)}{\partial \gamma} = 0$$

The estimates in (4.5) would differ very little from those in (4.4) if the magnitudes of $\frac{\partial \ln \Phi(\alpha,\beta)}{\partial \alpha}$ and $\frac{\partial \ln \Phi(\alpha,\beta)}{\partial \beta}$ were small relative to the magnitudes of $\frac{\partial \ln L(\alpha,\beta,\gamma)}{\partial \alpha}$ and $\frac{\partial \ln L(\alpha,\beta,\gamma)}{\partial \beta}$, respectively.

In order to find the estimates of α, β, and γ the value of σ^2 or the maximum constrained likelihood estimate of it must be available. For the work in this chapter it is assumed that σ^2 is known to be .01.

The general form of the beta prior distribution is given by equation (4.6).

$$g(\gamma) = \begin{cases} \dfrac{\gamma^{u-1}(1-\gamma)^{v-1}}{B(u,v)}, & 0 < \gamma < 1; \quad u,\ v > 0 \\ 0, & \text{elsewhere} \end{cases} \qquad (4.6)$$

Both correct and incorrect priors were considered for a limited number of cases. Table 4.1 indicates the assumed and actual prior combinations which were used. The values $\tilde{\bar{\gamma}}$ and $\bar{\gamma}$ are the corresponding assumed and actual prior means, respectively. $\tilde{\bar{\gamma}}$ was used in the specification of the Box-Lucas design.

Table 4.1 Assumed and actual priors used in simulation

Prior Parameters: Assumed u	Assumed v	Actual u_0	Actual v_0	$\tilde{\gamma}$	$\bar{\gamma}$
22.0	22.0	22.0	22.0	.5	.5
2.5	2.5	2.5	2.5	.5	.5
2.5	22.5	2.5	22.5	.1	.1
22.0	22.0	2.5	2.5	.5	.5
2.5	2.5	2.5	22.5	.5	.1

The priors in Table 4.1 are graphed in Figure 4.1.

Each combination in Table 4.1 was used with all combinations of $\alpha = 10$; $\beta = 1, 3$; and maximum $X = 16, 32$.

4.1 Box-Lucas Designs Versus Geometric-Spacing Designs

For both designs, the simulation procedure was as follows:

(1) A value of γ was generated from the actual prior beta distribution.

(2) Using this γ a data set was generated.

(3) Using the assumed prior distribution, maximum likelihood estimates of α, β, and γ were obtained.

(4) For the particular γ generated in step (1), the squared deviations of $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\gamma}$ from the actual values, were computed.

(5) Steps (1) to (4) were performed 2000 times for each situation, and the results averaged.

The estimated average mean square errors of $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\gamma}$ for the Box-Lucas design and the geometric-spacing design appear in Table 4.2.

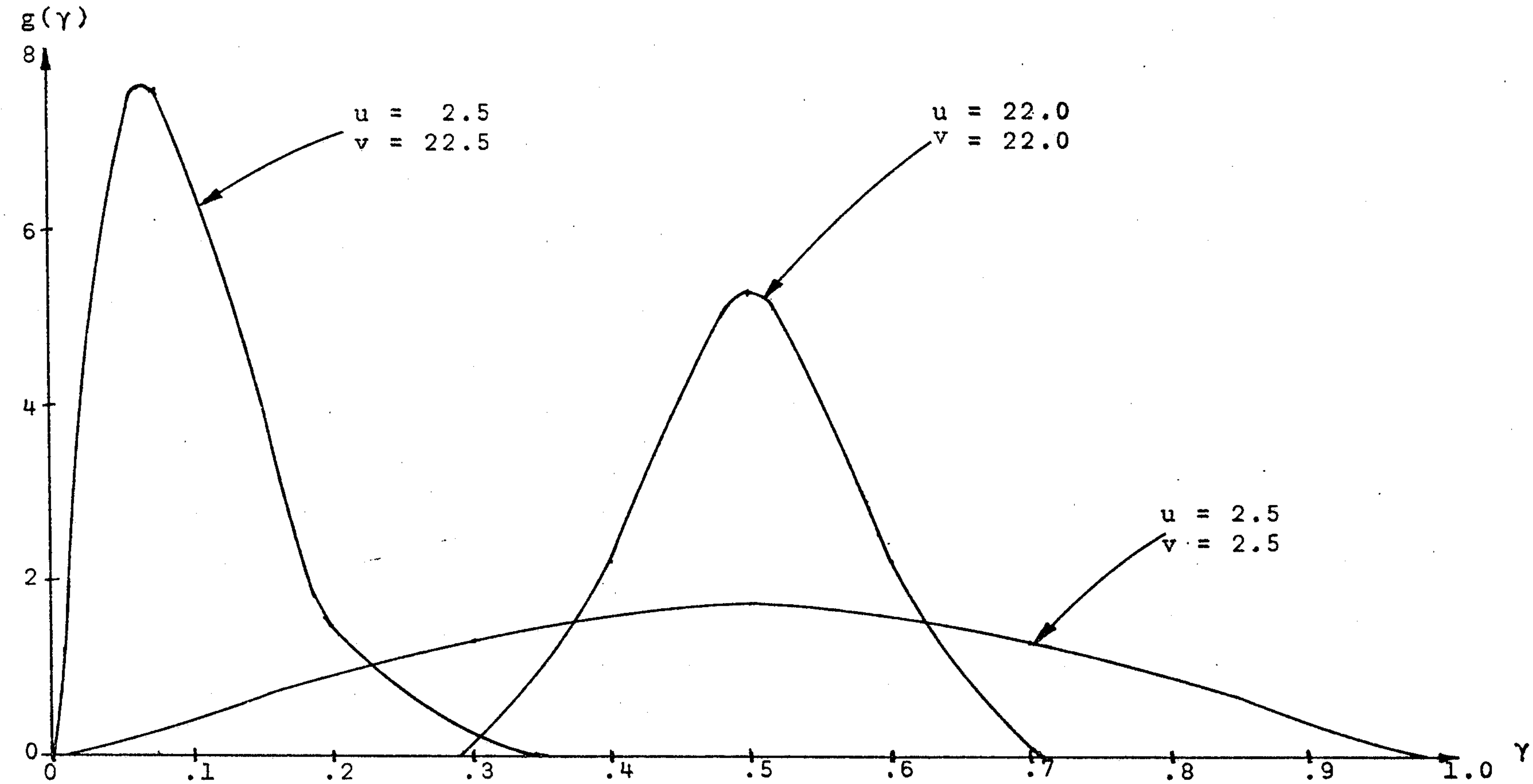

Figure 4.1 Priors given in Table 4.1

Table 4.2 Summary of average estimated mean square errors of $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\gamma}$ for selected assumed priors, actual priors, and sets of parameter values (e)

β = 1, maximum X = 16

Prior Distributions: Assumed Mean	Assumed Variance	Actual Mean	Actual Variance	Design Type	Average Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$
.5	.00555	.5	.00555	B	.002949	.006615	.002507
				G	.003510	.007456	.003212
.5	.04166	.5	.04166	B	.004963	.007840	.005284
				G	.008932	.011725	.006450
.1	.00346	.1	.00346	B	.002992	.006565	.001423
				G	.002129	.009164	.001802
.5	.00555	.5	.04166	B	.008448	.010012	.012294
				G	.015630	.015246	.016649
.5	.04166	.1	.00346	B	.003383	.006558	.014881
				G	.002691	.009484	.005565

(e) B = Box-Lucas design; G = geometric-spacing design. Results are averaged over 2000 data sets, with nine observations per data set.

Table 4.2 (continued)

$\beta = 3$, maximum $X = 16$

Prior Distributions Assumed Mean	Assumed Variance	Actual Mean	Actual Variance	Design Type	Average Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$
.5	.00555	.5	.00555	B	.003303	.006694	.000497
				G	.004255	.007478	.000757
.5	.04166	.5	.04166	B	.014098	.016381	.000735
				G	.012499	.014893	.000752
.1	.00346	.1	.00346	B	.003303	.006660	.000224
				G	.002347	.009320	.000328
.5	.00555	.5	.04166	B	.030476	.029360	.001829
				G	.033863	.032128	.001427
.5	.04166	.1	.00346	B	.003398	.006622	.002410
				G	.002467	.009461	.000384

Table 4.2 (continued)

$\beta = 1$, maximum $X = 32$

Prior Distributions				Design	Average Estimated Mean Square Error		
Assumed		Actual					
Mean	Variance	Mean	Variance	Type	$\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$
.5	.00555	.5	.00555	B	.002945	.006615	.002504
				G	.002571	.007830	.003146
.5	.04166	.5	.04166	B	.004168	.007347	.004891
				G	.003994	.008978	.005827
.1	.00346	.1	.00346	B	.002992	.006565	.001423
				G	.001757	.010665	.001745
.5	.00555	.5	.04166	B	.005286	.007801	.011286
				G	.008478	.011411	.014163
.5	.04166	.1	.00346	B	.003383	.006558	.014887
				G	.002113	.011206	.005184

Table 4.2 (continued)

$\beta = 3$, maximum X = 32

Prior Distributions: Assumed Mean	Assumed Variance	Actual Mean	Actual Variance	Design Type	Average Estimated Mean Square Error $\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$
.5	.00555	.5	.00555	B	.003295	.006693	.000497
				G	.002946	.007941	.000738
.5	.04166	.5	.04166	B	.007556	.010502	.000687
				G	.007681	.012604	.000693
.1	.00346	.1	.00346	B	.003303	.006660	.000224
				G	.001888	.010847	.000305
.5	.00555	.5	.04166	B	.012821	.014322	.001544
				G	.010172	.013691	.001092
.5	.04166	.1	.00346	B	.003398	.006622	.002412
				G	.001985	.010949	.000359

For the limited number of priors considered, the Box-Lucas design was generally as good as or better than the geometric-spacing design for estimating α except when the mean of the actual prior distribution was small. For estimating β the geometric-spacing design was never materially better than the Box-Lucas design and usually much worse. The geometric-spacing design was generally no better than the Box-Lucas design for estimating γ, except when the actual prior mean was .1 and the assumed prior mean was .5. In this case, geometric-spacing was much better.

For the Box-Lucas design, increasing the experimental range from 16 to 32 had little effect, except in those cases where the actual prior had significant positive probability near unity. In these cases, the accuracy of $\hat{\alpha}$ and $\hat{\beta}$ was higher for a maximum X of 32.

For the geometric-spacing design, the increase in experimental range increased the accuracy of $\hat{\alpha}$. The increase in range generally caused limited improvement in $\hat{\beta}$, except in cases where the actual prior was very diffuse. In these cases, the increase lowered the accuracy of $\hat{\beta}$. A limited increase in the accuracy of $\hat{\gamma}$ was present when the maximum X was increased from 16 to 32.

As was the case in chapter 3, the accuracy of $\hat{\gamma}$ was greater for β equal to three than for β equal to one. However, the accuracy of $\hat{\alpha}$ and $\hat{\beta}$ was lowered or essentially unchanged.

Intuitively, one would expect that the accuracy of $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\gamma}$ would be increasing functions of the tightness of correct priors. However, this relationship does not necessarily hold. In this simulation work, two correct priors with means of .5 are considered--one diffuse and the other moderately tight. For $\beta = 3$ and the geometric-spacing design, the diffuse prior yields a smaller average mean square error of $\hat{\gamma}$ than the tight prior. A partial justification for this apparent inconsistency may be seen by referring to the results for the geometric-spacing design with $\beta = 3$ in Table 3.11. Table 4.3 contains selected estimated mean square errors of $\hat{\gamma}$.

Table 4.3 Selected results from Table 3.11 for $\beta = 3$ and geometric-spacing design

Maximum X	γ_0	Estimated Mean Square Error of $\hat{\gamma}$
16	.1	.000336
	.3	.000850
	.5	.000874
	.7	.000534
	.9	.000382
32	.1	.000351
	.3	.000817
	.5	.000776
	.7	.000459
	.9	.000114

The mean square errors for $\hat{\gamma}$ are smaller when the true γ is near the extremes of the (0,1) interval than at the middle. The diffuse prior puts more weight at the extremes of the (0,1) interval and less near the middle than the tight prior. Thus, if the difference in weighting were the only consideration, the diffuse prior should yield greater accuracy.

The use of incorrect priors damages the performance of $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\gamma}$ relative to the use of correct priors. Battiste (1967) studied the use of prior information in a linear regression model. He found that the use of under-weighted, biased prior information was often preferable to using no prior information. It is suspected that a similar result holds here.

4.2 Effect of the Number of Simulations on the Stability of Results

In the determination of small sample properties, 2000 data sets were generated in each parameter-prior situation. This amount of sampling is not sufficient to adequately determine the small sample properties when the prior is diffuse. Although no work was done to verify it, it is suspected that 2000 simulations are not sufficient for any prior having significant positive probability near unity. In chapter 3 it was found that $\hat{\alpha}$ and $\hat{\beta}$ were very sensitive to $\hat{\gamma}$ for $\hat{\gamma}$ near unity. Thus it is important that the upper tail of any prior having significant positive probability near unity be sampled properly.

Table 4.4 contains results from Table 4.2 for $\beta = 3$, maximum $X = 16$, and the Box-Lucas design. In addition, the same parameter-prior situation is simulated again using a new set of random numbers. These results are also given in Table 4.4. Differences for given parameter-prior situations are attributable to sampling. Differences that appear when the actual prior is diffuse are large enough to indicate insufficient sampling.

Table 4.4 Selected results indicating sampling effects for $\beta = 3$, maximum X = 16, and the Box-Lucas design[f]

Prior Distributions				Random Number Set	Average Estimated Mean Square Error		
Assumed		Actual					
Mean	Variance	Mean	Variance		$\hat{\alpha}$	$\hat{\beta}$	$\hat{\gamma}$
.5	.00555	.5	.00555	1	.003303	.006694	.000497
				2	.003100	.006508	.000468
.5	.04166	.5	.04166	1	.014098	.016381	.000735
				2	.012116	.014356	.000658
.1	.00346	.1	.00346	1	.003303	.006660	.000224
				2	.003129	.006522	.000214
.5	.00555	.5	.04166	1	.030476	.029360	.001829
				2	.023031	.021677	.001622
.5	.04166	.1	.00346	1	.003398	.006622	.002410
				2	.003071	.006292	.002217

(f) All results are determined from 2000 data sets.

4.3 Summary and Conclusions

For the prior distributions considered, the overall performance of the Box-Lucas design exceeded that of the geometric-spacing design for estimating α and β. The evidence is not clear for γ. Further work is required to determine how much bias in the prior may be tolerated before geometric-spacing is to be preferred to Box-Lucas.

A tight prior may lead to a $\hat{\gamma}$ with lower accuracy than a diffuse prior. The experimental information on γ is greater for γ near the extremes of the (0,1) interval. The diffuse prior yields γ's near the extremes more often than the tight prior. If the prior information has small enough weight relative to the experimental information, the diffuse prior may lead to more accurate estimation of γ.

Relative to the use of correct priors, the use of incorrect priors lowered the accuracy of $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\gamma}$. As expected, the distinction is more prevalent for $\hat{\gamma}$.

Adequate sampling of the prior distribution is critical in obtaining reliable small sample results. For a diffuse prior, 2000 simulations are not sufficient. The sensitivity of $\hat{\alpha}$ and $\hat{\beta}$ to $\hat{\gamma}$ for $\hat{\gamma}$ near unity would seem to indicate that 2000 simulations are not sufficient for any prior having significant positive probability near unity.

The use of the prior information protects against a certain amount of variation in γ. In particular, the prior prevents a $\hat{\gamma}$ at a boundary of the parameter space.

The logical comparison of the effects of use and non-use of priors was not done. The reason for this omission is that, when the prior was not used in estimation, γ did not have a distribution.

5. COMPUTATIONAL PROCEDURES

For the simulation work in chapter 3, data sets were generated by GAUSS, a subroutine from IBM's System/360 Scientific Subroutine Package. The same generating seed was used for each parameter-design situation.

The estimation procedure is least squares with the additional restriction that $\hat{\gamma} \varepsilon (0,1)$. Written in sample form the model is

$$y_i = \hat{\alpha} - \hat{\beta}\hat{\gamma}^{X_i} + e_i, \; i = 1, 2, \ldots, n. \tag{5.1}$$

The value of $(\hat{\alpha},\hat{\beta},\hat{\gamma})$ that minimizes

$$Q = \sum_{i=1}^{n} e_i^2$$

$$= \sum_{i=1}^{n} (y_i - \hat{\alpha} + \hat{\beta}\hat{\gamma}^{X_i})^2$$

is desired. For $\hat{\gamma}$ fixed, the usual estimates for α and β are available. Letting $Z_i = \hat{\gamma}^{X_i}$,

$$\left.\begin{aligned} \hat{\alpha} &= \overline{y} + \hat{\beta}\,\overline{Z} \\ \hat{\beta} &= -\frac{\sum_{i=1}^{n} (Z_i - \overline{Z})(y_i - \overline{y})}{\sum_{i=1}^{n} (Z_i - \overline{Z})^2} \end{aligned}\right\} \tag{5.2}$$

Therefore for any $\hat{\gamma} \varepsilon (0,1)$, $\hat{\alpha}$, $\hat{\beta}$ and Q may be evaluated directly. Q as a function of $\hat{\gamma}$ is searched for its minimum value. In Figure 5.1 the correct estimate of γ is $\hat{\gamma}'$.

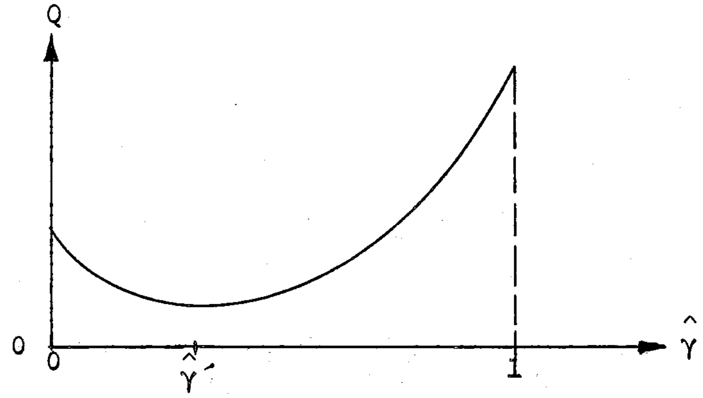

Figure 5.1 Error sum of squares as a function of $\hat{\gamma}$

An iteration technique reported by Spang (1962) for finding the minimum of a uni-modal function in two dimensions is used to find the minimum of $Q(\hat{\gamma})$. This technique has the advantage that it always converges to within prescribed error limits of the correct value in a fixed number of steps. For this work, twenty iterations were performed for each data set. The final estimate was at one end of an interval of length .000066 that contained the least squares estimate.

For some data sets, the $\hat{\gamma}$ that minimizes Q is small and the design is such that $\hat{\gamma}^X$ is essentially zero for all non-zero design points. If $\hat{\gamma}^X$ is small enough in magnitude, the result of this computation is replaced with a true zero by the computer for all $\hat{\gamma} < \hat{\gamma}^*$. The error sum of squares as seen by the computer is constant for $\hat{\gamma} < \hat{\gamma}^*$, so that there is no unique minimum for Q. Figure 5.2 illustrates the problem.

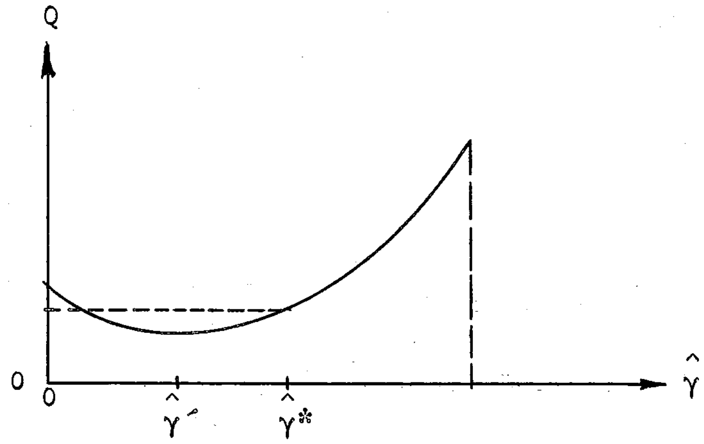

Figure 5.2 Error sum of squares when least squares estimate of γ is near zero

The curved line with the attached horizontal segment is Q as seen by the computer whereas the whole curved line is the true Q for this data set. $\hat{\gamma}'$ is the correct least squares estimate. $\hat{\gamma}^*$ is the estimate produced by the computing algorithm. The computing algorithm was arbitrarily set up to choose $\hat{\gamma}^*$.

For each parameter-design situation, the mean square errors of $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\gamma}$ were estimated using the general formula

$$\widehat{MSE}(\hat{\Theta}) = \frac{\sum_{i=1}^{m} (\hat{\Theta}_i - \Theta)^2}{m} \qquad (5.3)$$

where m was the number of estimates available; m = 1000 in section 3.1 and 500 less rejects in section 3.2.

All computations were performed in the double precision mode on a 360/65 IBM computer.

In chapter 4, small sample properties are determined for a limited number of cases.

Investigation of the small sample properties required the estimates of α, β, and γ for many data sets in each parameter-prior situation. For each data set, a new γ was generated from the beta prior.

The beta deviate generator depends on a relationship between a beta random variable and two chi-square random variables. The relationship is given by equation (5.4), where u and v are integral multiples of 0.5.

$$\text{Beta}(u,v) = \frac{\chi^2_{2u}}{\chi^2_{2u} + \chi^2_{2v}} \qquad (5.4)$$

The estimation procedure requires maximization of the natural log of the constrained likelihood function. For given γ, the same estimators for α and β (equation (5.2)), as were used in chapter 3, are appropriate. This result follows since the partials of lnL with respect to α and β do not involve the prior information. Assuming σ^2 is known to be .01, the values of α, β, and -lnL may be determined for a given γ. Thus the computational technique is to consider -lnL as a function of γ, and to determine the γ (and corresponding α and β) that minimizes -lnL using the minimization technique of Spang (1962).

The squared deviations of $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\gamma}$ from the actual values were computed for each data set and its corresponding generated γ. The results for the 2000 data sets generated in each parameter-prior situation were averaged.

The computations were performed in the double precision mode on a 360/75 IBM computer.

6. RECOMMENDATIONS FOR FURTHER RESEARCH

1. Use the determinant of the large sample variance-covariance matrix of $\hat{\alpha}$, $\hat{\beta}$, $\hat{\gamma}$ as the criterion for determining zones of preference in the $(\gamma_0, \tilde{\gamma})$ space for choosing between the geometric-spacing design and the Box-Lucas design. With such information at hand, an experimenter could make his choice based on his confidence in $\tilde{\gamma}$. Graphically, the results might appear as in Figure 6.1.

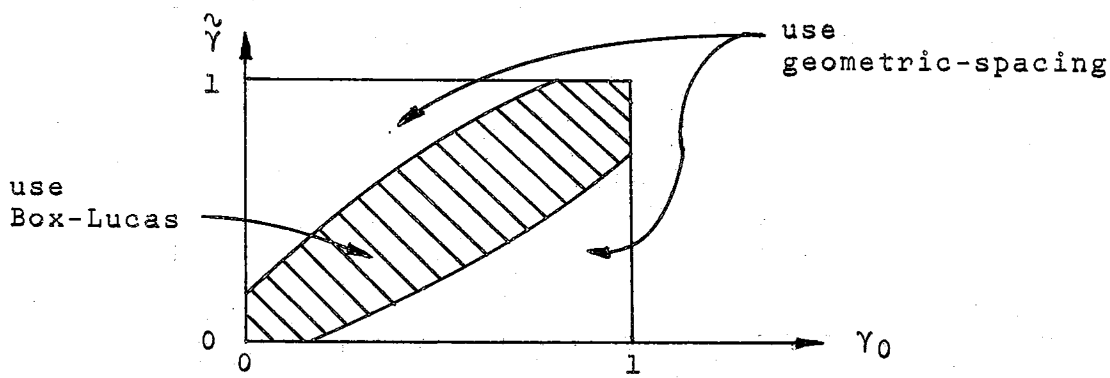

Figure 6.1 Zones of design preference in the $(\gamma_0, \tilde{\gamma})$ space

Determination of the region in Figure 6.1 could be done for various (β, maximum X) combinations.

2. Consider a compromise between the geometric-spacing design and the Box-Lucas design.

<u>Case (1)</u>: γ does not have a prior distribution. The experimenter picks a range $R = (\tilde{\gamma}_L, \tilde{\gamma}_U) \subset (0,1)$ that he is quite sure contains γ_0. In addition to design points

at 0, maximum X, and $X_{\tilde{\gamma}}$ as specified by Box & Lucas (1959), put design points at $X_{\tilde{\gamma}_L}$ and $X_{\tilde{\gamma}_U}$. With a total of nine observations this design would have three observations at 0, three at the maximum X and one each at the points $X_{\tilde{\gamma}_L}$, $X_{\tilde{\gamma}}$, $X_{\tilde{\gamma}_U}$.

For example, if $\tilde{\gamma}_L = .3$, $\tilde{\gamma} = .5$, and $X_{\tilde{\gamma}_U} = .7$, the design points (referring to Table 3.10) could be 0.0, .8306, 1.4425, 2.7503, and 16.0.

Case (2): γ has a known prior distribution. Use the same procedure as in Case (1) except $\tilde{\gamma}$ would be the mean of the prior and $\tilde{\gamma}_L$ and $\tilde{\gamma}_U$ would be at the lower and upper α percent points of the prior, respectively.

3. Consider the performance of the exponential model with respect to prediction. Compare estimated mean square error of prediction for the true model (exponential) with that for the simple linear regression model. The linear regression model may be preferred for γ near unity.

4. Consider sequential design, starting with something like a geometric-spacing design, which would be altered to Box-Lucas as more information became available on γ. A sequential design combined with the use of prior information in the estimation phase would seem to be a logical development.

5. Determine the effects of the use of incorrect priors if prior information is used in the estimation procedure.

6. In the framework of chapter 4, investigate the case where σ^2 must be estimated.

7. GENERAL SUMMARY AND CONCLUSIONS

The results of chapter 3 indicated that the equal-spacing design could not be recommended in place of the Box-Lucas design. When γ was guessed badly, both designs gave generally unacceptable results. In certain extreme cases both designs were such that the frequency distribution of $\hat{\gamma}$ was bimodal with essentially zero probability in the region of the true γ. When γ was guessed well, the Box-Lucas design was definitely better than the equal-spacing design.

The geometric-spacing design compared more favorably with the Box-Lucas design than the equal-spacing design. The geometric-spacing design protects the experimenter against a bad guess of γ. This design greatly decreased the chance of generating a $\hat{\gamma}$ at a boundary of the parameter space. However, in cases where the guessed γ was correct or only moderately off, the Box-Lucas design was somewhat better.

In chapter 4 it was assumed that prior information on γ was available in the form of a beta distribution. The use of correct prior information improves the accuracy of the estimators, relative to the use of incorrect priors. It is not possible to generate a $\hat{\gamma}$ at a boundary of the parameter space, as it was when prior information was not included in the estimation procedure. The use of biased or overweighted priors inflates the mean square errors of the estimators, particularly for $\hat{\gamma}$, relative to the performance of the estimators using the correct prior.

For estimating α and β the Box-Lucas design is generally better than the geometric-spacing design. The geometric-spacing design may be better for γ if the prior is badly biased.

From chapter 3 it is concluded that the geometric-spacing design offers protection against a bad $\tilde{\gamma}$, and would seem to be preferred unless the experimenter is confident that the assumed γ value is close to the true γ. A design more nearly resembling the Box-Lucas design might be preferable. Such a design is suggested in part 2, case (1) of chapter 6.

From chapter 4 it is concluded that available prior information should be incorporated into the estimation procedure, with the stipulation that care be taken in the weighting of this information. The geometric-spacing design offers some protection against a badly biased prior, but is dominated by the Box-Lucas design in most cases.

Possibly a very good strategy would be to use the design suggested in part 2, case (2) of chapter 6, with the prior information used in estimation of the parameters.

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9. APPENDIX

This chapter contains the derivation of large sample properties of $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\gamma}$.

9.1 Derivation of Large Sample Properties of $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\gamma}$ Without Prior Information on γ

The model is (replacing γ^{X_i} by Z_i)

$$Y_i = \alpha - \beta Z_i + \varepsilon_i, \quad i = 1, 2, \ldots, n, \tag{9.1}$$

with $\{\varepsilon_i\}$ independent and density function

$$f(y_i) = \frac{1}{\sqrt{2\pi}\,\sigma} e^{-\frac{1}{2\sigma^2}(y_i-\alpha+\beta Z_i)^2}, \quad i = 1, 2, \ldots, n \tag{9.2}$$

Therefore the likelihood function is

$$L(\alpha,\beta,\gamma) = \left(\frac{1}{2\pi}\right)^{\frac{n}{2}} \left(\frac{1}{\sigma}\right)^{n} e^{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i-\alpha+\beta Z_i)^2} \tag{9.3}$$

$$\ln L = K - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - \alpha + \beta Z_i)^2$$

where K is made up of terms not involving α, β or γ.

Taking all second order partial derivatives of ln L with respect to the parameters and computing the negative of their expectation yields the elements of the information matrix.

The identity $\frac{\partial \ln L}{\partial \gamma} = \frac{\partial \ln L}{\partial Z_i} \cdot \frac{\partial Z_i}{\partial \gamma}$, where $\frac{\partial Z_i}{\partial \gamma} = \frac{X_i Z_i}{\gamma}$, is used.

$$\frac{\partial^2 \ln L}{\partial \alpha^2} = -\frac{n}{\sigma^2}$$

$$-E\left(\frac{\partial^2 \ln L}{\partial \alpha^2}\right) = \frac{n}{\sigma^2}$$

$$\frac{\partial^2 \ln L}{\partial \alpha \ \partial \beta} = \frac{1}{\sigma^2} \sum_{i=1}^{n} Z_i$$

$$-E\left(\frac{\partial^2 \ln L}{\partial \alpha \ \partial \beta}\right) = -\frac{1}{\sigma^2} \sum_{i=1}^{n} Z_i$$

$$\frac{\partial^2 \ln L}{\partial \alpha \ \partial \gamma} = \frac{\beta^*}{\sigma^2} \sum_{i=1}^{n} X_i Z_i$$

$$-E\left(\frac{\partial^2 \ln L}{\partial \alpha \ \partial \gamma}\right) = -\frac{\beta^*}{\sigma^2} \sum_{i=1}^{n} X_i Z_i$$

$$\frac{\partial^2 \ln L}{\partial \beta^2} = -\frac{1}{\sigma^2} \sum_{i=1}^{n} Z_i^2$$

$$-E\left(\frac{\partial^2 \ln L}{\partial \beta^2}\right) = \frac{1}{\sigma^2} \sum_{i=1}^{n} Z_i^2$$

$$\frac{\partial^2 \ln L}{\partial \beta \ \partial \gamma} = -\frac{1}{\sigma^2} \sum_{i=1}^{n} \left(\frac{X_i Z_i \varepsilon_i}{\gamma} + \frac{\beta X_i Z_i^2}{\gamma}\right)$$

$$-E\left(\frac{\partial^2 \ln L}{\partial \beta \ \partial \gamma}\right) = \frac{\beta^*}{\sigma^2} \sum_{i=1}^{n} X_i Z_i^2$$

$$\frac{\partial^2 \ln L}{\partial \gamma^2} = -\frac{\beta^*}{\sigma^2} \sum_{i=1}^{n} \left(\frac{X_i^2 Z_i \varepsilon_i}{\gamma} + \frac{\beta X_i^2 Z_i^2}{\gamma} \right)$$

$$-E\left(\frac{\partial^2 \ln L}{\partial \gamma^2} \right) = \frac{\beta^{*2}}{\sigma^2} \sum_{i=1}^{n} X_i^2 Z_i^2$$

In the above equations, $\beta^* = \frac{\beta}{\gamma}$.

Therefore the information matrix is

$$V^{-1} = \frac{1}{\sigma^2} \begin{bmatrix} n & -\sum_{i=1}^{n} Z_i & -\beta^* \sum_{i=1}^{n} X_i Z_i \\ & \sum_{i=1}^{n} Z_i^2 & \beta^* \sum_{i=1}^{n} X_i Z_i^2 \\ \text{symmetric} & & \beta^{*2} \sum_{i=1}^{n} X_i^2 Z_i^2 \end{bmatrix} \qquad (9.4)$$

The inverse of V^{-1} is the large sample variance-covariance matrix for $\hat{\alpha}$, $\hat{\beta}$, $\hat{\gamma}$.

$$V = \frac{\sigma^2}{Q} \begin{bmatrix} V_{11} & V_{12} & V_{13} \\ & V_{22} & V_{23} \\ \text{symmetric} & & V_{33} \end{bmatrix} \qquad (9.5)$$

where,

$$Q = \beta^{*2} [nbf - a^2 f - bc^2 + 2acd - nd^2]$$

$$V_{11} = \beta^{*2} (bf - d^2)$$

$$V_{22} = \beta^{*2} (nf - c^2)$$

$$V_{33} = nb - a^2$$

$$V_{12} = \beta^{*2} (af - cd)$$

$$V_{13} = \beta^* (bc - ad)$$

$$V_{23} = \beta^* (ac - nd)$$

$$a = \sum_{i=1}^{n} Z_i, \quad b = \sum_{i=1}^{n} Z_i^2$$

$$c = \sum_{i=1}^{n} X_i Z_i, \quad d = \sum_{i=1}^{n} X_i Z_i^2$$

$$f = \sum_{i=1}^{n} X_i^2 Z_i^2$$

9.2 Large Sample Variances and Covariances When Box-Lucas Design is Used and $\tilde{\gamma}=\gamma_0$ and the Experimental Range Depends on $\tilde{\gamma}$

The basic design is $X_1 = 0$,

$$X_2 = -\frac{1}{\ln\gamma} + \frac{X_1 Z_1 - X_3 Z_3}{Z_1 - Z_3}, \qquad X_3 = \frac{\ln Z_3}{\ln\gamma} .$$

X_3 is to be located so that the expected response at X_3 achieves 100(1-p)% of the maximum change in the expected response from X_1. Therefore X_3 is determined from equation (9.6).

$$Z_3 = p \qquad (9.6)$$

or

$$X_3 = \frac{\ln p}{\ln\gamma}$$

Simplifying the expression for X_2 yields

$$X_2 = \frac{1}{\ln \gamma}\left(\frac{p - 1 - p \ln p}{1 - p}\right)$$

$$= \frac{K}{\ln \gamma}\text{, where } K = \frac{p - 1 - p \ln p}{1 - p} .$$

Therefore the Z_i have the values

$$Z_1 = 1, \quad Z_2 = e^K, \quad Z_3 = p .$$

From section 9.1,

$$\frac{\mathrm{Var}(\hat{\alpha})}{\sigma^2} = \frac{bf - d^2}{nbf - a^2f - bc^2 + 2acd - nd^2}$$

where

$$a = \frac{n}{3}(1 + e^K + p) \equiv \frac{n}{3} A$$

$$b = \frac{n}{3}(1 + e^{2K} + p^2) \equiv \frac{n}{3} B$$

$$c = \frac{n}{3 \ln\gamma}(Ke^K + p \ln p) \equiv \frac{n}{3 \ln\gamma} C$$

$$d = \frac{n}{3 \ln\gamma}(Ke^{2K} + p^2 \ln p) \equiv \frac{n}{3 \ln\gamma} D$$

$$f = \frac{n}{3(\ln\gamma)^2}(K^2e^{2K} + p^2 (\ln p)^2) \equiv \frac{n}{3(\ln\gamma)^2} F$$

Substituting the above equations into $\frac{\mathrm{Var}(\hat{\alpha})}{\sigma^2}$ and simplifying yields

$$\frac{\mathrm{Var}(\hat{\alpha})}{\sigma^2} = \frac{3(BF - D^2)}{n(3BF - A^2F - BC^2 + 2ACD - 3D^2)} \tag{9.7}$$

Similarly,

$$\frac{\mathrm{Var}(\hat{\beta})}{\sigma^2} = \frac{nf - c^2}{nbf - a^2f - bc^2 + 2acd - nd^2} \tag{9.8}$$

$$= \frac{9F - 3C^2}{n(3BF - A^2F - BC^2 + 2ACD - 3D^2)}$$

$$\frac{\mathrm{Cov}(\hat{\alpha},\hat{\beta})}{\sigma^2} = \frac{af - cd}{nbf - a^2f - bc^2 + 2acd - nd^2} \tag{9.9}$$

$$= \frac{3(AF - CD)}{n(3BF - A^2F - BC^2 + 2ACD - 3D^2)}$$

$$\frac{\mathrm{Var}(\hat{\gamma})}{\sigma^2} = \frac{nb - a^2}{\beta^{*2}(nbf - a^2f - bc^2 + 2acd - nd^2)} \tag{9.10}$$

$$= \frac{(\ln\gamma)^2}{n\beta^{*2}}\left(\frac{9B - 3A^2}{3BF - A^2F - BC^2 + 2ACD - 3D^2}\right)$$

$$\frac{\mathrm{Cov}(\hat{\alpha},\hat{\gamma})}{\sigma^2} = \frac{bc - ad}{\beta^*(nbf - a^2f - bc^2 + 2acd - nd^2)} \tag{9.11}$$

$$= \frac{\ln\gamma}{n\beta^*}\left(\frac{3(BC - AD)}{3BF - A^2F - BC^2 + 2ACD - 3D^2}\right)$$

$$\frac{\mathrm{Cov}(\hat{\beta},\hat{\gamma})}{\sigma^2} = \frac{ac - nd}{\beta^*(nbf - a^2f - bc^2 + 2acd - nd^2)} \tag{9.12}$$

$$= \frac{\ln\gamma}{n\beta^*}\left(\frac{3AC - 9D}{3BF - A^2F - BC^2 + 2ACD - 3D^2}\right)$$

Variances and covariances involving $\hat{\gamma}$ are functions of γ. The variance of $\hat{\gamma}$ is dependent on γ through

$$g(\gamma) = \frac{(\ln\gamma)^2}{\beta^{*2}} = \frac{\gamma^2(\ln\gamma)^2}{\beta^2} \quad .$$

$g(\gamma)$ is maximized for $\gamma = e^{-1} = .367879$.

$Cov(\hat{\alpha},\hat{\gamma})$ and $Cov(\hat{\beta},\hat{\gamma})$ are dependent on γ through

$$h(\gamma) = \frac{\ln\gamma}{\beta^*} = \frac{\gamma\ln\gamma}{\beta} \quad .$$

$h(\gamma)$ is maximized in absolute value for $\gamma = e^{-1}$.