RESPONSE SURFACE DESIGNS FOR THE DETECTION
OF MODEL INADEQUACY

by

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I. INTRODUCTION

1.1. Notation and General Remarks

Experimenters are frequently interested in exploring an unknown functional relationship

$$\eta = g(\xi_1, \xi_2, \ldots, \xi_k) \tag{1.1.1}$$

between a response η and quantitative variables $\xi_1, \xi_2, \ldots, \xi_k$. We shall assume that, although these variables are controlled and measured without error by the experimenter, the observable responses, y, are subject to random variation. In addition, we shall assume that the relationship (1.1.1) can be represented in a restricted region of interest, R, by a Taylor series expansion of some finite order. Essentially, this assumption allows the experimenter to approximate the relationship (1.1.1) by a graduating polynomial. Unfortunately, the specific order, as well as the parameters, of the graduating polynomial are usually unknown and must be determined from experimental observations. For purposes of standardization, experimenters sometimes find it useful to code the natural variables $\xi_1, \xi_2, \ldots, \xi_k$ (see Myers (1971)). We will denote the coded variables by $x_1, x_2, \ldots, x_k$.

Based upon operational constraints and prior knowledge, the experimenter intends to examine the use of the model

$$\eta_1(\underset{\sim}{x}) = \underset{\sim}{x}_1' \underset{\sim}{\beta}_1 \tag{1.1.2}$$

to represent the relationship (1.1.1) in a region of interest R, where the elements of the vector $\underset{\sim}{x}_1$ are functions of the coded variables

$$\underset{\sim}{x}' = (x_1, x_2, \ldots, x_k),$$

and $\underset{\sim}{\beta}_1$ is a vector containing p_1 parameters (notice that, vectors will be denoted by small, underscored, roman or greek letters; matrices will not be underscored but will be represented by capital roman letters). For example, if k = 2 and (1.1.2) is a second order polynomial then

$$\eta_1(\underset{\sim}{x}) = \beta_0 + x_1 \beta_1 + x_2 \beta_2 + x_1 \cdot x_2 \beta_{12} + x_1^2 \beta_{11} + x_2^2 \beta_{22}, \qquad (1.1.3)$$

$$\underset{\sim}{x}' = (1, x_1, x_2, x_1 \cdot x_2, x_1^2, x_2^2)$$

and $\underset{\sim}{\beta}_1' = (\beta_0, \beta_1, \beta_2, \beta_{12}, \beta_{11}, \beta_{22})$.

In this setting, the experimenter intends to fit model (1.1.2) using the method of least squares. An experiment is conducted obtaining n observations

$$\underset{\sim}{y}' = (y_1, y_2, \ldots, y_n)$$

at the points

$$(x_{1i}, x_{2i}, \ldots, x_{ki}); \; i = 1, 2, \ldots, n;$$

in a region of interest R. The experimenter assumes that

$$\underset{\sim}{y} = X_1 \underset{\sim}{\beta}_1 + \underset{\sim}{\varepsilon}$$

where X_1 is a $n \times p_1$ matrix whose ith row is a function of the variables $x_{1i}, x_{2i}, \ldots, x_{ki}$, and $\underset{\sim}{\varepsilon}$ is assumed to be a random vector with

$$E[\underset{\sim}{\varepsilon}] = \underset{\sim}{0} \text{ and } Var[\underset{\sim}{\varepsilon}] = \sigma^2 I_n$$

($\underset{\sim}{0}$ will be used to denote the null vector, and I_n will denote the

$n \times n$ identity matrix). For example, if $\eta_1(\underset{\sim}{x})$ is given by (1.1.3) then the ith row of X_1 is

$$\underset{\sim}{x}_{1i}' = (1, x_{1i}, x_{2i}, x_{1i} \cdot x_{2i}, x_{1i}^2, x_{2i}^2).$$

We will assume that $p_1 \leq n$ and that the rank of X_1 is p_1.

The points

$$(x_{1i}, x_{2i}, \ldots, x_{ki}),\ i = 1, 2, \ldots, n;$$

are referred to as the experimental design, and the matrix

$$D = \begin{bmatrix} x_{11} & x_{21} & \cdots & x_{k1} \\ x_{12} & x_{22} & \cdots & x_{k2} \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ x_{1n} & x_{2n} & \cdots & x_{kn} \end{bmatrix}^{n \times k}$$

is referred to as the design matrix.

It is well known (see Myers (1971)) that for model (1.1.2) the least squares estimators for $\underset{\sim}{\beta}_1$ and $\eta_1(\underset{\sim}{x})$ are

$$\hat{\underset{\sim}{\beta}}_1 = (X_1' X_1)^{-1} X_1' \underset{\sim}{y}$$

$$\text{and} \qquad \hat{\eta}_1(\underset{\sim}{x}) = \underset{\sim}{x}_1' \hat{\underset{\sim}{\beta}}_1 .$$

Furthermore, if (1.1.2) is the correct model,

$$E[\hat{\underset{\sim}{\beta}}_1] = \underset{\sim}{\beta}_1$$

$$\text{and} \qquad \mathrm{Var}[\hat{\underset{\sim}{\beta}}_1] = \sigma^2 (X_1' X_1)^{-1} . \qquad (1.1.4)$$

However, suppose that the true model is not given by (1.1.2). In particular, assume that the true model is

$$\eta(\underset{\sim}{x}) = \underset{\sim}{x}_1' \underset{\sim}{\beta}_1 + \underset{\sim}{x}_2' \underset{\sim}{\beta}_2, \qquad (1.1.5)$$

where the elements of $\underset{\sim}{x}_2$ are functions of the coded variables $\underset{\sim}{x}$, and $\underset{\sim}{\beta}_2$ is a vector containing p_2 additional parameters. We will sometimes refer to the assumed model (1.1.2) as the <u>proposed</u> or <u>lower order model</u> and the correct model (1.1.5) as the <u>true</u> or <u>higher order model</u>.

If the correct model is given by (1.1.5) then

$$\underset{\sim}{y} = X_1 \underset{\sim}{\beta}_1 + X_2 \underset{\sim}{\beta}_2 + \underset{\sim}{\epsilon}$$

where X_2 is a $n \times p_2$ matrix whose ith row is a function of the coded variables $\underset{\sim}{x}$. For example, if $k = 2$ and the lower order model is a second order polynomial while the higher order model is actually a third order polynomial then

$$\underset{\sim}{\beta}_2' = (\beta_{112}, \beta_{122}, \beta_{111}, \beta_{222})$$

and the ith row of X_2 is

$$\underset{\sim}{x}_{2i}' = (x_{1i}^2 \cdot x_{2i}, x_{1i} \cdot x_{2i}^2, x_{1i}^3, x_{2i}^3).$$

Now if the proposed model is not correct, the variance-covariance matrix for $\hat{\underset{\sim}{\beta}}_1$ is still given by (1.1.4). However, $\hat{\underset{\sim}{\beta}}_1$ is no longer unbiased. In fact,

$$E[\hat{\underset{\sim}{\beta}}_1] = \underset{\sim}{\beta}_1 + A \underset{\sim}{\beta}_2 \qquad (1.1.6)$$

where $$A = (X_1' X_1)^{-1} X_1' X_2.$$

The matrix A is usually referred to as the <u>alias matrix</u>.

It is important for the experimenter to verify the validity of his proposed model. This is sometimes done by using a preliminary test of one of the two hypotheses:

$$\begin{aligned} H_0:\ & E[\underset{\sim}{y}] = X_1 \underset{\sim}{\beta}_1 \\ \text{vs. } H_1:\ & E[\underset{\sim}{y}] \neq X_1 \underset{\sim}{\beta}_1 \end{aligned} \tag{1.1.7}$$

or

$$\begin{aligned} H_0:\ & \underset{\sim}{\beta}_2 = \underset{\sim}{0} \\ \text{vs. } H_1:\ & \underset{\sim}{\beta}_2 \neq \underset{\sim}{0}\ . \end{aligned} \tag{1.1.8}$$

With the assumption that the true model is given by (1.1.5), hypothesis (1.1.8) is equivalent to hypothesis (1.1.7). However, in general, the true model could be

$$\eta(\underset{\sim}{x}) = \underset{\sim}{x}_1' \underset{\sim}{\beta}_1 + \underset{\sim}{x}_2' \underset{\sim}{\beta}_2 + \underset{\sim}{x}_3' \underset{\sim}{\beta}_3$$

and these hypotheses would not be equivalent.

We will assume that the random vector $\underset{\sim}{\epsilon}$ is distributed as an n-variate Gaussian random vector with mean vector $\underset{\sim}{0}$ and variance-covariance matrix $\sigma^2 I_n$, i.e.,

$$\mathcal{L}(\underset{\sim}{\epsilon}) = N_n(\underset{\sim}{0}, \sigma^2 I_n).$$

Under this assumption, it is possible, provided the experiment is properly designed, to test hypothesis (1.1.7) or hypothesis (1.1.8) with a chi-square statistic, if σ^2 is known, or a F-ratio, if σ^2 is unknown. We will refer to these tests as tests for lack of fit. Since these tests are described in many statistical textbooks (see Myers (1971)), their analysis will not be discussed in detail here.

Under the assumption that the true model is given by (1.1.5), the non-centrality parameter of these tests is λ, where

$$\lambda = \sigma^{-2} \underset{\sim}{\beta}_2' L \underset{\sim}{\beta}_2.$$

The matrix of this quadratic form

$$L = X_2' [I_n - X_1 (X_1' X_1)^{-1} X_1'] X_2$$

will be referred to as the lack of fit matrix. The power of the lack of fit test is a function of λ and the degrees of freedom associated with the test statistic. In particular, the power is a monotone increasing function of λ.

It should be noted that the choice of which hypothesis, (1.1.7) or (1.1.8), to test, and possibly the test statistic, can be a complex matter. In general, this choice will affect the degrees of freedom associated with the test statistic, and hence the power of the test. Some of the factors influencing this choice are: (1) prior knowledge about the magnitude of higher order terms, (2) sample size limitations, and (3) the experimenter's underlying objectives.

1.2. The Problem

In general, the design problem is the selection of an experimental design that efficiently answers the experimenter's questions. This can be done by formulating some desirable design criteria, and then searching the class of permissible designs for a design that achieves these criteria, at least approximately, The class of permissible designs will be denoted by Δ. Essentially, Δ is a set containing all of the designs that an experimenter is willing to use. In this investigation, we shall assume that the number of observations, n, and the region of interest, R, are specified. Moreover, any design specifying n observations, all from the region R, will be assumed to be in Δ. It should be emphasized that it is the nature of the experimenter's questions and objectives that dictates whether one set of criteria is preferred over another. Let us examine criteria for the selection of an experimental design when the proposed model is given by (1.1.2) while the true model is given by (1.1.5).

1.2.1. General Considerations for the Selection of an Experimental Design

There are several properties of an experimental design that can influence our design selection. The three that we will be concerned with are:

1. the design's variance characteristics for both the lower and higher order models,
2. the design's fitted bias properties for the lower order model,

and 3. the design's power characteristics for the detection of model inadequacy.

Ideally, we would like to select designs that are optimum for all of these properties. In general, this is not possible; designs that are optimum for one of these characteristics are not likely to be optimum for the others. However, sometimes one of these properties is given primary consideration.

The variance properties of a design are a dominant consideration when the proposed model is known to be the true model. In this situation, $\hat{\underset{\sim}{\beta}}_1$ is unbiased, and

$$\mathrm{Var}[\hat{\underset{\sim}{\beta}}_1] = \sigma^2 (X_1' X_1)^{-1}.$$

Consequently, by design selection, we can influence the variances and covariances of $\hat{\underset{\sim}{\beta}}_1$. Several criteria for the selection of designs with good variance properties have been proposed. The two that we shall be concerned with are:

1. D-optimality--minimize the generalized variance of $\hat{\underset{\sim}{\beta}}_1$

and 2. V-optimality--minimize the variance of $\hat{\eta}_1(\underset{\sim}{x})$ averaged over the region of interest.

D-optimality has been extensively investigated (see St. John and Draper (1975) for a review of D-optimality). Since the generalized variance of $\hat{\underset{\sim}{\beta}}_1$ is

$$|\sigma^2 (X_1' X_1)^{-1}|,$$

designs that maximize

$$|X_1' X_1| \qquad (1.2.1)$$

are referred to as D-optimal for the lower order model.

The average variance of $\hat{\eta}_1(\underset{\sim}{x})$ can be expressed as

$$\Omega \int_R \mathrm{Var}[\hat{\eta}_1(\underset{\sim}{x})] \; dx_1 \cdot dx_2 \cdots dx_k$$
$$= \Omega\, \sigma^2 \int_R \underset{\sim}{x}_1' (X_1' X_1)^{-1} \underset{\sim}{x}_1 \; dx_1 \cdot dx_2 \cdots dx_k$$

$$= \sigma^2 \, \mathrm{Tr}\left\{ (X_1' X_1)^{-1} \, \Omega \int_R \underset{\sim}{x}_1 \, \underset{\sim}{x}_1' \quad dx_1 \cdot dx_2 \cdots dx_k \right\}$$

$$= \sigma^2 \, \mathrm{Tr}[(X_1' X_1)^{-1} M_{11}],$$

where $M_{11} = \Omega \int_R \underset{\sim}{x}_1 \, \underset{\sim}{x}_1' \quad dx_1 \cdot dx_2 \cdots dx_k$

and $\Omega^{-1} = \int_R dx_1 \cdot dx_2 \cdots dx_k$.

The average variance of $\hat{\eta}_1(\underset{\sim}{x})$ can be increased by increasing σ^2 and decreased by increasing n. Consequently, a standardized measure of a design's average variance characteristics for $\hat{\eta}_1(\underset{\sim}{x})$ is

$$V_1 = n/\sigma^2 \cdot \Omega \int_R \mathrm{Var}[\hat{\eta}_1(\underset{\sim}{x})] \quad dx_1 \cdot dx_2 \cdots dx_k$$

$$= n \, \mathrm{Tr}[(X_1' X_1)^{-1} M_{11}]. \qquad (1.2.2)$$

We will refer to a design as <u>V-optimal for the lower order model</u> if it minimizes V_1.

Now if the proposed model is not the true model, then the variance characteristics for the higher order model can be very important. The two measures of the design's variance properties for the higher order model that we will examine are:

1. $|X' X|$ (1.2.3)

and 2. $V_2 = n \, \mathrm{Tr}[(X' X)^{-1} M]$ (1.2.4)

where $X = [X_1 : X_2]$

$$\text{and} \quad M = \Omega \int_R \begin{bmatrix} \underset{\sim}{x}_1 \\ \underset{\sim}{x}_2 \end{bmatrix} \cdot [\underset{\sim}{x}_1', \underset{\sim}{x}_2'] \, dx_1 \cdot dx_2 \cdots dx_k .$$

The first of these properties, (1.2.3), is analogous to (1.2.1). Essentially, designs that maximize (1.2.3) minimize the generalized variance of the least squares estimate,

$$\hat{\underset{\sim}{\beta}} = (X' X)^{-1} X' \underset{\sim}{y},$$

for

$$\underset{\sim}{\beta}' = (\underset{\sim}{\beta}_1', \underset{\sim}{\beta}_2').$$

These designs will be referred to as D-Optimal for the higher order model. Likewise, the second property, V_2, is analogous to V_1; designs that minimize V_2 minimize the variance of

$$\hat{\eta}(\underset{\sim}{x}) = [\underset{\sim}{x}_1', \underset{\sim}{x}_2'] \, \hat{\underset{\sim}{\beta}}$$

averaged over the region of interest. These designs will be referred to as V-optimal for the higher order model.

Notice that, although D-optimality and V-optimality are both variance oriented criteria, in general, they are not equivalent. Essentially, D-optimality selects designs that have good variance properties for $\hat{\underset{\sim}{\beta}}_1$ (or $\hat{\underset{\sim}{\beta}}$) while V-optimality selects designs that have good average variance properties for $\hat{\eta}_1(\underset{\sim}{x})$ (or $\hat{\eta}(\underset{\sim}{x})$). Which of these variance criteria is preferred would depend upon the purpose of the experiment.

The fitted bias properties of a design can also be a dominant consideration when the proposed model is not the true model. In particular, this can occur when the higher order parameters provide a significant contribution to the response relationship, yet because of sample size limitations or simplicity, we still intend to fit the lower order model. In this case, $\hat{\beta}_1$ is no longer unbiased. Its expectation is given by (1.1.6).

One measure of the fitted bias properties of a design is the <u>average squared bias</u>

$$B = \Omega \int_R \{E[\hat{\eta}_1(\underset{\sim}{x})] - \eta(\underset{\sim}{x})\}^2 \, dx_1 \cdot dx_2 \cdots dx_k .$$

Box and Draper (1959) showed that

$$B = \underset{\sim}{\beta}_2' H \underset{\sim}{\beta}_2 \qquad (1.2.5)$$

where $H = M_{22} - M_{21} M_{11}^{-1} M_{12} + (A - M_{11}^{-1} M_{12})' M_{11} (A - M_{11}^{-1} M_{12})$

and $M_{ij} = \Omega \int_R \underset{\sim}{x}_i \underset{\sim}{x}_j' \, dx_1 \cdot dx_2 \cdots dx_k$, $i = 1, 2;\ j = 1, 2.$

They were also able to show that a necessary and sufficient condition for a design to <u>minimize</u> B is that

$$A = M_{11}^{-1} M_{12}.$$

Designs satisfying this condition are referred to as <u>minimum bias designs</u>.

The third property likely to influence our selection of an experimental design is the ability of a design to detect model inadequacy. This can be a dominant consideration in pilot experiments conducted for the explicit purpose of verifying an assumed model. We will assume that a lack of fit test will be used, and hence, we will use the non-centrality parameter of this test,

$$\lambda = \sigma^{-2} \underset{\sim}{\beta}_2' L \underset{\sim}{\beta}_2,$$

as a measure of a design's ability to detect model inadequacy.

Under this interpretation, a design is good for the detection of the higher order parameters if it maximizes the non-centrality parameter λ. If the $\underset{\sim}{\beta}_2$-space is one-dimensional, L is a scalar and λ is maximized by maximizing the scalar L. However, if the $\underset{\sim}{\beta}_2$-space is not one-dimensional, L is no longer a scalar, and λ cannot be maximized without knowing $\underset{\sim}{\beta}_2$.

To get around this difficulty, Folks (1958) assumed that $\underset{\sim}{\beta}_2$ was located on a particular line in the $\underset{\sim}{\beta}_2$-space, i.e.,

$$\underset{\sim}{\beta}_2 = (\text{constant})\ \underset{\sim}{1},$$

where $\underset{\sim}{1}$ is a vector of all ones. Under this assumption, he maximized the scalar $\underset{\sim}{1}' L \underset{\sim}{1}$.

The criterion

$$\underset{D \,\varepsilon\, \Delta}{\text{Max}} \; |L| \tag{1.2.6}$$

has been investigated by Atkinson (1972, 1973) for selecting designs that have good properties for the detection of lack of fit. We will refer to this criterion as <u>$|L|$-optimality</u>. Since

$$\text{Var}[\hat{\underset{\sim}{\beta}}_2] = \sigma^2 L^{-1}$$

where $\hat{\underset{\sim}{\beta}}_2$ is the least squares estimator for $\underset{\sim}{\beta}_2$, $|L|$-optimality selects designs that minimize the generalized variance of $\hat{\underset{\sim}{\beta}}_2$. Consequently, it has also been investigated for selecting designs that efficiently estimate subsets of parameters (see Kiefer (1959), and Hill and Hunter (1974)).

In terms of λ, since the volume of the hyperellipsoid in the $\underset{\sim}{\beta}_2$-space defined by $\lambda \leq \delta$ is simply

$$(\text{constant})\cdot|L|^{-\frac{1}{2}}$$

criterion (1.2.6) selects designs that minimize the volume of this hyperellipsoid for any $\delta > 0$. In this sense, $|L|$-optimality selects designs with tight, closed power contours. Note that this criterion does require $\underset{\sim}{\beta}_2$ to be estimable, or equivalently it requires the λ-contours to be closed. Because of operational constraints, this may not be feasible. Furthermore, as pointed out by Box and Draper (1959), it is possible for a design to have excellent overall lack of fit power properties without having closed power contours.

Another approach to the problem of maximizing λ without knowing $\underset{\sim}{\beta}_2$ is to assume that $\underset{\sim}{\beta}_2$ is a random vector and maximize the expected value of λ. If $\underset{\sim}{\beta}_2$ is a random vector,

$$E[\lambda] = \mathrm{Tr}\{L\ E[\underset{\sim}{\beta}_2\ \underset{\sim}{\beta}_2']\}. \tag{1.2.7}$$

Consequently, this approach selects designs that maximize (1.2.7). Note that this criterion does not require us to completely specify the underlying $\underset{\sim}{\beta}_2$-distribution. It is only necessary to evaluate $E[\underset{\sim}{\beta}_2\ \underset{\sim}{\beta}_2']$. Furthermore, it does not require $\underset{\sim}{\beta}_2$ to be estimable (L to be non-singular).

Of course, a possible weakness of this criterion is the motivation of an underlying $\underset{\sim}{\beta}_2$-distribution. However, an interesting and appealing example of this approach was given by Box and Draper (1959). They assumed that the orientation of the response surface with respect to the coordinate axes was a random variable, such that all possible orientations were equally likely. Equivalently, one could assume that the orientation of the coordinate axes with respect to the response surface is a random variable with all orientations equally likely. Under this assumption, Box and Draper obtained $E[\underset{\sim}{\beta}_2 \underset{\sim}{\beta}_2']$ by rotating the coordinate axes through an angle θ and averaging $\underset{\sim}{\beta}_2 \underset{\sim}{\beta}_2'$ over all θ.

As previously stated, we are sometimes justified in giving primary consideration to one of the three design properties--variance, fitted bias or power. Frequently, however, we would like to select designs that are good for a combined measure of these characteristics. In this spirit, Box and Draper (1959) investigated the selection of designs that minimize the <u>integrated expected mean squared error of the response surface</u>,

$$J = n/\sigma^2 \cdot \Omega \int_R E\{\hat{\eta}_1(\underset{\sim}{x}) - \eta(\underset{\sim}{x})\}^2 \; dx_1 \cdot dx_2 \cdots dx_k \; . \qquad (1.2.8)$$

This is sometimes referred to as <u>J-optimality</u>. This criterion appears to measure the combined variance and fitted bias properties of a design.

Under the assumption that the lower order model is used to fit the response surface, they showed that

$$J = V_1 + n/\sigma^2 \cdot B,$$

where V_1 and B are given by (1.2.2) and (1.2.5) respectively. We cannot minimize J without knowing $\underset{\sim}{\beta}_2$ unless the $\underset{\sim}{\beta}_2$-space is one-dimensional. To get around this difficulty, Box and Draper minimized the rotational average of J, the technique previously described for the maximization of λ.

From their investigation, they concluded that designs that minimize the rotational average of J were "nearly" minimum bias. From this they recommended the use of minimum bias designs.

This recommendation was disputed by Stigler (1971). He points out that their conclusion that minimum bias designs are nearly J-optimal stems from their concept of an operability region; this is the region in which it is possible to obtain observations. Box and Draper assumed that the region of interest was completely contained within the operability region. Their conclusion that minimum bias designs are nearly J-optimal appears to depend upon allowing the operability region to extend indefinitely beyond R. If the operability region and the region of interest are the same (as we shall assume in this investigation), it is not clear that minimum bias designs are nearly J-optimal. Stigler concludes that the variance properties of a design should not be ignored in favor of the design's fitted bias properties.

As an alternative, Stigler proposed the use of C-restricted D-optimality. A design is <u>C-restricted</u> <u>D-optimal</u> if it maximizes $|X_1' X_1|$ subject to the restriction that

$$|X_1' X_1| \leq C \cdot |X' X|, \qquad (1.2.9)$$

for some positive constant C specified by the experimenter. Since

$$|X' X| = |X_1' X_1| \cdot |L|,$$

the restriction (1.2.9) can be written as

$$|L| \geq C^{-1}.$$

Although this criterion seems very appealing, it appears difficult to use. In general, it is not clear how to choose C, and once C is specified, not only is this criterion difficult to optimize, it may require an unpractical number of observations.

Furthermore, C-restricted D-optimality ignores the fitted bias properties of a design. Although this may seem justified if C-restricted D-optimal designs have very good power for the detection of lack of fit, it should be emphasized that power properties are "average" properties. Although the power of the test may be .9, there is still a .1 probability of not detecting the higher order parameters, and the experimenter should be careful that, if these parameters are not detected, the fitted bias is not too large.

J-optimality and C-restricted D-optimality represent two approaches to selecting designs that have good variance, fitted bias and power properties. In general, this task is complicated by the fact that the relative importance of these three properties varies depending upon the purpose of the experiment and the experimenter's confidence in the validity of his proposed model.

1.2.2. The Seriousness of $\underset{\sim}{\beta}_2$

In this investigation, we will be concerned with the development and examination of criteria for the selection of designs that are good for detecting "model inadequacy." Although we will assume that the experimenter intends to use a lack of fit test to detect the presence of a higher order model, we will not equate "model inadequacy" with large values of the non-centrality parameter, λ. Instead we will allow the experimenter to define the significance of the additional higher order parameters, $\underset{\sim}{\beta}_2$, by the quadratic form

$$\tau = \sigma^{-2} \underset{\sim}{\beta}_2' T \underset{\sim}{\beta}_2 \qquad (1.2.10)$$

where T is a specified positive definite matrix. We will assume that the significance of $\underset{\sim}{\beta}_2$ is a monotone increasing function of τ. In order to emphasize the distinction between λ and τ and to avoid confusion with "statistical significance," we will use the phrase serious $\underset{\sim}{\beta}_2$ to refer to significant values of τ.

This definition of model inadequacy seems well motivated. In fact, there are two choices for τ that seem applicable for many experiments.

The first choice is motivated for judging whether the true response surface differs significantly from a class of models, such as the class of all second order polynomials. The primary difficulty in developing a definition for τ that provides a consistent mathematical interpretation of the degree that a surface departs from a class of models stems from the divergent interests of different experiments. For example, if we exhibit ten different curves and ask several experimenters to rank these curves according to their degree of departure from the class of straight lines, we would not be surprised if we obtained several different rankings. For his particular purpose, one experimenter may view convex curvature as more serious than concave while another may view curvature at the origin as more serious than curvature at the boundary of his experimental region.

For our purpose, we will judge the departure of a surface from a class of models by the average squared deviation of the true model from the best fitting model of the assumed class of models. Specifically, <u>the departure of the true surface $\eta(\underset{\sim}{x})$ from a class of models</u> $\mathcal{M}$ is defined to be

$$\tau_1 = \sigma^{-2}\,\Omega \int_R \{\eta_1^*(\underset{\sim}{x}) - \eta(\underset{\sim}{x})\}^2 \; dx_1 \cdot dx_2 \cdots dx_k \qquad (1.2.11)$$

where $\eta_1^*(\underset{\sim}{x})$ is the response at the point $\underset{\sim}{x}$ for the model in $\mathcal{M}$ that minimizes τ_1.

In this investigation, $\mathcal{M}$ will consist of all polynomials of degree d_1, and $\eta(\underset{\sim}{x})$ will be a polynomial of degree d_2. A geometric interpretation of τ_1 is illustrated in Figure 1.1 for $k = 1$, $d_1 = 1$ and $d_2 = 4$. In this figure, the region of interest is the interval $[-1, 1]$, and τ_1 measures the average squared deviation of the true fourth order polynomial from the best first order polynomial.

Box and Draper (1963) showed that

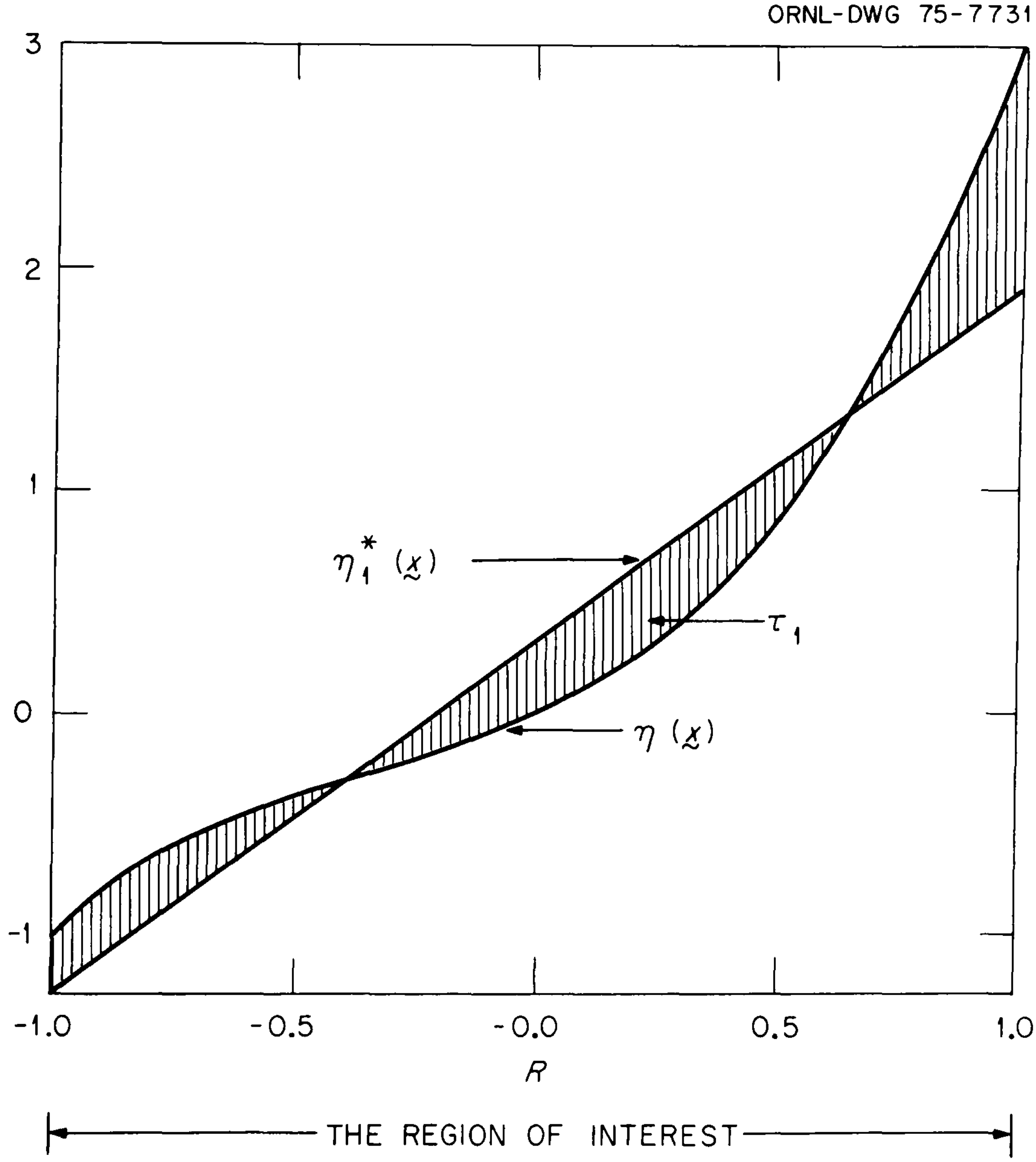

Figure 1.1. τ_1 for the Deviation of a Fourth Order Polynomial from its Best First Order Approximation

$$\tau_1 = \sigma^{-2} \underset{\sim}{\beta}_2' T_1 \underset{\sim}{\beta}_2 \tag{1.2.12}$$

$$\text{where } T_1 = [M_{22} - M_{21} M_{11}^{-1} M_{12}].$$

Thus for experiments in which the question of the degree of departure of a response surface from a class of models is important, a natural choice for T is T_1.

In other experiments, the experimenter is only indirectly interested in the departure of the surface from an assumed class of models. He is primarily interested in adequately estimating the response surface, and he considers departures from the assumed model to be serious only to the extent that they increase the departure of the <u>fitted</u> model from the true surface.

For these experiments, we saw that a measure of the departure of the fitted model from the true surface is the average mean squared error J, defined by (1.2.8). The $\underset{\sim}{\beta}_2$-dependent part of J is the average squared bias B, given by (1.2.5). Thus an appropriate definition for τ in this case is

$$\begin{aligned} \tau_2 &= \sigma^{-2}\,\Omega \int_R \{E[\hat{\eta}_1(\underset{\sim}{x})] - \eta(\underset{\sim}{x})\}^2 \; dx_1 \cdot dx_2 \cdots dx_k \\ &= \sigma^{-2} \underset{\sim}{\beta}_2' T_2 \underset{\sim}{\beta}_2 \end{aligned}$$

$$\text{where } T_2 = [A' M_{11} A - M_{21} A - A' M_{12} + M_{22}]. \tag{1.2.13}$$

Thus, T_2 is another choice for T.

Note that the seriousness associated with $\underset{\sim}{\beta}_2$ as measured by τ_2 depends upon the design as well as on $\underset{\sim}{\beta}_2$ itself and the region moments, M_{ij}. This reflects the fact that, under the philosophy that leads to the choice of τ_2, $\underset{\sim}{\beta}_2$ is "bad" only to the extent that it increases B, the departure of the expected fitted surface from the true surface. For one design the value of B associated with $\underset{\sim}{\beta}_2$ might be quite acceptable, while for another, the same $\underset{\sim}{\beta}_2$ might be completely unacceptable. This is in contrast to the choice of τ_1 in (1.2.12) where the seriousness associated with $\underset{\sim}{\beta}_2$ is unaffected by the design.

In addition to their natural motivations, we will show in Chapter II that these definitions for the seriousness of $\underset{\sim}{\beta}_2$ are "invariant" to model parameterization. Parameterization invariance is necessary to ensure a consistent definition for the seriousness of $\underset{\sim}{\beta}_2$.

1.2.3. The Scope of This Investigation

In this investigation, we will generally be concerned with the problem of selecting an experimental design when the proposed model is

$$\eta_1(\underset{\sim}{x}) = \underset{\sim}{x}_1' \underset{\sim}{\beta}_1$$

while the correct model may be

$$\eta(\underset{\sim}{x}) = \underset{\sim}{x}_1' \underset{\sim}{\beta}_1 + \underset{\sim}{x}_2' \underset{\sim}{\beta}_2 .$$

This problem will be approached using the concept, developed in the previous section, of allowing the experimenter to define the "seriousness of $\underset{\sim}{\beta}_2$" by the quadratic form

$$\tau = \sigma^{-2} \underset{\sim}{\beta}_2' \mathrm{T} \underset{\sim}{\beta}_2 .$$

In the next chapter, we will develop a family of criteria for design selection, the "$\Lambda(T)$ criteria." This development will emphasize the selection of designs that are good for detecting serious $\underset{\sim}{\beta}_2$. This is one way that the experimenter has of protecting against the possible inadequacy of his proposed model. However, if the experimenter's measure for the seriousness of $\underset{\sim}{\beta}_2$, τ, is affected by design selection, he can also protect against model inadequacy by minimizing τ. Consequently, we will also develop criteria to favor designs that tend to minimize τ while maintaining "reasonable" properties for the detection of model inadequacy.

Primary emphasis will be given to the use of τ_1 and τ_2 for measuring the seriousness of $\underset{\sim}{\beta}_2$ in polynomial regression models. In addition to developing the $\Lambda(T)$ criteria in Chapter II, we will also show that, for τ_1 and τ_2, these criteria are invariant to non-singular linear transformations of the region of interest. Therefore, the results in the subsequent chapters, where we restrict the region of interest to the k-dimensional cube or the unit sphere, apply also to any cuboidal or ellipsoidal region of interest.

In Chapter III, we will construct $\Lambda(T_1)$-optimal designs for cuboidal regions of interest and compare them with D-optimal designs for both the lower and higher order models, minimum bias designs and designs that maximize $|L|$. In particular, we will consider the following cases:

1. one-factor, first order vs. second order polynomial models and $n = 5, 9$;

2. one-factor, second order vs. third order polynomial models and $n = 6, 10$;

3. two-factor, first order vs. second order polynomial models and $n = 6$;

and 4. two-factor, second order vs. third order polynomial models and $n = 10$.

In Chapter IV, we will focus special attention on one particular member of the family of $\Lambda(T_1)$ criteria, the $\Lambda_2(T_1)$ criterion. We will obtain $\Lambda_2(T_1)$-optimal designs in a cuboidal region of interest for the following cases:

1. one-factor, first order vs. second order polynomial models and $n = 3 - 20$;

2. one-factor, second order vs. third order polynomial models and $n = 4 - 20$;

3. two-factor, first order vs. second order polynomial models and $n = 4 - 10$;

and 4. two-factor, second order vs. third order polynomial models and $n = 8 - 15$.

In Chapter V, we shall turn our attention to the $\Lambda(T_2)$ criteria, which are based on the use of τ_2 rather than τ_1 to define the seriousness of $\underset{\sim}{\beta}_2$. The presentation of Chapter V closely parallels that of Chapter III.

In Chapter VI, we give special attention to the $\Lambda_2(T_2,\frac{1}{2})$ criterion which is one of the criteria examined in Chapter V. The same cases that were considered for the $\Lambda_2(T_1)$ criterion in Chapter

IV will be considered here. For comparison, the $\Lambda_2(T_2,\frac{1}{2})$-optimal designs for two-factor, second order vs. third order polynomial models, n = 7 - 10, 12 - 14 and a circular region of interest will also be presented in Chapter VI. Power curves for the one-factor $\Lambda_2(T_1)$-optimal and $\Lambda_2(T_2,\frac{1}{2})$-optimal designs are also presented in Chapters IV and VI, respectively. They are provided to assist the experimenter in selecting an appropriate α-level and sample size for the lack of fit test.

II. DESIGN CRITERIA FOR THE DETECTION OF MODEL INADEQUACY

2.1. The $\Lambda(T)$ Criteria

In this section, we will propose several criteria for the selection of an experimental design, the $\Lambda(T)$ criteria. They are developed for the detection of model inadequacy. Their motivation is based upon the following assumptions:

1. the true surface has the form

$$\eta(\underset{\sim}{x}) = \underset{\sim}{x}_1' \underset{\sim}{\beta}_1 + \underset{\sim}{x}_2' \underset{\sim}{\beta}_2, \tag{2.1.1}$$

2. the proposed model, i.e., the one we anticipate fitting, has the form

$$\eta_1(\underset{\sim}{x}) = \underset{\sim}{x}_1' \underset{\sim}{\beta}_1, \tag{2.1.2}$$

3. a lack of fit test will be used to test the adequacy of the proposed model, (2.1.3)

and 4. the seriousness associated with $\underset{\sim}{\beta}_2$ is a monotone increasing function of

$$\tau = \sigma^{-2} \underset{\sim}{\beta}_2' T \underset{\sim}{\beta}_2 \tag{2.1.4}$$

where T is specified by the experimenter (see Section 1.2.2 for examples of T).

We shall occasionally refer to the model in assumption (2.1.1) as the <u>higher order model</u>, and the model in assumption (2.1.2) as the <u>lower order model</u>.

Assumption (2.1.3) provides us with a measure of the ability of a design to "detect" $\underset{\sim}{\beta}_2$, namely the non-centrality parameter

$$\lambda = \sigma^{-2} \underset{\sim}{\beta}_2' L \underset{\sim}{\beta}_2.$$

Geometrically, λ defines contours of equal power in the $\underset{\sim}{\beta}_2$-space. These will be referred to as the <u>λ-contours</u>. The region of minimum power defined by $\lambda = 0$ will be referred to as the <u>region of non-detectable bias</u>. This region is the $\underset{\sim}{\beta}_2$-subspace spanned by the orthonormal eigenvectors associated with the null eigenvalues of the lack of fit matrix, L. Hence if L is singular ($\underset{\sim}{\beta}_2$ is non-estimable), the region of non-detectable bias can contain points other than the origin. Not only does the lack of fit matrix determine the region of non-detectable bias, it also determines the general shape and orientation of the contours of equal power. Therefore, if the experimenter intends to use a lack of fit test, the structure of the lack of fit matrix can be important.

<u>2.1.1. An Example of the Effect of Design Selection Upon λ.</u>

To illustrate these ideas, suppose that the lower order model is a first order polynomial,

$$\eta_1(x) = \beta_0 + x\,\beta_1, \tag{2.1.5}$$

while the true surface is a third order polynomial,

$$\eta(x) = \beta_0 + x\,\beta_1 + x^2\,\beta_{11} + x^3\,\beta_{111}. \tag{2.1.6}$$

For this case, the $\underset{\sim}{\beta}_2$-space is two-dimensional with

$$\underset{\sim}{\beta}_2' = (\beta_{11}, \beta_{111}). \tag{2.1.7}$$

Now it is well known that, in order to fit a one-factor polynomial of degree d, the experiment must be conducted at no fewer than d + 1 distinct levels of the independent variable. Consequently, in order to fit the first order polynomial, we need observations at no fewer than two points, and in order to fit the third order polynomial, we need observations at no fewer than four points. However, if our experiment is conducted at only three distinct points, we can fit the first order model and still conduct a test for lack of fit, although the lack of fit matrix would be singular.

For example, consider the following class of designs defined by

$$D = \begin{bmatrix} \underset{\sim}{1} \\ \hline -\underset{\sim}{1} \\ \hline a\,\underset{\sim}{1} \\ \hline -a\,\underset{\sim}{1} \end{bmatrix} \begin{matrix} \}\, n_1 \text{ points at } 1 \\ \}\, n_1 \text{ points at } -1 \\ \}\, n_2 \text{ points at } a \\ \}\, n_2 \text{ points at } -a \end{matrix}$$

$$\text{with } 0 \leq a < 1 \quad \text{and} \quad n = 2(n_1 + n_2).$$

For these designs

$$L = 4n_1n_2(1-a^2)^2\, n^{-1} \begin{bmatrix} 1 & 0 \\ 0 & \dfrac{a^2 n}{2(a^2 n_2 + n_1)} \end{bmatrix}.$$

If $n_1 \neq 0$, $n_2 \neq 0$ and $a \neq 0$, this is a four-point design, and the lack of fit matrix is non-singular. Hence $\underset{\sim}{\beta}_2$ is estimable, or equivalently, L is non-singular, and we can fit the higher order model as well as conduct a test for lack of fit. If $n_1 \neq 0$, $n_2 \neq 0$ and $a = 0$, this is a three-point design with a singular lack of fit matrix. With this design, we cannot fit the higher order model, but, we can conduct a test for lack of fit. Finally if $n_1 = 0$ or $n_2 = 0$, this is a two-point design and $L = 0$. Hence although we can fit the lower order model with this design, we cannot conduct a test for lack of fit.

The $\underset{\sim}{\beta}_2$-space for the three and four-point designs are illustrated in Figure 2.1. Notice that for the four-point design, the region of non-detectable bias consists of only the point $\underset{\sim}{\beta}_2 = \underset{\sim}{0}$. This reflects the fact that L is non-singular. For the three-point design, the region of non-detectable bias is an entire line, the β_{111}/σ (cubic) axis, reflecting the fact that L is of rank one. Also note that the power contours for the four-point design are closed while the power contours for the three-point design parallel the region of non-detectable bias.

Since the power contours for the four-point design are closed and those for the three-point design are not, we might conclude that the four-point design has superior properties for the detection of lack of fit. However, in some ways, the power contours for the three-point design may be more desirable than those of the four-point design. This is illustrated in Figure 2.2 for $n_1 = n_2 = 1$. Notice that the three-point design is more sensitive to quadratic alternatives than the four-point design. Consequently, if we were more concerned about quadratic alternatives than cubic alternatives, we might prefer to use the three-point design.

This example was presented to emphasize the fact that by design selection we can control the general shape and tightness of the power contours, as well as the dimension of the region of non-detectable bias. However, we can also control the orientation of these contours.

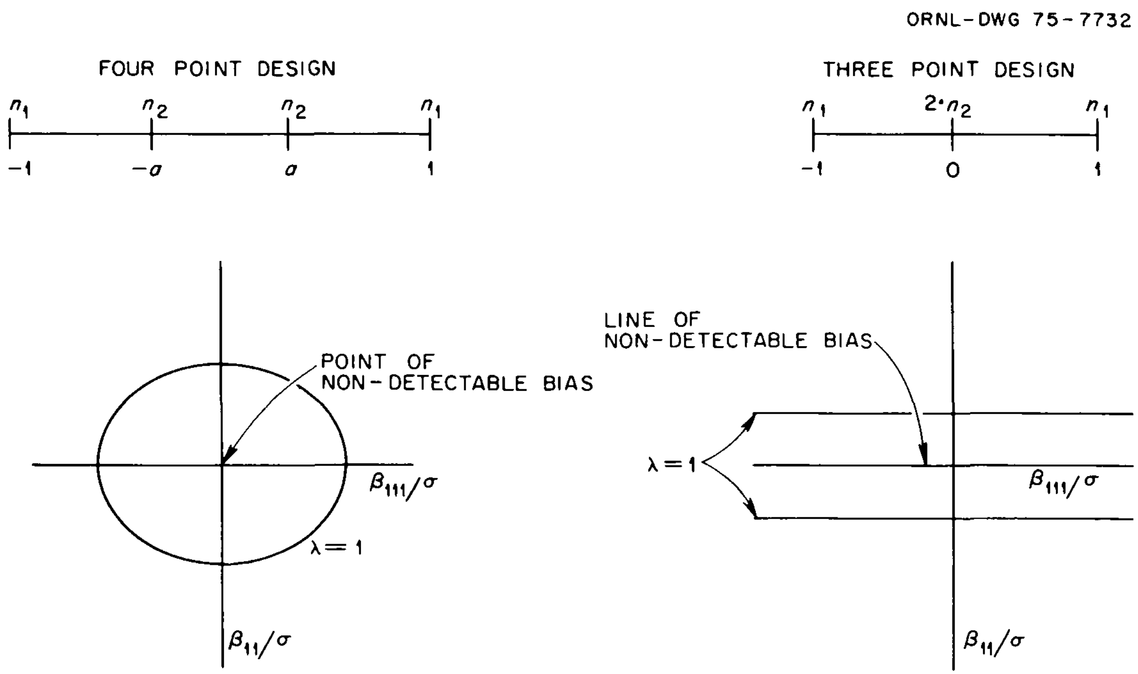

Figure 2.1. The $\underset{\sim}{\beta}_2$-Space for Three and Four Point Designs

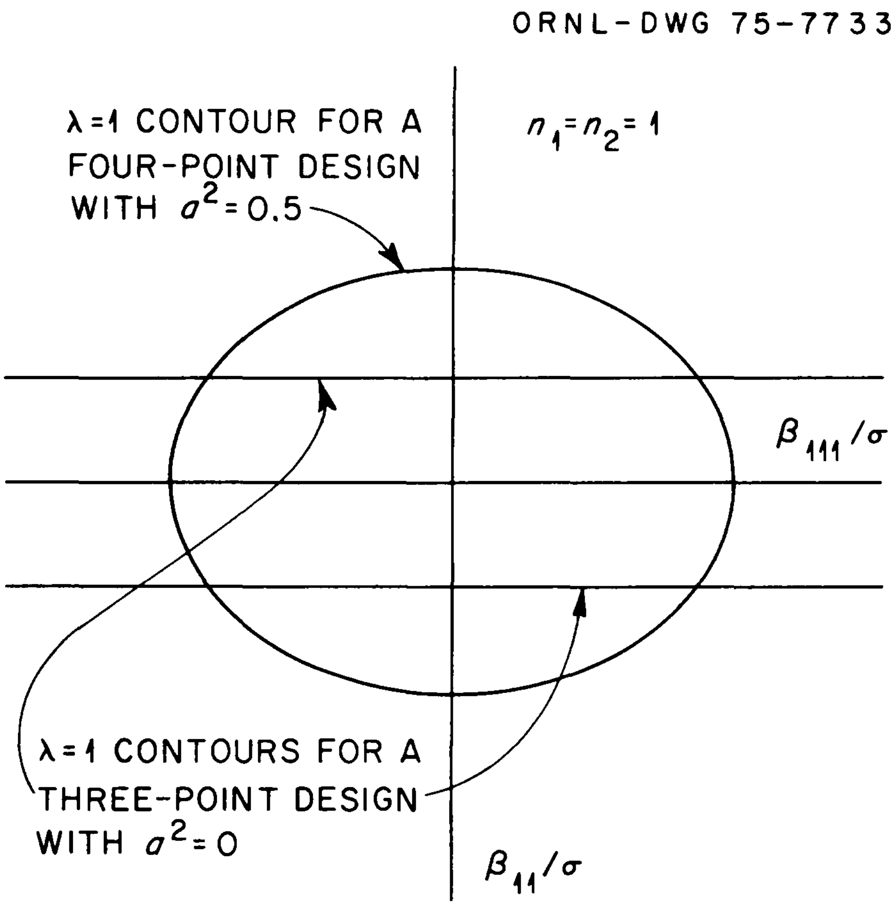

Figure 2.2. A Comparison of the Power Contours for Three and Four Point Designs

For example, consider the class of three-point designs with

$$D = \begin{bmatrix} \underset{\sim}{1} \\ \hdashline \underset{\sim}{-1} \\ \hdashline a\,\underset{\sim}{1} \end{bmatrix} \begin{matrix} \}\, n_1 \text{ points at } 1 \\ \}\, n_1 \text{ points at } -1 \\ \}\, 2n_2 \text{ points at } a \end{matrix}$$

where $-1 < a < 1$. For these designs,

$$L = \frac{4n_1n_2(1-a^2)^2}{n + a^2 2n_2} \begin{bmatrix} 1 & a \\ a & a^2 \end{bmatrix}.$$

We saw that, for $a = 0$, the power contours parallel the β_{111}/σ axis. However, as a moves between -1 and 1, the orientation of the power contours change. This is illustrated in Figure 2.3 for $a = 0$ and $a = .4$.

However, notice that for $a = 0$, the power contours are tighter to the line of non-detectable bias than for $a = .4$. Thus although we can control this orientation, in general, there is a tradeoff between the orientation and the tightness of the power contours.

The central question is: should we be concerned about power contour orientation? If we are not concerned about contour orientation, we would simply select the design with the "tightest" power contours. This is equivalent to selecting the design that maximizes the product of the non-zero eigenvalues of L.

For this investigation, we have assumed (assumption (2.1.4)) that the experimenter is able to measure the seriousness of alternatives by the quadratic form τ. This assumption provides us

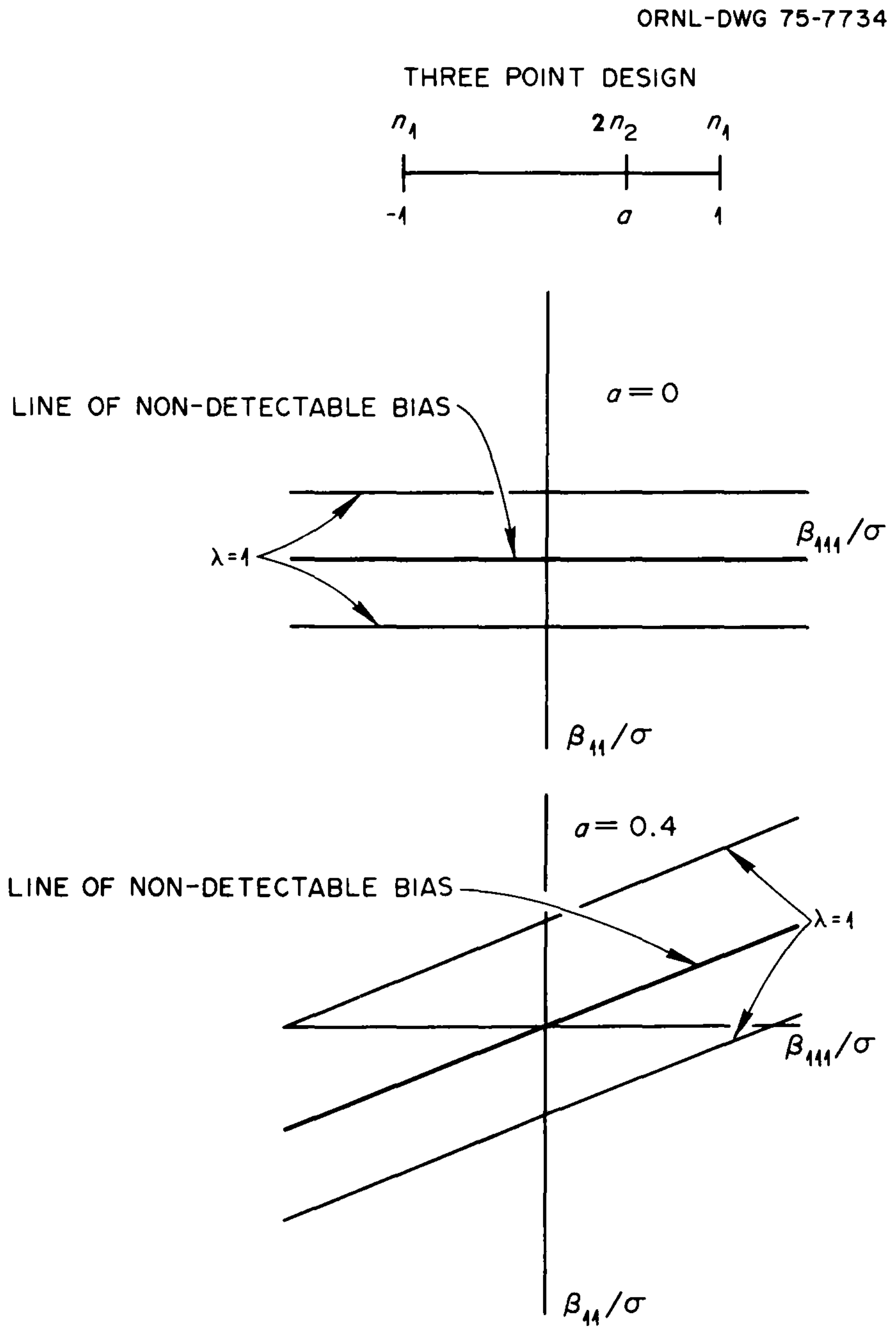

Figure 2.3. The Orientation of the λ-Contours for Three Point Designs with $a = 0$ and $a = .4$

with a means for judging the "goodness" of power contour orientation, as well as tightness.

2.1.2. $\Lambda_1(T)$-Optimality: A Mini-Max Criterion

In this section, we will examine several naturally suggested mini-max criteria. For this purpose, we will need the following theorem.

Theorem 2.1

Let $\underset{\sim}{\omega}' = (\omega_1, \omega_2, \ldots, \omega_r)$ be a r-dimensional real vector,

$\zeta_1 = \underset{\sim}{\omega}' Z_1 \underset{\sim}{\omega}$ be a positive semidefinite quadratic form,

$\zeta_2 = \underset{\sim}{\omega}' Z_2 \underset{\sim}{\omega}$ be a positive definite quadratic form,

and $\pi = \{\underset{\sim}{\omega} : \underset{\sim}{\omega}' Z_2 \underset{\sim}{\omega} = \delta, \delta > 0\}$

then

$$\underset{\underset{\sim}{\omega} \,\varepsilon\, \pi}{\mathrm{Min}} \zeta_1 = \delta \, Ch_{min}[Z_2^{-1} Z_1] \tag{2.1.8}$$

and

$$\underset{\underset{\sim}{\omega} \,\varepsilon\, \pi}{\mathrm{Max}} \zeta_1 = \delta \, Ch_{max}[Z_2^{-1} Z_1] \tag{2.1.9}$$

where $Ch_{min}[U]$ and $Ch_{max}[U]$ are the minimum and maximum characteristic roots of the matrix U, respectively.

Proof:

Since Z_2 is positive definite, it can be expressed as

$$Z_2 = Q' Z Q$$

where Q is an orthogonal matrix, i.e.,

$$Q' Q = I_r ,$$

and Z is a diagonal matrix with diagonal elements $z_1, z_2, \ldots, z_r$.

If $Z^{\frac{1}{2}}$ is a diagonal matrix with diagonal elements $\sqrt{z_1}, \sqrt{z_2}, \ldots, \sqrt{z_r}$ then the positive definite symmetric square root of Z_2 is

$$Z_2^{\frac{1}{2}} = Q' \, Z^{\frac{1}{2}} Q.$$

Notice that

$$Z_2 = Z_2^{\frac{1}{2}} Z_2^{\frac{1}{2}}, \text{ and } Z_2^{-1} = Z_2^{-\frac{1}{2}} Z_2^{-\frac{1}{2}}.$$

By the Rayleigh Principle (see Lancaster (1969)), the minimum value over the hypersphere defined by $\underset{\sim}{\omega}' \underset{\sim}{\omega} = \delta$ of any positive semidefinite quadratic form

$$\underset{\sim}{\omega}' \, U \, \underset{\sim}{\omega} \tag{2.1.10}$$

is simply $\delta \, Ch_{min}[U]$. Similarly the maximum value over this hypersphere for the quadratic form (2.1.10) is $\delta \, Ch_{max}[U]$. Thus, letting

$$\underset{\sim}{\gamma} = Z_2^{\frac{1}{2}} \underset{\sim}{\omega} \quad \text{and} \quad \pi_0 = \{\underset{\sim}{\gamma} : \underset{\sim}{\gamma}' \underset{\sim}{\gamma} = \delta\},$$

it follows that

$$\begin{aligned}
\underset{\underset{\sim}{\omega} \, \varepsilon \, \pi}{\text{Min}} \; \zeta_1 &= \underset{\underset{\sim}{\omega} \, \varepsilon \, \pi}{\text{Min}} \; \underset{\sim}{\omega}' \, Z_1 \, \underset{\sim}{\omega} \\
&= \underset{\underset{\sim}{\gamma} \, \varepsilon \, \pi_0}{\text{Min}} \; \underset{\sim}{\gamma}' \, Z_2^{-\frac{1}{2}} Z_1 \, Z_2^{-\frac{1}{2}} \underset{\sim}{\gamma} \\
&= \delta \, Ch_{min}[Z_2^{-\frac{1}{2}} Z_1 \, Z_2^{-\frac{1}{2}}] \\
&= \delta \, Ch_{min}[Z_2^{-1} \, Z_1],
\end{aligned}$$

and similarly,

$$\begin{aligned}
\underset{\underset{\sim}{\omega} \, \varepsilon \, \pi}{\text{Max}} \; \zeta_1 &= \underset{\underset{\sim}{\omega} \, \varepsilon \, \pi}{\text{Max}} \; \underset{\sim}{\omega}' \, Z_1 \, \underset{\sim}{\omega} \\
&= \underset{\underset{\sim}{\gamma} \, \varepsilon \, \pi_0}{\text{Max}} \; \underset{\sim}{\gamma}' \, Z_2^{-\frac{1}{2}} Z_1 \, Z_2^{-\frac{1}{2}} \underset{\sim}{\gamma} \\
&= \delta \, Ch_{max}[Z_2^{-\frac{1}{2}} Z_1 \, Z_2^{-\frac{1}{2}}]
\end{aligned}$$

$$= \delta \ Ch_{max}[Z_2^{-1} Z_1]$$

Q.E.D.

2.1.2.1. Maximize the Minimum Value of λ.--We have assumed that the "seriousness of $\underset{\sim}{\beta}_2$" is a monotone increasing function of

$$\tau = \sigma^{-2} \underset{\sim}{\beta}_2' T \underset{\sim}{\beta}_2 .$$

Conceptually, then, we suppose that the experimenter envisions some positive constant δ such that if $\tau \geq \delta$ then the seriousness associated with $\underset{\sim}{\beta}_2$ is unacceptable. We will refer to the region Φ defined by

$$\Phi = \{\underset{\sim}{\beta}_2 : \tau \geq \delta, \ \delta > 0\}$$

as the <u>region</u> <u>of</u> <u>unacceptably</u> <u>serious</u> $\underset{\sim}{\beta}_2$. One criterion which immediately comes to mind is to maximize the non-centrality parameter of the lack of fit test for "unacceptably serious $\underset{\sim}{\beta}_2$." Specifically, let us select the design in the class of permissible designs Δ that maximizes

$$\underset{\underset{\sim}{\beta}_2 \, \varepsilon \, \Phi}{\text{Min}} \ \lambda \quad . \qquad (2.1.11)$$

Before obtaining an analytical characterization of this criterion, it is useful to examine its geometric interpretation for a one-dimensional $\underset{\sim}{\beta}_2$-space (see Figure 2.4). For a one-dimensional $\underset{\sim}{\beta}_2$-space, the lack of fit and T matrices are scalars. Therefore, we can represent the λ and τ functions for any design $D \ \varepsilon \ \Delta$ as

$$\lambda_D = \sigma^{-2} \beta_2^2 L_D$$

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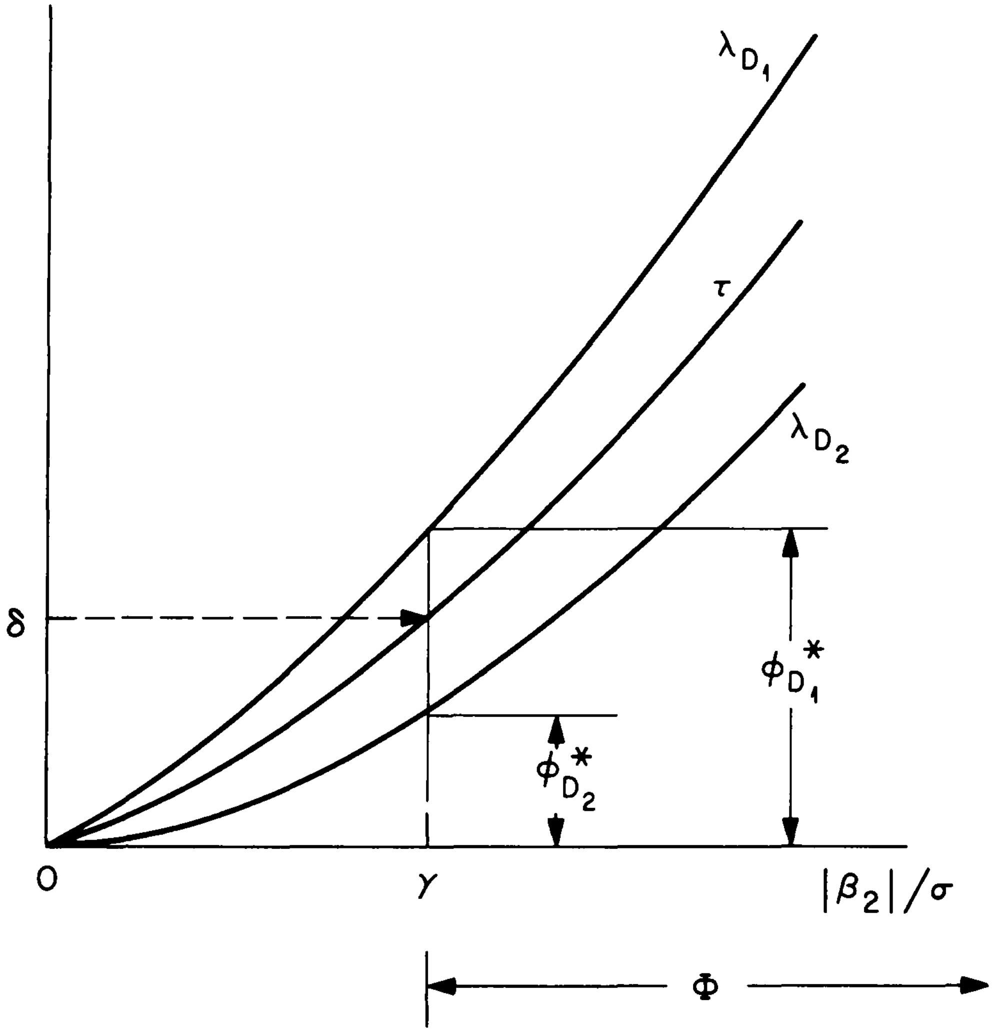

Figure 2.4. $\Lambda_1(T)$-Optimality: A Geometric Interpretation of Maximizing the Minimum Value of λ in the Region of Unacceptably Serious β_2, Φ, when τ is not Influenced by the Design

$$\text{and } \tau_D = \sigma^{-2} \beta_2^2 T_D \quad .$$

The region of unacceptably serious β_2, Φ, is then defined simply by the inequality

$$|\beta_2| / \sigma \geq \gamma_D,$$

$$\text{where } \gamma_D = (\delta / T_D)^{\frac{1}{2}} .$$

The "D" subscripts are added to emphasize that not only is the power of the lack of fit test design dependent, but the seriousness of β_2, and hence the region Φ, may also depend upon the design.

Now since τ and λ are monotone increasing functions of

$$|\beta_2| / \sigma,$$

the minimum value of λ will always occur at the boundary of the region Φ; namely, the minimum value of λ_D for $\beta_2 \varepsilon \Phi$ is

$$\phi_D^* = \gamma_D^2 L_D .$$

Notice that if the seriousness of β_2, as measured by τ, is not influenced by the design, γ_D is simply a constant, γ. Consequently, in this case, the design that maximizes the minimum value of λ for $\beta_2 \varepsilon \Phi$ is simply the design that maximizes L_D. When τ is design independent, the optimum design will always have the highest λ-function. This is illustrated in Figure 2.4; since

$$\phi_{D_1}^* > \phi_{D_2}^* ,$$

this criterion would select design D_1 over design D_2.

On the other hand, if τ is influenced by the design, the selection of a design is more complex (see Figure 2.5). If an experimenter decides to select a design which maximizes the power without regard for the magnitude of τ_D, he may obtain a design with excellent power properties but with an extremely large value for τ_D. On the other extreme, if an experimenter decides to select a design that minimizes τ_D, he may obtain a design with weak power properties.

Unless we are willing to accept one of these two extreme positions, and for some experiments we might, we should look for designs that provide a comfortable tradeoff between maximizing λ_D and minimizing τ_D. Criterion (2.1.11) provides such a tradeoff. This is illustrated in Figure 2.5. Although design D_1 has uniformly larger power than design D_2, it also has a uniformly larger τ-function. However design D_2, by sacrificing some power, has significantly reduced τ_D. Since

$$\phi^*_{D_2} > \phi^*_{D_1} ,$$

criterion (2.1.11) would select design D_2 over design D_1.

Now let us examine the analytical characterization of criterion (2.1.11) for a general $\underset{\sim}{\beta}_2$-space, i.e.,

$$\underset{D \,\varepsilon\, \Delta}{\text{Max}} \quad \underset{\underset{\sim}{\beta}_2 \,\varepsilon\, \Phi}{\text{Min}} \; \lambda \; . \tag{2.1.12}$$

For the case just examined, we observed that the minimum value of λ_D for unacceptably serious β_2 occurs at the boundary of the region Φ, namely at γ_D. Now suppose that the $\underset{\sim}{\beta}_2$-space is multi-dimensional and that the minimum value of λ is

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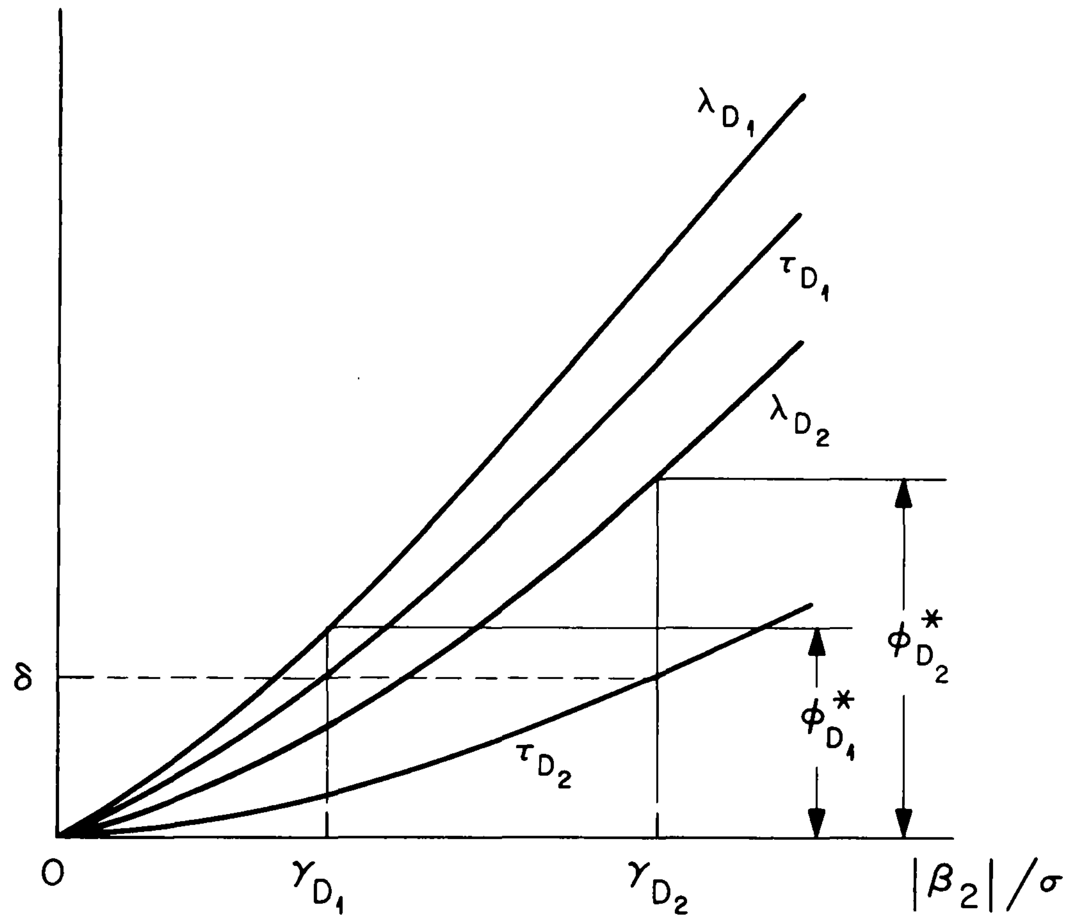

Figure 2.5. Λ_1(T)-Optimality: A Geometric Interpretation of Maximizing the Minimum Value of λ in the Region of Unacceptably Serious $\underset{\sim}{\beta}_2$, Φ, when τ is Influenced by the Design

$$\phi^* = \underset{\sim}{\gamma}' L \underset{\sim}{\gamma}$$

for some $\underset{\sim}{\gamma} \varepsilon \Phi$. If $\underset{\sim}{\gamma}$ is not on the boundary of Φ then there exists an ϵ such that $0 < \epsilon < 1$ and $(1-\epsilon)\underset{\sim}{\gamma} \varepsilon \Phi$, but

$$(1-\epsilon)^2 \underset{\sim}{\gamma}' L \underset{\sim}{\gamma} < \underset{\sim}{\gamma}' L \underset{\sim}{\gamma} = \phi^*$$

which contradicts the assumption that ϕ^* is the minimum value of λ for all $\underset{\sim}{\beta}_2 \varepsilon \Phi$. Thus even when the $\underset{\sim}{\beta}_2$-space is multi-dimensional, the minimum value of λ occurs on the boundary of the region Φ.

This implies that if Φ_0 is the region in the $\underset{\sim}{\beta}_2$-space defined by

$$\Phi_0 = \{\underset{\sim}{\beta}_2 : \tau = \delta,\ \delta > 0\}$$

then a design is optimum for criterion (2.1.12) if and only if it maximizes

$$\underset{\underset{\sim}{\beta}_2 \varepsilon \Phi_0}{\text{Min}} \lambda .$$

However, by (2.1.8) of Theorem 2.1, for any design $D \varepsilon \Delta$

$$\underset{\underset{\sim}{\beta}_2 \varepsilon \Phi_0}{\text{Min}} \lambda = \delta \, Ch_{min}[T^{-1} L]. \tag{2.1.13}$$

Consequently, since δ is a constant, a design maximizes the minimum value of λ for $\underset{\sim}{\beta}_2 \varepsilon \Phi$ if it maximizes $Ch_{min}[T^{-1} L]$.

The geometric interpretation of criterion (2.1.12) is illustrated in Figure 2.6 for the one-factor example considered in Section 2.1.1. In that example,

$$\underset{\sim}{\beta}_2' = (\beta_{11}, \beta_{111}).$$

The curve labeled "ϕ" in Figure 2.6 is the curve formed by projecting the contour $\tau = \delta$ onto the λ-surface. Criterion (2.1.12) selects

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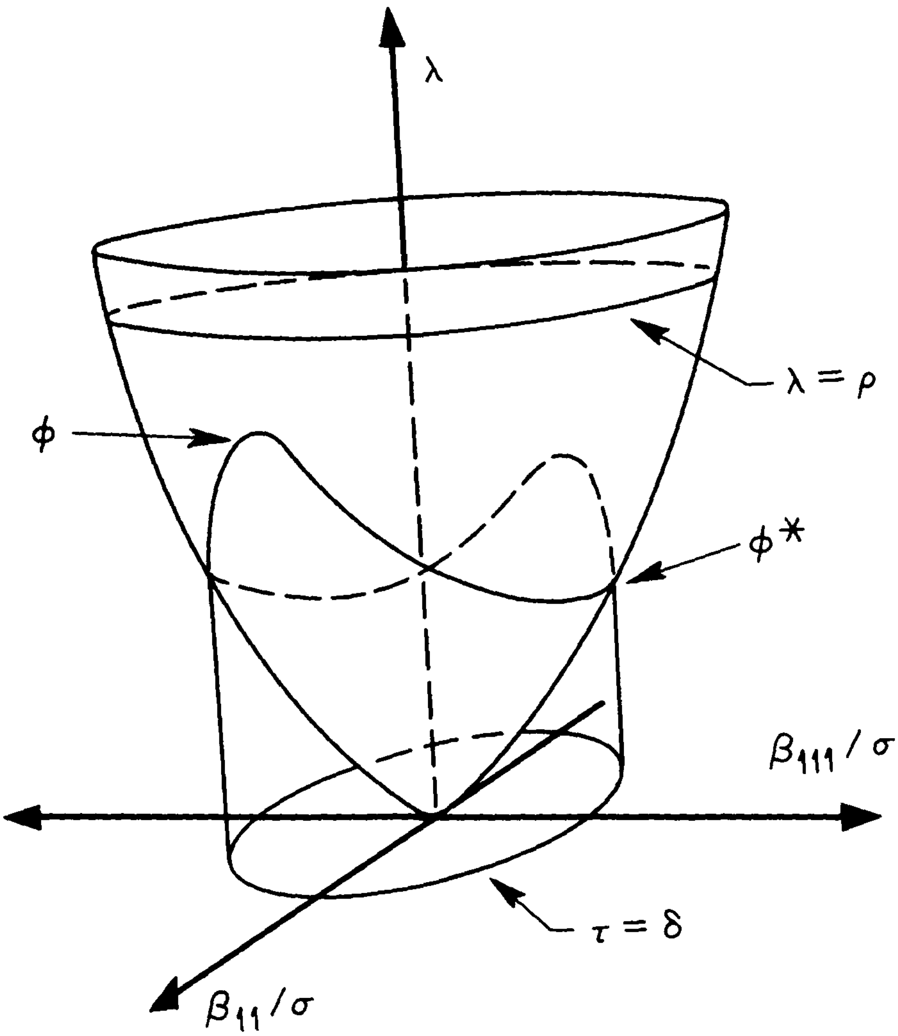

Figure 2.6. The Projection of the $\tau = \delta$ Contour onto the λ-Surface for a Two-Dimensional $\underset{\sim}{\beta}_2$-Space

designs that maximize ϕ^*, the minimum height of ϕ above the $\underset{\sim}{\beta}_2$-plane. Two properties of this criterion should be emphasized. First, it does not require the experimenter to explicitly specify δ, and second, this criterion does not distinguish between designs with a singular lack of fit matrix, since

$$Ch_{min}[T^{-1} L] = 0$$

if $|L| = 0$.

<u>2.1.2.2. Minimize the Maximum Value of τ.</u>--In the previous section, we supposed that the experimenter envisions some positive constant δ such that if $\tau \geq \delta$ then the seriousness associated with $\underset{\sim}{\beta}_2$ is unacceptable. Fortunately, we found that the selection of a design that maximizes the minimum value of λ for $\tau \geq \delta$ does not depend upon δ, and consequently, the experimenter is not required to explicitly specify δ. In a similar spirit, let us suppose that the experimenter envisions some positive constant ρ such that if $\lambda \leq \rho$ then the power of the lack of fit test is unacceptable. We will refer to the region Θ defined by

$$\Theta = \{\underset{\sim}{\beta}_2 : \lambda \leq \rho, \rho > 0\}$$

as the <u>region of poor power</u>.

If $\lambda > \rho$ and the magnitude of τ is very large, this fact is likely to be detected by the lack of fit test, and the experimenter can correct for it. However, we want to avoid the situation in which τ is large and $\lambda \leq \rho$. Consequently, we shall examine the selection of designs that minimize the maximum value of τ for $\lambda \leq \rho$. Specifically, let us examine the criterion

$$\underset{D \,\varepsilon\, \Delta}{\text{Min}} \quad \underset{\underset{\sim}{\beta_2} \,\varepsilon\, \Theta}{\text{Max}} \; \tau \tag{2.1.14}$$

where Δ is the class of permissible designs and Θ is a region of poor power.

Figure 2.7 illustrates the geometric interpretation of this criterion for a one-dimensional $\underset{\sim}{\beta_2}$-space. Since

$$\tau_D = \sigma^{-2} \beta_2^2 T_D$$

is a monotone increasing function of $|\beta_2| / \sigma$, the maximum value of τ for $\beta_2 \,\varepsilon\, \Theta$ occurs at the boundary of Θ, namely at

$$|\beta_2| / \sigma = \gamma_D = (\rho / L_D)^{\frac{1}{2}} .$$

Now, again, since τ is a monotone increasing function of $|\beta_2| / \sigma$ one way to reduce the magnitude of τ would be to select a design that makes the region of poor power as "tight" as possible, that is, to minimize γ_D. This would require us to maximize L_D, and if τ is design independent, we would simply select the design with the highest λ-function. However, if τ is influenced by the design, the design that maximizes L_D could have a large value for τ_D. Thus, we need to select a design that gives a good tradeoff between maximizing λ and minimizing τ. This is illustrated in Figure 2.7. Notice that although $\lambda_{D_1} > \lambda_{D_2}$, criterion (2.1.14) would select design D_2 over design D_1 since

$$\theta^*_{D_2} < \theta^*_{D_1} ,$$

where $\theta^*_{D_1}$ and $\theta^*_{D_2}$ are the maximum values of τ_{D_1} and τ_{D_2} respectively (see Figure 2.7).

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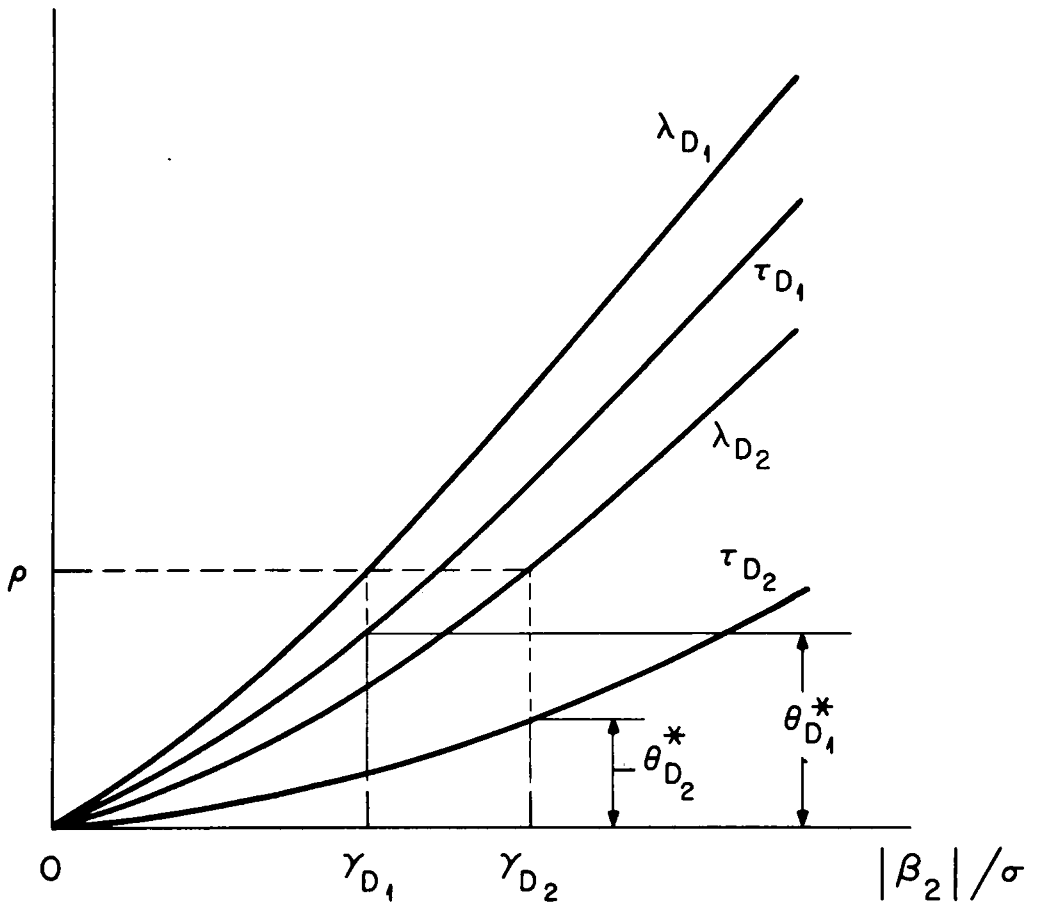

Figure 2.7. Minimizing the Maximum Seriousness Associated with $\underset{\sim}{\beta}_2$ in the Region of Poor Power, Θ

The geometric interpretation of this criterion for a two-dimensional $\underset{\sim}{\beta}_2$-space is illustrated in Figure 2.8. This is simply Figure 2.6 with the roles of λ and τ interchanged; instead of looking at the projection of the $\tau = \delta$ contour onto the λ-surface, we are now examining the projection θ of the $\lambda = \rho$ contour onto the τ-surface. The maximum value of τ for $\underset{\sim}{\beta}_2 \varepsilon \Theta$ is simply the maximum height, θ^*, of the curve θ above the $\underset{\sim}{\beta}_2$-plane.

The analytical characterization of this criterion is straightforward and parallels that of the previous section for criterion (2.1.12). In general, the maximum value of τ always occurs on the boundary of the region of poor power. Thus, if Θ_0 is the region in the $\underset{\sim}{\beta}_2$-space defined by

$$\Theta_0 = \{\underset{\sim}{\beta}_2 : \lambda = \rho,\ \rho > 0\}$$

then

$$\underset{\underset{\sim}{\beta}_2 \varepsilon \Theta}{\text{Max}} \ \tau = \underset{\underset{\sim}{\beta}_2 \varepsilon \Theta_0}{\text{Max}} \ \tau$$

However, this maximum is not defined if the $\lambda = \rho$ contour is not closed. So for this criterion we will require $|L| \neq 0$. By (2.1.9) of Theorem 2.1,

$$\underset{\underset{\sim}{\beta}_2 \varepsilon \Theta_0}{\text{Max}} \ \tau = \rho \ Ch_{max}[L^{-1} \ T].$$

Since ρ is assumed to be fixed, this criterion simply selects designs that minimize $Ch_{max}[L^{-1} \ T]$. Note that this criterion does not require the experimenter to explicitly specify ρ. Moreover, since

$$Ch_{max}[L^{-1} \ T] = \left[Ch_{min}[T^{-1} \ L]\right]^{-1},$$

it follows that criterion (2.1.14) is equivalent to criterion

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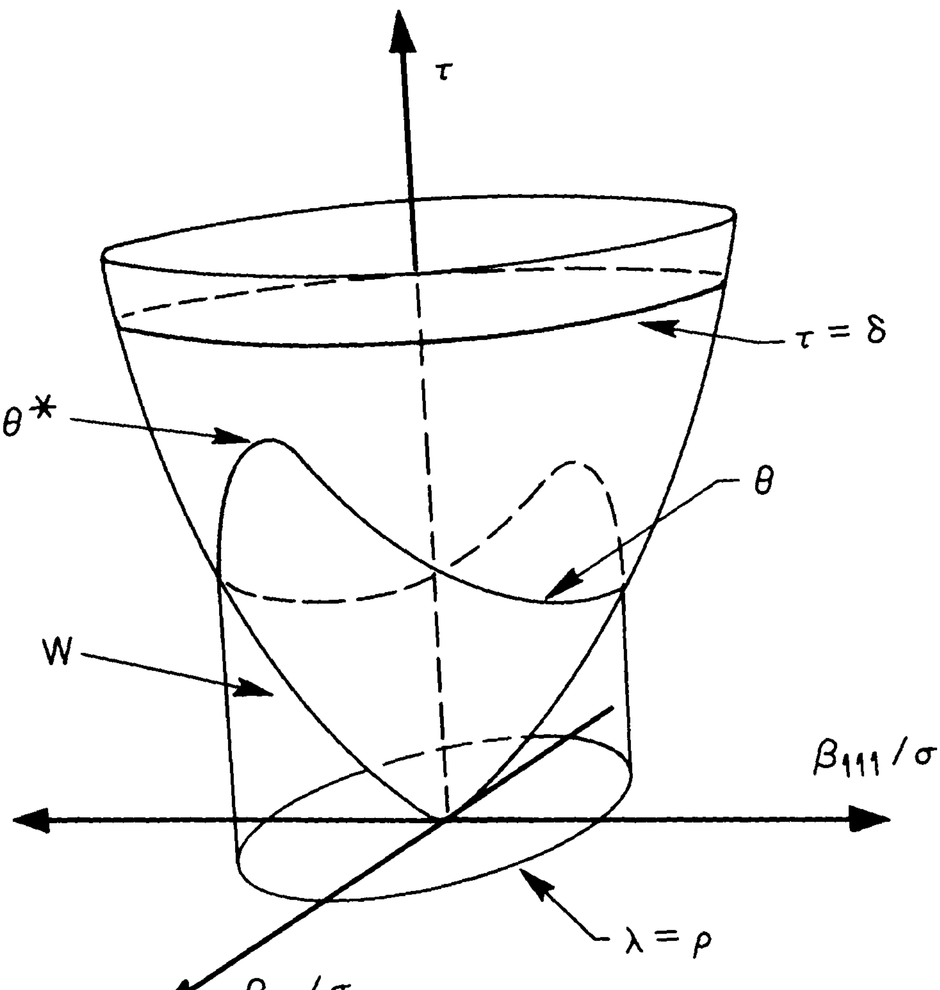


Figure 2.8. The Projection of the $\lambda = \rho$ Contour onto the τ-Surface for a Two-Dimensional $\underset{\sim}{\beta}_2$-Space

(2.1.12). In fact, not only do these criteria select the same optimal designs, they even give identical rankings for the class of permissible designs.

We will refer to a design as $\Lambda_1(T)$-optimal if it is optimal under either of the two previously described mini-max criteria. Specifically, a design is <u>$\Lambda_1(T)$-optimal</u> if it maximizes

$$\Lambda_1(T) = n^{-1} \, Ch_{\min}[T^{-1} L].$$

The factor "n^{-1}" is included to standardize $\Lambda_1(T)$ by the sample size.

2.1.3. $\Lambda_2(T,c)$-Optimality

In this section, and in Section 2.1.4, we will develop "average" analogs for $\Lambda_1(T)$-optimality. For this, we will need the following theorem.

<u>Theorem 2.2</u>

Let $\underset{\sim}{\omega}' = (\omega_1, \omega_2, \ldots, \omega_r)$ be a r-dimensional real vector,

$\zeta_1 = \underset{\sim}{\omega}' Z_1 \underset{\sim}{\omega}$ be a positive semidefinite quadratic form,

$\zeta_2 = \underset{\sim}{\omega}' Z_2 \underset{\sim}{\omega}$ be a positive definite quadratic form,

and $d\omega = d\omega_1 \cdot d\omega_2 \cdots d\omega_r$

then for any $\delta > 0$

$$\int_{\zeta_2 \leq \delta} \zeta_1 \; d\omega = \frac{\pi^{\frac{1}{2}r} \, \delta^{(\frac{1}{2}r + 1)}}{2(\frac{1}{2}r + 1)\cdot\Gamma(\frac{1}{2}r + 1)} \; |Z_2|^{-\frac{1}{2}} \, Tr[Z_2^{-1} Z_1], \qquad (2.1.15)$$

$$\lim_{\epsilon \to 0} \epsilon^{-1} \int_{\delta \le \zeta_2 \le \delta + \epsilon} \zeta_1 \, d\omega$$

$$= \frac{\pi^{\frac{1}{2}r} \delta^{\frac{1}{2}r}}{2\Gamma(\frac{1}{2}r + 1)} |Z_2|^{-\frac{1}{2}} \mathrm{Tr}[Z_2^{-1} Z_1], \qquad (2.1.16)$$

$$\lim_{\epsilon \to 0} \frac{\int_{\delta \le \zeta_2 \le \delta + \epsilon} \zeta_1 \, d\omega}{\int_{\delta \le \zeta_2 \le \delta + \epsilon} d\omega}$$

$$= r^{-1} \delta \, \mathrm{Tr}[Z_2^{-1} Z_1]. \qquad (2.1.17)$$

Proof:

Using the notation

$$\int_R C \, d\omega = \left[\int_R c_{ij} \, d\omega\right]^{r \times r}$$

for a matrix integral, where C is any $r \times r$ matrix, it is easily verified that

$$\int_R \underset{\sim}{\omega}' C \underset{\sim}{\omega} \, d\omega = \mathrm{Tr}\left[C \int_R \underset{\sim}{\omega} \underset{\sim}{\omega}' \, d\omega\right],$$

for any region R and matrix C. Now, using the result

$$\int_{\underset{\sim}{\omega}' \underset{\sim}{\omega} \le \delta} \underset{\sim}{\omega} \underset{\sim}{\omega}' \, d\omega = \Xi(\delta) \, I_r,$$

$$\text{where} \quad \Xi(\delta) = \frac{\pi^{\frac{1}{2}r}\,\delta^{(\frac{1}{2}r+1)}}{2(\frac{1}{2}r+1)\cdot\Gamma(\frac{1}{2}r+1)} ,$$

and the transformation $\underset{\sim}{\gamma} = Z_2^{\frac{1}{2}}\underset{\sim}{\omega}$, it follows that

$$\int_{\zeta_2 \le \delta} \zeta_1 \, d\omega = \int_{\underset{\sim}{\omega}' Z_2 \underset{\sim}{\omega} \le \delta} \underset{\sim}{\omega}' Z_1 \underset{\sim}{\omega} \, d\omega$$

$$= \int_{\underset{\sim}{\omega}' Z_2^{\frac{1}{2}} Z_2^{\frac{1}{2}} \underset{\sim}{\omega} \le \delta} \underset{\sim}{\omega}' Z_2^{\frac{1}{2}} Z_2^{-\frac{1}{2}} Z_1 Z_2^{-\frac{1}{2}} Z_2^{\frac{1}{2}} \underset{\sim}{\omega} \, d\omega$$

$$= |Z_2|^{-\frac{1}{2}} \int_{\underset{\sim}{\gamma}' \underset{\sim}{\gamma} \le \delta} \underset{\sim}{\gamma}' Z_2^{-\frac{1}{2}} Z_1 Z_2^{-\frac{1}{2}} \underset{\sim}{\gamma} \, d\gamma$$

$$= |Z_2|^{-\frac{1}{2}} \operatorname{Tr}\left\{ \int_{\underset{\sim}{\gamma}' \underset{\sim}{\gamma} \le \delta} \underset{\sim}{\gamma}\,\underset{\sim}{\gamma}' \, d\gamma \; Z_2^{-\frac{1}{2}} Z_1 Z_2^{-\frac{1}{2}} \right\}$$

$$= \Xi(\delta)\; |Z_2|^{-\frac{1}{2}} \operatorname{Tr}[Z_2^{-1} Z_1],$$

which proves (2.1.15).

The integral (2.1.16) is simply the first derivative with respect to δ of the integral (2.1.15), and it follows from the above result.

Since the volume of the hyperellipsoid defined by $\zeta_2 \le \delta$ is simply given by

$$\int_{\zeta_2 \le \delta} d\omega = \frac{\pi^{\frac{1}{2}r}\,\delta^{\frac{1}{2}r}}{\Gamma(\frac{1}{2}r+1)} \; |Z_2|^{-\frac{1}{2}} ,$$

it follows that

$$\int_{\delta \leq \zeta_2 \leq \delta + \epsilon} d\omega = \frac{\pi^{\frac{1}{2}r}}{\Gamma(\frac{1}{2}r + 1)} |Z_2|^{-\frac{1}{2}} [(\delta + \epsilon)^{\frac{1}{2}r} - \delta^{\frac{1}{2}r}] = g_1(\epsilon);$$

similarly, using (2.1.15), it follows that

$$\int_{\delta \leq \zeta_2 \leq \delta + \epsilon} \zeta_1 \ d\omega$$

$$= \frac{\pi^{\frac{1}{2}r}}{2(\frac{1}{2}r + 1)\cdot\Gamma(\frac{1}{2}r + 1)} |Z_2|^{-\frac{1}{2}} \mathrm{Tr}[Z_2^{-1} Z_1] \cdot [(\delta + \epsilon)^{(\frac{1}{2}r+1)} - \delta^{(\frac{1}{2}r+1)}]$$

$$= g_2(\epsilon) .$$

Then

$$g_2'(\epsilon) = \frac{\pi^{\frac{1}{2}r}}{2(\frac{1}{2}r + 1)\cdot\Gamma(\frac{1}{2}r + 1)} |Z_2|^{-\frac{1}{2}} \mathrm{Tr}[Z_2^{-1} Z_1] [(\tfrac{1}{2}r + 1) (\delta + \epsilon)^{\frac{1}{2}r}],$$

and

$$g_1'(\epsilon) = \frac{\pi^{\frac{1}{2}r}}{\Gamma(\frac{1}{2}r + 1)} |Z_2|^{-\frac{1}{2}} [\tfrac{1}{2}r (\delta + \epsilon)^{(\frac{1}{2}r - 1)}] .$$

Using L'Hospital's rule, we obtain

$$\lim_{\epsilon \to 0} \frac{g_2(\epsilon)}{g_1(\epsilon)} = \lim_{\epsilon \to 0} \frac{g_2'(\epsilon)}{g_1'(\epsilon)} = \lim_{\epsilon \to 0} \frac{\mathrm{Tr}[Z_2^{-1} Z_1]}{2(\frac{1}{2}r + 1)} \cdot \left[\frac{(\frac{1}{2}r+1) (\delta + \epsilon)^{\frac{1}{2}r}}{\frac{1}{2}r (\delta + \epsilon)^{(\frac{1}{2}r-1)}}\right]$$

$$= \lim_{\epsilon \to 0} \mathrm{Tr}[Z_2^{-1} Z_1] \frac{(\delta + \epsilon)}{r} = r^{-1} \delta \, \mathrm{Tr}[Z_2^{-1} Z_1],$$

which proves (2.1.17).

Q.E.D.

In the previous section, we saw that the mini-max criterion, $\Lambda_1(T)$-optimality, could be motivated from two different considerations, the "protection" and the "detection" of model inadequacy. First, we developed $\Lambda_1(T)$-optimality from detection considerations; we maximized the minimum value of the non-centrality parameter of the lack of fit test over the contour $\tau = \delta$. Then we motivated $\Lambda_1(T)$-optimality from protection considerations; we minimized the maximum seriousness of $\underset{\sim}{\beta}_2$ over the contour $\lambda = \rho$.

Now let us develop an average analog to maximizing the minimum value of the non-centrality parameter over the contour $\tau = \delta$. We have assumed that τ is a positive definite quadratic form. Thus, the τ-contours are closed, and T is non-singular. So, let us select designs that maximize the average value of the non-centrality parameter over the contour $\tau = \delta$, i.e.,

$$\max_{D \in \Delta} \lim_{\epsilon \to 0} \frac{\displaystyle\int_{\delta \le \tau \le \delta + \epsilon} \lambda \, d\beta_2}{\displaystyle\int_{\delta \le \tau \le \delta + \epsilon} d\beta_2} . \qquad (2.1.18)$$

Using (2.1.17) of Theorem 2.2, it follows that (2.1.18) is equal to

$$p_2^{-1} \delta \, \mathrm{Tr}[T^{-1} L]. \tag{2.1.19}$$

Hence this criterion is independent of δ, and it selects the designs that maximize

$$\mathrm{Tr}[T^{-1} L].$$

Figure 2.6 illustrates the geometric interpretation of this criterion for the one-factor example considered in the beginning of this chapter (the lower and higher order models were first and third order polynomials, respectively). In this figure, the curve labeled "ϕ" is the curve on the λ-surface formed by projecting the $\tau = \delta$ contour onto the λ-surface; this criterion maximizes the average height of ϕ above the $\underset{\sim}{\beta}_2$-plane.

This criterion seems well motivated in terms of power for the detection of model inadequacy. However, if the seriousness of $\underset{\sim}{\beta}_2$ is not design independent, then for each design, the $\tau = \delta$ contour can correspond to a different set of points in the $\underset{\sim}{\beta}_2$-space, and we must avoid sacrificing <u>protection</u> against model inadequacy (increasing τ) for <u>detection</u> of model inadequacy (increasing λ).

One measure of a design's ability to protect against model inadequacy is the "tightness" of its τ-contours as measured by the volume of the hyperellipsoid in the $\underset{\sim}{\beta}_2$-space defined by $\tau \leq \delta$. Hence we will weight the average value of λ over the contour $\tau = \delta$, (2.1.18), by the volume raised to some power of the hyperellipsoid defined by $\tau \leq \delta$. We will say that a design is

<u>$\Lambda_2(T,c)$-optimal</u> if it maximizes

$$\Lambda_2(T,c) = n^{-1} |T|^{-c} \operatorname{Tr}[T^{-1} L], \tag{2.1.20}$$

where the constant $c \geq 0$ is specified by the experimenter according to the degree of increased protection he wants against model inadequacy. Again, the factor "n^{-1}" is included to standardize $\Lambda_2(T,c)$ by the sample size. Of course, the factor $|T|^{-c}$ only affects experiments in which the seriousness of $\underset{\sim}{\beta}_2$ is design dependent.

Notice that, whereas $\Lambda_1(T)$-optimality required both T and L to be non-singular, $\Lambda_2(T,c)$-optimality only requires T to be non-singular. Consequently, this criterion can be used to select designs when, although we have enough degrees of freedom for lack of fit, we cannot completely estimate the higher order model.

This situation was illustrated by the example given in the beginning of this chapter when we used the three-point design

$$D = \begin{bmatrix} \underset{\sim}{1} \\ \hdashline -\underset{\sim}{1} \\ \hdashline a\underset{\sim}{1} \end{bmatrix} \begin{matrix} \}\, n_1 \text{ points at } 1 \\ \}\, n_1 \text{ points at } -1 \\ \}\, 2n_2 \text{ points at } a \end{matrix}$$

to fit a one-factor, first order polynomial when the higher order model was third order. The orientation of the τ and λ contours for $a = 0$ were illustrated in Figure 2.1. The geometric interpretation of $\Lambda_2(T,c)$ for this design is illustrated in Figure 2.9. If τ is design independent, $\Lambda_2(T,c)$-optimality maximizes the average height of ϕ, otherwise it maximizes the average height of ϕ

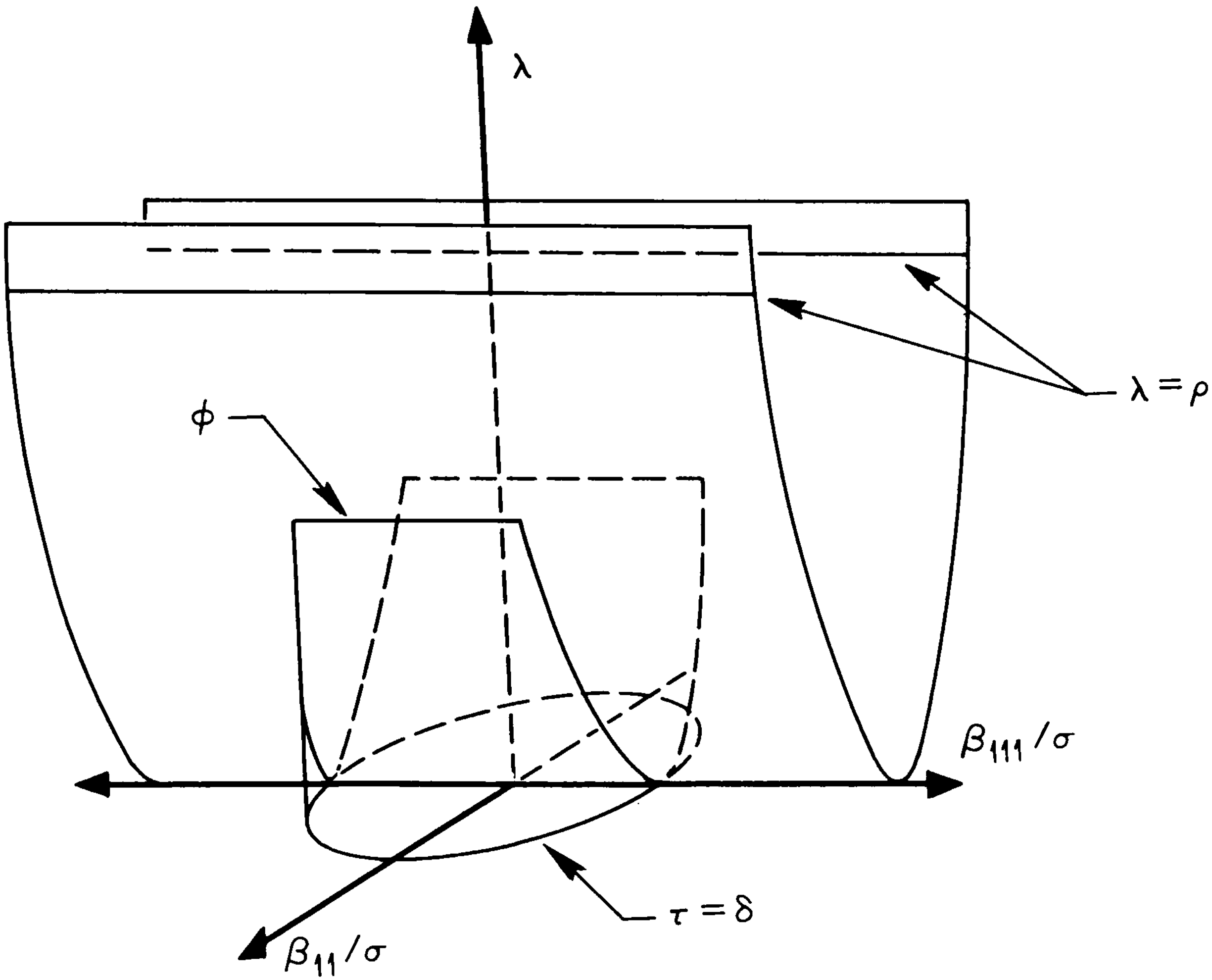


Figure 2.9. The Projection of the $\tau = \delta$ Contour onto the λ-Surface for a Two-Dimensional $\underset{\sim}{\beta}_2$-Space and a Singular Lack of Fit Matrix

weighted by the volume raised to the power 2c of the hyperellipsoid in the $\underset{\sim}{\beta}_2$-space defined by $\tau \leq \delta$.

From Figures 2.6 and 2.9, we can see that in order to maximize (2.1.20), we need to simultaneously perform several operations, We need to expand the $\tau = \delta$ contour, compress the λ-surface and simultaneously rotate both the $\tau = \delta$ contour and the λ-surface. Compressing the λ-surface and rotating the λ and τ contours is primarily influenced by the factor $\mathrm{Tr}[T^{-1} L]$ while the τ-contour expansion is primarily influenced by $|T|^{-c}$. The value of c chosen by the experimenter controls the degree of τ-contour expansion, i.e., the degree of increased protection against model inadequacy. The choice $c = 0$ corresponds to maximizing λ averaged over the contour $\tau = \delta$, possibly at the expense of the actual magnitude of τ. The choice $c = \frac{1}{2}$ has a particularly interesting geometric interpretation. $\Lambda_2(T,\frac{1}{2})$-optimality maximizes the surface area of the ellipsoidal shaped cylinder formed by the projection of the $\tau = \delta$ contour onto the λ-surface.

2.1.4 $\Lambda_3(T,c)$-Optimality

In the previous section, we developed an average analog to maximizing the minimum value of the non-centrality parameter over the contour $\tau = \delta$. In a similar manner, we can develop an integrated analog to criterion (2.1.14); instead of minimizing the maximum seriousness of $\underset{\sim}{\beta}_2$ over the contour $\lambda = \rho$, we will minimize the average value of τ over this contour. Specifically,

$$\operatorname*{Min}_{D \,\varepsilon\, \Delta} \quad \lim_{\epsilon \to 0} \quad \frac{\displaystyle\int_{\rho \le \lambda \le \rho + \epsilon} \tau \; d\beta_2}{\displaystyle\int_{\rho \le \lambda \le \rho + \epsilon} d\beta_2} \tag{2.1.21}$$

The development of this criterion will closely parallel the previous section. Obviously (2.1.21) closely resembles (2.1.18), and, whereas in the previous section we required the τ-contours to be closed, in this section, we must require the λ-contours to be closed, i.e., L to be non-singular.

Again using (2.1.17) of Theorem 2.2, it follows that (2.1.21) is equal to

$$p_2^{-1} \rho \operatorname{Tr}[L^{-1} T]. \tag{2.1.22}$$

Thus, a design minimizes the value of τ averaged over the contour $\lambda = \rho$ if it minimizes

$$\operatorname{Tr}[L^{-1} T],$$

and, as we have noted with the previous criteria, this criterion does not depend upon ρ.

Figure 2.8 illustrates the geometric interpretation of (2.1.21). The average value of τ given by (2.1.22) is simply the average height of the curve θ above the $\underset{\sim}{\beta}_2$-plane.

In the spirit of the previous section, we will generalize this criterion by weighting $\operatorname{Tr}[L^{-1} T]$ by the volume raised to some power of the hyperellipsoid in the $\underset{\sim}{\beta}_2$-space defined by $\lambda \le \rho$. We will refer to a design as $\Lambda_3(T,c)$-optimal if it minimizes

$$\Lambda_3(T,c) = |n^{-1} L|^{-c} \, \mathrm{Tr}[nL^{-1} T]; \qquad (2.1.23)$$

where the constant $c \geq 0$ is specified by the experimenter according to the added emphasis he wants to place on the tightness of the λ-contours. Again, the factor "n" was included to standardize $\Lambda_3(T,c)$ by the sample size.

From Figure 2.8, we can see that in order to minimize (2.1.23), we need to simultaneously perform several operations. We need to shrink the $\lambda = \rho$ contour, flatten the τ-surface, and simultaneously rotate both the $\lambda = \rho$ contour and the τ-surface. The compressing of the τ-surface and rotating the λ and τ contours is primarily influenced by $\mathrm{Tr}[L^{-1} T]$ while the shrinking of the λ-contours is primarily influenced by $|L|^{-c}$. The choice $c = 0$ corresponds to minimizing τ averaged over the $\lambda = \rho$ contour, possibly at the expense of the actual magnitude of λ. From (2.1.15) of Theorem 2.2, we can see that the choice $c = \frac{1}{2}$ corresponds to minimizing the value of τ integrated over the region of poor power defined by $\lambda \leq \rho$. Essentially, this choice for c maximizes the volume of the region "W" in Figure 2.8, defined by the projection of the contour $\lambda = \rho$ onto the τ-surface.

2.2. Invariance Properties for Non-Singular Linear Transformations

In this section, we will examine the effect of non-singular linear transformations upon the $\Lambda(T)$ criteria when $\eta_1(\underset{\sim}{x})$ and $\eta(\underset{\sim}{x})$

are polynomials containing all coefficients through orders d_1 and d_2 respectively. Additionally, since these criteria are functions of the T matrix, we will need to consider the effect of such transformations upon

$$\tau = \sigma^{-2} \underset{\sim}{\beta}_2' T \underset{\sim}{\beta}_2 .$$

Using the notation developed in Chapter I, consider the non-singular linear transformation

$$\underset{\sim}{z} = Q' \underset{\sim}{x} + \underset{\sim}{f} \tag{2.2.1}$$

mapping the $\underset{\sim}{x}$-variables into the new $\underset{\sim}{z}$-variables where Q is a non-singular $k \times k$ matrix and $\underset{\sim}{f}$ is a k-dimensional vector. This transformation maps the region of interest in the $\underset{\sim}{x}$-variables, denoted by R_x, into a region of interest in the $\underset{\sim}{z}$-variables, denoted by R_z. Transformations of this type include changes in scale, translations and rotations. For example, if $k = 2$,

$$z_1 = a_1 x_1 + a_2 x_2$$

and $$z_2 = b_1 x_1 + f_2$$

then

$$Q = \begin{pmatrix} a_1 & b_1 \\ a_2 & 0 \end{pmatrix}$$

and $$\underset{\sim}{f}' = (0, f_2).$$

Essentially, a criterion for the selection of an experimental design is said to be <u>invariant to non-singular linear transformations</u> if for <u>any</u> transformation of the form (2.2.1) then, whenever D_x

is an optimal design in the $\underset{\sim}{x}$-variables,

$$D_z = D_x Q + \underset{\sim}{1} \underset{\sim}{f}'$$

is an optimal design in the $\underset{\sim}{z}$-variables. We will show that whenever an experimenter intends to use a polynomial of degree d_1 to represent the true response surface, which is a polynomial of degree $d_2 \geq d_1$, then all of the criteria examined in this investigation are invariant to non-singular linear transformations, i.e., for

1. D-optimality,
2. V-optimality,
3. $|L|$-optimality,
4. all of the $\Lambda(T)$ criteria for τ_1 and τ_2

and 5. the minimum bias criterion.

So let us suppose that the experimenter intends to use a polynomial containing <u>all</u> coefficients through order d_1 to represent the true response surface. Furthermore, let us suppose that, in the $\underset{\sim}{x}$-variables, the true response surface is a polynomial of order $d_2 \geq d_1$ given by

$$\eta(\underset{\sim}{x}) = \underset{\sim}{x}_*' \underset{\sim}{\beta}$$

$$\text{where } \underset{\sim}{x}_*' = (\underset{\sim}{x}_1', \underset{\sim}{x}_2')$$

$$\text{and } \underset{\sim}{\beta}' = (\underset{\sim}{\beta}_1', \underset{\sim}{\beta}_2').$$

Now since $\underset{\sim}{z}$ is a non-singular transformation of $\underset{\sim}{x}$, it follows that the true response model in the $\underset{\sim}{z}$-variables, given by

$$\mu(\underset{\sim}{z}) = \eta(\underset{\sim}{x}) \text{ where } \underset{\sim}{x} = (Q')^{-1} [\underset{\sim}{z} - \underset{\sim}{f}],$$

is also a polynomial of order d_2. So we can express $\mu(\underset{\sim}{z})$ as

$$\mu(z) = \underset{\sim}{z}_*' \underset{\sim}{\gamma} .$$

Without loss of generality, we will suppose that the coefficients in $\underset{\sim}{z}_*$ and $\underset{\sim}{x}_*$ are ordered so that the ith order coefficients appear before the coefficients of order i + 1. Moreover, let us partition $\underset{\sim}{z}_*$ and $\underset{\sim}{\gamma}$ as

$$\underset{\sim}{z}_*' = (\underset{\sim}{z}_1', \underset{\sim}{z}_2')$$

$$\text{and} \quad \underset{\sim}{\gamma}' = (\underset{\sim}{\gamma}_1', \underset{\sim}{\gamma}_2')$$

where $\mu_1(\underset{\sim}{z}) = \underset{\sim}{z}_1' \underset{\sim}{\gamma}_1$ is a polynomial of order d_1.

It is easily seen that the coefficients in $\underset{\sim}{z}_*$ are simply polynomials in $\underset{\sim}{x}$ of order less than or equal to d_2; thus,

$$\underset{\sim}{z}_* = P' \underset{\sim}{x}_*$$

for some matrix P. Moreover, the coefficients in $\underset{\sim}{z}_1$ are polynomials in $\underset{\sim}{x}$ of order less than or equal to d_1 and $\eta_1(\underset{\sim}{x})$ is a polynomial containing all coefficients through order d_1; thus, P can be expressed as

$$P = \begin{bmatrix} P_1 & P_2 \\ 0 & P_3 \end{bmatrix}$$

$$\text{where} \quad P_1 = \begin{bmatrix} \begin{pmatrix} 1 & \underset{\sim}{f}' \\ \underset{\sim}{0} & Q \end{pmatrix} & Q_2 \\ 0 & Q_3 \end{bmatrix} .$$

For example, if $k = 2$, $d_1 = 1$ and $d_2 = 2$,

$$\underset{\sim}{f}' = (f_1, f_2),$$

$$\text{and} \quad Q = \begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \end{bmatrix}$$

$$\text{then} \qquad P_1 = \begin{bmatrix} 1 & f_1 & f_2 \\ 0 & a_1 & b_1 \\ 0 & a_2 & b_2 \end{bmatrix},$$

$$P_2 = \begin{bmatrix} f_1 f_2 & f_1^2 & f_2^2 \\ (a_1 f_2 + b_1 f_1) & 2f_1 a_1 & 2f_2 b_1 \\ (a_2 f_2 + b_2 f_1) & 2f_1 a_2 & 2f_2 b_2 \end{bmatrix},$$

$$\text{and} \qquad P_3 = \begin{bmatrix} (a_1 b_2 + a_2 b_1) & 2a_1 a_2 & 2b_1 b_2 \\ a_1 b_1 & a_1^2 & b_1^2 \\ a_2 b_2 & a_2^2 & b_2^2 \end{bmatrix}.$$

In what follows, we will need to show that if Q is non-singular then P is non-singular. In order to prove this, we will use the following lemma.

<u>Lemma 2.1</u>

Given $\underset{\sim}{x}_*$ and $\underset{\sim}{z}_* = P' \underset{\sim}{x}_*$ as defined above, let

$$M^x = \Omega_x \int_{R_x} \underset{\sim}{x}_* \underset{\sim}{x}_*' \quad dx_1 \cdot dx_2 \cdots dx_k$$

$$\text{and} \quad M^z = \Omega_z \int_{R_z} \underset{\sim}{z}_* \underset{\sim}{z}_*' \quad dz_1 \cdot dz_2 \cdots dz_k$$

where Ω_x^{-1} and Ω_z^{-1} are the volumes of the regions of interest , R_x and R_z, in the $\underset{\sim}{x}$ and $\underset{\sim}{z}$ variables respectively, and $\Omega_x^{-1} > 0$ then

$$1. \quad M^z = P' M^x P \tag{2.2.2}$$

$$\text{and} \quad 2. \quad |M^z| > 0. \tag{2.2.3}$$

Proof:

Since $\underset{\sim}{z} = Q' \underset{\sim}{x} + \underset{\sim}{f}$, and $|Q| \neq 0$, it follows that

$$\Omega_z^{-1} = J_0 \, \Omega_x^{-1} > 0,$$

where J_0 is the absolute value of $|Q|$. This ensures that M^z is well defined. Since $\underset{\sim}{z}_* = P' \underset{\sim}{x}_*$, it follows that

$$\begin{aligned} M^z &= \Omega_z \int_{R_z} \underset{\sim}{z}_* \underset{\sim}{z}_*' \, dz_1 \cdot dz_2 \cdots dz_k \\ &= J_0^{-1} \, \Omega_x \int_{R_z} \underset{\sim}{z}_* \underset{\sim}{z}_*' \, dz_1 \cdot dz_2 \cdots dz_k \\ &= J_0^{-1} \, \Omega_x \, P' \int_{R_x} J_0 \, \underset{\sim}{x}_* \underset{\sim}{x}_*' \, dx_1 \cdot dx_2 \cdots dx_k \, P \\ &= P' \, \Omega_x \int_{R_x} \underset{\sim}{x}_* \underset{\sim}{x}_*' \, dx_1 \cdot dx_2 \cdots dx_k \, P \\ &= P' M^x P, \end{aligned}$$

so that (2.2.2) follows. The result (2.2.3) was given by Evans (1974). Specifically, let $\underset{\sim}{c}$ be any non-zero vector of dimension $p = p_1 + p_2$. Since $\underset{\sim}{c} \neq \underset{\sim}{0}$ and $\underset{\sim}{c}' \underset{\sim}{z}_*$ is a polynomial in $\underset{\sim}{z}$, $\underset{\sim}{c}' \underset{\sim}{z}_* \neq 0$ almost everywhere. Thus, since $\Omega_z^{-1} > 0$, it follows that

$$\underset{\sim}{c}' M^z \underset{\sim}{c} = \Omega_z \int_{R_z} \underset{\sim}{c}' \underset{\sim}{z}_* \underset{\sim}{z}_*' \underset{\sim}{c} \, dz_1 \cdot dz_2 \cdots dz_k$$

$$= \Omega_z \int_{R_z} (\underset{\sim}{c}' \underset{\sim}{z}_*)^2 \; dz_1 \cdot dz_2 \cdots dz_k > 0.$$

This implies that M^z is positive definite, so that $|M^z| > 0$.

Q.E.D.

From this we obtain the following theorem.

Theorem 2.3

If Q is non-singular then P, P_1 and P_3 are all non-singular.

Proof:

By Lemma 2.1, $|M^z| = |P' M^x P| = |P|^2 |M^x|$ and $|M^z| > 0$. Therefore, $|P|^2 > 0$ and $|M^x| > 0$; moreover,

$$|P|^2 = |M^z| / |M^x|,$$

and P is non-singular. Since $|P| = |P_1| \cdot |P_3|$, P_1 and P_3 are also non-singular.

Q.E.D.

Now $\mu(\underset{\sim}{z}) = \eta(\underset{\sim}{x}) = \underset{\sim}{x}_1' \underset{\sim}{\beta}_1 + \underset{\sim}{x}_2' \underset{\sim}{\beta}_2$; also

$$\begin{aligned} \mu(\underset{\sim}{z}) &= \underset{\sim}{z}_1' \underset{\sim}{\gamma}_1 + \underset{\sim}{z}_2' \underset{\sim}{\gamma}_2 \\ &= \underset{\sim}{x}_1' P_1 \underset{\sim}{\gamma}_1 + (\underset{\sim}{x}_1' P_2 + \underset{\sim}{x}_2' P_3) \underset{\sim}{\gamma}_2 \\ &= \underset{\sim}{x}_1' (P_1 \underset{\sim}{\gamma}_1 + P_2 \underset{\sim}{\gamma}_2) + \underset{\sim}{x}_2' P_3 \underset{\sim}{\gamma}_2. \end{aligned}$$

Since two polynomials are identical only if their coefficients are identical, we obtain

$$\underset{\sim}{\beta}_1 = P_1 \underset{\sim}{\gamma}_1 + P_2 \underset{\sim}{\gamma}_2$$

$$\text{and } \underset{\sim}{\beta}_2 = P_3 \underset{\sim}{\gamma}_2 \quad .$$

Thus, since P_1 and P_2 are non-singular,

$$\underset{\sim}{\gamma}_1 = P_1^{-1}\,\underset{\sim}{\beta}_1 - P_1^{-1}\,P_2\,P_3^{-1}\,\underset{\sim}{\beta}_2$$

$$\text{and } \underset{\sim}{\gamma}_2 = P_3^{-1}\,\underset{\sim}{\beta}_2.$$

In terms of the observation vector, this transformation can be written as:

$$\begin{aligned}\underset{\sim}{y} &= X\,\underset{\sim}{\beta} + \underset{\sim}{\epsilon}\\ &= [X\ P]\ [P^{-1}\,\underset{\sim}{\beta}] + \underset{\sim}{\epsilon}\\ &= Z\,\underset{\sim}{\gamma} + \underset{\sim}{\epsilon}\\ &= Z_1\,\underset{\sim}{\gamma}_1 + Z_2\,\underset{\sim}{\gamma}_2 + \underset{\sim}{\epsilon}\end{aligned}$$

$$\text{where } Z_1 = X_1\,P_1$$

$$\text{and } Z_2 = X_1\,P_2 + X_2\,P_3\ ;$$

We can now show that D-optimality and V-optimality are invariant to non-singular linear transformations.

Theorem 2.4

D-optimality is invariant to non-singular linear transformations.

Proof:

Since $Z = X\,P$, $|Z'\,Z| = |P|^2\,|X'\,X|$.

Thus, by Theorem 2.4, $|P|^2 > 0$ and the result of this theorem follows.

Q.E.D.

Theorem 2.5

V-optimality is invariant to non-singular linear transformations.

Proof:

Using (2.2.2) of Lemma 2.1 and the fact that $Z = X\,P$, it follows that

$$Tr[(Z'\ Z)^{-1}\ M^{z}] \ = \ Tr[P^{-1}\ (X'\ X)^{-1}\ (P')^{-1}\ P'\ M^{x}\ P]$$

$$= \ Tr[(X'\ X)^{-1}\ M^{x}]\ .$$

Thus V-optimality is invariant to non-singular linear transformations. Q.E.D.

In order to show that $|L|$-optimality is invariant to non-singular linear transformations, we will use the following lemma.

Lemma 2.2

$$L_z \ = \ P_3'\ L_x\ P_3$$

$$\text{where} \quad L_z \ = \ Z_2'\ [I_n - Z_1(Z_1'Z_1)^{-1}\ Z_1']\ Z_2$$

$$\text{and} \quad L_x \ = \ X_2'\ [I_n - X_1(X_1'X_1)^{-1}\ X_1']\ X_2\ .$$

Proof:

$$\begin{aligned}
L_z &= Z_2\ [I_n - Z_1(Z_1'Z_1)^{-1}\ Z_1']\ Z_2 \\
&= (X_1P_2 + X_2P_3)'[I_n - X_1P_1(P_1'X_1'X_1P_1)^{-1}\ P_1'X_1']\ (X_1P_2 + X_2P_3) \\
&= P_2'X_1'\ [I_n - X_1(X_1'X_1)^{-1}\ X_1']\ X_1P_2 \ + \\
&\qquad P_2'X_1'\ [I_n - X_1(X_1'X_1)^{-1}\ X_1]\ X_2P_3 \ + \\
&\qquad P_3'X_2'\ [I_n - X_1(X_1'X_1)^{-1}\ X_1']\ X_1P_2 \ + \\
&\qquad P_3'X_2'\ [I_n - X_1(X_1'X_1)^{-1}\ X_1']\ X_2P_3 \\
&= P_2'\ [X_1' - X_1']\ X_1P_2 \ + \ P_2'\ [X_1' - X_1']\ X_2P_3 \ + \\
&\qquad P_3'X_2'\ [X_1 - X_1]\ P_2 \ + \ P_3'\ L_x\ P_3 \\
&= P_3'\ L_x\ P_3.
\end{aligned}$$

Thus,

$$L_z = P_3' L_x P_3,$$

and the result of this lemma follows.

Q.E.D.

Theorem 2.6

$|L|$-optimality is invariant to non-singular linear transformations.

Proof:

By the previous lemma, $|L_z| = |P_3' L_x P_3| = |P_3|^2 |L_x|$, and by Theorem 2.4, $|P_3|^2 > 0$. Thus the result of this theorem follows.

Q.E.D.

Now let us examine the effect of this transformation upon τ. Let

$$\tau_x = \sigma^{-2} \underset{\sim}{\beta}_2' T^x \underset{\sim}{\beta}_2$$

$$\text{and } \tau_z = \sigma^{-2} \underset{\sim}{\gamma}_2' T^z \underset{\sim}{\gamma}_2$$

be the values of τ in the $\underset{\sim}{x}$-variables and $\underset{\sim}{z}$-variables respectively. T^x and T^z are the T matrices in the $\underset{\sim}{x}$-variables and $\underset{\sim}{z}$-variables respectively. We will say that <u>τ is invariant under non-singular linear transformations</u> if for any transformation of the form (2.2.1),

$$\tau_x = \tau_z$$

for all $\underset{\sim}{\beta}_2$ (or equivalently for all $\underset{\sim}{\gamma}_2$ since $\underset{\sim}{\gamma}_2 = P_3^{-1}\underset{\sim}{\beta}_2$). Since

$$\tau_x = \sigma^{-2} \underset{\sim}{\beta}_2' (P_3')^{-1} P_3' T^x P_3 (P_3)^{-1} \underset{\sim}{\beta}_2 = \sigma^{-2} \underset{\sim}{\gamma}_2' P_3' T^x P_3 \underset{\sim}{\gamma}_2,$$

a sufficient condition for τ to be invariant under non-singular linear transformations is: $$T^z = P_3' T^x P_3. \qquad (2.2.4)$$

Without loss of generality, we will assume that T^x is symmetric, so that this condition is necessary, as well as sufficient, for τ to be invariant under non-singular linear transformations. In what follows, we will partition M^x and M^z (defined in Lemma 2.1) as:

$$M^x = \begin{bmatrix} M^x_{11} & M^x_{12} \\ M^x_{21} & M^x_{22} \end{bmatrix} \quad \text{and} \quad M^z = \begin{bmatrix} M^z_{11} & M^z_{12} \\ M^z_{21} & M^z_{22} \end{bmatrix},$$

so that,

$$M^x_{ij} = \Omega_x \int_{R_x} \underset{\sim}{x}_i \underset{\sim}{x}_j' \, dx_1 \cdot dx_2 \cdots dx_k$$

$$\text{and} \quad M^z_{ij} = \Omega_z \int_{R_z} \underset{\sim}{z}_i \underset{\sim}{z}_j' \, dz_1 \cdot dz_2 \cdots dz_k ,$$

$$i = 1, 2; \; j = 1, 2.$$

We will now show that T_1 and T_2 satisfy condition (2.2.4).

<u>Theorem 2.7</u>

τ_1 is invariant under non-singular linear transformations.

Proof:

Using Lemma 2.1, we obtain

$$M^z_{11} = [P_1' M^x_{11} P_1],$$

$$M^z_{12} = [P_1' M^x_{12} P_3 + P_1' M^x_{11} P_2],$$

$$\text{and} \quad M^z_{22} = [P_2' M^x_{11} P_2 + P_3' M^x_{21} P_2 + P_2' M^x_{12} P_3 + P_3' M^x_{22} P_3].$$

Thus,

$$\begin{aligned}
T^z &= M^z_{22} - M^z_{21}(M^z_{11})^{-1} M^z_{12} \\
&= [P_2' M^x_{11} P_2 + P_3' M^x_{21} P_2 + P_2' M^x_{12} P_3 + P_3' M^x_{22} P_3] \\
&\qquad - [P_3' M^x_{21} P_1 + P_2' M^x_{11} P_1] [P_1^{-1}(M^x_{11})^{-1} (P_1')^{-1}] \\
&\qquad\qquad \cdot [P_1' M^x_{12} P_3 + P_1' M^x_{11} P_2] \\
&= [P_2' M^x_{11} P_2 + P_3' M^x_{21} P_2 + P_2' M^x_{12} P_3 + P_3' M^x_{22} P_3] \\
&\qquad - [P_3' M^x_{21}(M^x_{11})^{-1} + P_2'] \cdot [M^x_{12} P_3 + M^x_{11} P_2] \\
&= [P_2' M^x_{11} P_2 + P_3' M^x_{21} P_2 + P_2' M^x_{12} P_3 + P_3' M^x_{22} P_3] \\
&\qquad - [P_3' M^x_{21}(M^x_{11})^{-1} M^x_{12} P_3 + P_3' M^x_{21} P_2 + P_2' M^x_{12} P_3 \\
&\qquad\qquad + P_2' M^x_{11} P_2] \\
&= [P_3' M^x_{22} P_3 - P_3' M^x_{21}(M^x_{11})^{-1} M^x_{12} P_3] \\
&= P_3' T^x P_3.
\end{aligned}$$

Q.E.D.

Theorem 2.8

τ_2 is invariant under non-singular linear transformations.

Proof:

Let $A_z = (Z_1' Z_1)^{-1} Z_1' Z_2$ be the alias matrix in the $\underset{\sim}{z}$-variables. Then, it is easily shown that

$$A_z = P_1^{-1} [P_2 + A_x P_3]$$

where

$$A_x = (X_1' X_1)^{-1} X_1' X_2$$

is the alias matrix in the $\underset{\sim}{x}$-variables. Now using Lemma 2.1, we obtain

$$
\begin{aligned}
T_2^z &= A_z' M_{11}^z A_z - A_z' M_{12}^z - M_{21}^z A_z + M_{22}^z \\
&= \{(P_2 + A_x P_3)'(P_1')^{-1} P_1' M_{11}^x P_1 P_1^{-1}(P_2 + A_x P_3) \\
&\qquad - (P_2 + A_x P_3)'(P_1')^{-1}[P_1' M_{11}^x P_2 + P_1' M_{12}^x P_3] \\
&\qquad - [P_2' M_{11}^x P_1 + P_3' M_{21}^x P_1] P_1^{-1} (P_2 + A_x P_3) \\
&\qquad + [P_2' M_{11}^x P_2 + P_3' M_{21}^x P_2 + P_2' M_{12}^x P_3 + P_3' M_{22}^x P_3]\} \\
&= \{[P_2' M_{11}^x P_2 + P_2' M_{11}^x A_x P_3 + P_3' A_x' M_{11}^x P_2 + P_3' A_x' M_{11}^x A_x P_3] \\
&\qquad - [P_2' M_{11}^x P_2 + P_2' M_{12}^x P_3 + P_3' A_x' M_{11}^x P_2 + P_3' A_x' M_{12}^x P_3] \\
&\qquad - [P_2' M_{11}^x P_2 + P_3' M_{21}^x P_2 + P_2' M_{11}^x A_x P_3 + P_3' M_{21}^x A_x P_3] \\
&\qquad + [P_2' M_{11}^x P_2 + P_3' M_{21}^x P_2 + P_2' M_{12}^x P_3 + P_3' M_{22}^x P_3]\} \\
&= \{P_3' A_x' M_{11}^x A_x P_3 - P_3' A_x' M_{12}^x P_3 - P_3' M_{21}^x A_x P_3 + P_3' M_{22}^x P_3\} \\
&= P_3' [A_x' M_{11}^x A_x - A_x' M_{12}^x - M_{21}^x A_x + M_{22}^x] P_3 \\
&= P_3' T_2^x P_3.
\end{aligned}
$$

Q.E.D.

It is interesting to note that if we measure the seriousness of $\underset{\sim}{\beta}_2$ by

$$\tau = \sigma^{-2} \underset{\sim}{\beta}_2' \underset{\sim}{\beta}_2, \tag{2.2.5}$$

τ will not be invariant under non-singular linear transformations. Since we view the seriousness of the bias as an innate property of an experiment, the use of (2.2.5) as a measure of the seriousness of $\underset{\sim}{\beta}_2$ seems inconsistent. We will now show that, if τ is invariant under non-singular linear transformations, the $\Lambda(T)$ criteria are also invariant.

Theorem 2.9

If τ is invariant under non-singular linear transformations of the form

$$\underset{\sim}{z} = Q' \underset{\sim}{x} + \underset{\sim}{f}$$

mapping the region of interest R_x into R_z, and if a design D_x is $\Lambda_1(T)$-optimal, $\Lambda_2(T,c)$-optimal or $\Lambda_3(T,c)$-optimal in R_x then

$$D_z = D_x Q + \underset{\sim}{1} \underset{\sim}{f}'$$

is $\Lambda_1(T)$-optimal, $\Lambda_2(T,c)$-optimal or $\Lambda_3(T,c)$-optimal in R_z, respectively.

Proof:

Since τ is invariant under non-singular linear transformations,

$$T^z = P_3' T^x P_3,$$

and by Lemma 2.2, $$L_z = P_3' L_x P_3.$$

Thus $$(T^z)^{-1} L_z = P_3^{-1} (T^x)^{-1} L_x P_3, \qquad (2.2.6)$$

so that $(T^z)^{-1} L_z$ and $(T^x)^{-1} L_x$ have the same characteristic roots. From this, it follows that

$$Ch_{min}[(T^z)^{-1} L_z] = Ch_{min}[(T^x)^{-1} L_x],$$

and thus if D_x is $\Lambda_1(T)$-optimal in R_x, D_z is $\Lambda_1(T)$-optimal in R_z.

The relationship (2.2.6) also implies that

$$Tr[(T^z)^{-1} L_z] = Tr[(T^x)^{-1} L_x]$$

$$\text{and} \quad Tr[(L_z)^{-1} T^z] = Tr[(L_x)^{-1} T^x].$$

In additon, since

$$|T^z| = |P_3|^2 \, |T^x|$$

$$\text{and} \quad |L_z| = |P_3|^2 \, |L_x|$$

where $|P_3|^2$ is a positive constant,

$$\Lambda_2(T^z,c) = |P_3|^{-2c} \, |T^x|^{-c} \, n^{-1} \, Tr[(T^x)^{-1} \, L_x] = |P_3|^{-2c} \, \Lambda_2(T^x,c)$$

and similarly,

$$\Lambda_3(T^z,c) = |P_3|^{-2c} \, |n^{-1}L_x|^{-c} \, n \, Tr[L_x^{-1} \, T^x] = |P_3|^{-2c} \, \Lambda_3(T^x,c).$$

Therefore, if D_x is $\Lambda_2(T,c)$-optimal (or $\Lambda_3(T,c)$-optimal) in R_x then D_z is $\Lambda_2(T,c)$-optimal (or $\Lambda_3(T,c)$-optimal) in R_z.

Q.E.D.

Theorem 2.10

If D_x is a minimum bias design in R_x,

$$D_z = D_x \, Q + \underset{\sim}{f}$$

is a minimum bias design in R_z.

Proof:

Let A_x and A_z be the alias matrices for D_x and D_z respectively:, as we observed in the proof of Theorem 2.8,

$$A_z = P_1^{-1} \, (P_2 + A_x \, P_3).$$

Also, by (2.2.2) of Lemma 2.1,

$$M_{11}^z = P_1' \, M_{11}^x \, P_1$$

$$\text{and} \quad M_{12}^z = P_1' \, (M_{11}^x \, P_2 + M_{12}^x \, P_3),$$

and since D_x is a minimum bias design, $A_x = (M_{11}^x)^{-1} \, M_{12}^x$.

Thus $(M_{11}^{z})^{-1} M_{12}^{z} = P_1^{-1}(M_{11}^{x})^{-1}(M_{11}^{x} P_2 + M_{12}^{x} P_3) = P_1^{-1}(P_2 + A_x P_3)$.

Therefore, $(M_{11}^{z})^{-1} M_{12}^{z} = A_z$, so D_z is minimum bias for R_z.

Q.E.D.

2.3. Effects of Moment Preserving Rotations

In the previous section, we found that, if τ is invariant under non-singular linear transformations of the form

$$\underset{\sim}{z} = Q' \underset{\sim}{x} + \underset{\sim}{f}$$

and D_x is $\Lambda(T)$-optimal in R_x then

$$D_z = D_x Q + \underset{\sim}{1} \underset{\sim}{f}'$$

is $\Lambda(T)$-optimal in R_z, and we were able to show that τ_1 and τ_2 are both invariant under non-singular linear transformations.

Let us now consider the transformation

$$\underset{\sim}{z} = Q' \underset{\sim}{x}$$

where Q is orthogonal. We will say that Q preserves the region moments of R_x if $M^x = M^z$. For example, any orthogonal rotation preserves the region moments of a hypersphere, and a 90°, 180° or 270° orthogonal rotation preserves the region moments of a square.

Theorem 2.11

Let D_0 be the design obtained from design D_1 by

$$D_0 = D_1 \; Q$$

where Q preserves the region moments of R then, for τ_1 or τ_2, the characteristic polynomials of $[T^{-1} L]$ for D_0 and D_1 are identical.

Proof:

Consider the transformation $\underset{\sim}{z} = Q' \underset{\sim}{x}$. For this transformation,

$$P_2 = 0,$$

$$\underset{\sim}{z}_1' = \underset{\sim}{x}_1' P_1,$$

$$\text{and} \quad \underset{\sim}{z}_2' = \underset{\sim}{x}_2' P_3.$$

So if A_0 and A_1 are the alias matrices of D_0 and D_1 respectively then

$$A_0 = P_1^{-1} A_1 P_3. \tag{2.3.1}$$

Since Q preserves the region moments of R, it follows that

$$M_{ij}^x = M_{ij}^z, \; i = 1, 2; \; j = 1, 2.$$

Hence by Lemma 2.1,

$$M_{11}^x = P_1' M_{11}^x P_1,$$

$$M_{12}^x = P_1' M_{12}^x P_3,$$

$$\text{and} \quad M_{22}^x = P_3' M_{22}^x P_3.$$

This implies that

$$M_{11}^x = (P_1')^{-1} M_{11}^x (P_1)^{-1},$$

$$M_{12}^x = (P_1')^{-1} M_{12}^x (P_3)^{-1},$$

$$\text{and} \quad M_{22}^x = (P_3')^{-1} M_{22}^x (P_3)^{-1}.$$

From this result we obtain,

$$[M_{22} - M_{21} M_{11}^{-1} M_{12}] = [P_3' M_{22} P_3 - P_3' M_{21} M_{11}^{-1} M_{12} P_3]$$

$$= P_3' T_1 P_3,$$

and by (2.3.1), if T_2^0 and T_2^1 are the T_2 matrices for D_0 and D_1

respectively,

$$T_2^o = A_0' M_{11} A_0 - A_0' M_{12} - M_{21} A_0 + M_{22}$$

$$= P_3' A_1' (P_1')^{-1} M_{11} P_1^{-1} A_1 P_3 - P_3' A_1' (P_1')^{-1} M_{12}$$
$$- M_{21} P_1^{-1} A_1 P_3 + M_{22}$$

$$= P_3' A_1 M_{11} A_1 P_3 - P_3' A_1 M_{12} P_3 - P_3' M_{21} A_1 P_3$$
$$+ P_3' M_{22} P_3$$

$$= P_3' T_2^1 P_3.$$

Thus,

$$T_1 = (P_3')^{-1} T_1 (P_3)^{-1} \tag{2.3.2}$$

$$\text{and } T_2^1 = (P_3')^{-1} T_2^o (P_3)^{-1}. \tag{2.3.3}$$

Also, by Lemma 2.2, if L_0 and L_1 are the lack of fit matrices for D_0 and D_1 respectively then

$$L_1 = (P_3')^{-1} L_0 (P_3)^{-1}. \tag{2.3.4}$$

Finally, from (2.3.2), (2.3.3) and (2.3.4), we obtain

$$T_1^{-1} L_1 = P_3 T_1^{-1} (P_3') (P_3')^{-1} L_0 P_3^{-1}$$

$$= P_3 T_1^{-1} L_0 P_3^{-1},$$

$$\text{and } (T_2^1)^{-1} L_1 = P_3 (T_2^o)^{-1} P_3' (P_3')^{-1} L_o P_3^{-1}$$

$$= P_3 (T_2^o)^{-1} L_0 P_3^{-1} .$$

Hence $[(T_1)^{-1} L_1]$ and $[(T_2^1)^{-1} L_1]$ are by definition similar to

$[(T_1)^{-1} L_o]$ and $[(T_2^o)^{-1} L_o]$ respectively, and the results of this theorem follow.

Q.E.D.

Corollary 2.1

For τ_1 or τ_2, the characteristic polynomials of $[T\ L^{-1}]$ for designs D_o and D_1 are identical.

Proof:

This follows immediately from Theorem 2.11, since if H_o and H_1 are any non-singular, similar matrices then H_o^{-1} is similar to H_1^{-1}.

Q.E.D.

Theorem 2.11 and its corollary appear to be a very useful result. They imply that, for τ_1 and τ_2, if D_1 is $\Lambda_1(T)$-optimal, $\Lambda_2(T,0)$-optimal or $\Lambda_3(T,0)$-optimal then the design D_o obtained by

$$D_o = D_1 Q$$

is also optimal provided that Q does not alter the region moments of R and D_o is permissible, i.e., $D_o \varepsilon \Delta$. Furthermore, in the proof of the preceding theorem, we observed that

$$T_2^o = P_3' T_2^1 P_3,$$

$$\text{and} \quad L_o = P_3' L_1 P_3.$$

Then using these results, and the following theorem, it is easily shown that this property also holds for D-optimality, $|L|$-optimality, and $\Lambda_2(T,c)$-optimality and $\Lambda_3(T,c)$-optimality for any positive constant c.

Theorem 2.12

For the non-singular linear transformation, $\underset{\sim}{z} = Q' \underset{\sim}{x}$, if Q is orthogonal then $|P|^2 = 1$, $|P_1|^2 = 1$, and $|P_3|^2 = 1$.

Proof:

In the proof of theorem 2.3, we observed that for any non-singular transformation mapping R_x into R_z,

$$|P|^2 = |M^z| \ / \ |M^x|, \tag{2.3.5}$$

where M^x and M^z are the region moment matrices in the $\underset{\sim}{x}$-variables and $\underset{\sim}{z}$-variables respectively. So let R_x be the hypersphere defined by

$$R_x = \{\underset{\sim}{x} : \underset{\sim}{x}' \underset{\sim}{x} \leq 1\}.$$

Then since Q is orthogonal,

$$R_z = \{\underset{\sim}{z} : \underset{\sim}{z}' \underset{\sim}{z} \leq 1\},$$

and moreover, $M^x = M^z$. This together with (2.3.5) implies that $|P|^2 = 1$. Also since the order of the polynomial is arbitrary, $|P_1|^2 = 1$. Finally, since $|P|^2 = |P_1|^2 \cdot |P_3|^2$, we obtain $|P_3|^2 = 1$.

Q.E.D.

2.4. Effects of Augmenting a Design Upon the $\Lambda(T)$ Criteria

Now let us turn our attention to the effects of augmenting an existing design with one additonal observation. The approach used in this section has been used previously to obtain useful characterizations of D-optimality and to develop algorithms for obtaining D-optimal designs, see Wynn (1970), Dykstra (1971), and Mitchell (1972, 1974).

Now consider the problem of augmenting

$$X = [X_1 : X_2]$$

with one observation taken at

$$\underset{\sim}{x}_*' = (\underset{\sim}{x}_1', \underset{\sim}{x}_2').$$

Since we have the freedom of taking this observation anywhere in the region of interest, the problem is to determine the point in R that optimizes our design criterion.

Let us represent the augmented X matrix by

$$W = \begin{bmatrix} X_1 & \vdots & X_2 \\ & \vdots & \\ \underset{\sim}{x}_1' & \vdots & \underset{\sim}{x}_2' \end{bmatrix} = [W_1 : W_2].$$

For simplicity, we will also use the notation:

$$L_1 = X_2' [I_n - X_1 (X_1' X_1)^{-1} X_1'] X_2,$$

$$L_2 = W_2' [I_{n+1} - W_1 (W_1' W_1)^{-1} W_1'] W_2,$$

$$A_1 = (X_1' X_1)^{-1} X_1' X_2,$$

$$A_2 = (W_1' W_1)^{-1} W_1' W_2,$$

$$\text{and} \quad a = \underset{\sim}{x}_1' (X_1' X_1)^{-1} \underset{\sim}{x}_1.$$

The following lemmas express L_2 and L_2^{-1} in terms of A_1, L_1, and $\underset{\sim}{x}_*$.

<u>Lemma 2.3</u>

$$L_2 = L_1 + \frac{1}{1+a} \cdot (A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2) \cdot (A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)'$$

Proof:

$$\text{Since,} \quad (W_1' W_1)^{-1} = (X_1' X_1 + \underset{\sim}{x}_1 \underset{\sim}{x}_1')^{-1}$$

$$= (X_1' X_1)^{-1} - \frac{1}{1+a} \cdot (X_1' X_1)^{-1} \underset{\sim}{x}_1 \underset{\sim}{x}_1' (X_1' X_1)^{-1},$$

$$L_2 = W_2' W_2 - W_2 W_1 (W_1' W_1)^{-1} W_1' W_2$$

$$= X_2' X_2 + \underset{\sim}{x}_2 \underset{\sim}{x}_2' - (X_2' X_1 + \underset{\sim}{x}_2 \underset{\sim}{x}_1')$$
$$\cdot [(X_1' X_1)^{-1} - \frac{1}{1+a} (X_1' X_1)^{-1} \underset{\sim}{x}_1 \underset{\sim}{x}_1' (X_1' X_1)^{-1}]$$
$$\cdot (X_1' X_2 + \underset{\sim}{x}_1 \underset{\sim}{x}_2')$$

$$= X_2' X_2 - X_2' X_1 (X_1' X_1)^{-1} X_1' X_2 + \underset{\sim}{x}_2 \underset{\sim}{x}_2'$$
$$- \underset{\sim}{x}_2 \underset{\sim}{x}_1' (X_1' X_1)^{-1} \underset{\sim}{x}_1 \underset{\sim}{x}_2' - X_2' X_1 (X_1' X_1)^{-1} \underset{\sim}{x}_1 \underset{\sim}{x}_2'$$
$$+ \frac{1}{1+a} X_2' X_1 (X_1' X_1)^{-1} \underset{\sim}{x}_1 \underset{\sim}{x}_1' (X_1' X_1)^{-1} X_1' X_2$$
$$+ \frac{1}{1+a} X_2' X_1 (X_1' X_1)^{-1} \underset{\sim}{x}_1 \underset{\sim}{x}_1' (X_1' X_1)^{-1} \underset{\sim}{x}_1 \underset{\sim}{x}_2'$$
$$- \underset{\sim}{x}_2 \underset{\sim}{x}_1' (X_1' X_1)^{-1} X_1' X_2$$
$$+ \frac{1}{1+a} \underset{\sim}{x}_2 \underset{\sim}{x}_1' (X_1' X_1)^{-1} \underset{\sim}{x}_1 \underset{\sim}{x}_1' (X_1' X_1)^{-1} X_1' X_2$$
$$+ \frac{1}{1+a} \underset{\sim}{x}_2 \underset{\sim}{x}_1' (X_1' X_1)^{-1} \underset{\sim}{x}_1 \underset{\sim}{x}_1' (X_1' X_1)^{-1} \underset{\sim}{x}_1 \underset{\sim}{x}_2'$$

$$= L_1 + (1-a)\underset{\sim}{x}_2 \underset{\sim}{x}_2' - A_1' \underset{\sim}{x}_1 \underset{\sim}{x}_2' + \frac{1}{1+a} A_1' \underset{\sim}{x}_1 \underset{\sim}{x}_1' A_1$$
$$+ \frac{a}{1+a} A_1' \underset{\sim}{x}_1 \underset{\sim}{x}_2' - \underset{\sim}{x}_2 \underset{\sim}{x}_1' A_1 + \frac{a}{1+a} \underset{\sim}{x}_2 \underset{\sim}{x}_1' A_1$$
$$+ \frac{a^2}{1+a} \underset{\sim}{x}_2 \underset{\sim}{x}_2'$$

$$= L_1 + \frac{1}{1+a} \underset{\sim}{x}_2 \underset{\sim}{x}_2' + \frac{1}{1+a} A_1' \underset{\sim}{x}_1 \underset{\sim}{x}_1' A_1$$
$$+ \left(\frac{1}{1+a} - 1\right) [A_1' \underset{\sim}{x}_1 \underset{\sim}{x}_2' + \underset{\sim}{x}_2 \underset{\sim}{x}_1' A_1]$$

$$= L_1 + \frac{1}{1+a} (A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2) \cdot (A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)'.$$

Q.E.D.

Lemma 2.4

$$L_2^{-1} = L_1^{-1} - \frac{L_1^{-1}(A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)(A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)' L_1^{-1}}{1 + a + (A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)' L_1^{-1}(A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)}$$

Proof:

This is an immediate consequence of the preceding lemma and the fact that for any vector $\underset{\sim}{Y}$ and non-singular matrix H,

$$(H + \underset{\sim}{Y}\underset{\sim}{Y}')^{-1} = H^{-1} - \frac{H^{-1}\underset{\sim}{Y}\underset{\sim}{Y}'H^{-1}}{1 + \underset{\sim}{Y}' H^{-1} \underset{\sim}{Y}} .$$

Q.E.D.

The following theorem provides a useful expression for $\Lambda_2(T,c)$-optimality, if τ is design independent.

Theorem 2.13

$$Tr[T^{-1} L_2] = Tr[T^{-1} L_1] + \frac{1}{1+a}(A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)' T^{-1}(A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)$$

Proof: Using Lemma 2.3,

$$\begin{aligned} Tr[T^{-1} L_2] &= Tr[T^{-1}\{L_1 + \frac{1}{1+a}(A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)(A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)'\}] \\ &= Tr[T^{-1} L_1] + \frac{1}{1+a} Tr[T^{-1}(A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)(A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)'] \\ &= Tr[T^{-1} L_1] + \frac{1}{1+a}(A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)' T^{-1}(A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2). \end{aligned}$$

Q.E.D.

Hence, if τ is not design dependent, for the $\Lambda_2(T,c)$ criterion, we simply select the point that maximizes

$$(1 + \underset{\sim}{x}_1' (X_1' X_1)^{-1} \underset{\sim}{x}_1)^{-1} \cdot (A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)' T^{-1}(A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2).$$

The following theorem provides a similar expression for $|L|$-optimality.

Theorem 2.14

$$|L_2| = |L_1| \cdot [1 + \frac{1}{1+a} (A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)' L_1^{-1} (A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)]$$

Proof:

Using Lemma 2.3 and the fact that, for any non-singular matrix H and vector $\underset{\sim}{Y}$,

$$\frac{|H + \underset{\sim}{Y} \underset{\sim}{Y}'|}{|H|} = 1 + \underset{\sim}{Y}' H^{-1} \underset{\sim}{Y},$$

$$|L_2| = |L_1 + \frac{1}{1+a} (A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2) (A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)'|$$

$$= |L_1| \cdot [1 + \frac{1}{1+a} (A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)' L_1^{-1} (A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)].$$

Q.E.D.

This theorem implies that we can maximize $|L_2|$ given L_1 by taking our observation at the point that maximizes

$$\frac{1}{1+a} (A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2)' L_1^{-1} (A_1' \underset{\sim}{x}_1 - \underset{\sim}{x}_2).$$

Similar results may hold for design dependent τ (such as τ_2), but we have not pursued them here because of the extensive algebra that appears to be necessary.

III. AN EXAMINATION OF THE VARIANCE, BIAS AND POWER PROPERTIES OF OF $\Lambda(T_1)$-OPTIMAL DESIGNS FOR CUBOIDAL REGIONS OF INTEREST

3.1. Introduction

In Section 1.2.2, τ_1 was introduced as a measure of the inherent departure of the true surface $\eta(\underset{\sim}{x})$ from an assumed class of models $\mathcal{M}$. We defined τ_1, the average squared deviation of the true model from the best fitting model of the assumed class of models, by

$$\tau_1 = \sigma^{-2}\,\Omega \int_R [\eta_1^*(\underset{\sim}{x}) - \eta(\underset{\sim}{x})]^2 \; dx_1 \cdot dx_2 \cdots dx_k$$

where $\eta_1^*(\underset{\sim}{x})$ is the response at the point $\underset{\sim}{x}$ for the model in $\mathcal{M}$ that minimizes τ_1 (the "best" model). We indicated that

$$\tau_1 = \sigma^{-2}\,\underset{\sim}{\beta}_2'\, T_1\, \underset{\sim}{\beta}_2,$$

where the elements of the $p_2 \times p_2$ matrix

$$T_1 = [M_{22} - M_{21}\, M_{11}^{-1}\, M_{12}]$$

are functions of the region of interest and not of the design.

In Section 2.1, we developed the $\Lambda(T)$ criteria. They were motivated primarily for experiments in which the detection of the deviation of the true response surface from a model is of fundamental importance. However, it is important to determine if the designs that they select have adequate variance properties for both the lower and higher order models and adequate fitted bias properties for the lower order model. In this chapter, we will attempt to characterize the variance, bias and power properties of the $\Lambda_1(T_1)$-optimal, $\Lambda_2(T_1,c)$-optimal, and $\Lambda_3(T_1,c)$-optimal designs for $c = 0$ and $c = \frac{1}{2}$. The general approach will be to compare the properties of these designs with those of designs generally considered to have very good variance, bias, or power properties. Appendix B contains a summary of the design characteristics that will be examined in this chapter.

For the variance comparison, we will use D-optimal designs for both the lower and higher order models. These designs will be obtained using the computational algorithm described in Appendix A. They will be used to calculate the "D-efficiencies" E_1 and E_2, which are defined as follows for any given design D_0:

$$E_1 = \left[\frac{|X_1' X_1|_{D_0}}{\underset{D \in \Delta}{\text{Max}} |X_1' X_1|} \right]^{p_1^{-1}} \tag{3.1.1}$$

$$E_2 = \left[\frac{|X' X|_{D_0}}{\underset{D \in \Delta}{\text{Max}} |X' X|} \right]^{(p_1 + p_2)^{-1}} . \tag{3.1.2}$$

E_1 will be referred to as the D-efficiency for the lower order model, and E_2 will be referred to as the D-efficiency for the higher order model.

Minimum bias designs will be used for the bias comparison. Since minimum bias designs are not unique, we must impose secondary conditions for their selection. Our approach is to attempt to select minimum bias designs that exhibit optimum variance and power properties. This is not always an easy task. Hence, we will sometimes examine more than one minimum bias design and use minimum bias designs contained in the literature, when available.

Of course, as far as a comparison of the power properties for the lack of fit test are concerned, $\Lambda(T)$-optimal designs are considered optimum. However, it has been suggested that the designs that maximize $|L|$ possess very good power properties (see Atkinson (1972)). So, we will include these designs in the comparisons; we will refer to them as the $|L|$-optimal designs. Like the D-optimal designs, the $|L|$-optimal designs were found using the computational algorithm described in Appendix A.

Because of the invariance results of Chapter II, all of these designs are invariant to non-singular linear transformations. Thus, although we will restrict our region of interest to the hypercube defined by

$$-1 \leq x_i \leq 1, \; i = 1, 2, \ldots, k; \tag{3.1.3}$$

the results of this chapter apply to any region of interest that can be expressed as a non-singular linear transformation of (3.1.3).

The results of this chapter are primarily empirical. We will restrict our attention not only to cuboidal regions of interest, but also to the following two cases:

1. the proposed model is a first order polynomial while the true model is a second order polynomial, (3.1.4)

and 2. the proposed model is a second order polynomial while the true model is a third order polynomial. (3.1.5)

For both of these cases, T_1 is a diagonal matrix. For case (3.1.4), the diagonal elements of T_1 are:

$$\begin{aligned} &1 / 9 \text{ for the } \beta_{ij},\ i \neq j, \text{ terms,} \\ &\text{and } 4 / 45 \text{ for the } \beta_{ii} \text{ terms.} \end{aligned} \qquad (3.1.6)$$

For case (3.1.5), the diagonal elements of T_1 are:

$$\begin{aligned} &1 / 27 \text{ for the } \beta_{ijk},\ i \neq j \neq k, \text{ terms,} \\ &4 / 135 \text{ for the } \beta_{iij}, \beta_{iji}, \beta_{jii},\ i \neq j, \text{ terms,} \\ &\text{and } 4 / 175 \text{ for the } \beta_{iii} \text{ terms.} \end{aligned} \qquad (3.1.7)$$

3.2. One-Factor $\Lambda(T_1)$-Optimal Designs for Polynomial Models and $c = 0, \frac{1}{2}$

In this section, we will examine one-factor $\Lambda(T_1)$-optimal designs. The closed interval $[-1, 1]$ is used as the region of interest; however, because of the invariance results of Section 2.2, the results of this section apply to any region of interest of the form $[a, b]$, where $a < b$. We will examine designs for the following cases: (1) first order vs. second order polynomial models and $n = 5, 9$; and (2) second order vs. third order polynomial models and $n = 6, 10$.

For both of these cases, the $\underset{\sim}{\beta}_2$-space is one-dimensional, and the $\Lambda(T_1)$ criteria can be summarized as:

1. $\Lambda_1(T_1)$-optimality-- $\underset{D \in \Delta}{\text{Max}}\ L / T_1$,
2. $\Lambda_2(T_1,c)$-optimality-- $\underset{D \in \Delta}{\text{Max}}\ L / T_1^{1+c}$

and 3. $\Lambda_3(T_1,c)$-optimality-- $\underset{D \, \varepsilon \, \Delta}{\text{Max}} \; L^{1+c} / T_1$, where $c \geq 0$.

Since T_1 is not influenced by the design, all of these criteria are equivalent to $|L|$-optimality. We simply select designs that maximize the scalar L. Consequently, in this section, we will refer to these criteria collectively as $\Lambda(T_1)$-optimality. Note that if T were not independent of the design, the $\Lambda(T)$ criteria would be distinct.

3.2.1. One-Factor $\Lambda(T_1)$-Optimal Designs for First Order vs. Second Order Polynomial Models and n = 5, 9

First let us consider the case when the proposed model is a first order polynomial,

$$\eta_1(x) = \beta_0 + x\,\beta_1,$$

and the true model is second order,

$$\eta(x) = \beta_0 + x\,\beta_1 + x^2\beta_{11}.$$

In general, since L is a function of n variables, it is difficult to maximize analytically. By using a design optimization algorithm, however, it is easily optimized for reasonable values of n. We will examine this case for two values of n, n = 5 and n = 9.

The minimum bias designs that are presented in this section were selected after examining all minimum bias designs of the form:

$$D = \begin{bmatrix} a\,\underset{\sim}{1} \\ \hline -a\,\underset{\sim}{1} \\ \hline \underset{\sim}{0} \end{bmatrix} \begin{matrix} \} \; n_1 \text{ points} \\ \} \; n_1 \text{ points} \\ \} \; n_2 \text{ points} \end{matrix}$$

for $a^2 \leq 1$ and $n_1 = 1, 2, \ldots, (n-1)/2$. The minimum bias designs for n = 5 and n = 9 that are presented had the best variance and the best power properties among all minimum bias designs of this form.

3.2.1.1. The n = 5 Designs.--The n = 5 designs, and some of their properties, are contained in Table 3.1. The notation (:) denotes a replication factor. For example,

$$[\pm 1.0\ (2),\ 1.0]$$

is abbreviated notation for the design

$$[+1.0,\ +1.0,\ -1.0,\ -1.0,\ +1.0].$$

The D-efficiencies listed in Table 3.1 were computed using the values of the determinants associated with the D-optimal designs given in this table. These determinants are:

1. $|n^{-1} X_1' X_1| = .96$ for the first order D-optimal design,

and 2. $|n^{-1} X' X| = .128$ for the second order D-optimal design.

Table 3.1 indicates that the $\Lambda(T_1)$-optimal design for this case has a fairly high D-efficiency for the second order polynomial model, but a somewhat low D-efficiency for the first order model. The average variances of $\hat{\eta}_1(\underset{\sim}{x})$ and $\hat{\eta}(\underset{\sim}{x})$ (V_1 and V_2) for the $\Lambda(T_1)$-optimal design indicate that it does have excellent variance properties for the second order polynomial model. In fact, the $\Lambda(T_1)$-optimal design has a smaller average variance for the second order polynomial, V_2, than either the 2nd order D-optimal design or the minimum bias design.

As far as the bias is concerned, the T_2 column indicates that the $\Lambda(T_1)$-optimal design is nearly minimum bias. This is illustrated in Figure 3.1. Notice that for this case, the D-optimal designs have rather poor bias properties.

TABLE 3.1.

A Comparison of Some Characteristics of the One-Factor $\Lambda(T_1)$-Optimal Design for First Order vs. Second Order Models and n = 5.

Design	n^{-1} L	T_2	Standardized Average Variances V_1	V_2	D-Efficiencies E_1	E_2
1st Order D-Optimal [± 1.0 (2), 1.0]	.00000	.533333	1.3889	∞	1.0000	1.0000
2nd Order D-Optimal [± 1.0 (2), 0.0]	.16000	.306667	1.4167	3.3333	0.9129	1.0000
Minimum Bias [± .912871, 0.0 (3)]	.16667	.088889	2.0000	2.5333	0.5893	0.7571
$\Lambda(T_1)$-Optimal [± 1.0, 0.0 (3)]	.24000	.093333	1.8333	2.2222	0.6455	0.9086

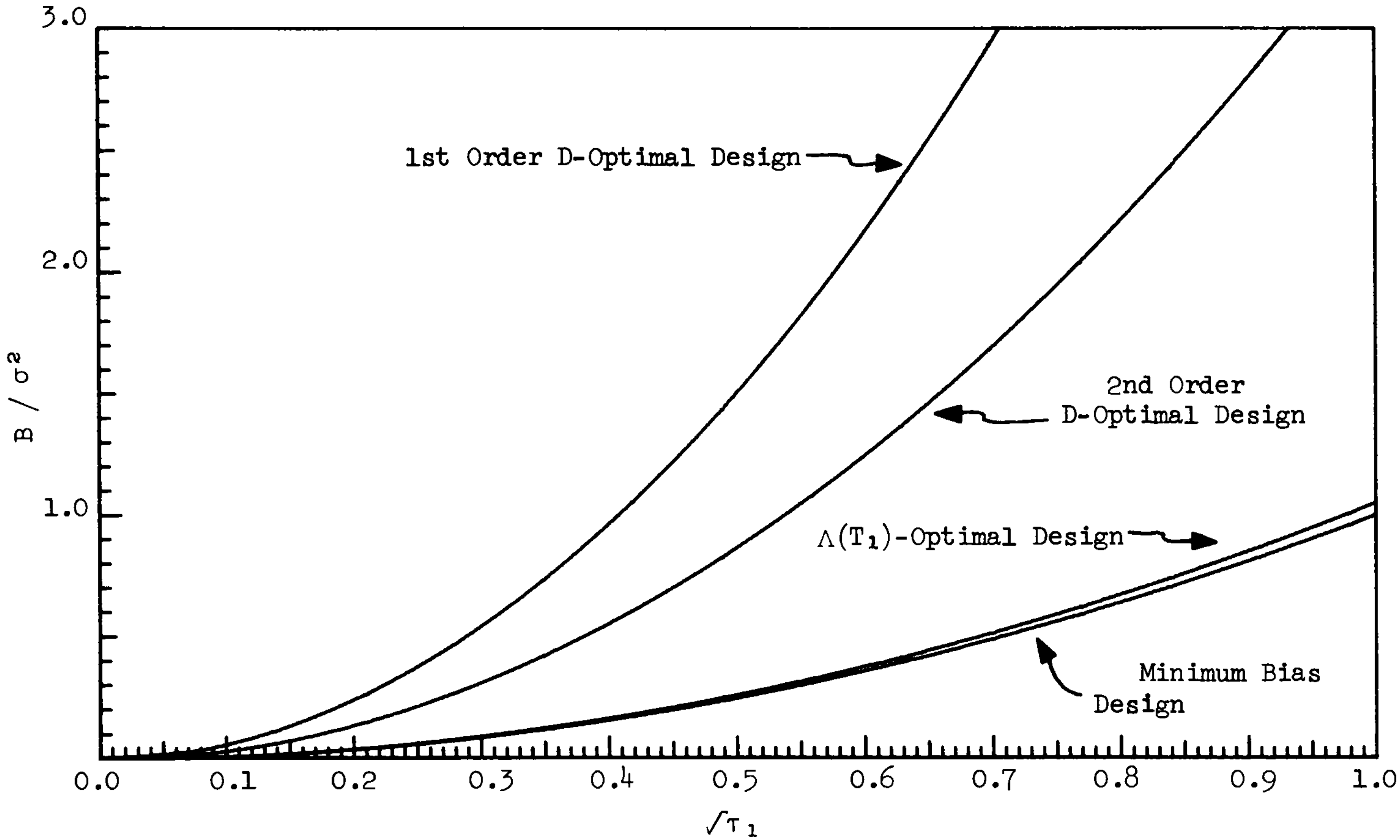


Figure 3.1. A Comparison of the Bias Functions for One-Factor $\Lambda(T_1)$-Optimal Designs for First Order vs. Second Order Models and $n = 5$

The power of the lack of fit test for these designs is illustrated in Figure 3.2 for $\alpha = .05$ (α is the probability of rejecting H_0 when H_0 is correct). These power curves are based upon an F-test in which the residual mean square for the higher order model is used in the denominator. When the $\underset{\sim}{\beta}_2$-space is one-dimensional and the T matrix is design independent, as it is in this section, the $\Lambda(T)$ criteria simply select the design with the highest power curve.

For this case, it appears that the $\Lambda(T_1)$-optimal design has exceptionally good properties. It has the best power properties; it is nearly minimum bias, and it has excellent variance properties.

3.2.1.2. The n = 9 Designs.--The n = 9 designs and some of their properties are given in Table 3.2. The standardized determinants for the D-optimal designs listed in this table are:

1. $|n^{-1} X_1' X_1| = .98765$ for the first order D-optimal design,

and 2. $|n^{-1} X' X| = .14400$ for the second order D-optimal design.

This table appears to be very similar to Table 3.1, for the n = 5 designs. The $\Lambda(T_1)$-optimal design for n = 9 has a high D-efficiency for the second order model, and again, the $\Lambda(T_1)$-optimal design has the smallest average variance for prediction of the second order model.

The bias and power functions for these designs are illustrated in Figures 3.3 and 3.4 respectively. The power properties of the $\Lambda(T_1)$-optimal design are optimum, and again, it appears that the $\Lambda(T_1)$-optimal design is nearly minimum bias.

As we observed for the n = 5, $\Lambda(T_1)$-optimal design, it appears that the n = 9, $\Lambda(T_1)$-optimal design has exceptionally good properties.

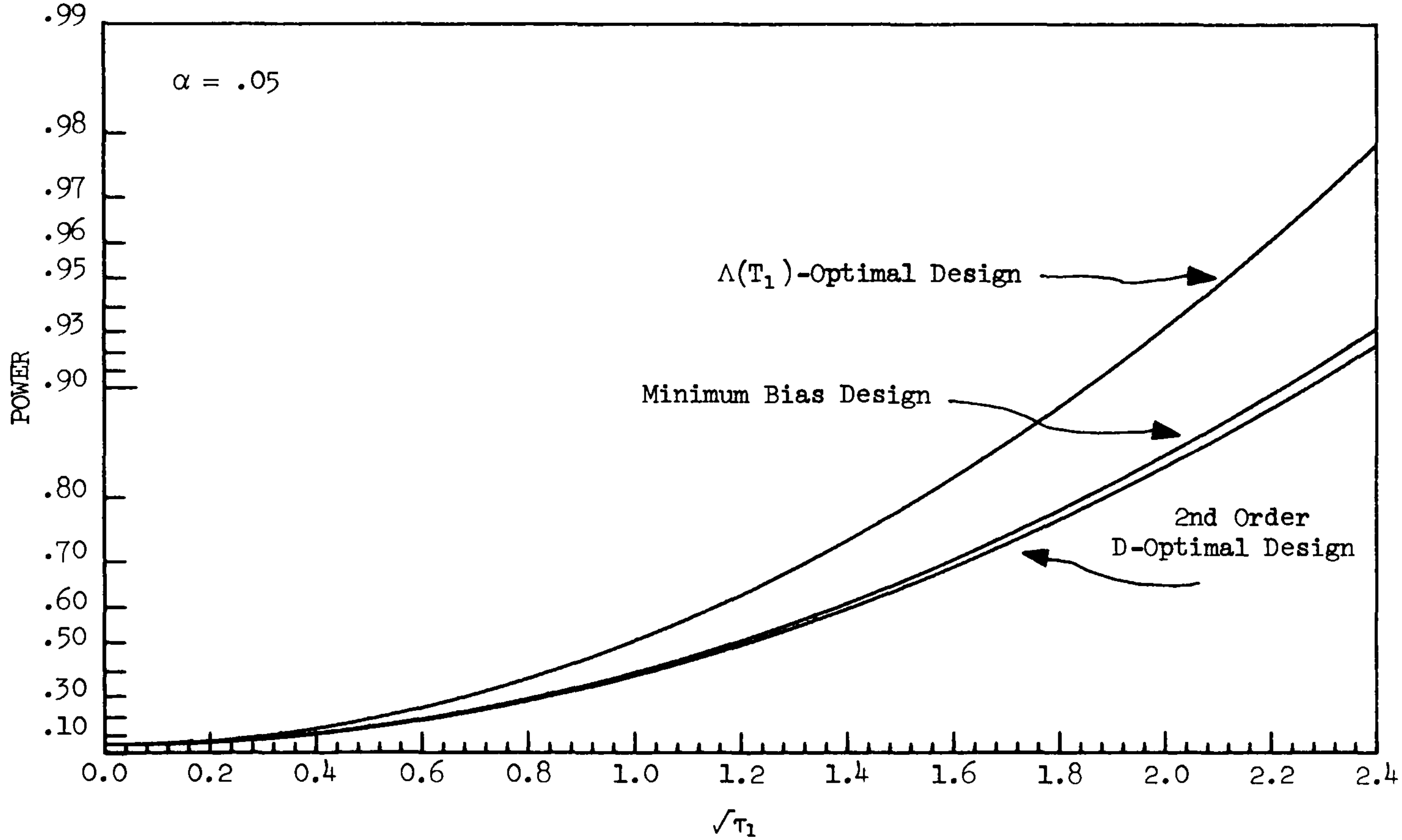


Figure 3.2. A Comparison of the Power Functions for One-Factor $\Lambda(T_1)$-Optimal Designs for First Order vs. Second Order Models and n = 5

TABLE 3.2.

A Comparison of Some Characteristics of the One-Factor $\Lambda(T_1)$-Optimal Design for First Order vs. Second Order Models and $n = 9$.

			Standardized Average Variances		D-Efficiencies	
Design	$n^{-1} L$	T_2	V_1	V_2	E_1	E_2
1st Order D-Optimal [± 1.0 (4), 1.0]	.00000	.533333	1.3500	∞	1.0000	0.0000
2nd Order D-Optimal [± 1.0 (3), 0.0 (3)]	.22222	.200000	1.5000	2.4000	0.8216	1.0000
Minimum Bias [± .866025 (2), 0.0 (5)]	.13889	.088889	2.0000	2.6400	0.5809	0.6786
$\Lambda(T_1)$-Optimal [± 1.0 (2), 0.0 (5)]	.24691	.101235	1.7500	2.1600	0.6708	0.9048

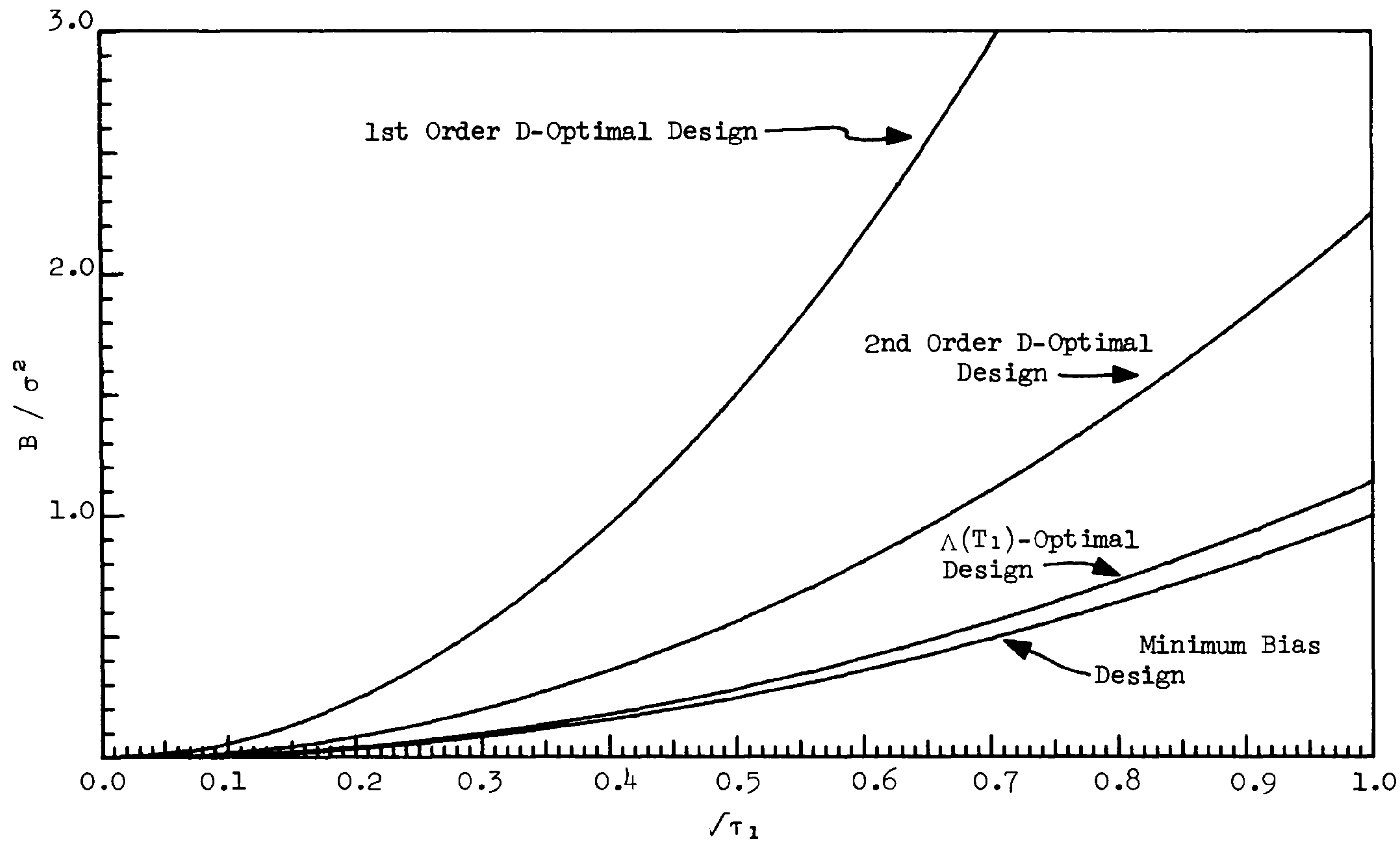


Figure 3.3. A Comparison of the Bias Functions for One-Factor $\Lambda(T_1)$-Optimal Designs for First Order vs. Second Order Models and $n = 9$

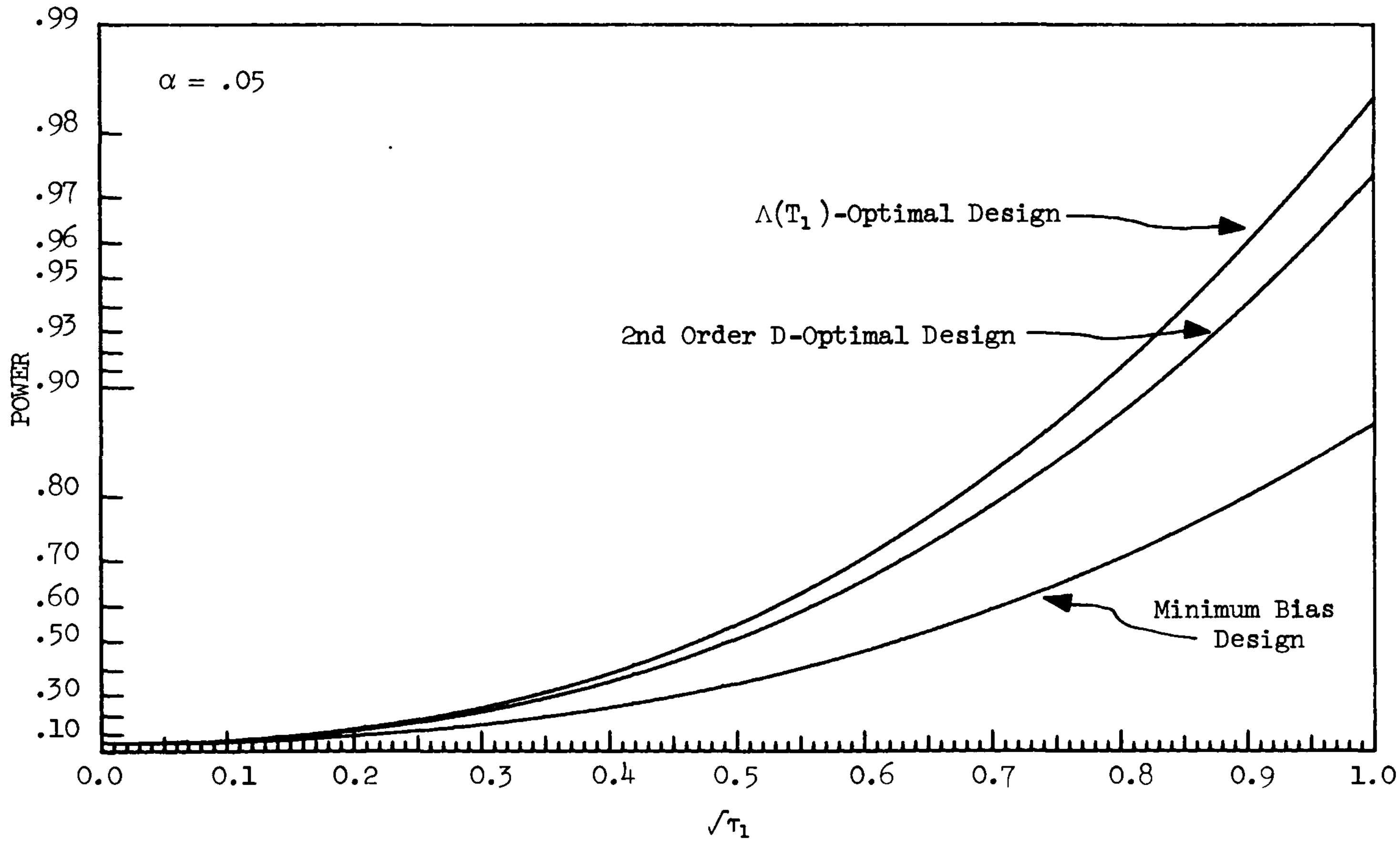


Figure 3.4. A Comparison of the Power Functions for One-Factor $\Lambda(T_1)$-Optimal Designs for First Order vs. Second Order Models and $n = 9$

It has the best power properties; it is nearly minimum bias, and it has excellent variance properties.

3.2.2. One-Factor $\Lambda(T_1)$-Optimal Designs for Second Order vs. Third Order Polynomial Models and n = 6, 10

Now let us examine the $\Lambda(T_1)$-optimal designs when the proposed model is second order,

$$\eta_1(x) = \beta_0 + x\,\beta_1 + x^2\beta_{11},$$

and the true model is third order,

$$\eta(x) = \beta_0 + x\,\beta_1 + x^2\beta_{11} + x^3\beta_{111}.$$

As in the previous section, the $\underset{\sim}{\beta}_2$-space is one-dimensional, and consequently, the $\Lambda(T_1)$ criteria are all equivalent to $|L|$-optimality. Again, we will examine this case for two value of n, n = 6 and n = 10.

The minimum bias designs that are presented in this section were selected after examining all one-factor, second order vs. third order minimum bias designs of the form:

$$D = \begin{bmatrix} a\,\underset{\sim}{1} \\ \hline -a\,\underset{\sim}{1} \\ \hline \frac{1}{2}\,\underset{\sim}{1} \\ \hline -\frac{1}{2}\,\underset{\sim}{1} \end{bmatrix} \begin{matrix} \}\, n_1 \text{ points} \\ \}\, n_1 \text{ points} \\ \}\, n_2 \text{ points} \\ \}\, n_2 \text{ points} \end{matrix}$$

for $n_1 = 1, 2, \ldots, (\frac{1}{2}n-1)$ and $a^2 \leq 1$. The minimum bias designs that are presented for n = 6 and n = 10 had the best variance and the best power properties among all minimum bias designs of this form.

3.2.2.1. The n = 6 Designs.--Table 3.3 contains the n = 6 designs and some of their characteristics. The value of the standardized determinants for the D-optimal designs listed in this table are:

1. $|n^{-1} X_1' X_1| = .14815$ for the second order D-optimal design,

and 2. $|n^{-1} X' X| = .40454 \times 10^{-2}$ for the third order D-optimal design.

For n = 6, there are two distinctly different third order D-optimal designs. Third order D-optimal Design (1) appears to be superior to third order D-optimal Design (2) in all respects except E_1, the D-efficiency for the second order polynomial.

The variance characteristics for the $\Lambda(T_1)$-optimal design seem to be very good. In fact, the D-efficiency of this design for the third order polynomial is very high, and although the D-efficiency for the second order polynomial seems somewhat low, it is only slightly lower than the efficiency of D-optimal Design (1) for the second order polynomial.

The bias properties of these designs are illustrated in Figure 3.5, and the power properties of these designs are illustrated in Figure 3.6 for $\alpha = .05$. As we noted in the previous section, again the $\Lambda(T_1)$-optimal design appears to have very good bias properties.

3.2.2.2. The n = 10 Designs.--Table 3.4 contains the n = 10 designs and some of their characteristics. The value of the standardized determinants for the D-optimal designs listed in this table are:

1. $|n^{-1} X_1' X_1| = .144$ for the second order D-optimal design,

and 2. $|n^{-1} X' X| = .47186 \times 10^{-2}$ for the third order D-optimal

TABLE 3.3.

A Comparison of Some Characteristics of the One-Factor $\Lambda(T_1)$-Optimal Design for Second Order vs. Third Order Models and $n = 6$.

Design	$n^{-1}L$	T_2	Standardized Average Variances V_1	V_2	D-Efficiencies E_1	E_2
2nd Order D-Optimal [$\pm$ 1.0 (2), 0.0 (2)]	.000000	.076190	2.40000	∞	1.0000	0.0000
3rd Order D-Optimal--Design (1) [$\pm$ 1.0, $\pm\sqrt{.2}$ (2)]	.060952	.032653	2.46429	3.00000	0.7652	1.0000
3rd Order D-Optimal--Design (2) [$\pm$ 1.0, 1.0, $\sqrt{.2}$, $-\sqrt{.2}$ (2)]	.047407	.055121	2.69445	3.85714	0.8320	1.0000
Minimum Bias [$\pm$ .902652, $\pm$ .5 (2)]	.032945	.022857	3.16991	3.86370	0.5941	0.7092
$\Lambda(T_1)$-Optimal [$\pm$ 1.0, $\pm$ .5 (2)]	.062500	.030357	2.60000	3.08571	0.7500	0.9913

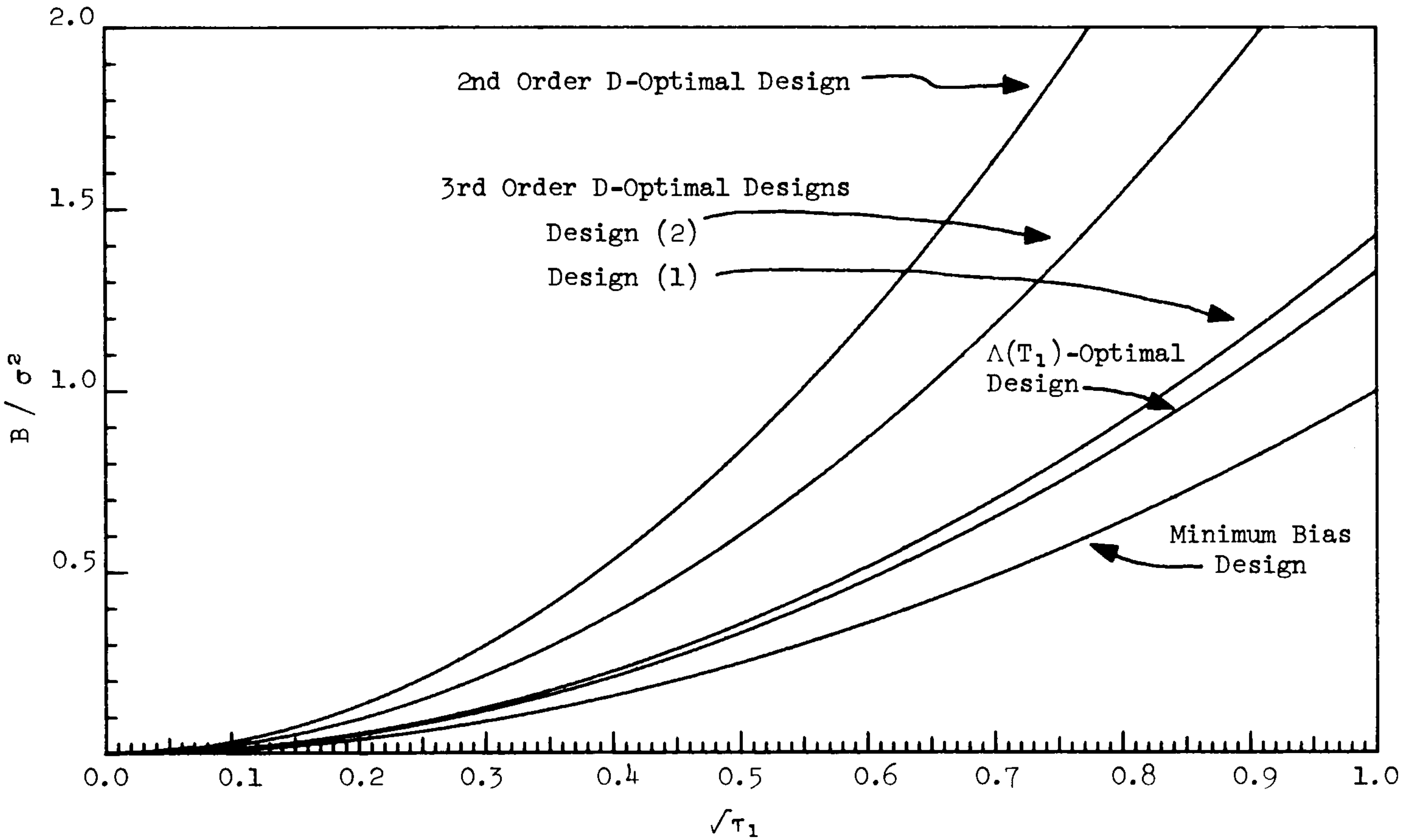


Figure 3.5. A Comparison of the Bias Functions for One-Factor $\Lambda(T_1)$-Optimal Designs for Second Order vs. Third Order Models and $n = 6$

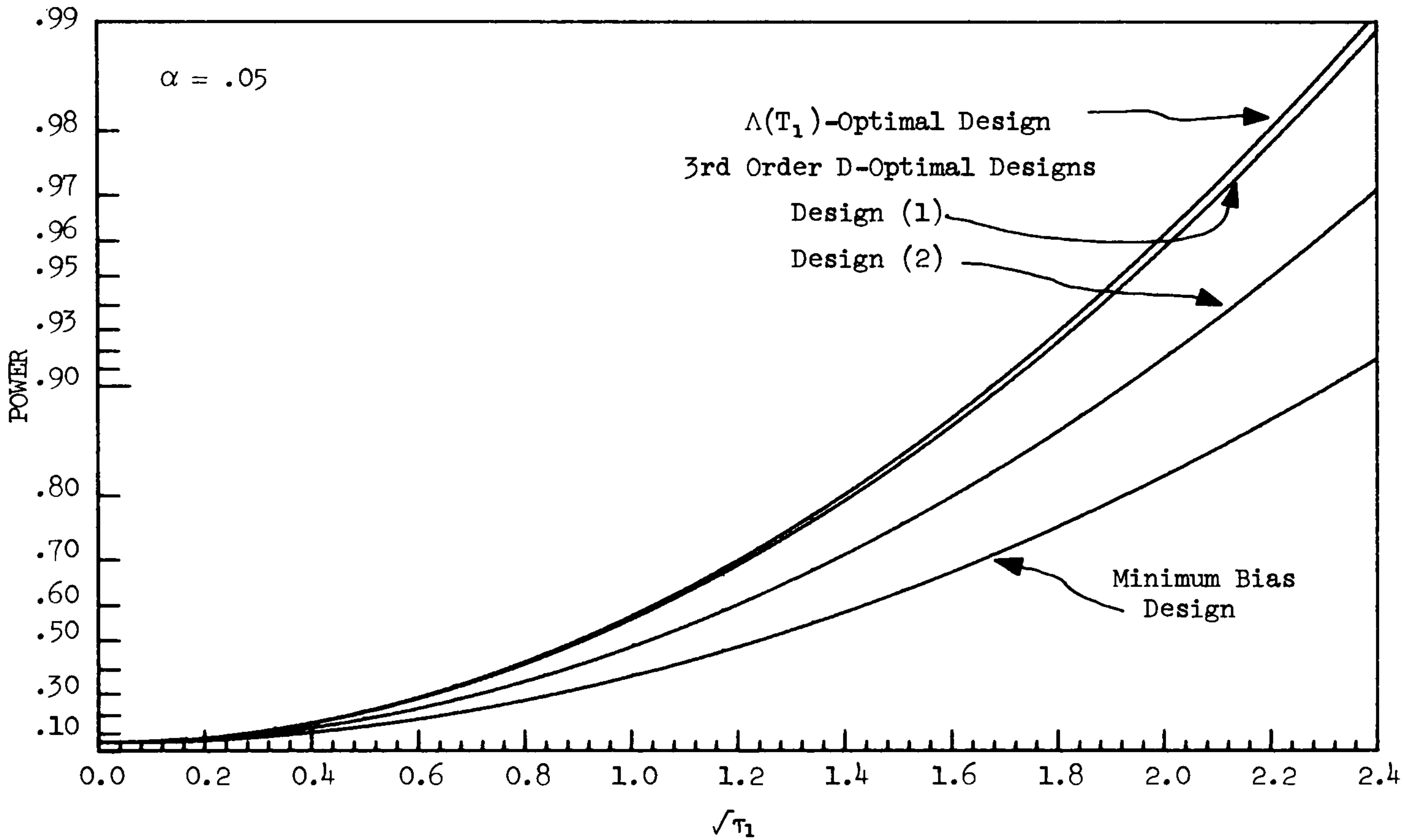


Figure 3.6. A Comparison of the Power Functions for One-Factor $\Lambda(T_1)$-Optimal Designs for Second Order vs. Third Order Models and n = 6

TABLE 3.4. A Comparison of Some Characteristics of the One-Factor $\Lambda(T_1)$-Optimal Design for Second Order vs. Third Order Models and n = 10.

			Standardized Average Variances		D-Efficiencies	
Design	$n^{-1} L$	T_2	V_1	V_2	E_1	E_2
2nd Order D-Optimal [$\pm$ 1.0 (3), 0.0 (4)]	.000000	.076190	2.2222	∞	1.0000	0.0000
†3rd Order D-Optimal--Design (1) [$\pm$ 1.0 (2), $\pm\sqrt{.2}$ (3)	.059077	.038321	2.4466	3.0952	0.8216	1.0000
†3rd Order D-Optimal--Design (2) [$\pm$ 1.0 (3), $\pm\sqrt{.2}$ (2)]	.045177	.054045	2.8513	4.0476	0.8985	1.0000
†3rd Order D-Optimal--Design (3) [$\pm$ 1.0 (2), 1.0, $\pm\sqrt{.2}$ (2), $\sqrt{.2}$]	.051200	.049642	2.6019	3.5714	0.8618	1.0000
Minimum Bias [$\pm$ .981491, $\pm$ .5]	.049933	.022857	2.9840	3.4417	0.6055	0.7626
$\Lambda(T_1)$-Optimal [$\pm$ 1.0, $\pm$ .513578 (3)]	.061465	.035054	2.6693	3.2396	0.7960	0.9862

† There are three distinctly different 3rd order, one-factor D-optimal designs for n = 10.

design.

For this case, there are three D-optimal designs for the third order polynomial. D-optimal Design (1) appears to be better than either of the other two third order D-optimal designs except for the D-efficiency for fitting the second order polynomial, E_1. Furthermore, except for E_1, D-optimal Design (2) appears to be superior to D-optimal Design (3) for the third order model.

Again, the variance properties of the $\Lambda(T_1)$-optimal design are very good for the third order model and acceptable for the second order model. The bias and power functions for these designs are illustrated in Figures 3.7 and 3.8 respectively. These figures seem to be very similar to Figures 3.5 and 3.6 for the n = 6 designs.

3.3. Two-Factor $\Lambda(T_1)$-Optimal Designs for Polynomial Models and $c = 0, \frac{1}{2}$

In the previous section, we examined the variance, bias and power characteristics of one-factor $\Lambda(T_1)$-optimal designs for first order vs. second order and second order vs. third order polynomials. We found that the $\Lambda(T_1)$-optimal designs appeared to have good variance, as well as power, properties for both values of n considered. Yet for these cases, the $\underset{\sim}{\beta}_2$-space was one-dimensional which together with the design independence of T_1 made all of the $\Lambda(T_1)$ criteria equivalent to $|L|$-optimality. Hence it is of interest to examine the properties of these designs for a multi-dimensional $\underset{\sim}{\beta}_2$-space.

In this section, we will examine the properties of two-factor

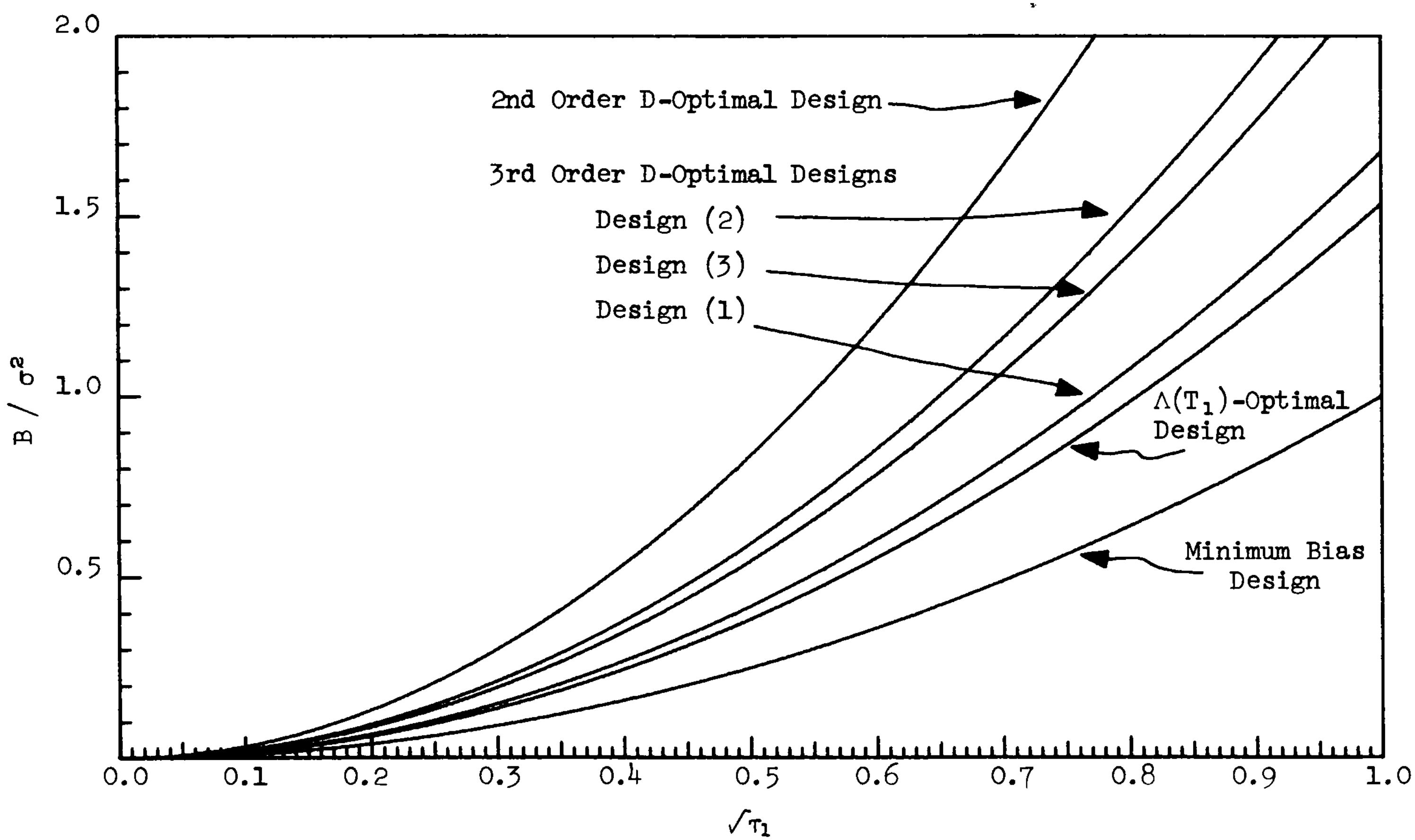


Figure 3.7. A Comparison of the Bias Functions for One-Factor $\Lambda(T_1)$-Optimal Designs for Second Order vs. Third Order Models and n = 10

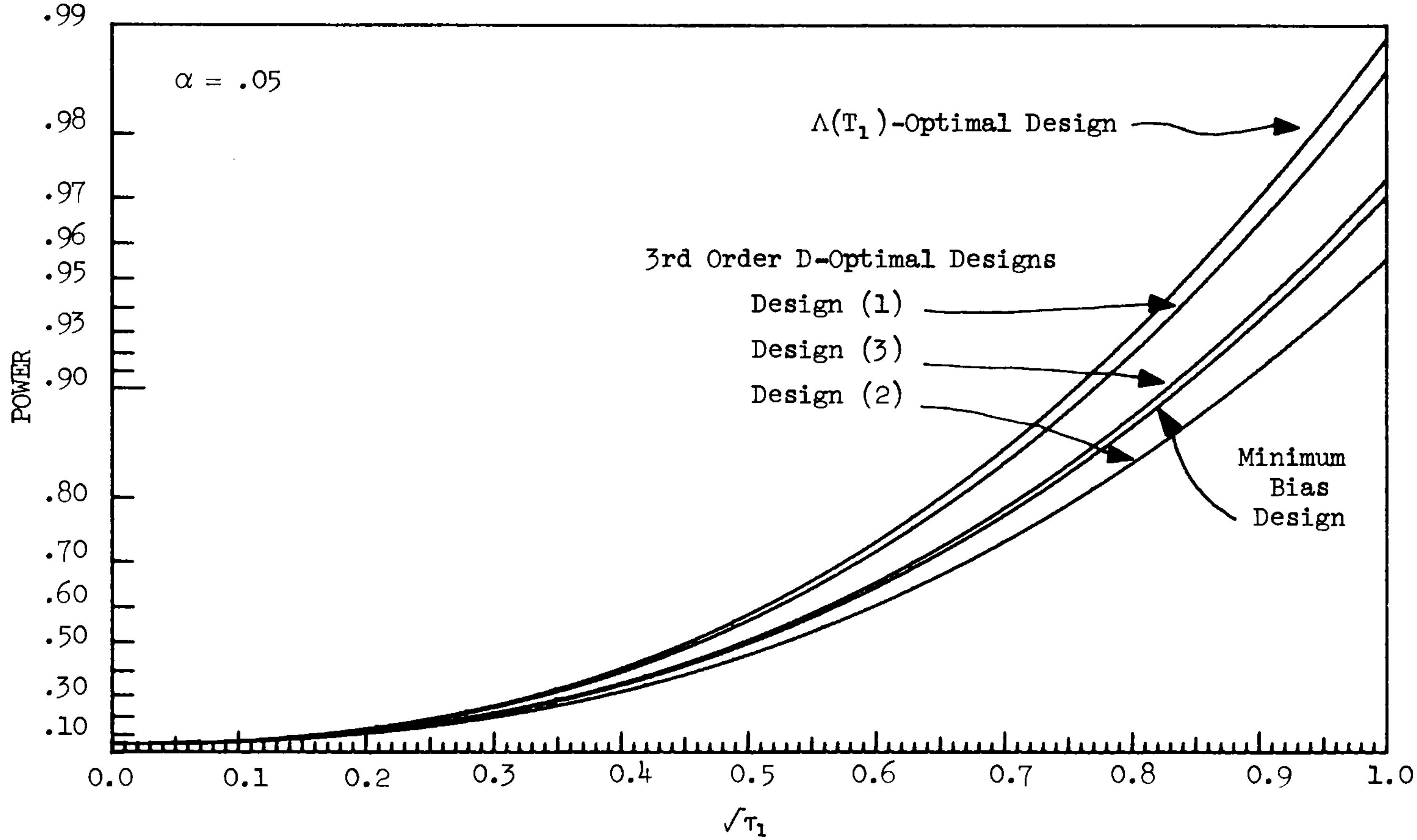


Figure 3.8. A Comparison of the Power Functions for One-Factor $\Lambda(T_1)$-Optimal Designs for Second Order vs. Third Order Models and n = 10

$\Lambda_1(T_1)$-optimal, $\Lambda_2(T_1,c)$-optimal, and $\Lambda_3(T_1,c)$-optimal designs for $c = 0$ and $c = \frac{1}{2}$. Since T_1 is not influenced by the design, the value of c does not effect the selection of a $\Lambda_2(T_1,c)$-optimal design. Consequently, $\Lambda_2(T_1,0)$-optimality is equivalent to $\Lambda_2(T_1,\frac{1}{2})$-optimality, and we will use the abbreviated notation $\Lambda_2(T_1)$ for $\Lambda_2(T_1,c)$.

The region of interest will now be the square defined by

$$-1 \leq x_i \leq 1, \ i = 1, 2;$$

and the β_2-space will be multi-dimensional. The lack of fit and T matrices are no longer scalars, and in general, none of the $\Lambda(T)$ criteria, nor $|L|$-optimality, are equivalent. Hence we now have a rather large choice of optimal designs.

Since these designs are difficult to obtain and evaluate, we will concentrate our interest on the following two cases:

1. the proposed model is a first order polynomial while the true model is a second order polynomial and $n = 6$,

and 2. the proposed model is a second order polynomial while the true model is a third order polynomial and $n = 10$.

We will be examining minimum-point designs for the higher order model, as there are 6 parameters in the second order polynomial and ten parameters in the third order polynomial. Although the $\Lambda_2(T_1,c)$ criterion does not require a non-singular lack of fit matrix, $\Lambda_1(T_1)$-optimality, $\Lambda_3(T_1,c)$-optimality, and $|L|$-optimality do. Since we intend to collectively examine all of the $\Lambda(T_1)$ criteria, this requires us to examine designs with at least enough observations to fit the higher order model.

Since, in this section, the $\underset{\sim}{\beta}_2$-space is multi-dimensional, we cannot determine the average squared bias,

$$B = \Omega \int_R \{E[\hat{\eta}_1(\underset{\sim}{x})] - \eta(\underset{\sim}{x})\}^2 \, dx_1 \cdot dx_2 \cdots dx_k,$$

or the non-centrality parameter

$$\lambda = \sigma^{-2} \underset{\sim}{\beta}_2' \, L \, \underset{\sim}{\beta}_2,$$

without knowing $\underset{\sim}{\beta}_2$. Consequently, we will examine the following two bias and power characteristics:

1. the maximum value of B / σ^2 and minimum value of λ for $\tau_1 = \delta$,

and 2. the average value of B / σ^2 and λ for $\tau_1 = \delta$.

By Theorem 2.1, for $\tau_1 = \delta$, the maximum value of B / σ^2 is $\delta \cdot Ch_{max}[T_1^{-1} T_2]$ and the minimum value of λ is $\delta \cdot Ch_{min}[T_1^{-1} L]$. Also, by (2.1.17) of Theorem 2.2, for $\tau_1 = \delta$, the average value of B / σ^2 and λ are $p_2^{-1} \delta \cdot Tr[T_1^{-1} T_2]$ and $p_2^{-1} \delta \cdot Tr[T_1^{-1} L]$, respectively. In addition, we will examine the relationship between these bias properties and the Euclidean norm of the T_2 matrix,

$$\|T_2\| = \left[\sum_{i,j} t_{ij}^2 \right]^{\frac{1}{2}} .$$

3.3.1. Two-Factor $\Lambda(T_1)$-Optimal Designs for First Order vs. Second Order Polynomial Models and n = 6

First let us examine the two-factor $\Lambda(T_1)$-optimal designs when the proposed model is a first order polynomial,

$$\eta_1(\underset{\sim}{x}) = \beta_0 + x_1 \beta_1 + x_2 \beta_2,$$

while the true model is a second order polynomial,

$$\eta(\underset{\sim}{x}) = \beta_0 + x_1\beta_1 + x_2\beta_2 + x_1x_2\beta_{12} + x_1^2\beta_{11} + x_2^2\beta_{22}.$$

For this case, the $\underset{\sim}{\beta}_2$-space is three-dimensional with

$$\underset{\sim}{\beta}_2' = (\beta_{12}, \beta_{11}, \beta_{22}),$$

$$\text{and} \quad T_1 = \begin{bmatrix} 1/9 & & 0 \\ & 4/45 & \\ 0 & & 4/45 \end{bmatrix}.$$

The $\Lambda(T_1)$ criteria can be summarized as:

1. $\Lambda_1(T_1)$-optimality--maximize the smallest characteristic root of the symmetric matrix

$$\begin{bmatrix} 9\,\ell_{11} & & * \\ 3\sqrt{45/2}\,\ell_{21} & 45/4\,\ell_{22} & \\ 3\sqrt{45/2}\,\ell_{31} & 45/4\,\ell_{32} & 45/4\,\ell_{33} \end{bmatrix},$$

2. $\Lambda_2(T_1)$-optimality--maximize

$$[9\,\ell_{11} + 45/4(\ell_{22} + \ell_{33})],$$

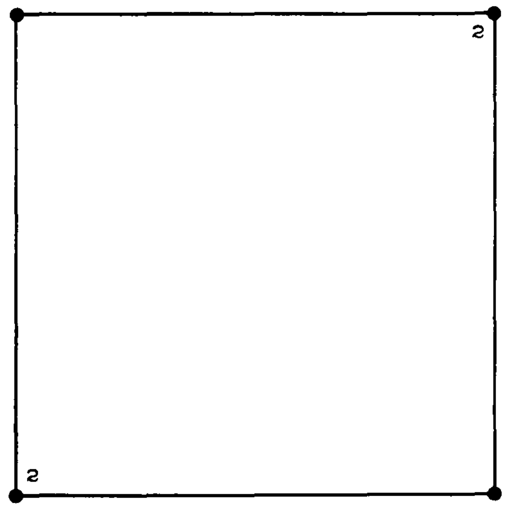
3. $\Lambda_3(T_1,c)$-optimality--minimize

$$|L|^{-c}\,[\ell_{11}^{-}/9 + 4/45(\ell_{22}^{-} + \ell_{33}^{-})],$$

where $L = [\ell_{ij}]$ and $L^{-1} = [\ell_{ij}^{-}]$.

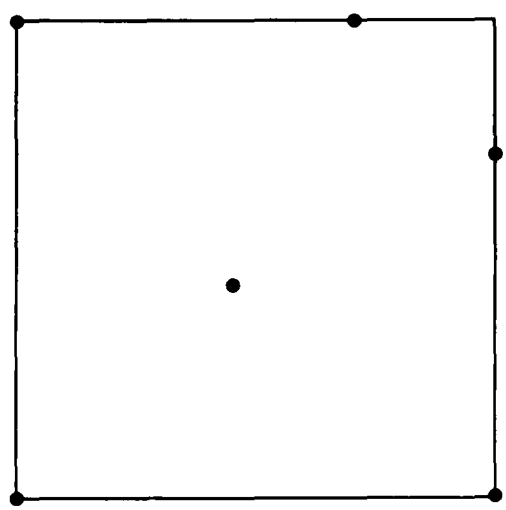
The first and second order D-optimal designs and the $|L|$-optimal design are given in Figure 3.9. The values of the standardized determinants for the D-optimal designs are:

1. $|n^{-1} X_1' X_1| = .88889$ for the first order D-optimal design,



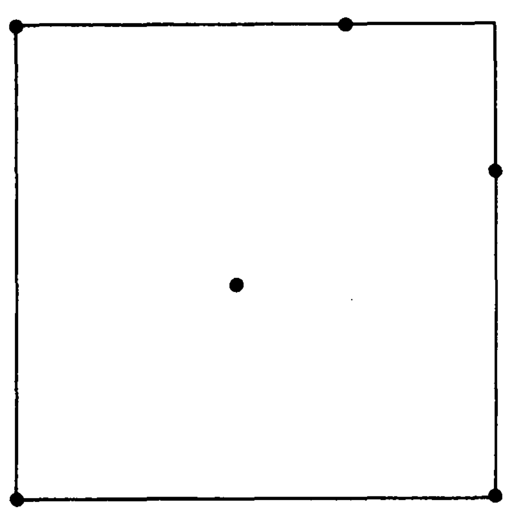
1st Order D-Optimal Design

1.000000	1.000000
1.000000	1.000000
-1.000000	-1.000000
-1.000000	-1.000000
1.000000	-1.000000
-1.000000	1.000000



2nd Order D-Optimal Design

-1.000000	1.000000
-1.000000	-1.000000
1.000000	-1.000000
-0.131500	-0.131500
1.000000	0.394400
0.394400	1.000000



|L|-Optimal Design

-1.000000	1.000000
-1.000000	-1.000000
1.000000	-1.000000
-0.111311	-0.111311
1.000000	0.346685
0.346685	1.000000

Figure 3.9. Two-Factor D-Optimal and |L|-Optimal Designs for First Order vs. Second Order Models and n = 6

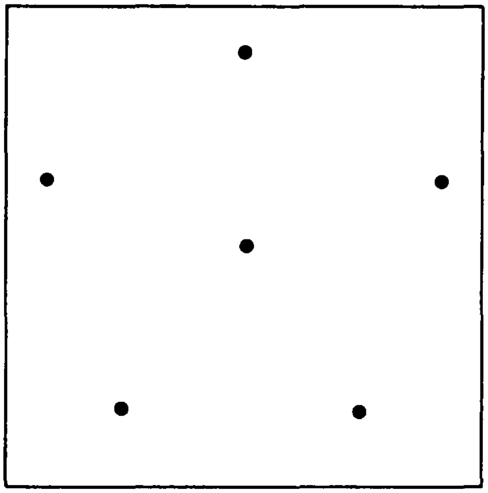
and 2. $|n^{-1} X' X| = .57385 \times 10^{-2}$ for the second order D-optimal design.

The second order D-optimal design was given by Hartley and Ruud (1969) and also by Box and Draper (1971). We will examine two minimum bias designs, given by Lawrence (1964). They are illustrated in Figure 3.10. The $\Lambda_1(T_1)$-optimal and $\Lambda_2(T_1)$-optimal designs are given in Figure 3.11, and the $\Lambda_3(T_1,c)$-optimal designs for $c = 0$ and $c = \frac{1}{2}$ are given in Figure 3.12.

Some of the properties of these designs are given in Table 3.5. The variance properties for the second order polynomial, listed in Table 3.5, indicate that the $\Lambda_2(T_1)$-optimal design, the first order D-optimal design, and the minimum bias hexagon all have a singular lack of fit matrix. Although we can conduct a lack of fit test with these designs, they cannot be used to fit the second order model.

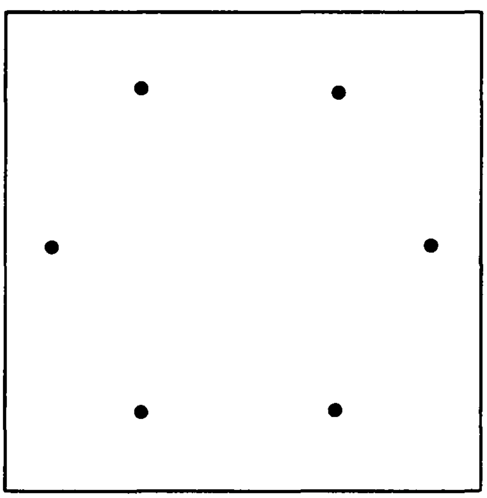
As expected, the $|L|$-optimal design has a very high D-efficiency for the second order model. However, the $\Lambda_1(T_1)$-optimal, $\Lambda_3(T_1,0)$-optimal and $\Lambda_3(T_1,\frac{1}{2})$-optimal designs do nearly as well. In fact, the average variances of these designs for the second order model, V_2, are smaller than any of the other designs listed in Table 3.5. For the first order polynomial, the variance properties of the $\Lambda(T_1)$-optimal designs are very good.

Now let us examine the fitted bias properties of these designs. For this case, the bias matrix (T_2) is no longer a scalar. Hence, for a given seriousness of inherent departure from the first order model, as measured by τ_1, there is a range of fitted bias. We will



Minimum Bias Pentagon
plus Center Point

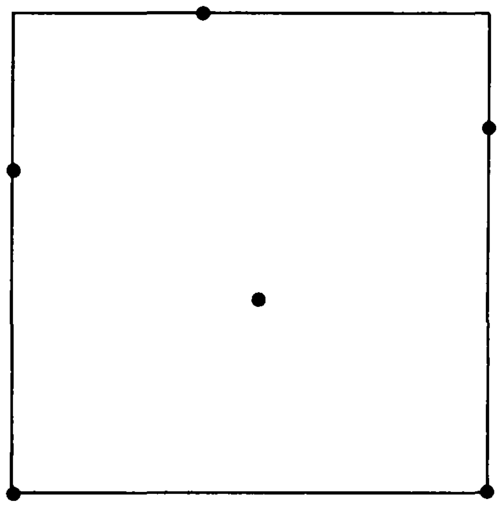
0.000000	0.894427
0.850651	0.276393
-0.850651	0.276393
0.525731	-0.723607
-0.525731	-0.723607
0.000000	0.000000



Minimum Bias
Hexagon

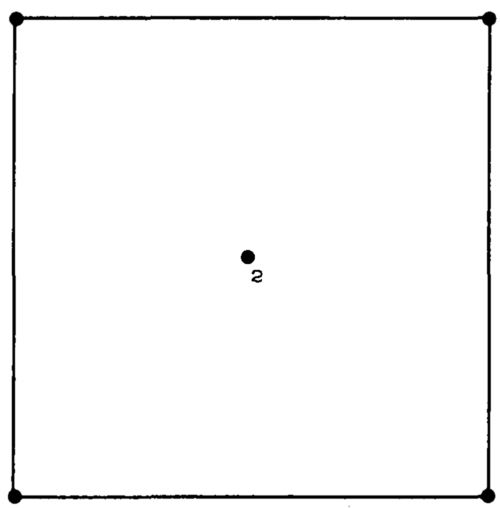
0.816497	0.000000
-0.816497	0.000000
0.408248	-0.707107
-0.408248	0.707107
0.408248	0.707107
-0.408248	-0.707107

Figure 3.10. Two-Factor Minimum Bias Designs for
First Order vs. Second Order Models and n = 6



$\Lambda_1(T_1)$-Optimal Design

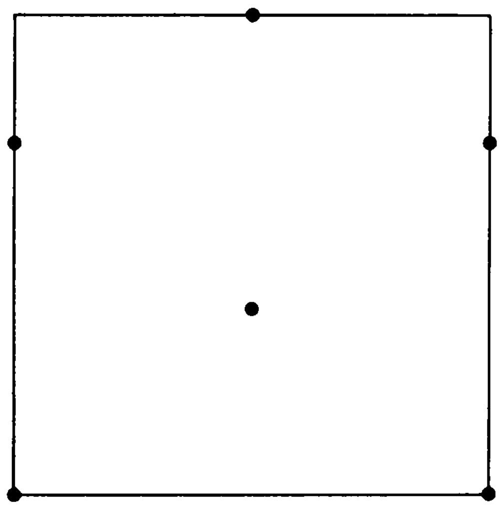
-1.000000	-1.000000
1.000000	-1.000000
-0.244338	1.000000
-1.000000	0.340729
1.000000	0.532605
0.022593	-0.212873



$\Lambda_2(T_1)$-Optimal Design

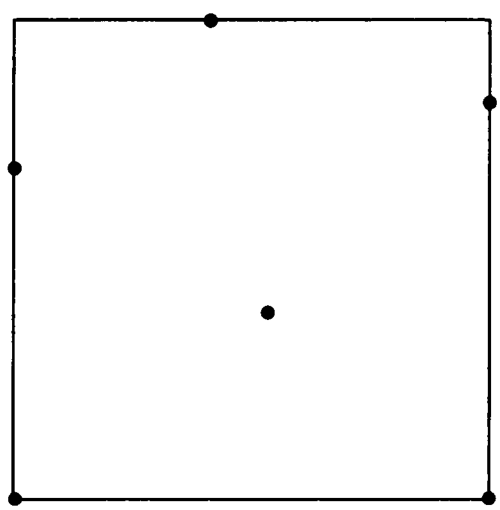
1.000000	-1.000000
-1.000000	1.000000
1.000000	1.000000
-1.000000	-1.000000
0.000000	0.000000
0.000000	0.000000

Figure 3.11. Two-Factor $\Lambda_1(T_1)$-Optimal and $\Lambda_2(T_1)$-Optimal Designs for First Order vs. Second Order Models and $n = 6$



$\Lambda_3(T_1,0)$-Optimal Design

0.000000	1.000000
-1.000000	-1.000000
1.000000	-1.000000
0.000000	-0.207743
-1.000000	0.471890
1.000000	0.471890



$\Lambda_3(T_1,\frac{1}{2})$-Optimal Design

-1.000000	-1.000000
1.000000	-1.000000
-0.169037	1.000000
-1.000000	0.402792
1.000000	0.726860
0.057933	-0.169608

Figure 3.12. Two-Factor $\Lambda_3(T_1,c)$-Optimal Designs for First Order vs. Second Order Models and n = 6

TABLE 3.5.

A Comparison of Some Characteristics of Two-Factor $\Lambda(T_1)$-Optimal Designs for First Order vs. Second Order Models and n = 6.

Design	$\lvert n^{-1} L\rvert$	$\lVert T_2\rVert$	Standardized Average Variances V_1	V_2	D-Efficiencies E_1	E_2
1st Order D-Optimal	$.00000 \times 10^{0}$	1.10039	1.7500	∞	1.0000	0.0000
2nd Order D-Optimal	$.11959 \times 10^{-1}$	0.40539	1.9694	4.9043	0.8572	1.0000
$\lvert L\rvert$-Optimal	$.12089 \times 10^{-1}$	0.40095	1.9802	4.8838	0.8526	0.9983
Minimum Bias Hexagon	$.00000 \times 10^{0}$	0.16777	3.0000	∞	0.5946	0.0000
Minimum Bias Pentagon plus Center Point	$.39506 \times 10^{-3}$	0.16777	3.0000	7.3333	0.5946	0.4439
$\Lambda_1(T_1)$-Optimal	$.10293 \times 10^{-1}$	0.32587	2.0855	4.6914	0.8115	0.9403
$\Lambda_2(T_1)$-Optimal	$.00000 \times 10^{0}$	0.34211	2.0000	∞	0.8409	0.0000
$\Lambda_3(T_1,0)$-Optimal	$.10595 \times 10^{-1}$	0.32573	2.0786	4.6517	0.7575	0.9452
$\Lambda_3(T_1,\frac{1}{2})$-Optimal	$.11213 \times 10^{-1}$	0.36464	2.0361	4.6863	0.8270	0.9660

examine three bias properties of these designs: the maximum and average bias as a function of τ_1, and the Euclidean norm of the T_2 matrix. The maximum fitted bias for a given value of τ_1 is given in Figure 3.13, and the average bias for a given value of τ_1 is illustrated in Figure 3.14. Notice that, for this case, these figures agree completely with the Euclidean norm of T_2, given in Table 3.5.

As with the fitted bias, the power of the lack of fit test varies for a given value of τ_1. Hence, we will examine two power properties: the minimum and the average value of the non-centrality parameter of the lack of fit test, λ, for a given value of τ_1. The minimum value of λ for a given value of τ_1 is illustrated in Figure 3.15, and the average value of λ for a given value of τ_1 is illustrated in Figure 3.16. The designs with a singular lack of fit matrix are not illustrated in Figure 3.15 since the minimum power for these designs is always equal to α, regardless of the seriousness of inherent bias.

3.3.1.1. The $\Lambda_1(T_1)$-Optimal Design.--The $\Lambda_1(T_1)$-optimal design was constructed to maximize the minimum value of the non-centrality parameter for $\tau_1 = \delta$, and Figure 3.15 indicates that this design is clearly superior with this respect. In addition, the $\Lambda_1(T_1)$-optimal design has excellent variance properties for fitting the second order model, and good variance properties for the lower order model. The bias properties of this design are essentially indistinguishable from those of the $\Lambda_3(T_1,0)$-optimal design. However, although Figures 3.13 and 3.14 indicate that the bias properties of the

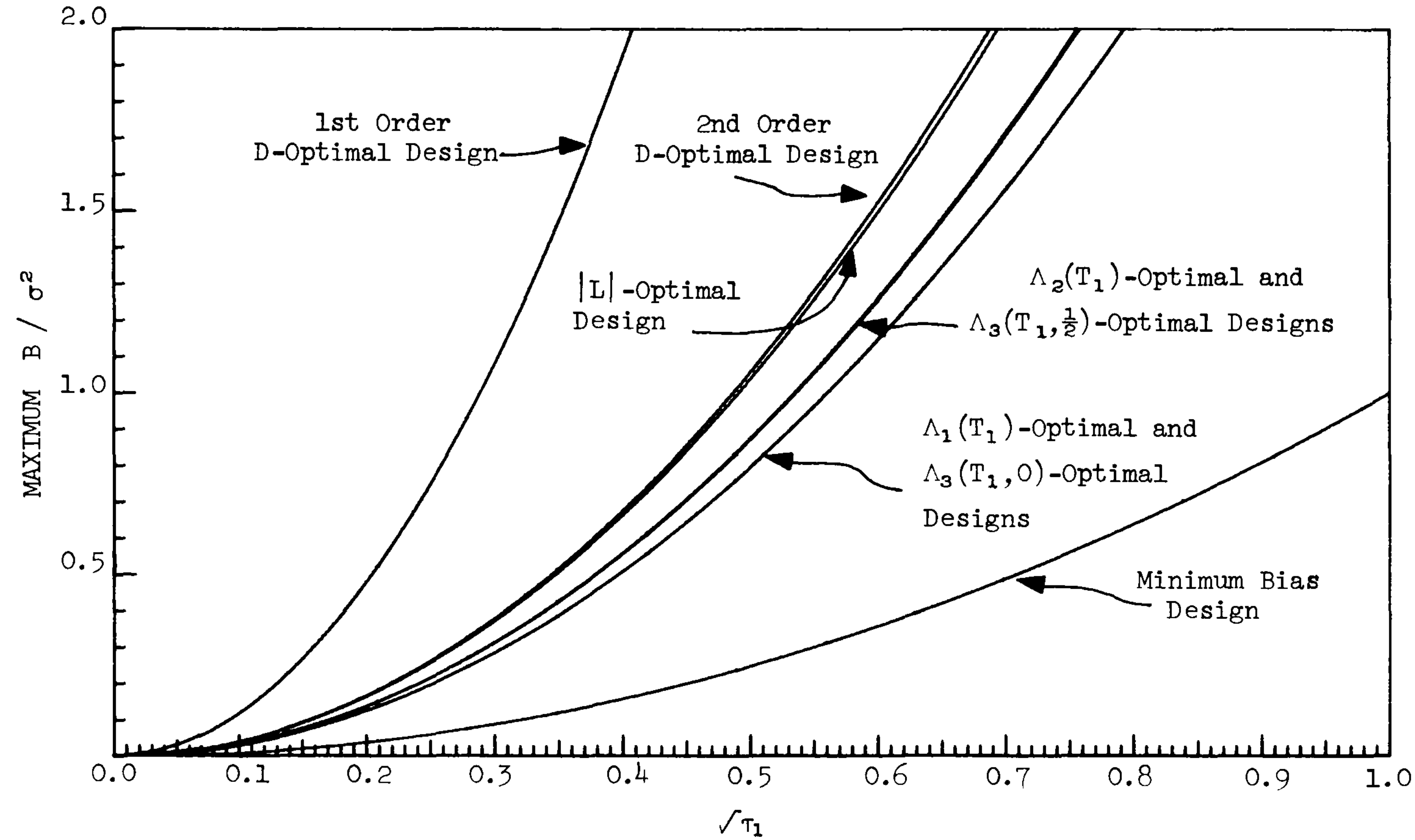


Figure 3.13. The Maximum Bias for Two-Factor $\Lambda(T_1)$-Optimal Designs for First Order vs. Second Order Models and n = 6

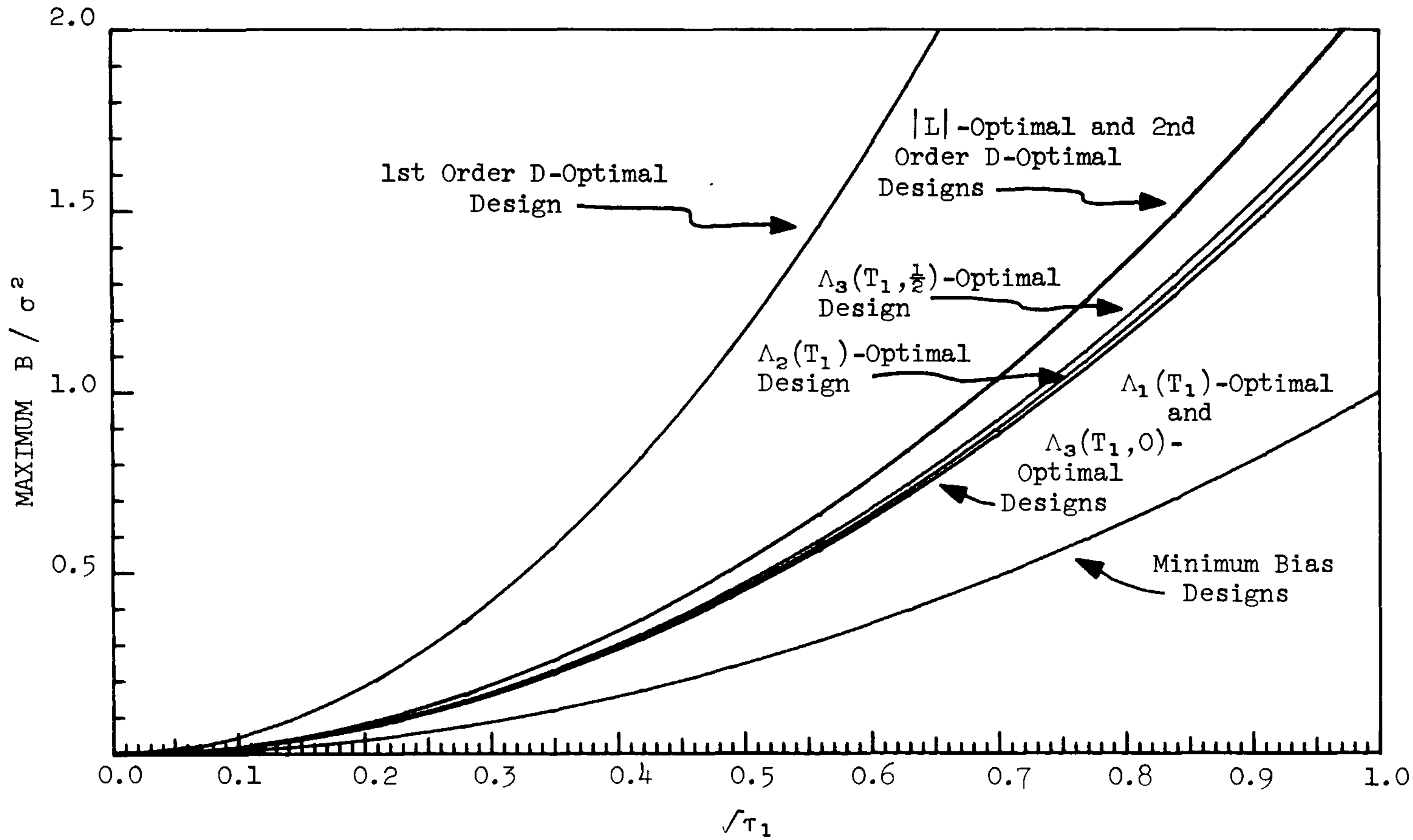


Figure 3.14. The Average Bias for Two-Factor $\Lambda(T_1)$-Optimal Designs for First Order vs. Second Order Models and $n = 6$

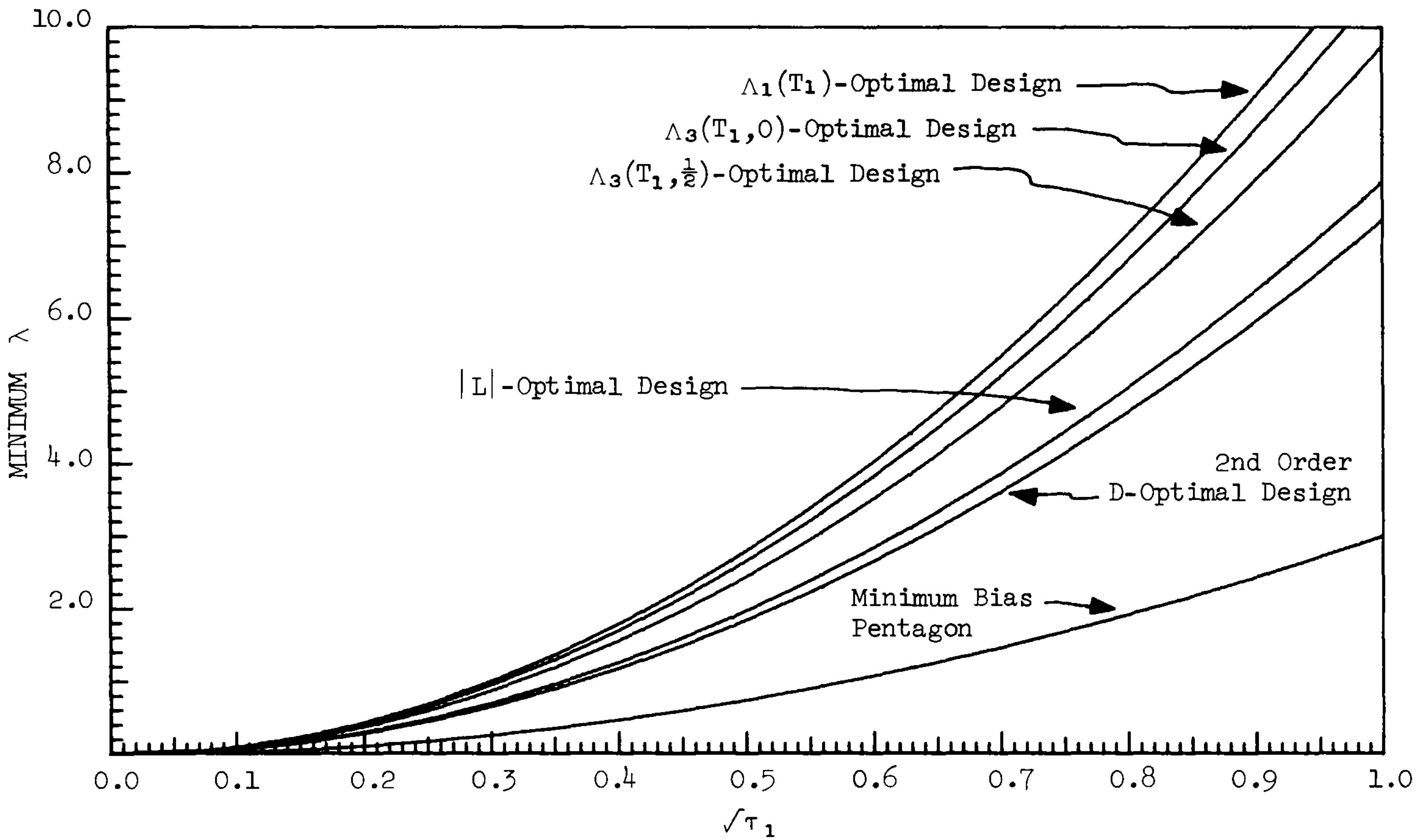


Figure 3.15. The Minimum Value of the Non-Centrality Parameter for Two-Factor $\Lambda(T_1)$-Optimal Designs for First Order vs. Second Order Models and n = 6

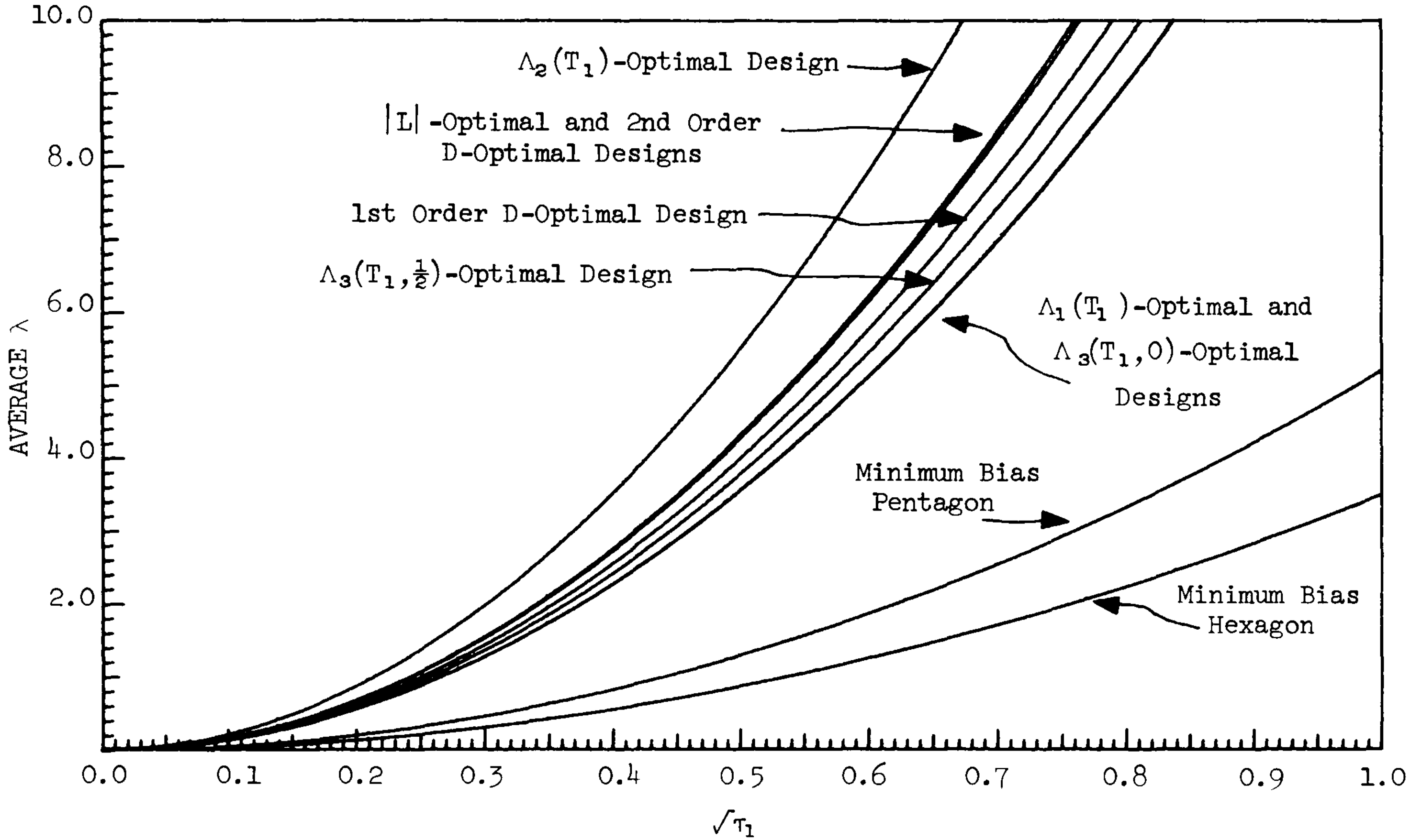


Figure 3.16. The Average Value of the Non-Centrality Parameter for Two-Factor $\Lambda(T_1)$-Optimal Designs for First Order vs. Second Order Models and n = 6

$\Lambda_1(T_1)$-optimal and $\Lambda_3(T_1,0)$-optimal designs are better than those of the other non-minimum bias designs examined in this section, the bias characteristics of the minimum bias designs are clearly superior to those of the non-minimum bias designs in this section. The maximum bias properties of the non-minimum bias designs (Figure 3.13) appear to be particularly poor.

3.3.1.2. The $\Lambda_2(T_1)$-Optimal Design.--The $\Lambda_2(T_1)$ criterion selects designs that maximize

$$\mathrm{Tr}[T_1^{-1} L].$$

Since (by (2.1.17) of Theorem 2.2) the average value of λ for $\tau_1 = \delta$ is

$$p_2^{-1}\, \delta\, \mathrm{Tr}[T_1^{-1} L],$$

the $\Lambda_2(T_1)$-optimal design maximizes the average value of λ for $\tau_1 = \delta$ (see Figure 3.16). However, the $\Lambda_2(T_1)$-optimal design examined in this section is singular for the higher order model. Hence, for this design, the minimum value of λ for $\tau_1 = \delta$ is always zero, regardless of the magnitude of δ. The bias properties of the $\Lambda_2(T_1)$-optimal design are fair, and it has slightly better variance properties for the lower order model than any of the other $\Lambda(T_1)$-optimal designs examined in this section. Furthermore, the $\Lambda_2(T_1)$-optimal design is completely symmetric about the origin; that is, any 90°, 180° or 270° rotation of this design results in the same design. The other $\Lambda(T_1)$-optimal designs do not possess this symmetry property. Finally, it should be noted that the design selected by the $\Lambda_2(T_1)$ criterion is one which has been recommended as a good design for fitting a first order model and conducting a lack of fit test (see Draper and Herzberg (1971), and Myers (1971)).

3.3.1.3. The $\Lambda_3(T_1,c)$-Optimal Designs.--The $\Lambda_3(T_1,c)$-optimal designs for $c = 0$ and $c = \frac{1}{2}$ were illustrated in Figure 3.12. The use of c for $\Lambda_3(T_1,c)$-optimality was proposed to allow the experimenter to increase $|L|$. However, Figure 3.12 indicates that, for this case, the $c = 0$ and $c = \frac{1}{2}$ designs are very similar. Now as we noted in 3.3.1.1, the properties of the $\Lambda_3(T_1,0)$-optimal design are very similar to those of the $\Lambda_1(T_1)$-optimal design, and the remarks made in that section apply to the $\Lambda_3(T_1,0)$-optimal design as well. In summary, the $\Lambda_3(T_1,c)$-optimal designs have excellent power and variance properties for the higher order model, and fair bias and variance properties for the lower order model.

3.3.2. Two-Factor $\Lambda(T_1)$-Optimal Designs for Second Order vs. Third Order Polynomial Models and n = 10

Now let us examine two-factor designs when the proposed model is a second order polynomial,

$$\eta_1(\underset{\sim}{x}) = \beta_0 + x_1\beta_1 + x_2\beta_2 + x_1x_2\beta_{12} + x_1^2\beta_{11} + x_2^2\beta_{22},$$

while the true model is a third order polynomial,

$$\eta(\underset{\sim}{x}) = \beta_0 + x_1\beta_1 + x_2\beta_2 + x_1x_2\beta_{12} + x_1^2\beta_{11} + x_2^2\beta_{22} + x_1^2x_2\beta_{112} + x_1x_2^2\beta_{122} + x_1^3\beta_{111} + x_2^3\beta_{222}.$$

For this case, the $\underset{\sim}{\beta}_2$-space is four-dimensional with

$$\underset{\sim}{\beta}_2' = (\beta_{112}, \beta_{122}, \beta_{111}, \beta_{222})$$

$$\text{and} \quad T_1 = \begin{bmatrix} 4/135 & & & 0 \\ & 4/135 & & \\ 0 & & 4/175 & \\ & & & 4/175 \end{bmatrix}.$$

The $\Lambda(T_1)$ criteria can be summarized as:

1. $\Lambda_1(T_1)$-optimality--maximize the smallest characteristic root of the symmetric matrix

$$\frac{1}{4}\begin{bmatrix} 135\,\ell_{11} & & & * \\ 135\,\ell_{21} & 135\,\ell_{22} & & \\ 15\sqrt{105}\,\ell_{31} & 15\sqrt{105}\,\ell_{32} & 175\,\ell_{33} & \\ 15\sqrt{105}\,\ell_{41} & 15\sqrt{105}\,\ell_{42} & 175\,\ell_{43} & 175\,\ell_{44} \end{bmatrix}$$

2. $\Lambda_2(T_1)$-optimality--maximize

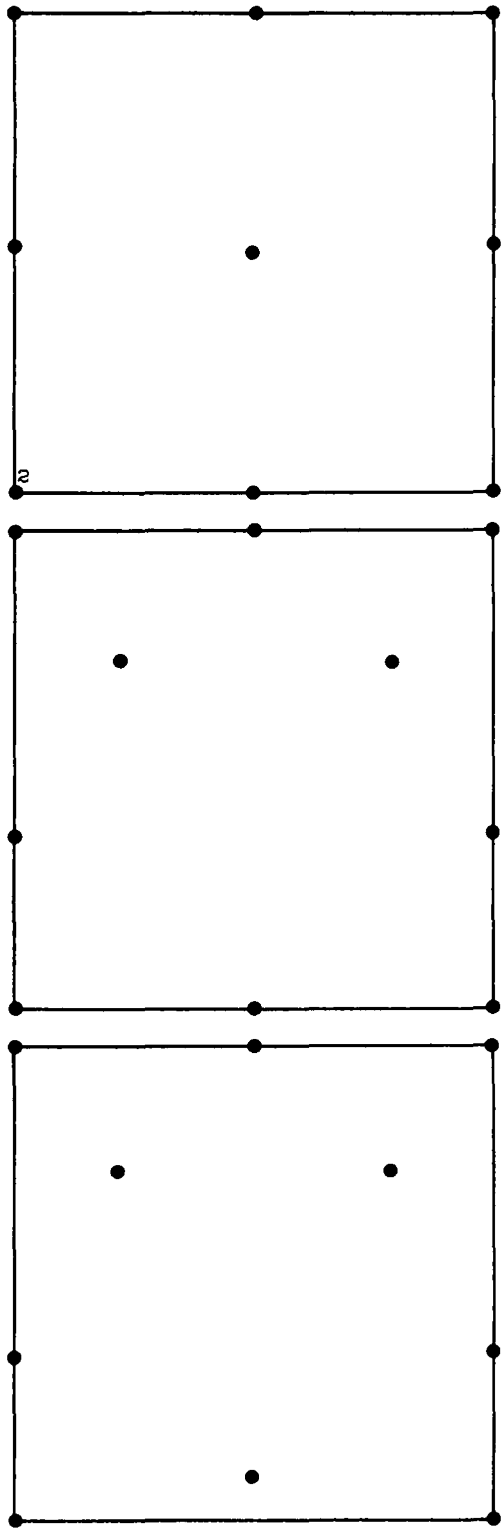
$$\tfrac{1}{4}\,[135(\ell_{11} + \ell_{22}) \;+\; 175(\ell_{33} + \ell_{44})]$$

3. $\Lambda_3(T_1,c)$-optimality--minimize

$$4\,|L|^{-c}\,[(\ell^{-}_{11} + \ell^{-}_{22})/135 \;+\; (\ell^{-}_{33} + \ell^{-}_{44})/175],$$

where $L = [\ell_{ij}]$ and $L^{-1} = [\ell^{-}_{ij}]$ (note that we are using the abbreviated notation $\Lambda_2(T_1)$ for $\Lambda_2(T_1,c)$ since the value of c has no effect on the selection of a $\Lambda_2(T_1,c)$-optimal design when the T matrix is design independent).

The n = 10 designs for this case are given in Figures 3.17 - 3.20. The D-optimal, $|L|$-optimal and the $\Lambda(T_1)$-optimal designs were obtained using the design optimization algorithm described in Appendix A. The minimum bias square plus hexagon was referred to by Lawrence (1964) (his specifications for the square and hexagon radius were incorrect), and the minimum bias square plus star and center points was given by



2nd Order D-Optimal Design

2^2 plus

-1.000000	-1.000000
-1.000000	0.099329
0.099329	-1.000000
1.000000	0.016983
0.016983	1.000000
-0.024346	-0.024346

3rd Order D-Optimal Design

2^2 plus

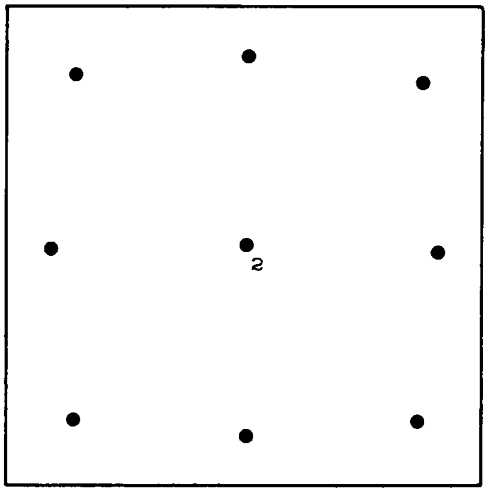
1.000000	-0.292770
-1.000000	-0.292770
0.000000	1.000000
0.000000	-1.000000
-0.577350	0.487950
0.577350	0.487950

$|L|$-Optimal Design

2^2 plus

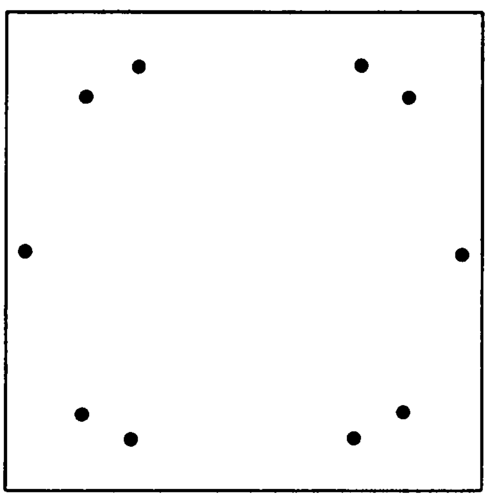
1.000000	-0.307739
-1.000000	-0.307739
0.000000	1.000000
0.000000	-0.842161
-0.579597	0.520421
0.579597	0.520421

Figure 3.17. Two-Factor D-Optimal and $|L|$-Optimal Designs for Second Order vs. Third Order Models and n = 10



Minimum Bias
Square plus Star
and Center Points

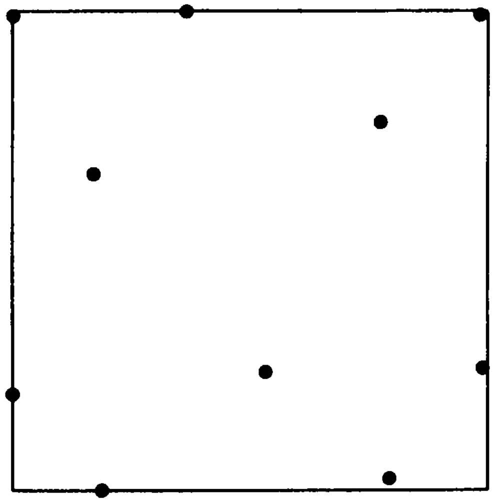
0.738000	-0.738000
-0.738000	0.738000
0.738000	0.738000
-0.738000	-0.738000
0.830000	0.000000
-0.830000	0.000000
0.000000	0.830000
0.000000	-0.830000
0.000000	0.000000
0.000000	0.000000



Minimum Bias
Square plus Hexagon

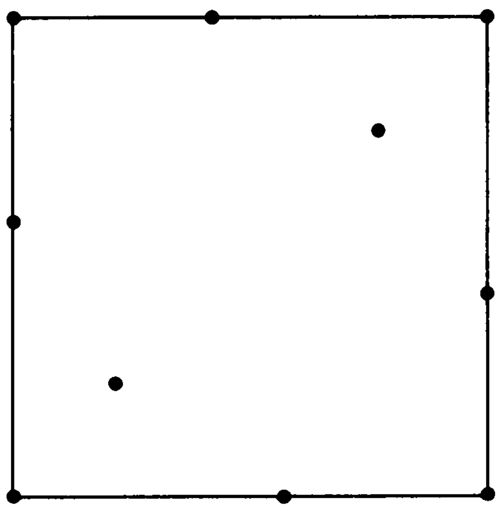
0.694868	-0.694868
-0.694868	0.694868
0.694868	0.694868
-0.694868	-0.694868
0.954179	0.000000
-0.954179	0.000000
0.477089	-0.826343
-0.477089	0.826343
0.477089	0.826343
-0.477089	-0.826343

Figure 3.18. Two-Factor Minimum Bias Designs for Second Order vs. Third Order Models and n = 10



$\Lambda_1(T_1)$-Optimal Design

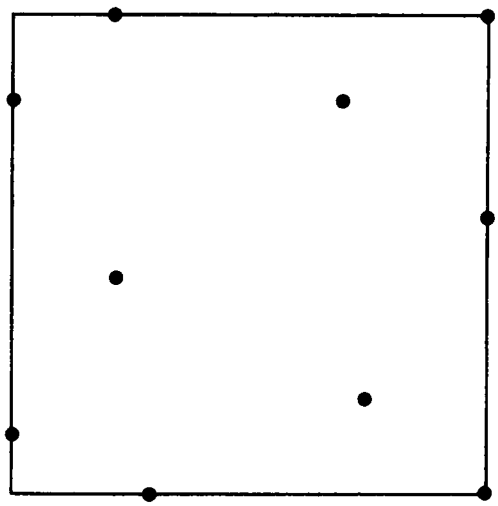
0.999861	0.999853
-1.000000	0.999995
0.999176	-0.499174
0.638045	-0.945769
-0.270702	1.000000
-1.000000	-0.596319
-0.620133	-1.000000
-0.650772	0.356077
0.573316	0.572929
0.072904	-0.504351



$\Lambda_2(T_1)$-Optimal Design

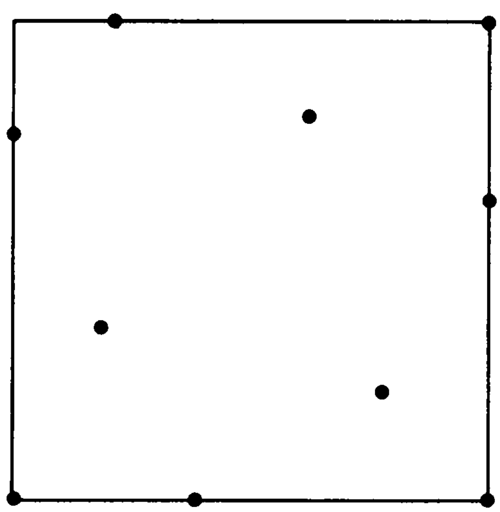
1.000000	-1.000000
-1.000000	1.000000
1.000000	1.000000
-1.000000	-1.000000
1.000000	-0.162432
-1.000000	0.162432
-0.162432	1.000000
0.162432	-1.000000
0.562434	0.562434
-0.562434	-0.562434

Figure 3.19. Two-Factor $\Lambda_1(T_1)$-Optimal and $\Lambda_2(T_1)$-Optimal Designs for Second Order vs. Third Order Models and n = 10



$\Lambda_3(T_1,0)$-Optimal Design

1.000000	1.000000
1.000000	-1.000000
-0.559576	1.000000
-1.000000	0.646074
-1.000000	-0.770436
-0.391261	-1.000000
1.000000	0.148482
0.382493	0.638766
-0.597240	-0.098917
0.516805	-0.597615



$\Lambda_3(T_1,\frac{1}{2})$-Optimal Design

1.000000	1.000000
-1.000000	-1.000000
1.000000	-1.000000
-1.000000	0.607708
-0.607708	1.000000
1.000000	0.239565
-0.239565	-1.000000
0.278879	0.656844
-0.656844	-0.278879
0.577463	-0.577463

Figure 3.20. Two-Factor $\Lambda_3(T_1,c)$-Optimal Designs for Second Order vs. Third Order Models and n = 10

Draper and Lawrence (1965) (see Figure 3.18).

Some of the properties for these designs are given in Table 3.6. The D-efficiencies were computed using the determinants of the second and third order D-optimal designs illustrated in Figure 3.17. Their determinants are:

1. $|n^{-1} X_1' X_1| = .94605 \times 10^{-2}$ for the second order D-optimal design,

and 2. $|n^{-1} X' X| = .60012 \times 10^{-7}$ for the third order D-optimal design.

The variance properties listed in this table for the third order polynomial indicate that the second order D-optimal design, the $\Lambda_2(T_1)$-optimal design, and both minimum bias designs are singular for the third order model.

As far as the bias and power properties of these designs are concerned, we will proceed as we did in the previous section. The maximum bias for a given inherent departure from the second order model (τ_1) and the average bias for a given value of τ_1 are illustrated in Figures 3.21 and 3.22 respectively. In general, these figures indicate that the bias properties of the minimum bias designs are considerably better than the bias properties of the other designs examined in this section. Moreover, as we noted in the previous section, Figures 3.21 and 3.22 agree completely with the Euclidean norm of T_2, given in Table 3.6.

The maximum and average value of the non-centrality parameter are illustrated in Figures 3.23 and 3.24 respectively. Notice that the

TABLE 3.6.

A Comparison of Some Characteristics of Two-Factor $\Lambda(T_1)$-Optimal Designs for Second Order vs. Third Order Models and n = 10.

Design	$\lvert n^{-1} L \rvert$	$\lVert T_2 \rVert$	Standardized Average Variances V_1	V_2	D-Efficiencies E_1	E_2
2nd Order D-Optimal	$.00000 \times 10^{0}$	.18013	4.3405	∞	1.0000	0.0000
3rd Order D-Optimal	$.10631 \times 10^{-4}$	.16357	4.6946	10.5772	0.9175	1.0000
$\lvert L \rvert$-Optimal	$.11494 \times 10^{-4}$	.15102	4.6494	9.3166	0.8927	0.9914
Minimum Bias Square plus Hexagon	$.00000 \times 10^{0}$	.05292	343.3100	∞	0.2336	0.0000
Minimum Bias Square plus Star and Center Points	$.00000 \times 10^{0}$	.05292	6.7981	∞	0.4356	0.0000
$\Lambda_1(T_1)$-Optimal	$.67083 \times 10^{-5}$	.11151	4.8142	8.9351	0.7814	0.8673
$\Lambda_2(T_1)$-Optimal	$.00000 \times 10^{0}$	.14003	4.5462	∞	0.9246	0.0000
$\Lambda_3(T_1,0)$-Optimal	$.97678 \times 10^{-5}$	.11653	4.6875	8.5594	0.8090	0.9194
$\Lambda_3(T_1,\frac{1}{2})$-Optimal	$.11212 \times 10^{-4}$	.13316	4.6767	8.7118	0.8408	0.9540

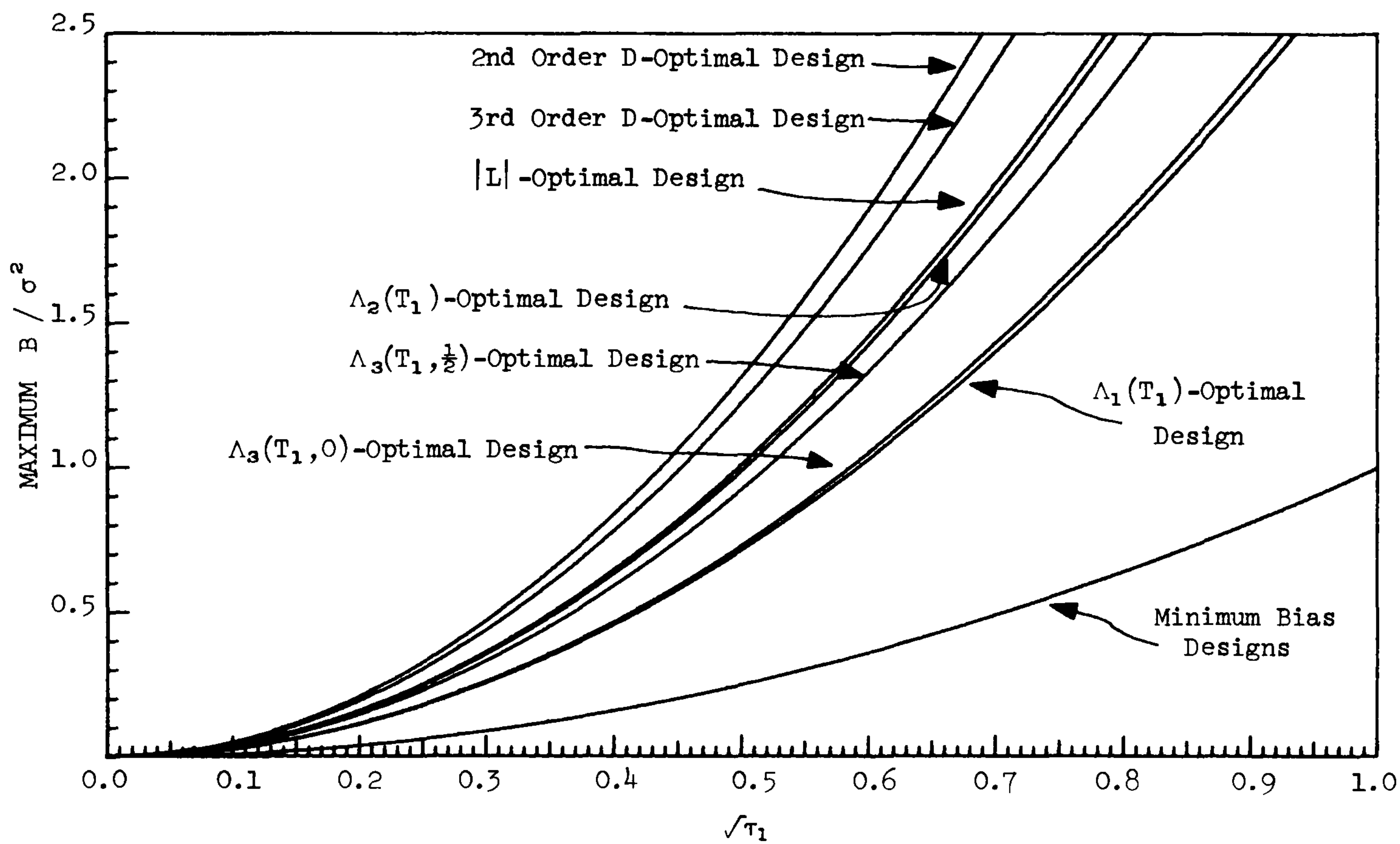


Figure 3.21. The Maximum Bias for Two-Factor $\Lambda(T_1)$-Optimal Designs for Second Order vs. Third Order Models and n = 10

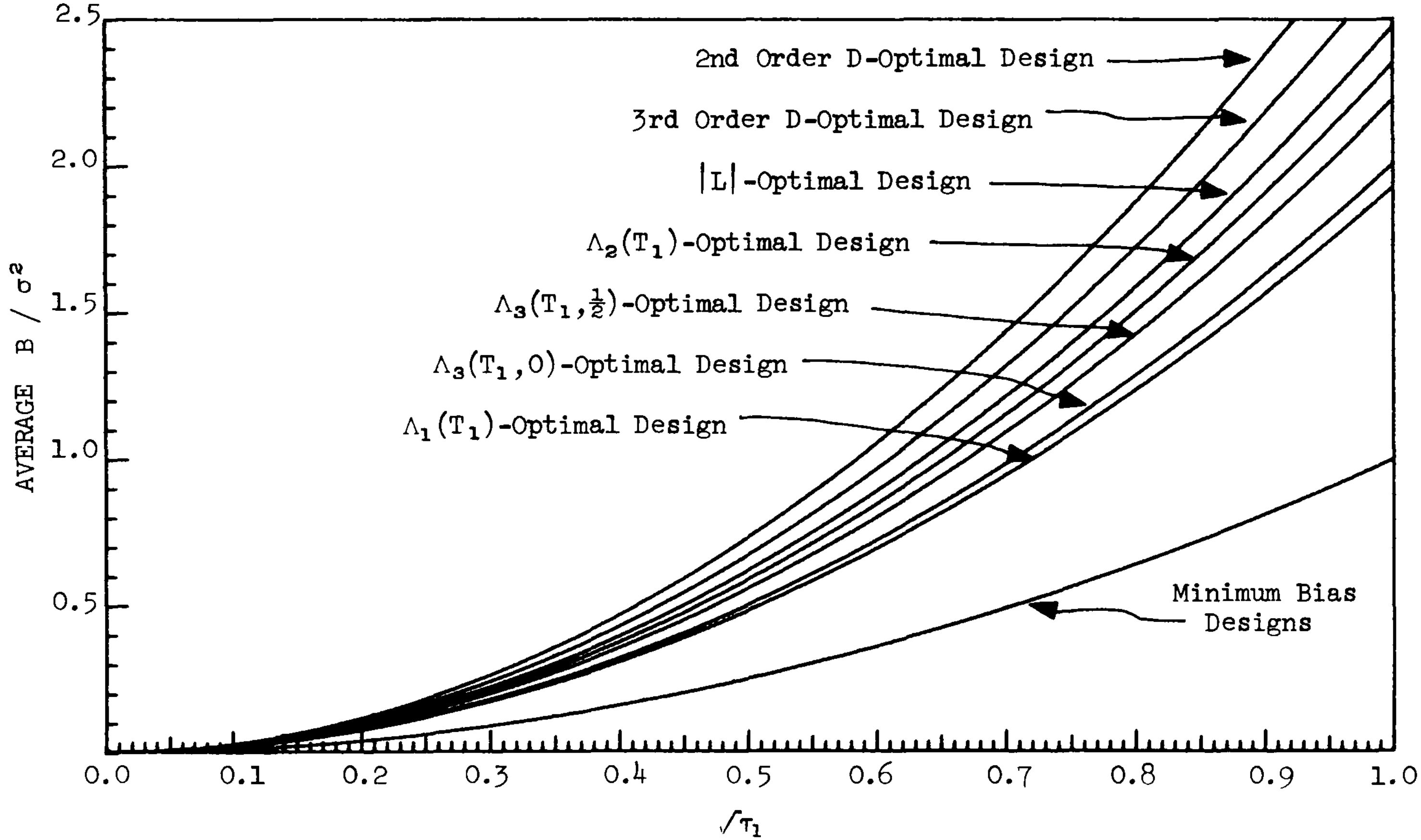


Figure 3.22. The Average Bias for Two-Factor $\Lambda(T_1)$-Optimal Designs for Second Order vs. Third Order Models and n = 10

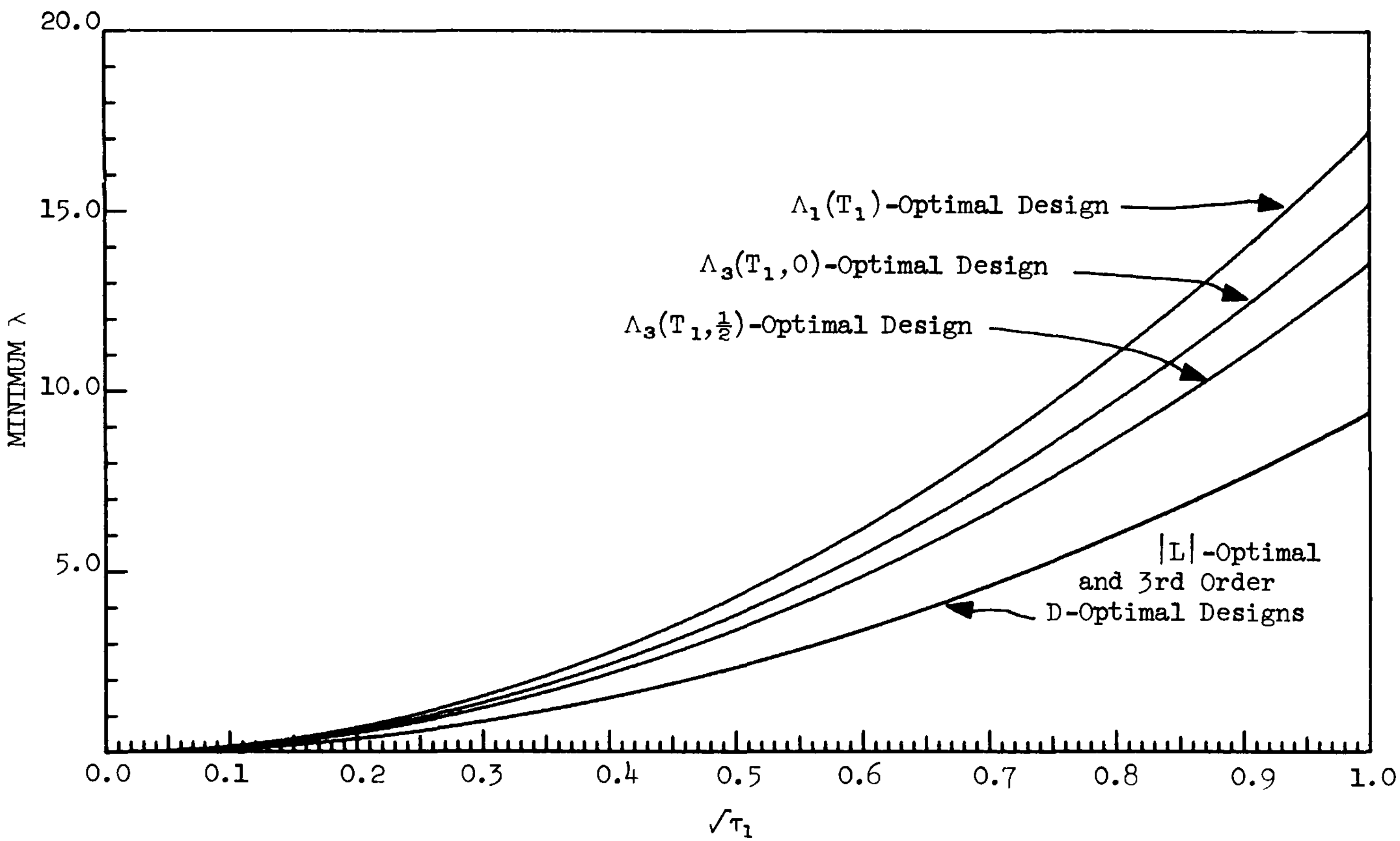


Figure 3.23. The Minimum Value of the Non-Centrality Parameter for Two-Factor $\Lambda(T_1)$-Optimal Designs for Second Order vs. Third Order Models and $n = 10$

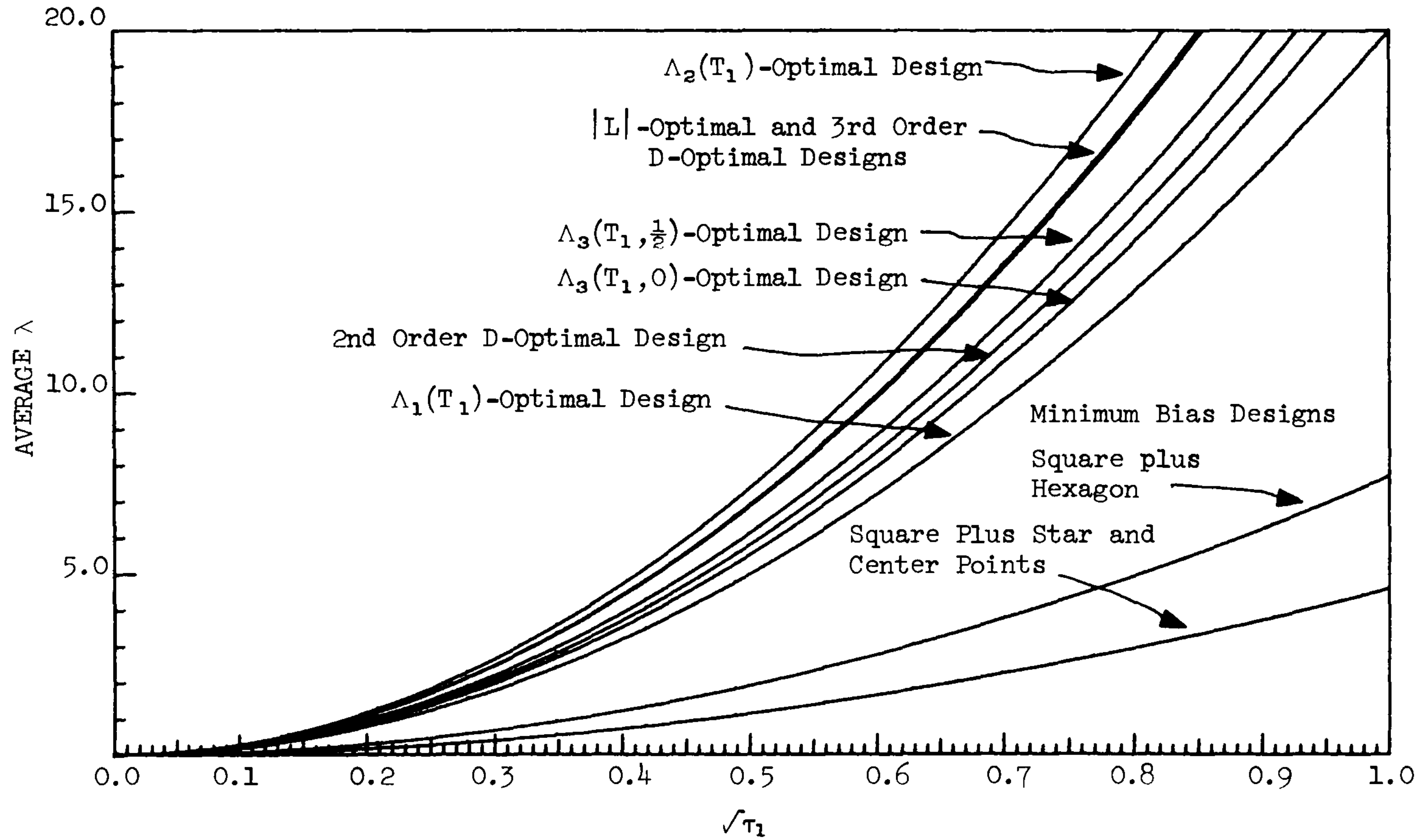


Figure 3.24. The Average Value of the Non-Centrality Parameter for Two-Factor $\Lambda(T_1)$-Optimal Designs for Second Order vs. Third Order Models and n = 10

power properties of the $|L|$-optimal and third order D-optimal designs are nearly identical. This is not unexpected since the design patterns, illustrated in Figure 3.17, for these designs are very similar.

3.3.2.1. The $\Lambda_1(T_1)$-Optimal Design.--The $\Lambda_1(T_1)$-optimal design maximizes the minimum value of λ for a given value of τ_1 (see Figure 3.23). This design also has good average variance properties for prediction of the lower order model (V_1), very good average variance properties for prediction of the higher order model (V_2), and fair bias properties. In fact, for this design, the average variance for prediction of the higher order model is smaller than either the $|L|$-optimal or third order D-optimal designs. However, although the $\Lambda_1(T_1)$-optimal design has better bias properties than any of the other non-minimum bias designs given in this section, this design is not nearly minimum bias.

3.3.2.2. The $\Lambda_2(T_1)$-Optimal Design.--The $\Lambda_2(T_1)$-optimal design maximizes the average value of λ for a given value of τ_1 (see Figure 3.24). However, this design is singular for the higher order model, and hence, the minimum value of λ for $\tau_1 = \delta$ is always zero for this design. In addition, although the bias properties for the $\Lambda_2(T_1)$-optimal design are not very good, it has good variance properties for the lower order model. In 3.3.1.2 we noted that the $\Lambda_2(T_1)$-optimal design for first order vs. second order models was more symmetric than any of the other $\Lambda(T_1)$-optimal designs. For this case, it also appears that the $\Lambda_2(T_1)$-optimal design is more symmetric than any of the other $\Lambda(T_1)$-optimal designs.

3.3.2.3. The $\Lambda_3(T_1,c)$-Optimal Designs.--For this case, the $\Lambda_3(T_1,0)$-optimal and $\Lambda_3(T_1,\frac{1}{2})$-optimal designs are very similar. Furthermore, as we noted in Section 3.3.1, the $\Lambda_3(T_1,c)$-optimal designs appear to be very similar to the $\Lambda_1(T_1)$-optimal design. In summary, the properties of the $\Lambda_3(T_1,c)$-optimal designs for this case appear to be quite good. Like the $\Lambda_1(T_1)$-optimal design, their bias properties are only fair, but their variance properties are good for the lower order model and very good for the higher order model.

3.4. Summary

In this chapter, we have attempted to examine the variance, bias and power properties of the $\Lambda(T_1)$ criteria by comparing $\Lambda(T_1)$-optimal designs with D-optimal designs for both the lower and higher order models, minimum bias designs, and designs that maximize $|L|$. Furthermore, we noted that, since $|T_1|^{-c}$ is always a constant, the use of c has no effect upon the selection of a $\Lambda_2(T_1,c)$-optimal design, and hence, we have used the abbreviated notation $\Lambda_2(T_1)$ for $\Lambda_2(T_1,c)$.

In general, it appears that, in addition to selecting designs that have certain optimum properties for the detection of lack of fit, the designs selected by the $\Lambda(T_1)$ criteria also have good variance and fair bias properties. In particular, the cases examined in this chapter suggest the following observations:

1. $\Lambda(T_1)$-optimal designs have good variance properties for the lower order model,

2. $\Lambda(T_1)$-optimal designs have very good variance properties for the higher order model, except for the $\Lambda_2(T_1)$-optimal designs which may be singular for the higher order model,

3. the bias properties of $\Lambda(T_1)$-optimal designs are only fair; however, $\Lambda(T_1)$-optimal designs give a substantial improvement over D-optimal designs for the lower order model in this respect,

4. the $\Lambda_1(T_1)$-optimal and $\Lambda_3(T_1,0)$-optimal designs are very similar, both in pattern and in properties. They have good variance properties for the lower order model and very good variance properties for the higher order model.

This last observation is possibly very useful since the two-factor $\Lambda_1(T_1)$-optimal designs were computationally very difficult to obtain. It should be emphasized that these observations are based solely upon the empirical evidence presented in this chapter. Thus, since we have examined only a few cases, at this time, we cannot be certain that these observations will hold in general.

IV. $\Lambda_2(T_1)$-OPTIMAL DESIGNS FOR CUBOIDAL REGIONS OF INTEREST

4.1. Introduction

In the preceding chapter, we compared $\Lambda(T_1)$-optimal designs with D-optimal, $|L|$-optimal and minimum bias designs for cuboidal regions of interest. We observed that, for one-factor, first order vs. second order and second order vs. third order polynomial models, all of the $\Lambda(T_1)$ criteria were equivalent to $|L|$-optimality, and their variance and fitted bias properties appeared to be good overall. However, for the equivalent two-factor models, the $\Lambda(T_1)$-optimal designs were distinct, and we summarized the weak and strong points of each criterion.

The purpose of this chapter is to single out one of the $\Lambda(T_1)$ criteria and investigate the types of designs that it leads to. The $\Lambda_2(T_1)$ criterion was selected for this purpose for two reasons. First, this is the only $\Lambda(T_1)$ criteria that can be applied when the sample size is not large enough for fitting the higher order model; and second, the investigations in the preceding chapter indicated that $\Lambda_2(T_1)$-optimality is easier to numerically optimize than either $\Lambda_1(T_1)$-optimality or $\Lambda_3(T_1,c)$-optimality.

In Chapter II, we saw that $\Lambda_2(T_1)$-optimality maximizes the average value of the non-centrality parameter, λ, over any τ-contour. However, in Chapter III, we observed that $\Lambda_2(T_1)$-optimal designs also appear to have very good properties for fitting the lower order model. Thus, the designs presented in this chapter, are well recommended when the experimenter has considerable confidence in the lower order model, but wants to know if he is wrong. Furthermore, we observed that these designs may be singular for the higher order model. Thus, if the experimenter intends to use a $\Lambda_2(T_1)$-optimal design that is singular for the higher order model, he should be willing to augment his design if he finds that his assumption in the validity of the lower order model is incorrect.

4.2. One-Factor $\Lambda_2(T_1)$-Optimal Designs

In this section, we will obtain one-factor $\Lambda_2(T_1)$-optimal designs for the region of interest defined by

$$-1 \leq x \leq 1.$$

However, because of the invariance results of Section 2.2, these designs can be scaled for any region of interest defined by

$$a \leq x \leq b,$$

where $a < b$.

In addition, for the one-factor cases considered in this section, it is easily shown that the transformation $z = -x$ is a "moment preserving transformation" (see Section 2.3). Thus, by Theorem 2.11, it follows that for the one-factor cases considered in Sections 4.2.1 and 4.2.2, if D is a $\Lambda_2(T_1)$-optimal design then -D is also a $\Lambda_2(T_1)$-optimal design.

4.2.1. One-Factor $\Lambda_2(T_1)$-Optimal Designs for First Order vs. Second Order Polynomial Models

Table 4.1 contains the one-factor $\Lambda(T_1)$-optimal designs, and some of their properties, for first order vs. second order polynomial models and n = 3 - 20. The n = 5 and n = 9 designs were examined in Section 3.2.1. The designs listed in this table appear to follow the pattern:

$$[\pm\ 1.0\ (n_o),\ 0.0\ (2n_o)] \qquad \text{for } n = 4n_o,$$

$$[\pm\ 1.0\ (n_o),\ 0.0\ (2n_o+1)] \qquad \text{for } n = 4n_o + 1,$$

$$[+\ 1.0\ (n_o+1),\ -1.0\ (n_o),\ a\ (2n_o+1)] \qquad \text{for } n = 4n_o + 2,$$

and $$[\pm\ 1.0\ (n_o+1),\ 0.0\ (2n_o+1)] \qquad \text{for } n = 4n_o + 3,$$

where $a \leq .070741$.

Except for the minimum-point, n = 3, design the properties of these designs appear to be fairly homogeneous. The ranges for some of their properties appear to be:

$$V_2 \quad 2.1333\text{--}2.2944,$$

$$V_1 \quad 1.5833\text{--}1.8333,$$

$$n^{-1}\,L \quad 0.2383\text{--}0.2500,$$

and $$T_2 \quad 0.0933\text{--}0.1456.$$

These designs were motivated primarily for the detection of model inadequacy. In deciding which design to use, it is important that the experimenter selects an α-level and sample size that will provide him with the power he wants for the detection of what he considers to be serious model inadequacy. Figures 4.1 through 4.4 are provided for that purpose. The power curves presented in these figures are based upon an F-test for lack of fit in which the residual

TABLE 4.1

One-Factor $\Lambda_2(T_1)$-Optimal Designs for First Order vs. Second Order Models

	Design							Standardized Average Variances	
	n_1	n_2	n_3						
	-1.0	a	1.0						
n	n_1	n_2	n_3	a	$\Lambda_2(T_1,0)$	$n^{-1}L$	T_2	V_1	V_2
3	1	1	1	.000000	2.5000	.22222	.20000	1.5000	2.4000
4	1	2	1	.000000	2.8125	.25000	.11667	1.6667	2.1333
5	1	3	1	.000000	2.7000	.24000	.09333	1.8333	2.2222
6	1	3	2	.070741	2.6805	.23830	.11533	1.8104	2.2944
7	2	3	2	.000000	2.7551	.24490	.14558	1.5833	2.1778
8	2	4	2	.000000	2.8125	.25000	.11667	1.6667	2.1333
9	2	5	2	.000000	2.7778	.24691	.10123	1.7500	2.1600
10	2	5	3	.040840	2.7666	.24592	.11597	1.7152	2.1868
11	3	5	3	.000000	2.7893	.24793	.13388	1.6111	2.1511
12	3	6	3	.000000	2.8125	.25000	.11667	1.6667	2.1333
13	3	7	3	.000000	2.7959	.24852	.10533	1.7222	2.1460
14	3	7	4	.028874	2.7893	.24794	.11628	1.6910	2.1600
15	4	7	4	.000000	2.8000	.24889	.12889	1.6250	2.1429
16	4	8	4	.000000	2.8125	.25000	.11667	1.6667	2.1333
17	4	9	4	.000000	2.8028	.24913	.10773	1.7083	2.1407
18	4	9	5	.022364	2.7985	.24876	.11643	1.6813	2.1493
19	5	9	5	.000000	2.8047	.24931	.12613	1.6333	2.1393
20	5	10	5	.000000	2.8125	.25000	.11667	1.6667	2.1333

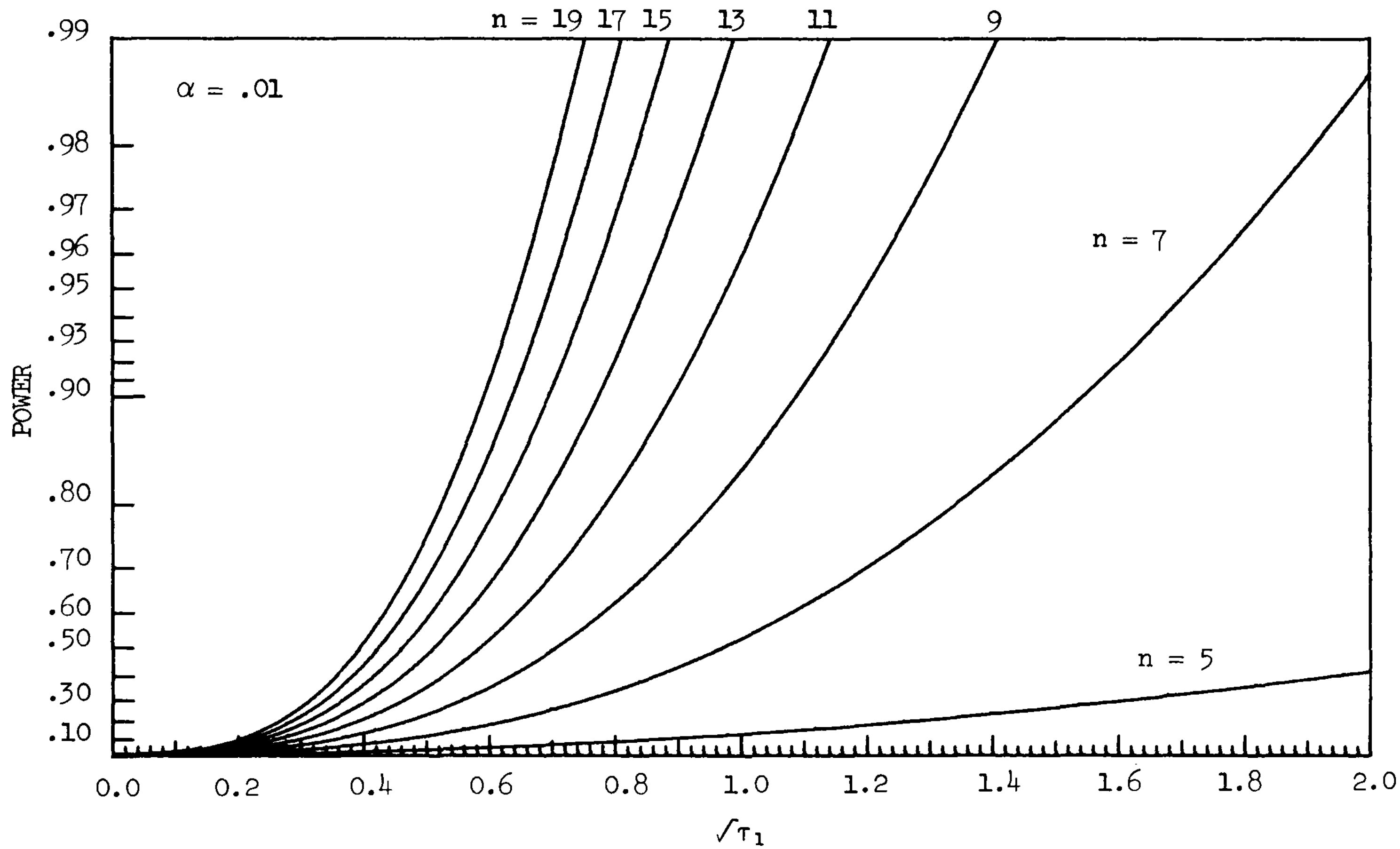


Figure 4.1. Power Functions for One-Factor $\Lambda_2(T_1)$-Optimal Designs for First Order vs. Second Order Models and $\alpha = .01$

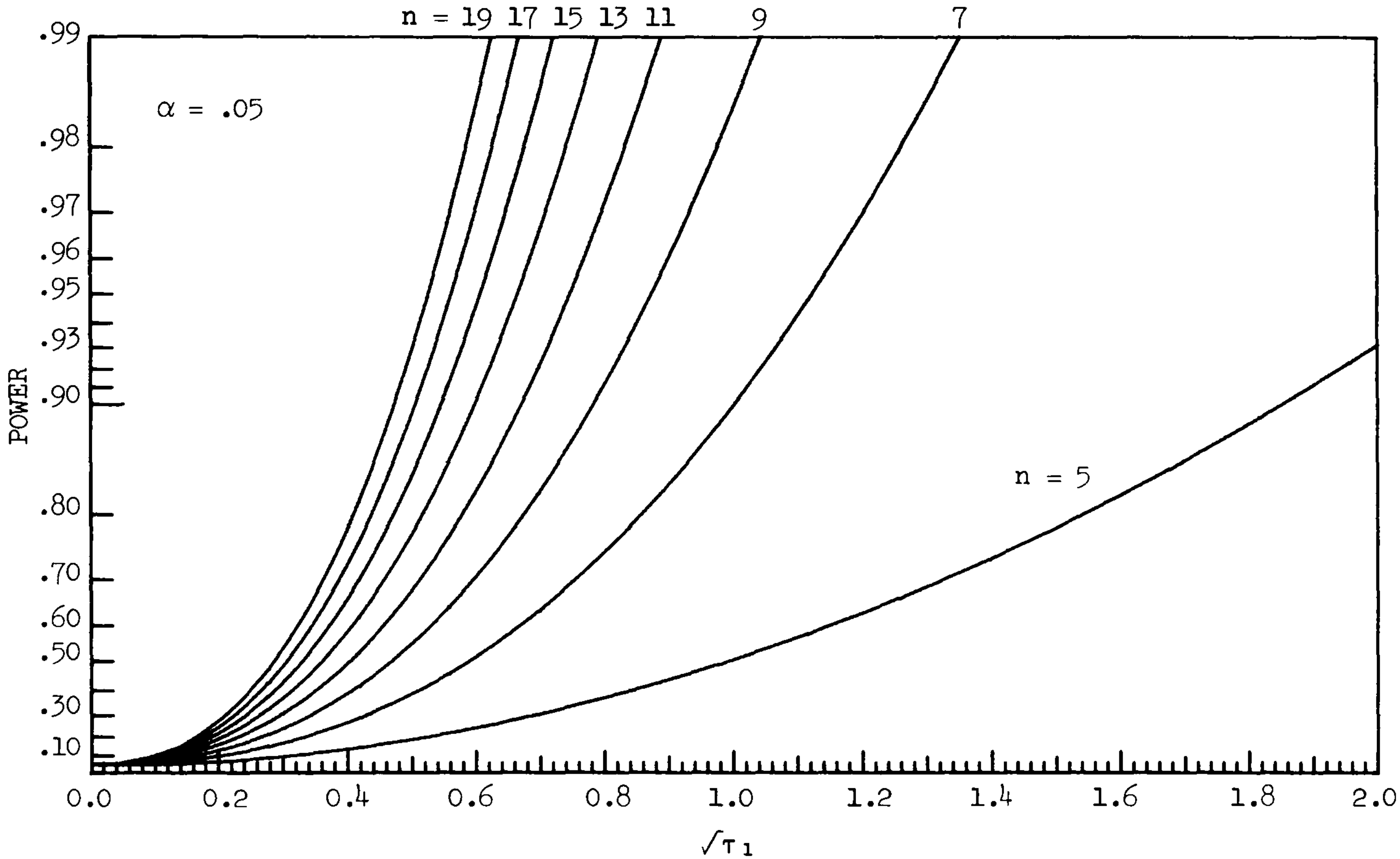


Figure 4.2. Power Functions of the One-Factor $\Lambda_2(T_1)$-Optimal Designs for First Order vs. Second Order Polynomials and $\alpha = .05$

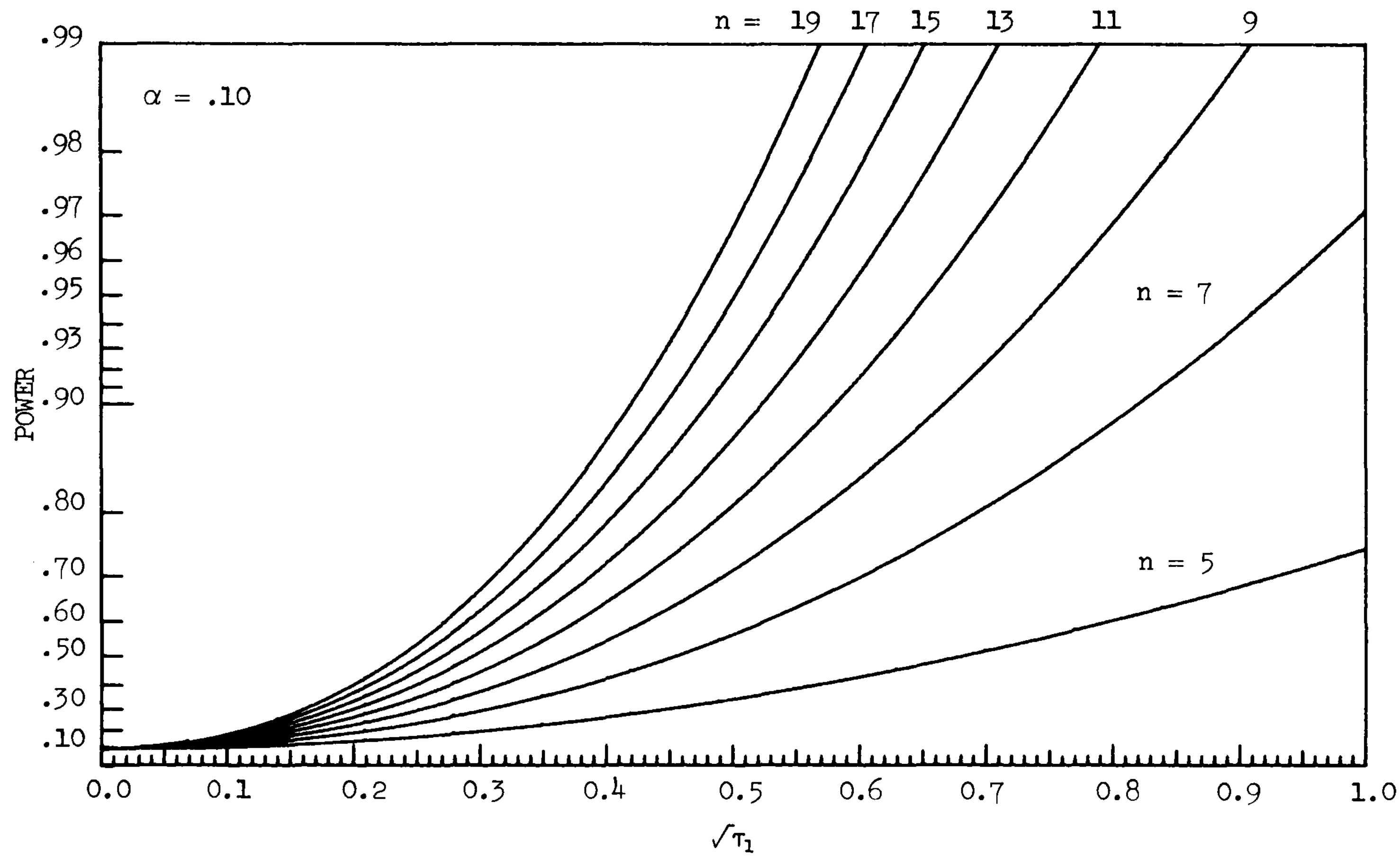


Figure 4.3. Power Functions for One-Factor $\Lambda_2(T_1)$-Optimal Designs for First Order vs. Second Order Models and $\alpha = .10$

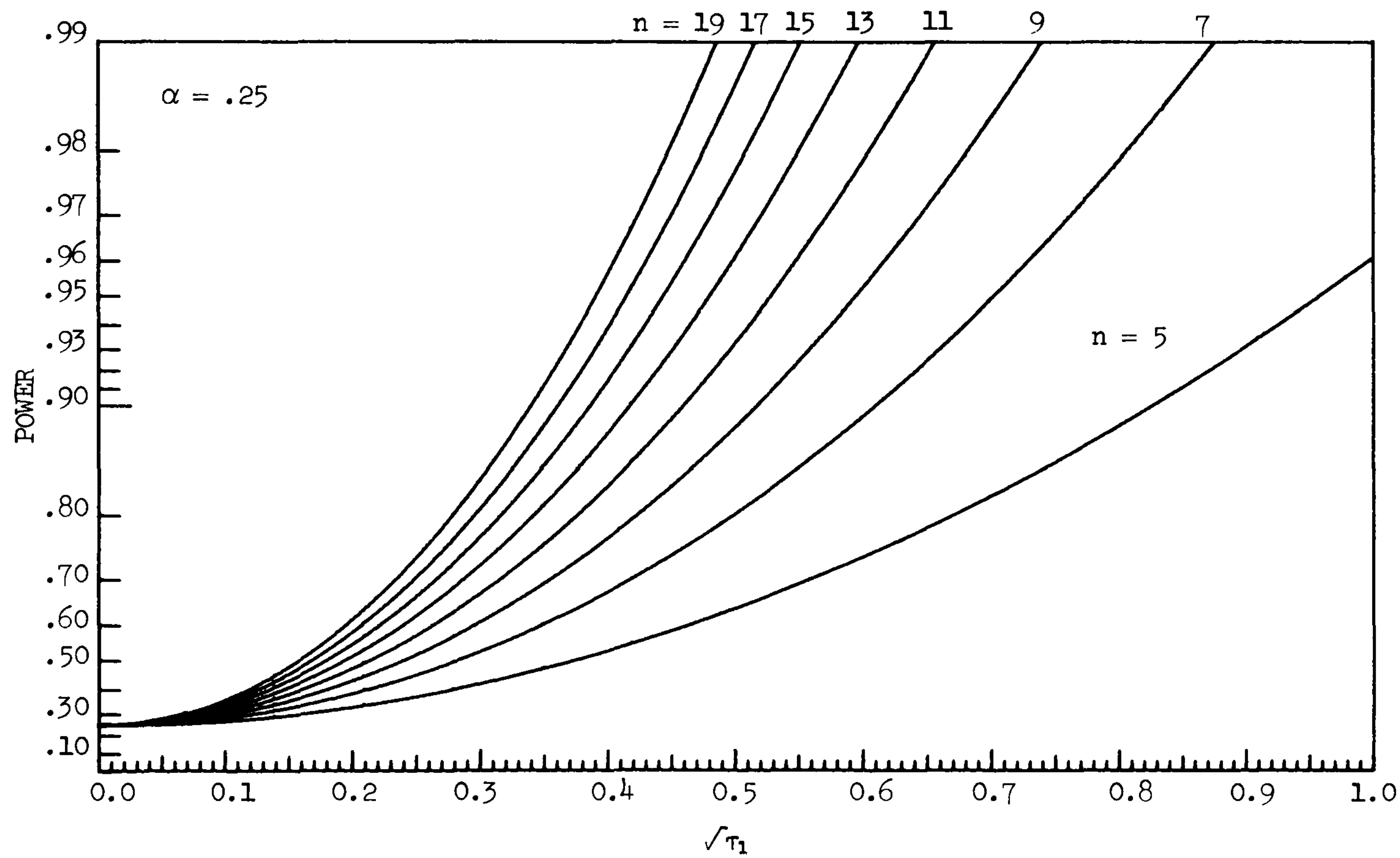


Figure 4.4. Power Functions for One-Factor $\Lambda_2(T_1)$-Optimal Designs for First Order vs. Second Order Models and α = .25

mean square for the higher order model is used in the denominator.

In using these figures, it is helpful to recall that

$$\tau_1 = \sigma^{-2}\,\Omega \int_{-1}^{1} [\eta_1^*(x) - \eta(x)]^2\,dx\ ,$$

where $\eta(x) = \beta_0 + x\,\beta_1 + x^2\beta_{11}$ is the true second order polynomial, and $\eta_1^*(x)$ is the "best" fitting first order approximation to $\eta(x)$. τ_1 measures the ratio of the average squared departure of the response surface to the variance. Thus, $\sqrt{\tau_1}$ can be though of as the "standard deviation" associated with the difference between $\eta(x)$ and its best linear approximation, relative to the error standard deviation σ. In this case, τ_1 can also be expressed in terms of β_{11} as

$$\tau_1 = 4/45(\beta_{11}^2\ /\ \sigma^2).$$

As an example, suppose that we have chosen $\alpha = .25$ and we want a .75 probability of detecting the second order coefficient β_{11} when the root mean squared deviation of the true model from its best first order approximation is $\frac{1}{2}\sigma$. Then using Figure 4.4, we see that a $\Lambda_2(T_1)$-optimal design with $n \geq 7$ will give us the needed power.

4.2.2. One-Factor $\Lambda_2(T_1)$-Optimal Designs for Second Order vs. Third Order Polynomial Models

Table 4.2 contains the one-factor $\Lambda_2(T_1)$-optimal designs, and some of their properties, for second order vs. third order polynomial models and n = 4 - 20. The n = 6 and n = 10 designs were examined

TABLE 4.2

One-Factor $\Lambda_2(T_1)$-Optimal Designs for Second Order vs. Third Order Models

Design

n_1 n_2 n_3 n_4

-1.0 -a b 1.0

n	n_1	n_2	n_3	n_4	a	b	$\Lambda_2(T_1,0)$	n^{-1} L	T_2	Standardized Average Variances V_1	V_2
4	1	1	1	1	.529883	.529883	2.4806	.05670	.042432	2.9369	3.6853
5	1	1	2	1	.488430	.548650	2.4947	.05702	.043274	2.8229	3.5818
6	1	2	2	1	.500000	.500000	2.7344	.06250	.030357	2.6000	3.0857
7	1	2	3	1	.476193	.504738	2.6450	.06046	.029428	2.6564	3.1431
8	1	3	3	1	.478240	.478240	2.6477	.06052	.025331	2.6574	3.0760
9	2	2	3	2	.504339	.541550	2.5462	.05820	.041334	2.8182	3.5285
10	2	3	3	2	.513578	.513578	2.6891	.06146	.035054	2.6693	3.2396
11	2	3	4	2	.495744	.519133	2.6903	.06149	.033770	2.6456	3.1948
12	2	4	4	2	.500000	.500000	2.7344	.06250	.030357	2.6000	3.0857
13	2	4	5	2	.486410	.502781	2.7071	.06188	.029357	2.6125	3.0870
14	2	5	5	2	.488381	.488381	2.7076	.06189	.027307	2.6093	3.0506
15	3	4	5	3	.504513	.523706	2.6681	.06098	.035907	2.6849	3.2737
16	3	5	5	3	.508795	.508795	2.7161	.06208	.033255	2.6330	3.1687
17	3	5	6	3	.497392	.511929	2.7165	.06209	.032219	2.6211	3.1400
18	3	6	6	3	.500000	.500000	2.7344	.06250	.030357	2.6000	3.0857
19	3	6	7	3	.490488	.501968	2.7214	.06220	.029528	2.6040	3.0787
20	3	7	7	3	.492070	.492070	2.7215	.06221	.028183	2.6007	3.0537

in Section 3.2.2. The designs in this table appear to follow the pattern:

$[\pm 1.0\ (n_o),\ \pm .5\ (2n_o)]$ for $n = 6n_o$,

$[\pm 1.0\ (n_o),\ -a\ (2n_o),\ b\ (2n_o+1)]$ for $n = 6n_o + 1$,

$[\pm 1.0\ (n_o),\ \pm a\ (2n_o+1)]$ for $n = 6n_o + 2$,

$[\pm 1.0\ (n_o+1),\ -a\ (2n_o),\ b\ (2n_o+1)]$ for $n = 6n_o + 3$,

$[\pm 1.0\ (n_o+1),\ \pm a\ (2n_o+1)]$ for $n = 6n_o + 4$,

and $[\pm 1.0\ (n_o+1),\ -a\ (2n_o+1),\ b\ (2n_o+2)]$ for $n = 6n_o + 5$,

where a and b are approximately equal to .5.

Except for the n = 4 and n = 5 designs, the properties for these designs appear to be fairly homogeneous. The ranges for some of their properties are:

V_2 3.0506--3.2737

V_1 2.6000--2.8182

$n^{-1} L$ 0.0582--0.0625

and T_2 0.0282--0.0413

Figures 4.5 through 4.8 are provided for choosing the sample size and α-level for the lack of fit test. For this case,

$$\tau_1 = 4/175(\beta_{111}^2 / \sigma^2).$$

4.3. Two-Factor $\Lambda_2(T_1)$-Optimal Designs for Square Regions of Interest

In this section, we will obtain two-factor $\Lambda_2(T_1)$-optimal designs for a region of interest defined by

$$-1 \leq x_i \leq 1,\ i = 1,\ 2. \qquad (4.3.1)$$

However, because of the invariance results of Section 2.2, the designs

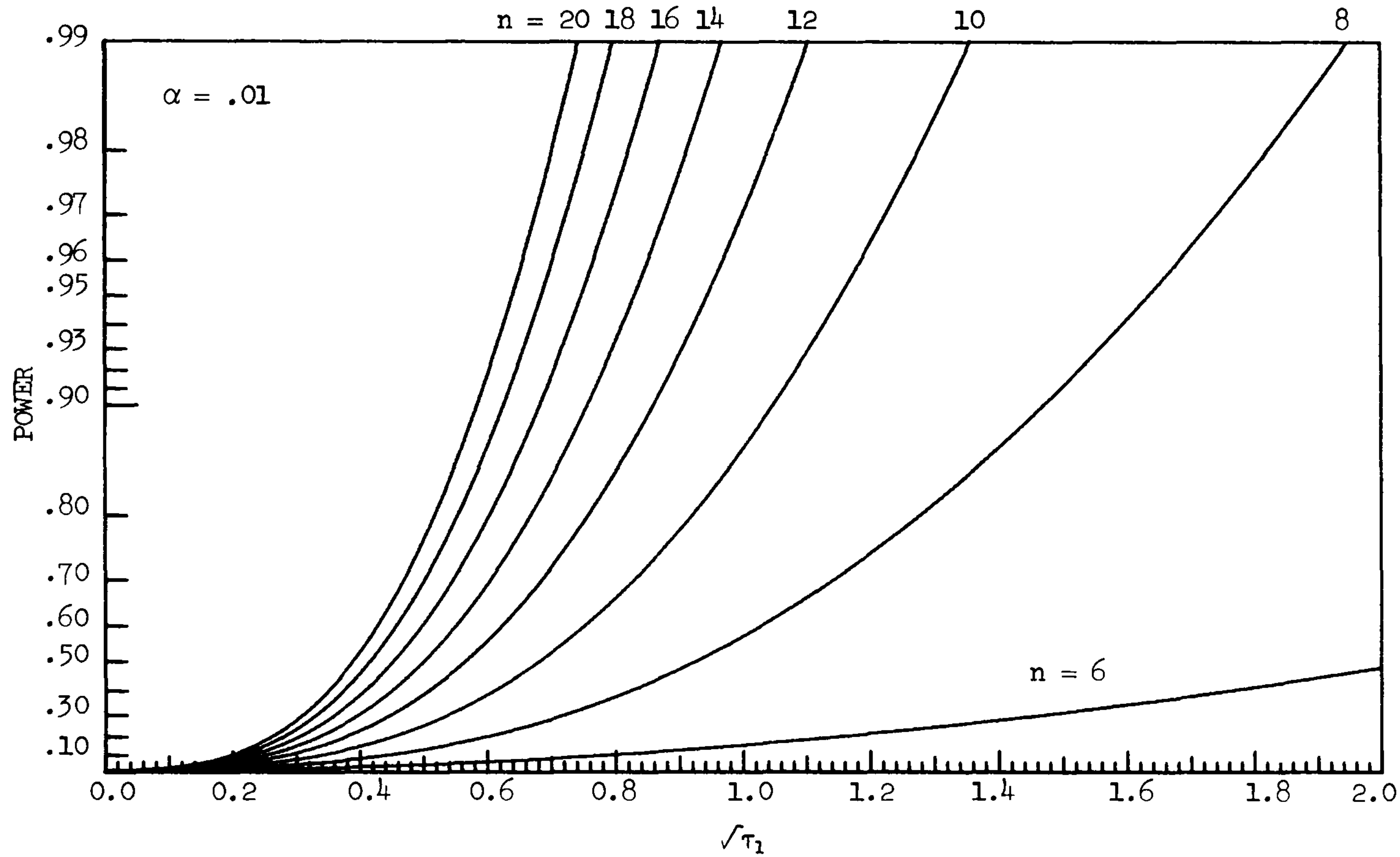


Figure 4.5. Power Functions for One-Factor $\Lambda_2(T_1)$-Optimal Designs for Second Order vs. Third Order Models and $\alpha = .01$

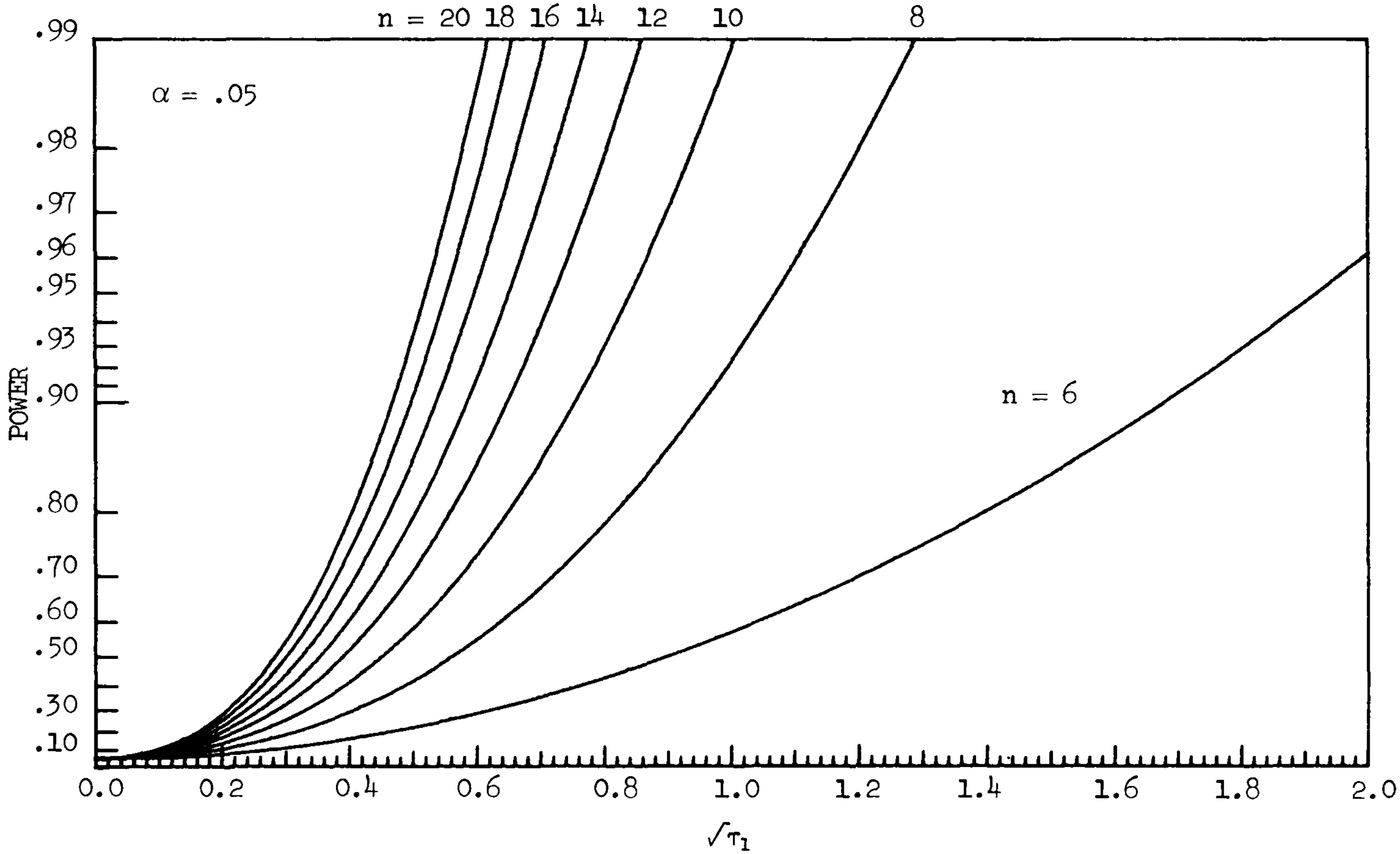


Figure 4.6. Power Functions for One-Factor $\Lambda_2(T_1)$-Optimal Designs for Second Order vs. Third Order Models and $\alpha = .05$

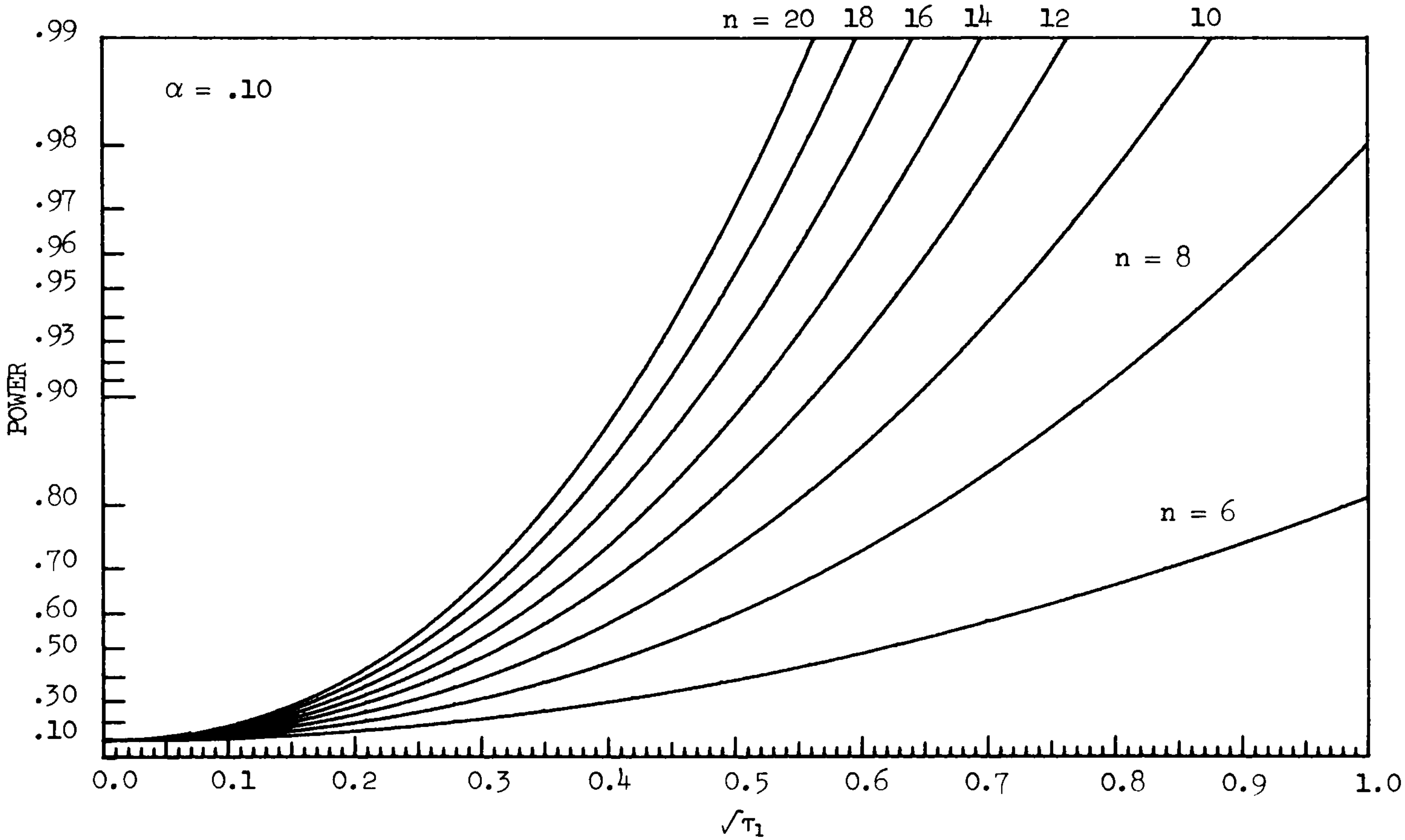


Figure 4.7. Power Functions for One-Factor $\Lambda_2(T_1)$-Optimal Designs for Second Order vs. Third Order Models and $\alpha = .10$

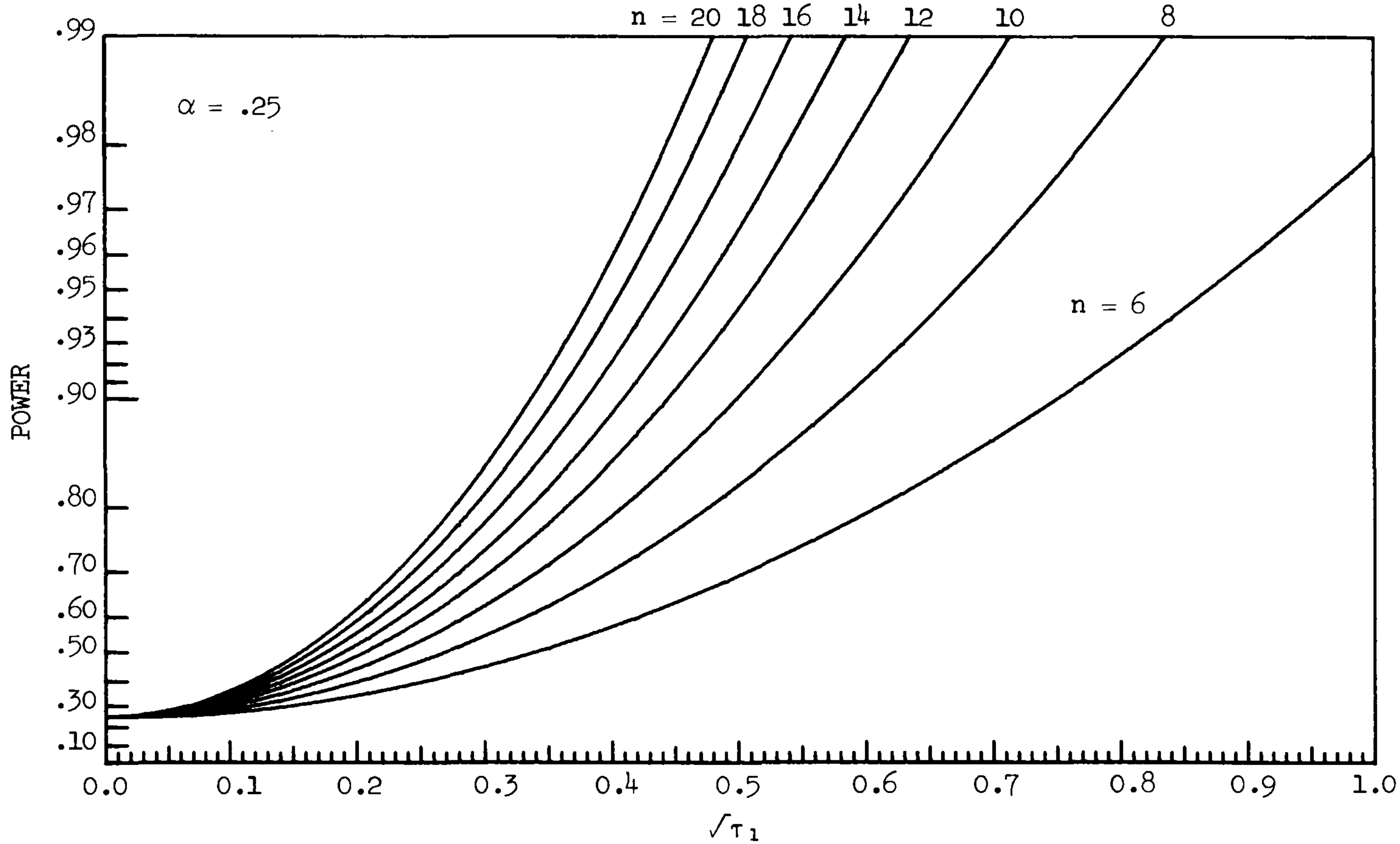


Figure 4.8. Power Functions of the One-Factor $\Lambda_2(T_1)$-Optimal Designs for Second Order vs. Third Order Polynomials and α = .25

given in this section can be scaled for any region of interest that can be expressed as a non-singular linear transformation of (4.3.1), such as

$$a_i \leq x_i \leq b_i, \ i = 1, 2.$$

Furthermore, it is easy to see that any 90°, 180° or 270° orthogonal rotation preserves the region moments of a square. Thus, by Theorem 2.11, it follows that any 90°, 180° or 270° orthogonal rotation of the optimal designs presented in Sections 4.3.1 and 4.3.2 are also optimal.

4.3.1. Two-Factor $\Lambda_2(T_1)$-Optimal Designs for First Order vs. Second Order Polynomial Models and Square Regions of Interest

Table 4.3 contains the two-factor $\Lambda_2(T_1)$-optimal designs for first order vs. second order polynomial models and a square region of interest. The n = 6 design was examined in Section 3.3.1. It is interesting to note that these designs are of the type recommended by Draper and Herzberg (1971) and also by Myers (1971) for fitting a first order model and conducting a lack of fit test.

The variance, bias and power properties for the n = 4 design are somewhat different from the other designs in Table 4.3. This is probably due to the fact that the n = 4 design is concentrated on only four design points while the other designs are concentrated on five design points. Excluding the n = 4 design, the ranges of the design properties listed in Table 4.3 are:

$$V_1 \quad 1.8333\text{--}2.1607$$

$$\text{and} \quad \|T_2\| \quad 0.2473\text{--}0.5434$$

TABLE 4.3

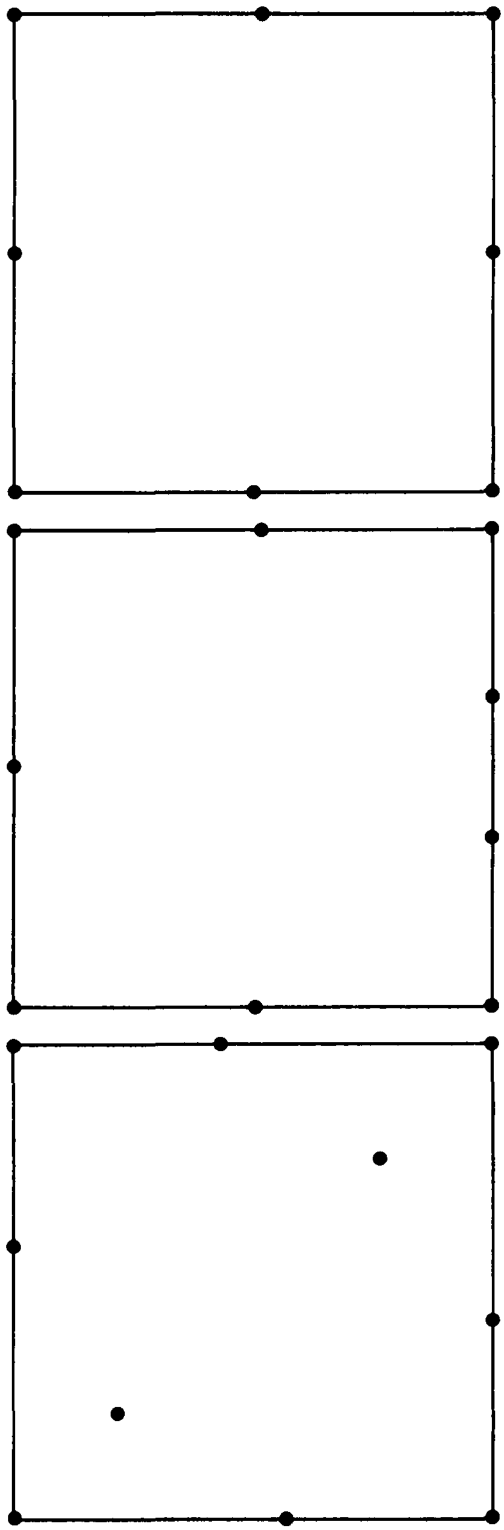
Two-Factor $\Lambda_2(T_1)$-Optimal Designs for First Order vs. Second Order Models

n	Design	$\Lambda_2(T_1,0)$	$\|T_2\|$	V_1	$\|n^{-1} X_1' X_1\|$
4	2^2	9.0000	.98808	1.6667	1.00000
5	2^2 plus one center point	10.8000	.54341	1.8333	0.64000
6	2^2 plus two center points	11.0000	.34211	2.0000	0.44444
7	2^2 plus three center points	10.6530	.24730	2.1667	0.36253
8	2^2 plus two center points and opposite corner points	10.4062	.52119	2.0000	0.50000
9	2^2 plus three center points and opposite corner points	10.5556	.39038	2.1250	0.39506
10	Two replicates of the n = 5 design	10.8000	.54341	1.8333	0.64000

Notice that all of these designs are singular for the second order model.

4.3.2. Two-Factor $\Lambda_2(T_1)$-Optimal Designs for Second Order vs. Third Order Polynomial Models and Square Regions of Interest

Figures 4.9 through 4.11 contain the two-factor $\Lambda_2(T_1)$-optimal designs for second order vs. third order polynomial models and a square region of interest and $n = 8$-15. Some of the properties for these designs are contained in Table 4.4. The $n = 10$ design was examined in Section 3.3.2. Notice that for $n \leq 10$, these designs are singular for the third order model, but for $n \geq 11$, they appear to have reasonable variance properties for the third order model.



n = 8

2^2 plus

1.000000	0.000000
-1.000000	0.000000
0.000000	1.000000
0.000000	-1.000000

n = 9

2^2 plus

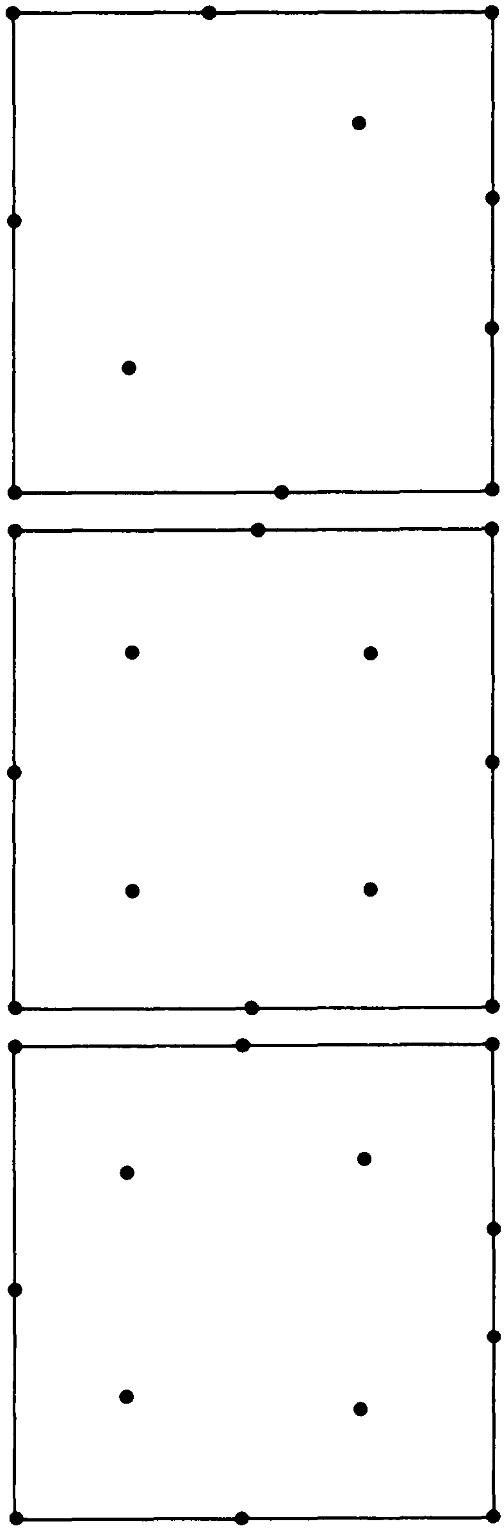
1.000000	-0.326856
1.000000	0.326856
-1.000000	0.000000
0.008101	1.000000
0.008101	-1.000000

n = 10

2^2 plus

1.000000	-0.162432
-1.000000	0.162432
-0.162432	1.000000
0.162432	-1.000000
0.526434	0.526434
-0.526434	-0.526434

Figure 4.9. Two-Factor $\Lambda_2(T_1)$-Optimal Designs for Second Order vs. Third Order Models and n = 8-10



n = 11

2^2 plus

-1.000000	0.133499
0.139958	-1.000000
1.000000	-0.337364
1.000000	0.212748
-0.191295	1.000000
0.469354	0.584257
-0.536432	-0.510439

n = 12

2^2 plus

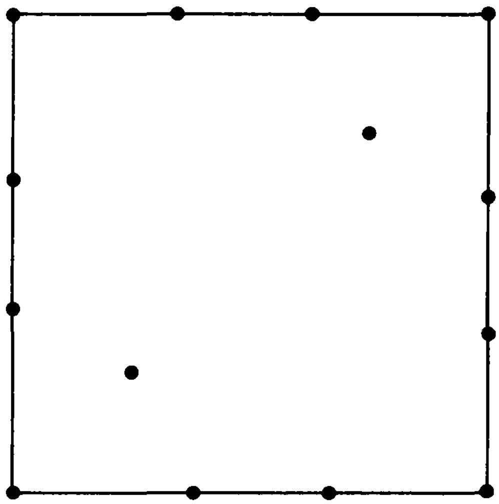
1.000000	0.000000
-1.000000	0.000000
0.000000	1.000000
0.000000	-1.000000
0.518117	-0.518117
-0.518117	0.518117
0.518117	0.518117
-0.518117	-0.518117

n = 13

2^2 plus

-1.000000	0.000000
1.000000	-0.260913
1.000000	0.260913
-0.042615	1.000000
-0.042615	-1.000000
0.478641	-0.553677
0.478641	0.553677
-0.536936	0.503105
-0.536936	-0.503105

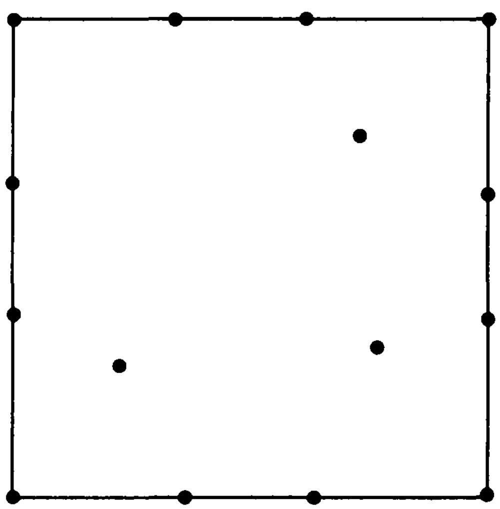
Figure 4.10. Two-Factor $\Lambda_2(T_1)$-Optimal Designs for Second Order vs. Third Order Models and n = 11-13



n = 14

2^2 plus

-1.000000	-0.230798
1.000000	0.230798
-0.230798	-1.000000
0.230798	1.000000
-1.000000	0.335094
1.000000	-0.335094
0.335094	-1.000000
-0.335094	1.000000
0.518914	0.518914
-0.518914	-0.518914



n = 15

2^2 plus

-1.000000	-0.236953
1.000000	0.273963
0.236953	1.000000
-0.273963	-1.000000
-1.000000	0.335892
1.000000	-0.275394
0.275394	-1.000000
-0.335892	1.000000
0.466078	0.545495
-0.545495	-0.466078
0.548258	-0.548258

Figure 4.11. Two-Factor $\Lambda_2(T_1)$-Optimal Designs for Second Order vs. Third Order Models and n = 14-15

TABLE 4.4

Characteristics of the Two-Factor $\Lambda_2(T_1)$-Optimal Designs for Second Order vs. Third Order Models and n = 8-15

n	$\Lambda_2(T_1,0)$	$\lvert n^{-1} L\rvert$	T_2	$\lvert n^{-1} X_1' X_1\rvert$	$\lvert n^{-1} X' X\rvert$	V_1	V_2
† 8	11.2500	$.00000 \times 10^{0}$	.16852	$.8789 \times 10^{-2}$	$.0000 \times 10^{0}$	5.9556	∞
† 9	11.2909	$.00000 \times 10^{0}$	.15988	$.6911 \times 10^{-2}$	$.0000 \times 10^{0}$	6.2308	∞
† 10	11.7961	$.00000 \times 10^{0}$	.14003	$.5909 \times 10^{-2}$	$.0000 \times 10^{0}$	4.5462	∞
11	11.6784	$.51752 \times 10^{-5}$	.13318	$.5168 \times 10^{-2}$	$.2674 \times 10^{-7}$	4.6907	17.1025
12	11.8666	$.20369 \times 10^{-4}$	.11761	$.3858 \times 10^{-2}$	$.7858 \times 10^{-7}$	4.1561	7.3873
13	11.7298	$.21343 \times 10^{-4}$	.11261	$.3555 \times 10^{-2}$	$.7588 \times 10^{-7}$	4.2652	7.4802
14	11.7647	$.15286 \times 10^{-4}$	.11297	$.4096 \times 10^{-2}$	$.6259 \times 10^{-7}$	4.0946	10.3771
15	11.6381	$.21664 \times 10^{-4}$	.10993	$.3567 \times 10^{-2}$	$.7727 \times 10^{-7}$	4.6766	8.4933

† These designs are singular for the third order model.

V. AN EXAMINATION OF THE VARIANCE, BIAS AND POWER PROPERTIES OF $\Lambda(T_2)$-OPTIMAL DESIGNS FOR CUBOIDAL REGIONS OF INTEREST

5.1. Introduction

In Chapter III, we examined the variance, bias and power properties of the $\Lambda(T)$ criteria for τ_1. In this chapter, we will perform a similar examination of the $\Lambda(T)$ criteria for

$$\tau_2 = \sigma^{-2}\,\Omega \int_R \{E[\hat{\eta}_1(\underset{\sim}{x})] - \eta(\underset{\sim}{x})\}^2 \; dx_1 \cdot dx_2 \cdots dx_k$$

$$= \sigma^{-2}\, \underset{\sim}{\beta}_2'\, T_2\, \underset{\sim}{\beta}_2,$$

where $T_2 = [A'\, M_{11}\, A - A'\, M_{12} - M_{21}\, A + M_{22}]$.

The structure and notation used in this chapter will closely parallel that used in Chapter III (see Appendix B for a partial summary of the notation used in this chapter).

Recall that τ_1 measures the average squared deviation of the true model from its best approximation within an assumed class of models, whereas τ_2 measures the average squared deviation of the true model from the fitted model. As a result, τ_1 is not influenced by the design whereas τ_2 is.

In this chapter, we will examine the following criteria:

1. $\Lambda_1(T_2)$-optimality-- $\underset{D\,\varepsilon\,\Delta}{\text{Max}}\ \text{Ch}_{\min}[T_2^{-1}\, L]$, (5.1.1)

2. $\Lambda_2(T_2,c)$-optimality-- $\underset{D\,\varepsilon\,\Delta}{\text{Max}}\ |T_2|^{-c}\ \text{Tr}[T_2^{-1}\, L]$, (5.1.2)

and 3. $\Lambda_3(T_2,c)$-optimality-- $\underset{D\,\varepsilon\,\Delta}{\text{Min}}\ |L|^{-c}\ \text{Tr}[L^{-1}\, T_2]$, (5.1.3) for $c = 0$ and $c = \frac{1}{2}$. We shall collectively refer to these criteria as the $\Lambda(T_2)$ criteria.

5.2. One-Factor $\Lambda(T_2)$-Optimal Designs for Polynomial Models and $c = 0, \frac{1}{2}$

In this section, we will examine one-factor $\Lambda(T_2)$-optimal designs for $c = 0$ and $c = \frac{1}{2}$. The closed interval $[-1, 1]$ is used as the region of interest; however, because of the invariance results of Section 2.2, the results of this section apply to any region of interest of the form $[a, b]$, where $a < b$. We will examine the one-factor, first order vs. second order polynomial models for $n = 5$, 9, and the one-factor, second order vs. third order polynomial models for $n = 6$, 10.

For all of these cases, the $\underset{\sim}{\beta}_2$-space is one-dimensional, and the $\Lambda(T_2)$ criteria for $c = 0$ and $c = \frac{1}{2}$ can be summarized as:

1. $\Lambda_1(T_2)$, $\Lambda_2(T_2,0)$, and $\Lambda_3(T_2,0)$-optimality--

$$\underset{D \,\varepsilon\, \Delta}{\text{Max}} \; L \,/\, T_2, \tag{5.2.1}$$

2. $\Lambda_2(T_2,\frac{1}{2})$-optimality--

$$\underset{D \,\varepsilon\, \Delta}{\text{Max}} \; L \,/\, T_2^{3\div 2}, \tag{5.2.2}$$

3. $\Lambda_3(T_2,\frac{1}{2})$-optimality--

$$\underset{D \,\varepsilon\, \Delta}{\text{Max}} \; L^{3\div 2} \,/\, T_2. \tag{5.2.3}$$

5.2.1. One-Factor $\Lambda(T_2)$-Optimal Designs for First Order vs. Second Order Polynomial Models and $n = 5, 9$

In general, we cannot expect criteria (5.2.1) - (5.2.3) to select

The same optimal designs. However, for this case, these criteria do select the same optimal design for n = 5 and n = 9. Furthermore, these designs are the $\Lambda(T_1)$-optimal designs examined in Section 3.2.1. We recall that these designs were exceptional among those examined in Chapter III, in that they were nearly minimum bias.

5.2.2. One-Factor $\Lambda(T_2)$-Optimal Designs for Second Order vs. Third Order Polynomial Models and n = 6, 10

5.2.2.1. The n = 6 Designs.--The one-factor, n = 6, $\Lambda(T_2)$-optimal designs are given in Table 5.1. Their bias and power functions are illustrated in Figures 5.1 and 5.2 respectively. The power curves in Figure 5.2 are based upon an F-test in which the residual mean square for the higher order model is used in the denominator. For this case, there seems to be little difference among the $\Lambda(T_2)$-optimal designs.

On the whole, the n = 6, $\Lambda(T_2)$-optimal designs seem to have good variance, bias and power properites. Their strongest competitor is the $|L|$-optimal design (this is also the $\Lambda(T_1)$-optimal design). However, although this design has slightly better variance properties, its bias properties are not quite as good as those of the $\Lambda(T_2)$-optimal designs. Notice that the second order D-optimal and third order D-optimal Design (2) appear to have very poor bias properties.

Table 5.1 illustrates the use of c for achieving tradeoffs between maximizing the power (n^{-1} L) and minimizing the fitted bias (T_2). $\Lambda_3(T_2,\frac{1}{2})$-optimality maximizes (5.2.3), thereby emphasizing

TABLE 5.1. A Comparison of Some Characteristics of One-Factor $\Lambda(T_2)$-Optimal Designs for Second Order vs. Third Order Models and n = 6

Design	n^{-1} L	T_2	Standardized Average Variances V_1	V_2	D-Efficiencies E_1	E_2
2nd Order D-Optimal [$\pm$ 1.0 (2), 0.0 (2)]	.000000	.076190	2.4000	∞	1.0000	0.0000
3rd Order D-Optimal--Design (1) [$\pm$ 1.0, $\pm\sqrt{.2}$ (2)]	.060952	.032653	2.4643	3.0000	0.7652	1.0000
3rd Order D-Optimal--Design (2) [$\pm$ 1.0, 1.0, $\sqrt{.2}$, $-\sqrt{.2}$ (2)]	.047407	.055121	2.6945	3.8571	0.8320	1.0000
Minimum Bias [$\pm$ .902652, $\pm$ .5 (2)]	.032945	.022857	3.1699	3.8637	0.5941	0.7092
$\lvert L \rvert$-Optimal [$\pm$ 1.0, $\pm$ .5 (2)]	.062500	.030357	2.6000	3.0857	0.7500	0.9913
$\Lambda_1(T_2)$-Optimal, $\Lambda_2(T_2,0)$-Optimal and $\Lambda_3(T_2,0)$-Optimal [$\pm$ 1.0, $\pm$ .538690 (2)]	.061676	.029328	2.7609	3.2365	0.7357	0.9458
$\Lambda_2(T_2,\frac{1}{2})$-Optimal [$\pm$ .983792, $\pm$ .536212 (2)]	.055652	.027211	2.8308	3.3197	0.7094	0.9236
$\Lambda_3(T_2,\frac{1}{2})$-Optimal [$\pm$ 1.0, $\pm$ .529462 (2)]	.062021	.029528	2.7165	3.1926	0.7393	0.9788

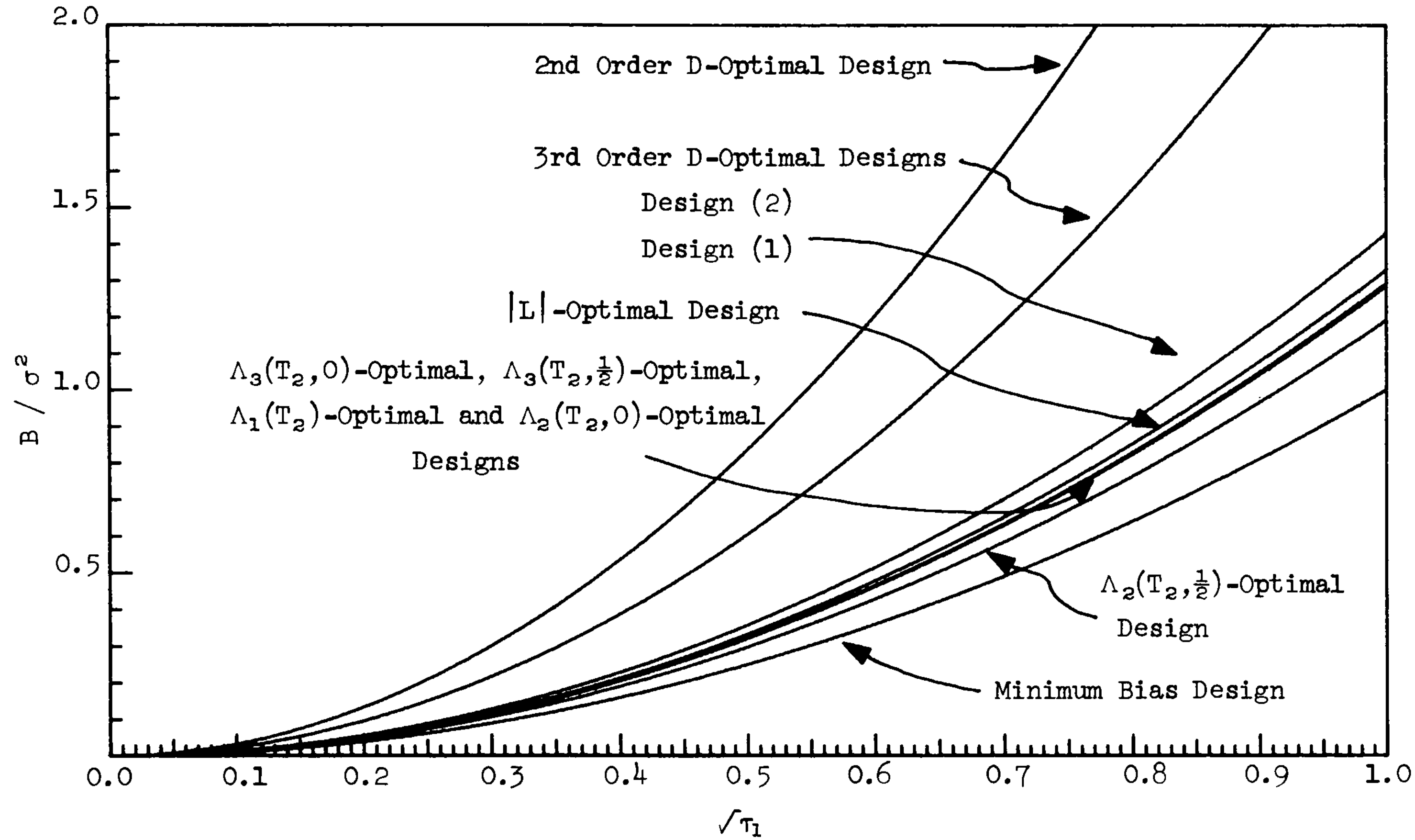


Figure 5.1. A Comparison of the Bias Functions for One-Factor $\Lambda(T_2)$-Optimal Designs for Second Order vs. Third Order Models and $n = 6$

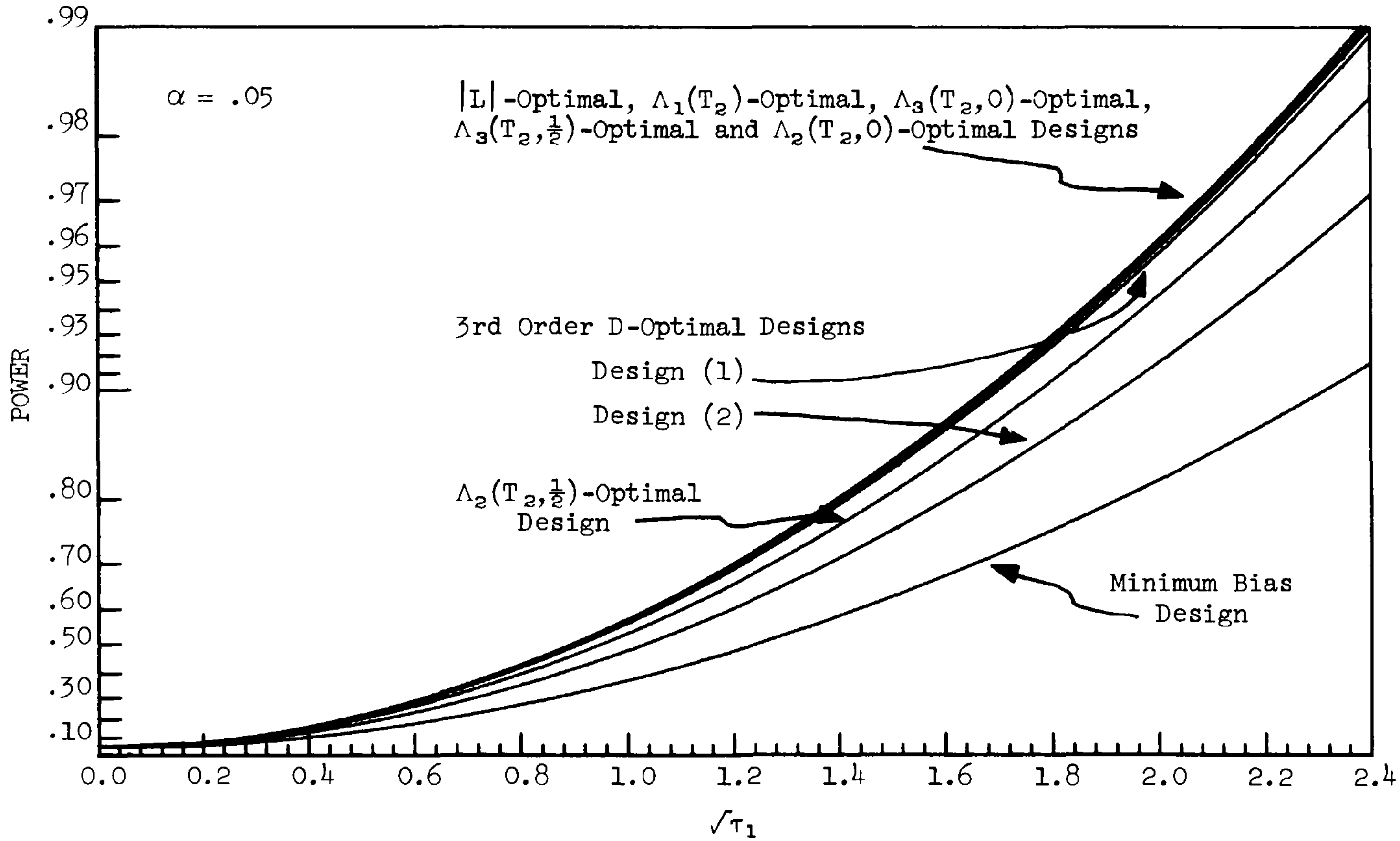


Figure 5.2. A Comparison of the Power Functions for One-Factor $\Lambda(T_2)$-Optimal Designs for Second Order vs. Third Order Models and $n = 6$

power for the detection of model inadequacy at the possible expense of increased fitted bias. On the other hand, $\Lambda_2(T_2,\frac{1}{2})$-optimality maximizes (5.2.2), thereby emphasizing bias protection at the possible expense of decreased power. $\Lambda_1(T_2)$, $\Lambda_2(T_2,0)$, and $\Lambda_3(T_2,0)$-optimality all maximize (5.2.1); as a result, they have selected a design with bias and power properties between those of the $\Lambda_2(T_2,\frac{1}{2})$-optimal and $\Lambda_3(T_2,\frac{1}{2})$-optimal designs.

5.2.2.2. The n = 10 Designs.--The one-factor, n = 10, $\Lambda(T_2)$-optimal designs for c = 0 and c = $\frac{1}{2}$ are given in Table 5.2. Their bias and power functions are illustrated in Figures 5.3 and 5.4 respectively. Again, as we noted for the n = 6 designs, the bias and variance properties of the $\Lambda(T_2)$-optimal designs are almost indistinguishable. On the whole, the $\Lambda(T_2)$-optimal designs appear to have very good power and bias properties, very good variance properties for the higher order model, but only fair variance properties for the lower order model.

The major differences between the n = 6 and n = 10 designs appear to be in their variance and bias properties. The variance properties of the n = 10, $\Lambda(T_2)$-optimal designs are not as good for the lower order model as those noted for the n = 6 designs. However, the bias properties of the $\Lambda(T_2)$-optimal, n = 10 designs are much better than those noted for the n = 6 designs. In fact, the n = 10, $\Lambda(T_2)$-optimal designs are nearly minimum bias. They appear to have obtained a very favorable tradeoff between their variance and bias properties.

TABLE 5.2. A Comparison of Some Characteristics of One-Factor $\Lambda(T_2)$-Optimal Designs for Second Order vs. Third Order Models and n = 10

Design	n^{-1} L	T_2	Standardized Average Variances V_1	V_2	D-Efficiencies E_1	E_2
2nd Order D-Optimal [$\pm$ 1.0 (3), 0.0 (4)]	.000000	.076190	2.2222	∞	1.0000	0.0000
3rd Order D-Optimal--Design (1) [$\pm$ 1.0 (2), $\pm\sqrt{.2}$ (3)]	.059077	.038321	2.4466	3.0952	0.8216	1.0000
3rd Order D-Optimal--Design (2) [$\pm$ 1.0 (3), $\pm\sqrt{.2}$ (2)]	.045177	.054045	2.8513	4.0476	0.8985	1.0000
3rd Order D-Optimal--Design (3) [$\pm$ 1.0 (2), 1.0, $\pm\sqrt{.2}$ (2), $\sqrt{.2}$]	.051200	.049642	2.6019	3.5714	0.8618	1.0000
Minimum Bias [$\pm$ .981491, $\pm$ .5 (4)]	.049933	.022857	2.9840	3.4417	0.6055	0.7626
$\|L\|$-Optimal [$\pm$ 1.0 (2), $\pm$ .513578 (3)]	.061465	.035054	2.6693	3.2396	0.7960	0.9862
$\Lambda_1(T_2)$-Optimal, $\Lambda_2(T_2,0)$-Optimal and $\Lambda_3(T_2,0)$-Optimal [$\pm$ 1.0, $\pm$ .479005 (4)]	.056830	.023182	2.8313	3.2392	0.6325	0.8139
$\Lambda_2(T_2,\frac{1}{2})$-Optimal [$\pm$ 1.0, $\pm$ .484603 (4)]	.056716	.023145	2.8400	3.2481	0.6319	0.8129
$\Lambda_3(T_2,\frac{1}{2})$-Optimal [$\pm$ 1.0, $\pm$ .474383 (4)]	.056901	.023218	2.8249	3.2329	0.6330	0.8146

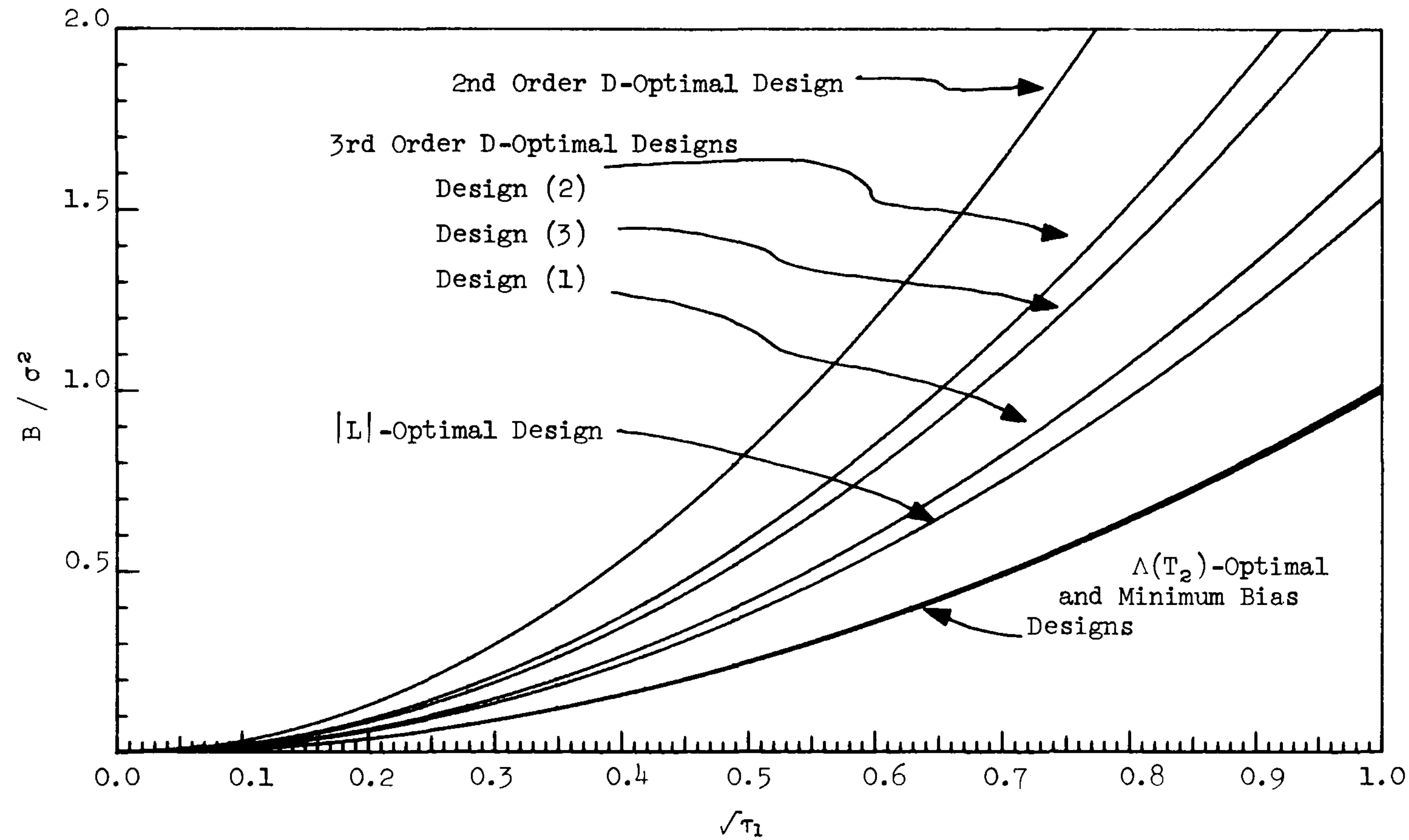


Figure 5.3. A Comparison of the Bias Functions for One-Factor $\Lambda(T_2)$-Optimal Designs for Second Order vs. Third Order Models and n = 10

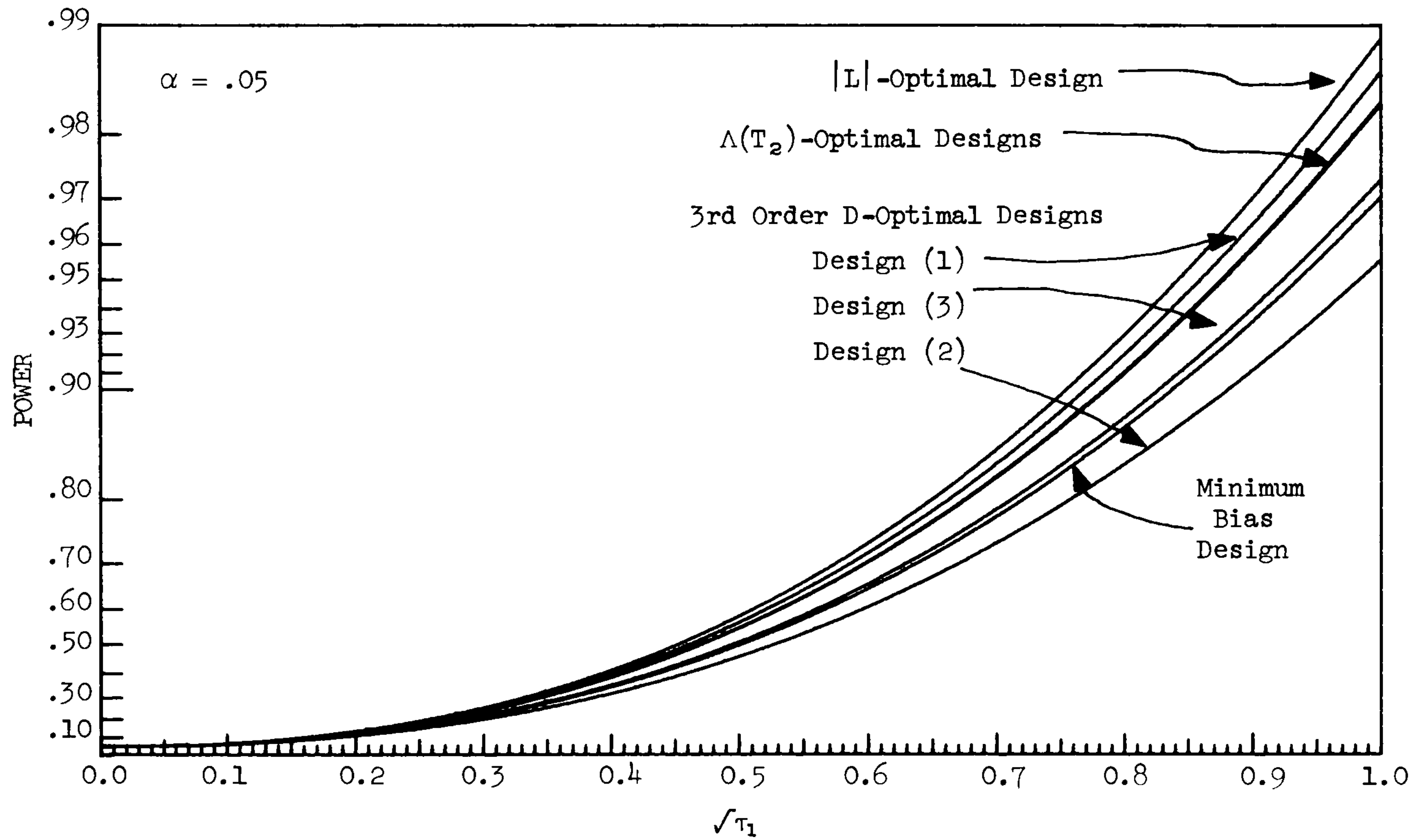


Figure 5.4. A Comparison of the Power Functions for One-Factor $\Lambda(T_2)$-Optimal Designs for Second Order vs. Third Order Models and n = 10

Notice that for this case, the $|L|$-optimal design (this is also the $\Lambda(T_1)$-optimal design) is not as competitive as it was for the $n = 6$ case. It still has slightly better variance and power properties, but its bias properties are considerably worse.

5.3. Two-Factor $\Lambda(T_2)$-Optimal Designs for Polynomial Models and $c = 0, \frac{1}{2}$

In this section, we will examine the $\Lambda(T_2)$ criteria (5.1.1) -- (5.1.3) for the square region of interest defined by

$$-1 \leq x_i \leq 1, \quad i = 1, 2. \tag{5.3.1}$$

However, because of the invariance results of Section 2.2, these results are applicable for any region of interest that can be expressed as a non-singular linear transformation of (5.3.1). Furthermore, because of Theorems 2.11 and 2.12, any 90°, 180° or 270° rotation of the optimal designs given in Sections 5.3.1 and 5.3.2 are also optimal.

5.3.1. Two-Factor $\Lambda(T_2)$-Optimal Designs for First Order vs. Second Order Polynomial Models and $n = 6$

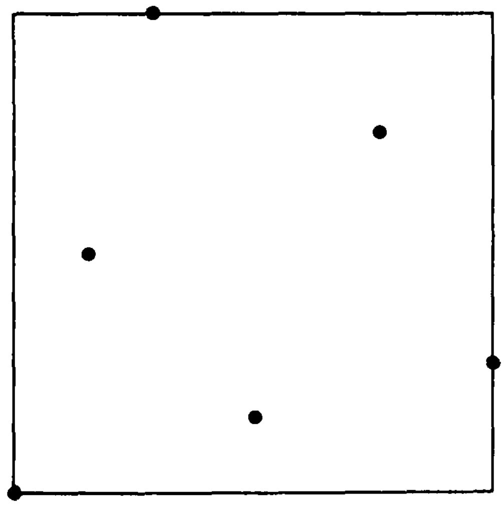
First let us examine the two-factor $\Lambda(T_2)$-optimal designs when the lower order model is first order,

$$\eta_1(\underset{\sim}{x}) = \beta_0 + x_1 \beta_1 + x_2 \beta_2,$$

while the higher order model is second order,

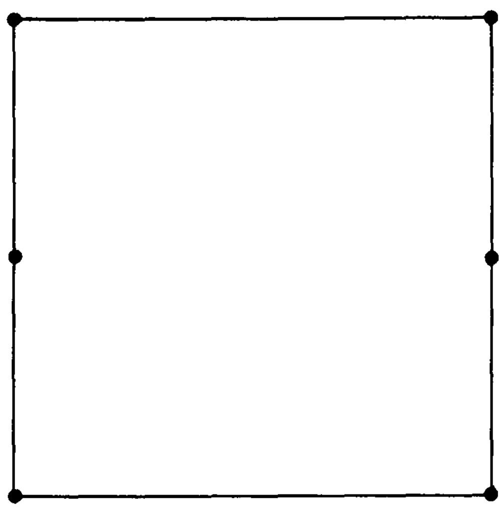
$$\eta(\underset{\sim}{x}) = \beta_0 + x_1 \beta_1 + x_2 \beta_2 + x_1 x_2 \beta_{12} + x_1^2 \beta_{11} + x_2^2 \beta_{22} .$$

The $n = 6$, $\Lambda(T_2)$-optimal designs for this case are illustrated in Figures 5.5 -- 5.6. Some of their properties are given in Table 5.3.



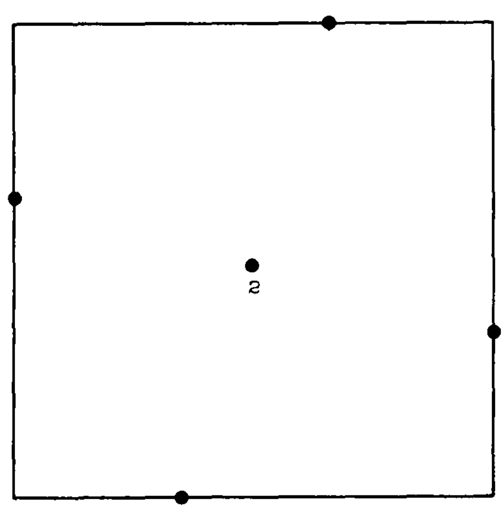
$\Lambda_1(T_2)$-Optimal Design

-1.000000	-1.000000
1.000000	-0.466230
-0.466230	1.000000
0.564405	0.564405
0.009629	-0.689963
-0.689963	0.009629



$\Lambda_2(T_2,0)$-Optimal Design

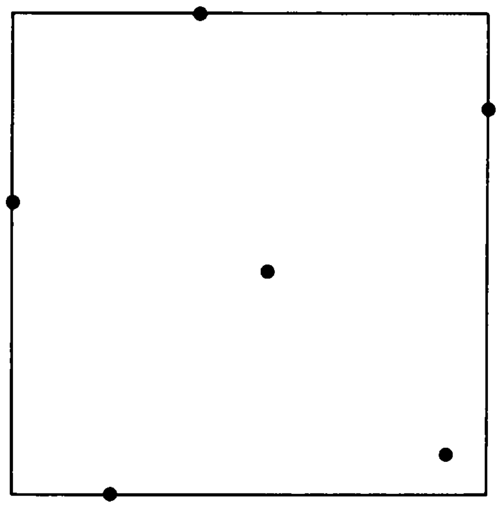
1.000000	-1.000000
-1.000000	1.000000
1.000000	1.000000
-1.000000	-1.000000
1.000000	0.000000
-1.000000	0.000000



$\Lambda_2(T_2,\frac{1}{2})$-Optimal Design

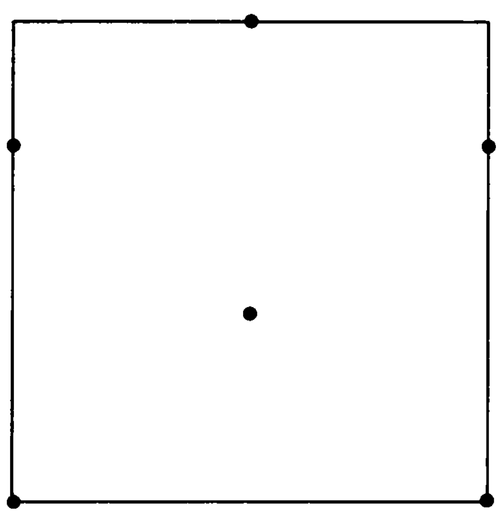
1.000000	-0.311446
-1.000000	0.311446
-0.311446	-1.000000
0.311446	1.000000
0.000000	0.000000
0.000000	0.000000

Figure 5.5. Two-Factor $\Lambda_1(T_2)$-Optimal and $\Lambda_2(T_2,c)$-Optimal Designs for First Order vs. Second Order Models and $n = 6$



$\Lambda_3(T_2,0)$-Optimal Design

-1.000000	0.239931
-0.239931	1.000000
1.000000	0.625280
-0.625280	-1.000000
0.092138	-0.092138
0.885426	-0.885426



$\Lambda_3(T_2,\frac{1}{2})$-Optimal Design

-1.000000	-1.000000
1.000000	-1.000000
0.000000	1.000000
1.000000	0.530517
-1.000000	0.530517
0.000000	-0.218569

Figure 5.6. Two-Factor $\Lambda_3(T_2,c)$-Optimal Designs for First Order vs. Second Order Models and $n = 6$

TABLE 5.3

A Comparison of Some Characteristics of Two-Factor $\Lambda(T_2)$-Optimal Designs for First Order vs. Second Order Models and n = 6

Design	$\lvert n^{-1} L\rvert$	$\lVert T_2\rVert$	Standardized Average Variances V_1	V_2	D-Efficiencies E_1	E_2
1st Order D-Optimal	$.00000 \times 10^{0}$	1.10039	1.7500	∞	1.0000	0.0000
2nd Order D-Optimal	$.11959 \times 10^{-1}$	0.40539	1.9694	4.9043	0.8572	1.0000
$\lvert L\rvert$-Optimal	$.12089 \times 10^{-1}$	0.40095	1.9802	4.8838	0.8526	0.9983
Minimum Bias Hexagon	$.00000 \times 10^{0}$	0.16777	3.0000	∞	0.5946	0.0000
Minimum Bias Pentagon plus Center Point	$.39506 \times 10^{-3}$	0.16777	3.0000	7.3333	0.5946	0.4439
$\Lambda_1(T_2)$-Optimal	$.16377 \times 10^{-2}$	0.26497	2.4036	6.0911	0.7207	0.6396
$\Lambda_2(T_2,0)$-Optimal	$.00000 \times 10^{0}$	0.65997	1.8333	∞	0.9086	0.0000
$\Lambda_2(T_2,\frac{1}{2})$-Optimal	$.00000 \times 10^{0}$	0.16889	2.8232	∞	0.6228	0.0000
$\Lambda_3(T_2,0)$-Optimal	$.60681 \times 10^{-2}$	0.23078	2.2363	4.6531	0.6895	0.8218
$\Lambda_3(T_2,\frac{1}{2})$-Optimal	$.10911 \times 10^{-1}$	0.33262	2.0557	4.6416	0.8194	0.9557

The D-optimal, $|L|$-optimal and minimum bias designs referred to in Table 5.3 were illustrated in Figures 3.9 and 3.10. The second order D-optimal design was given by Hartley and Ruud (1969) and also by Box and Draper (1971). The minimum bias designs were obtained from Lawrence (1964). The other designs were obtained using the computational algorithm described in Appendix A.

The maximum and average bias properties of these designs are illustrated in Figures 5.7 and 5.8. The $\Lambda_2(T_2,\frac{1}{2})$-optimal design is nearly minimum bias, and the $\Lambda_1(T_2)$-optimal and $\Lambda_3(T_2,0)$-optimal designs appear to have good fitted bias properties relative to the remaining designs. The minimum and average value of λ for a given value of τ_1 are illustrated in Figures 5.9 and 5.10. These figures illustrate some of the tradeoffs between maximizing λ and minimizing the fitted bias, τ_2. While the $\Lambda_2(T_2,\frac{1}{2})$-optimal design is nearly minimum bias, its power and variance properties are not as good as those of the other $\Lambda_1(T_2)$-optimal designs. Similarly, although the $\Lambda_2(T_2,0)$-optimal and $\Lambda_3(T_2,\frac{1}{2})$-optimal designs have good power and variance properties, their bias properties seem poor.

5.3.1.1. The $\Lambda_1(T_2)$-optimal Design.--The $\Lambda_1(T_2)$-optimal design appears to have only fair variance and power properties for the detection of a given level of inherent departure (it still has good power properties in the sense defined by its own criterion). This is partly excused by its good bias properties, relative to most of the other designs. However, the variance and power properties of the $\Lambda_3(T_2,0)$-optimal design, which has nearly the same bias properties,

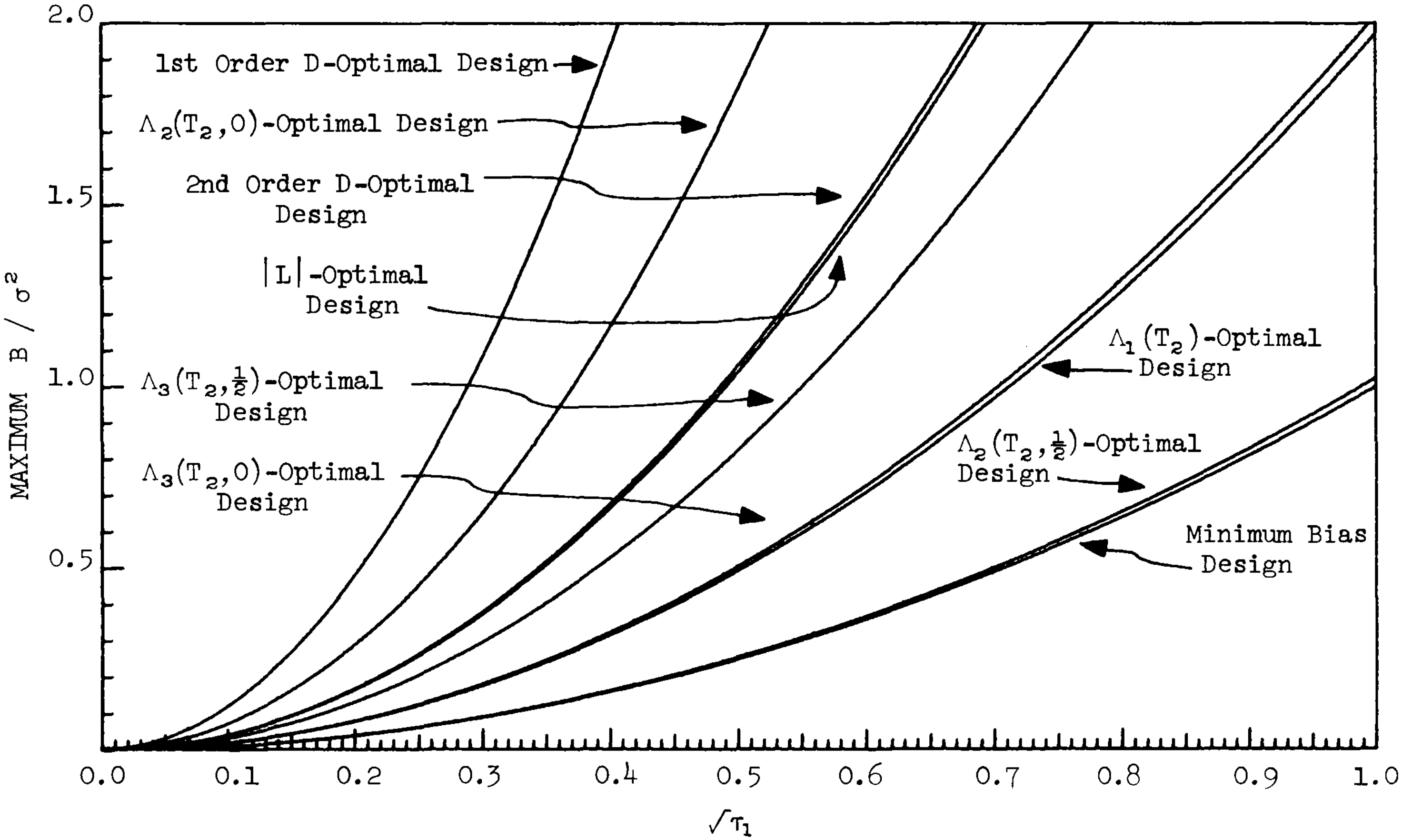


Figure 5.7. The Maximum Bias for Two-Factor $\Lambda(T_2)$-Optimal Designs for First Order vs. Second Order Models and $n = 6$

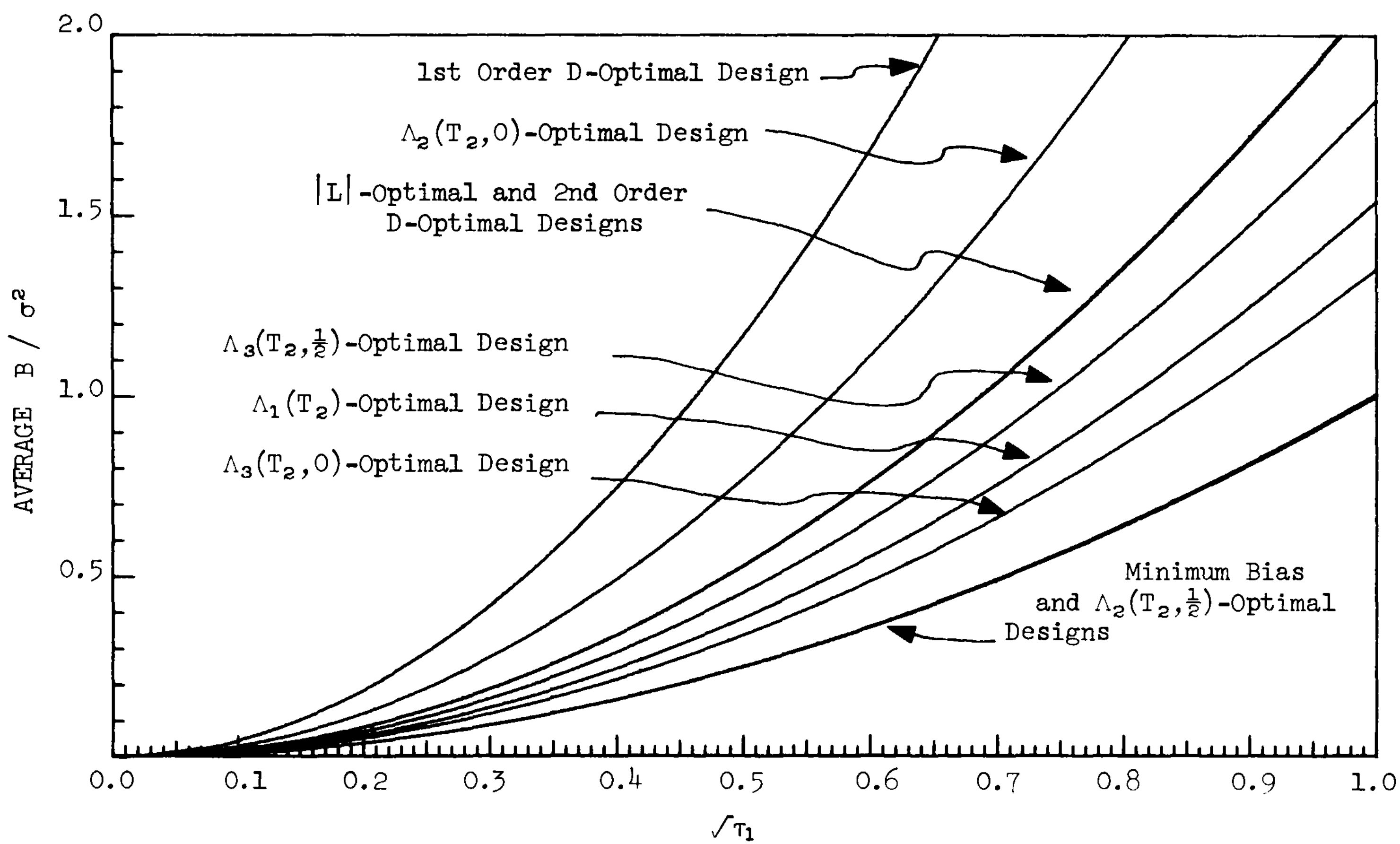


Figure 5.8. The Average Bias for Two-Factor $\Lambda(T_2)$-Optimal Designs for First Order vs. Second Order Models and n = 6

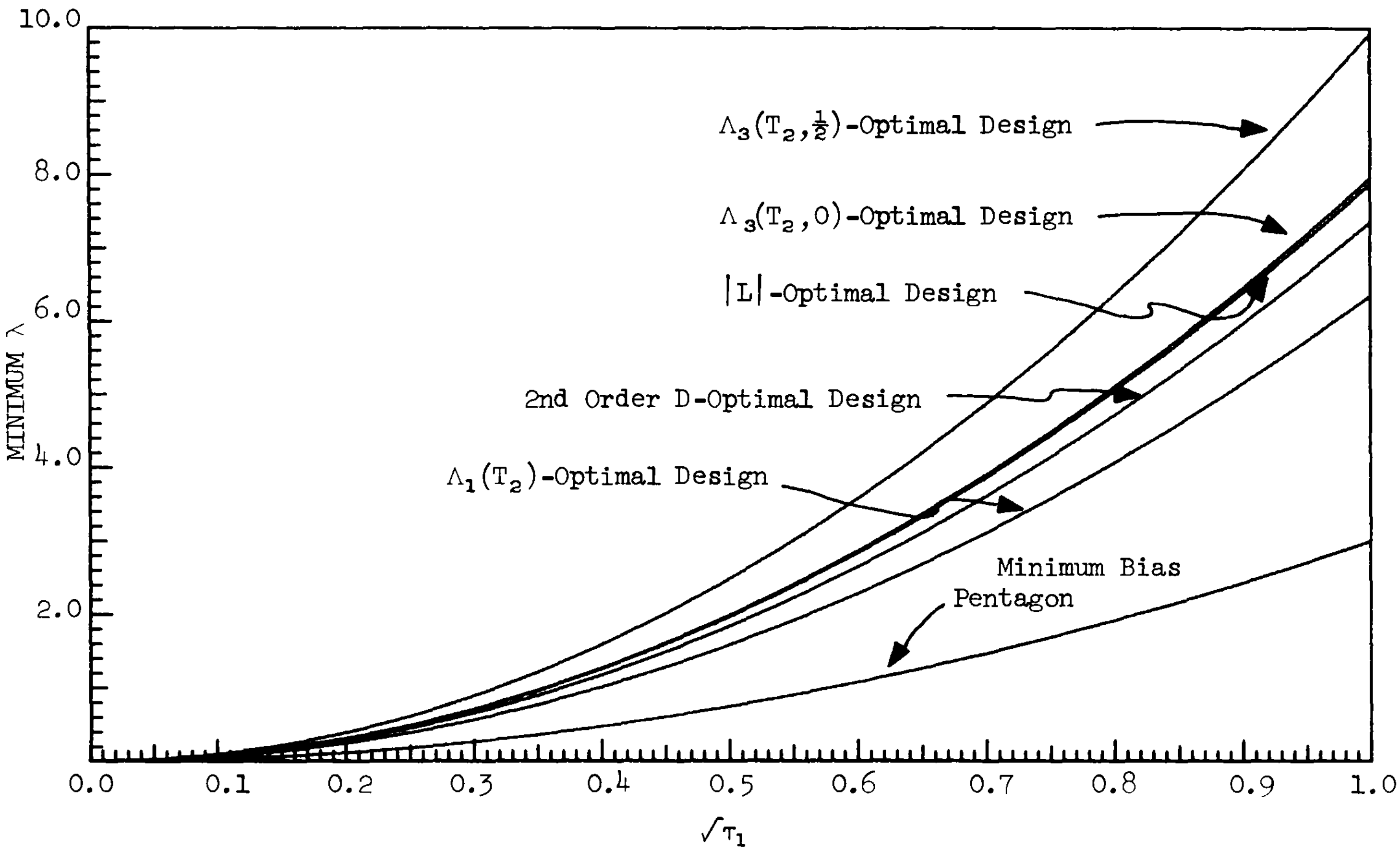


Figure 5.9. The Minimum Value of the Non-Centrality Parameter for Two-Factor $\Lambda(T_2)$-Optimal Designs for First Order vs. Second Order Models and n = 6

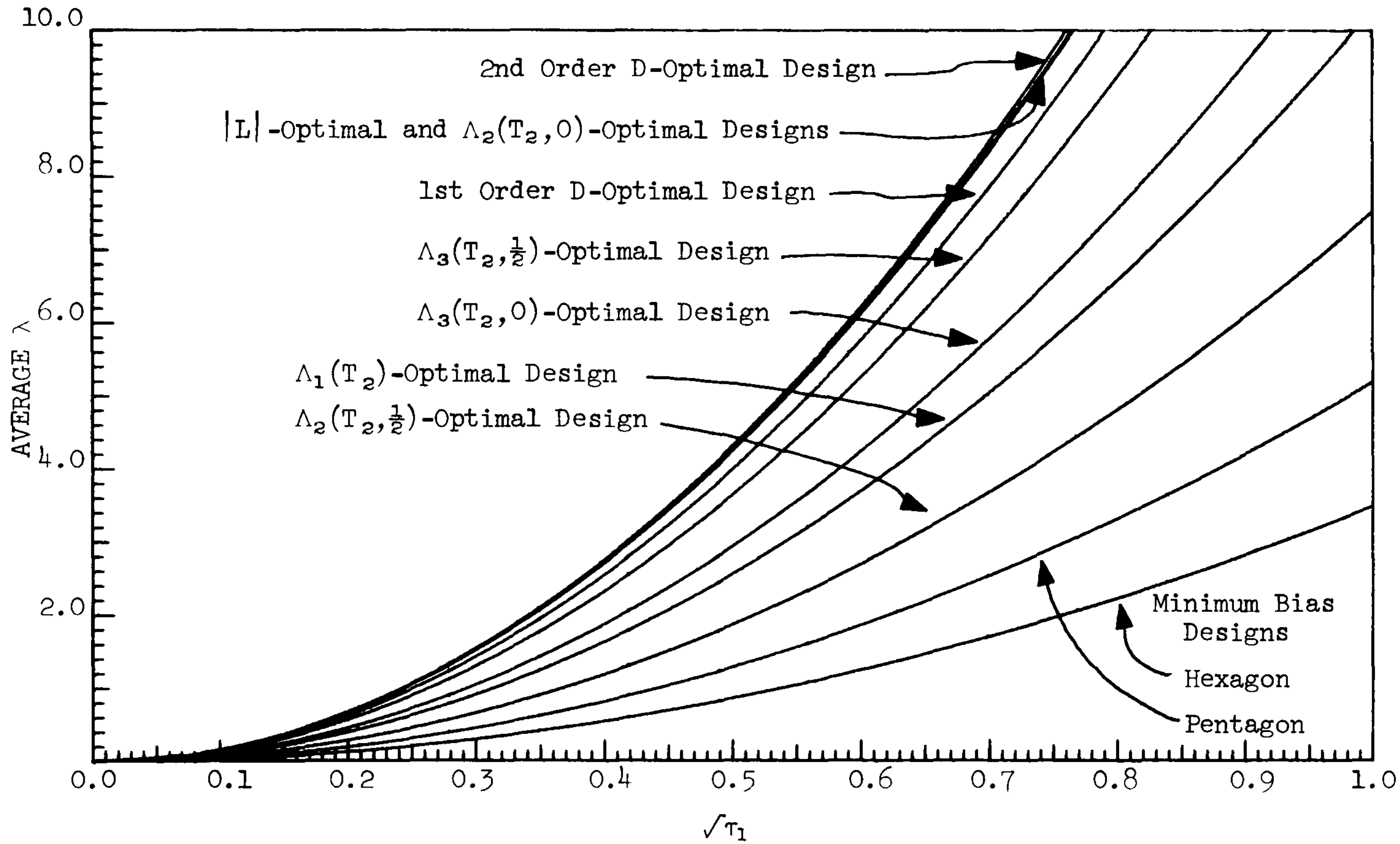


Figure 5.10. The Average Value of the Non-Centrality Parameter for Two-Factor $\Lambda(T_2)$-Optimal Designs for First Order vs. Second Order Models and $n = 6$

are better than those of the $\Lambda_1(T_2)$-optimal design.

5.3.1.2. The $\Lambda_2(T_2,c)$-Optimal Designs.--The use of c with this criterion appears to have a large effect upon the selection of a $\Lambda_2(T_2,c)$-optimal design. The $c = 0$ design has very poor bias properties but has excellent properties for the average value of λ for a given level of inherent bias, τ_1. On the other hand, the $c = \frac{1}{2}$ design is nearly minimum bias but has somewhat poor power properties for the detection of a given level of inherent bias. Both of these designs are singular for the higher order model. This may be partly excused by the fact that the $c = 0$ design has excellent variance properties for the lower order model while the $c = \frac{1}{2}$ design is nearly minimum bias. It should be noted that the $c = \frac{1}{2}$ design, which is nearly minimum bias, appears to be superior to the minimum bias designs examined in Table 5.3.

5.3.1.3. The $\Lambda_3(T_2,c)$-Optimal Designs.--The effect of changing c from 0 to $\frac{1}{2}$ is not as marked for the $\Lambda_3(T_2,c)$ criterion as it is for the $\Lambda_2(T_2,c)$ criterion. The $c = 0$ design was motivated for minimizing the average value of τ_2 over the contour $\lambda = \rho$. So it is not surprising that its bias properties are superior to those of the $c = \frac{1}{2}$ design. On the other hand, the power properties of the $c = \frac{1}{2}$ design are better than those of the $c = 0$ design. The variance properties for these designs are very good. In fact, it is somewhat surprising that for these designs, the value of V_2 (the standardized average variance of $\hat{\eta}(\underset{\sim}{x})$) is smaller than the values of V_2 for the $|L|$-optimal and second order D-optimal designs. On the whole, the

$\Lambda_3(T_2,c)$-optimal designs appear to have achieved a very favorable combination of variance, bias and power properties.

5.3.2. Two-Factor $\Lambda(T_2)$-Optimal Designs for Second Order vs. Third Order Polynomial Models and n = 10

Now let us examine the two-factor $\Lambda(T_2)$-optimal designs when the lower order model is second order,

$$\eta_1(\underline{x}) = \beta_0 + x_1\beta_1 + x_2\beta_2 + x_1x_2\beta_{12} + x_1^2\beta_{11} + x_2^2\beta_{22},$$

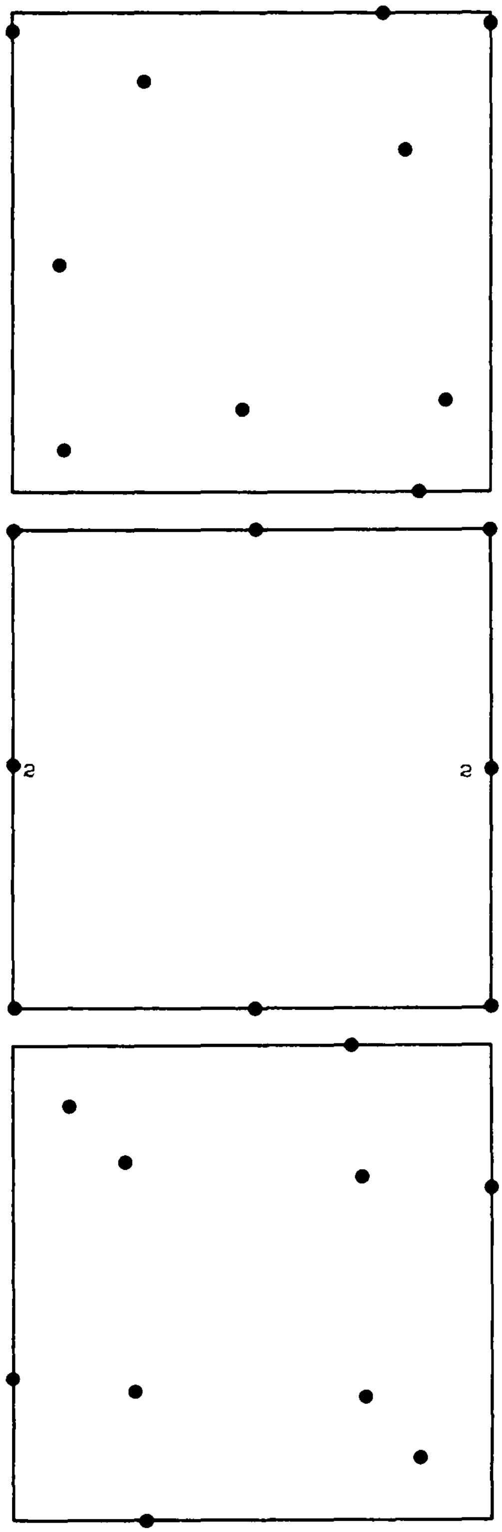
while the higher order model is third order,

$$\eta(\underline{x}) = \beta_0 + x_1\beta_1 + x_2\beta_2 + x_1x_2\beta_{12} + x_1^2\beta_{11} + x_2^2\beta_{22}$$
$$+ x_1^2x_2\beta_{112} + x_1x_2^2\beta_{122} + x_1^3\beta_{111} + x_2^3\beta_{222}.$$

The n = 10, $\Lambda(T_2)$-optimal designs for this case are given in Figures 5.11 and 5.12. Their variance properties are given in Table 5.4. The D-optimal, $|L|$-optimal and minimum bias designs referred to in this table were illustrated in Figures 3.17 and 3.18. The minimum bias square plus hexagon was referred to by Lawrence (1964), and the minimum bias square plus star and center points was given by Draper and Lawrence (1965) (see Figure 3.18). The other designs in Table 5.4 were obtained using the computational algorithm described in Appendix A.

The bias properties of these designs are illustrated in Figures 5.13 and 5.14. Again, the $\Lambda_2(T_2,\frac{1}{2})$-optimal design is nearly minimum bias. The power properties of these designs are illustrated in Figures 5.15 and 5.16.

5.3.2.1. The $\Lambda_1(T_2)$-Optimal Design.--The properties of the



$\Lambda_1(T_2)$-Optimal Design

-1.000000	0.867889
1.000000	0.924484
0.719391	-1.000000
-0.813399	-0.867889
0.840298	-0.615980
-0.815280	-0.034501
-0.452410	0.758708
0.550231	0.981357
0.662626	0.455502
0.042078	-0.648530

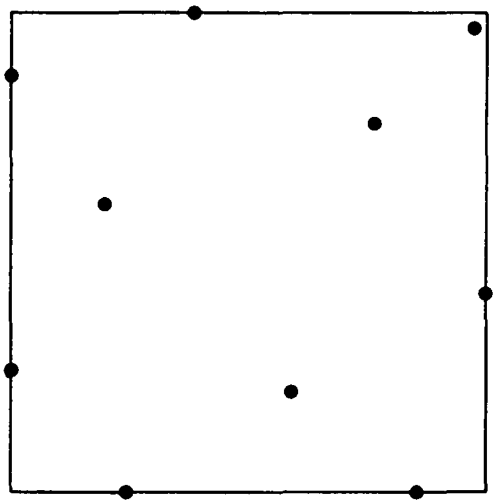
$\Lambda_2(T_2,0)$-Optimal Design

1.000000	-1.000000
-1.000000	1.000000
1.000000	1.000000
-1.000000	-1.000000
1.000000	0.000000
-1.000000	0.000000
0.000000	1.000000
0.000000	-1.000000
1.000000	0.000000
-1.000000	0.000000

$\Lambda_2(T_2,\frac{1}{2})$-Optimal Design

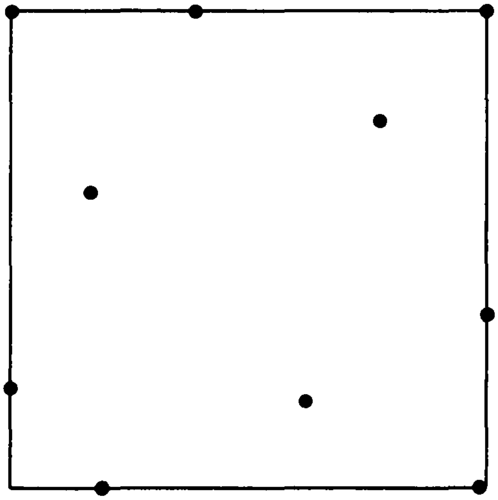
0.762200	-0.762200
-0.762200	0.762200
0.530722	-0.530722
-0.530722	0.530722
0.479968	0.479968
-0.479968	-0.479968
1.000000	0.430135
0.430135	1.000000
-1.000000	-0.430135
-0.430135	-1.000000

Figure 5.11. Two-Factor $\Lambda_1(T_2)$-Optimal and $\Lambda_2(T_2,c)$-Optimal Designs for Second Order vs. Third Order Models and $n = 10$



$\Lambda_3(T_2,0)$-Optimal Design

0.565407	0.565407
0.965907	0.965907
-1.000000	0.761426
0.761426	-1.000000
-1.000000	-0.536984
-0.536984	-1.000000
1.000000	-0.262358
-0.262358	1.000000
0.196796	-0.636435
-0.636435	0.196796



$\Lambda_3(T_2,\frac{1}{2})$-Optimal Design

-1.000000	1.000000
1.000000	1.000000
1.000000	-0.242237
0.965268	-1.000000
-0.238920	1.000000
-1.000000	-0.586223
-0.599062	-1.000000
0.590574	0.586255
-0.673500	0.268744
0.224939	-0.657209

Figure 5.12. Two-Factor $\Lambda_3(T_2,c)$-Optimal Designs for Second Order vs. Third Order Models and n = 10

TABLE 5.4

A Comparison of Some Characteristics of Two-Factor $\Lambda(T_2)$-Optimal Designs for Second Order vs. Third Order Models and n = 10

Design	$\lvert n^{-1} L\rvert$	$\lVert T_2\rVert$	Standardized Average Variances V_1	V_2	D-Efficiencies E_1	E_2
2nd Order D-Optimal	$.00000 \times 10^{0}$	.18013	4.3405	∞	1.0000	0.0000
3rd Order D-Optimal	$.10631 \times 10^{-4}$	.16357	4.6946	10.5772	0.9175	1.0000
$\lvert L\rvert$-Optimal	$.11494 \times 10^{-4}$	.15102	4.6494	9.3166	0.8927	0.9914
Minimum Bias Square plus Hexagon	$.00000 \times 10^{0}$	.05292	343.3100	∞	0.2336	0.0000
Minimum Bias Square plus Star and Center Points	$.00000 \times 10^{0}$	.05292	6.7981	∞	0.4356	0.0000
$\Lambda_1(T_2)$-Optimal	$.15452 \times 10^{-5}$	.08833	5.7321	10.1397	0.6564	0.8204
$\Lambda_2(T_2,0)$-Optimal	$.00000 \times 10^{0}$	.15002	5.9722	∞	0.9306	0.0000
$\Lambda_2(T_2,\frac{1}{2})$-Optimal	$.00000 \times 10^{0}$	.05469	6.0680	∞	0.5418	0.0000
$\Lambda_3(T_2,0)$-Optimal	$.63352 \times 10^{-5}$	.08652	4.9467	8.6362	0.7441	0.8364
$\Lambda_3(T_2,\frac{1}{2})$-Optimal	$.10908 \times 10^{-4}$	.12659	4.6801	8.6234	0.8356	0.9479

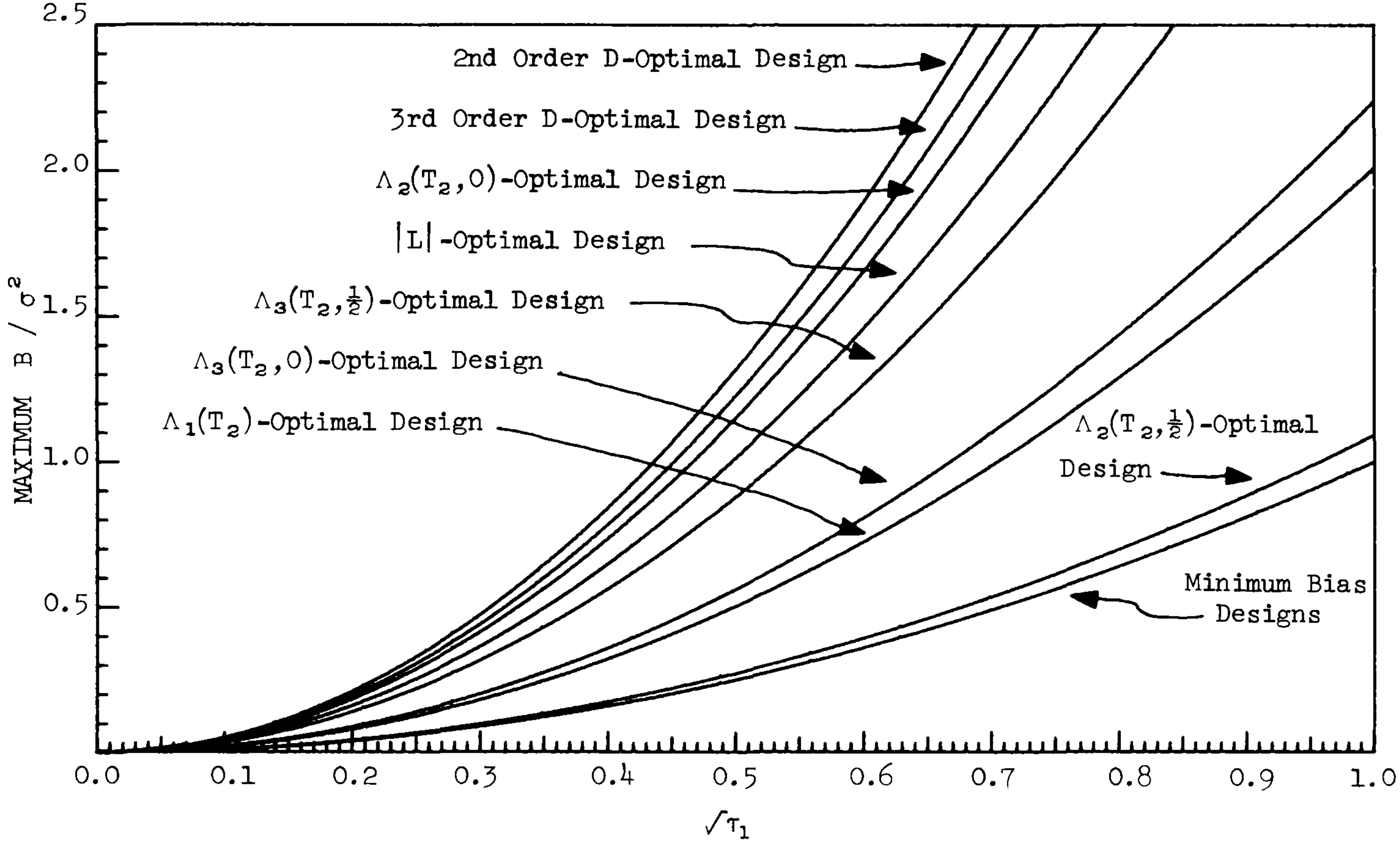


Figure 5.13. The Maximum Bias for Two-Factor $\Lambda(T_2)$-Optimal Designs for Second Order vs. Third Order Models and $n = 10$

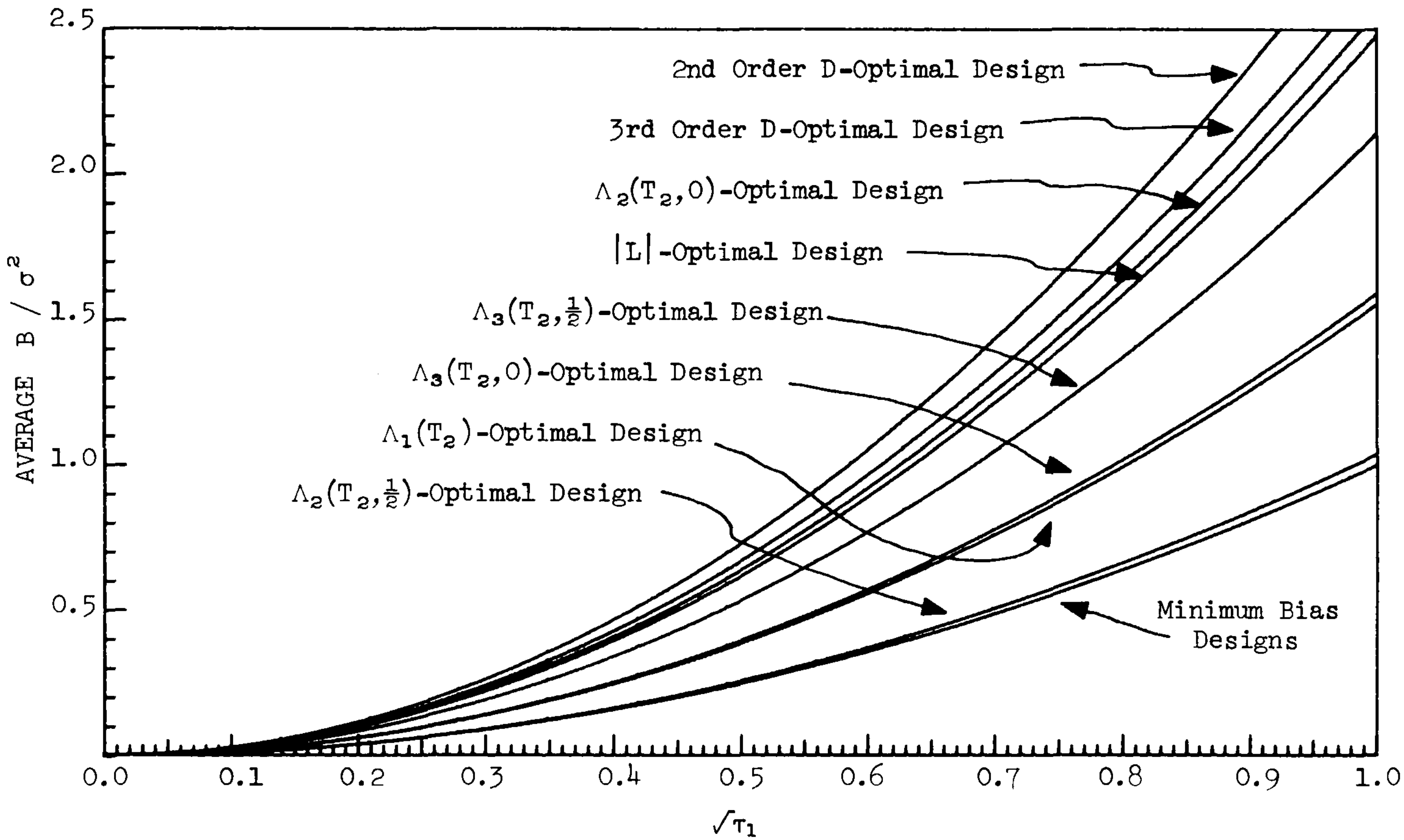


Figure 5.14. The Average Bias for Two-Factor $\Lambda(T_2)$-Optimal Designs for Second Order vs. Third Order Models and n = 10

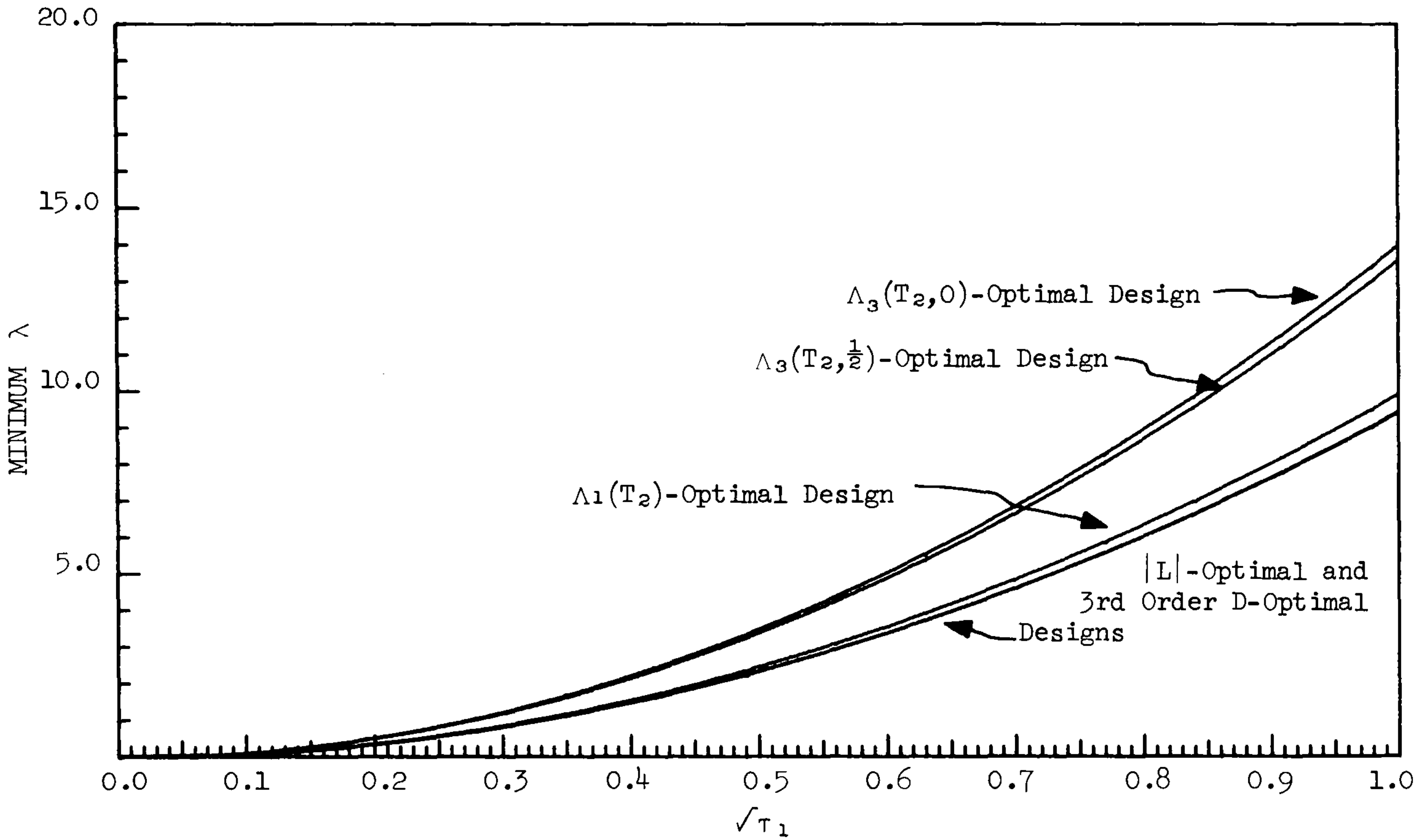


Figure 5.15. The Minimum Value of the Non-Centrality Parameter for Two-Factor $\Lambda(T_2)$-Optimal Designs for Second Order vs. Third Order Models and n = 10

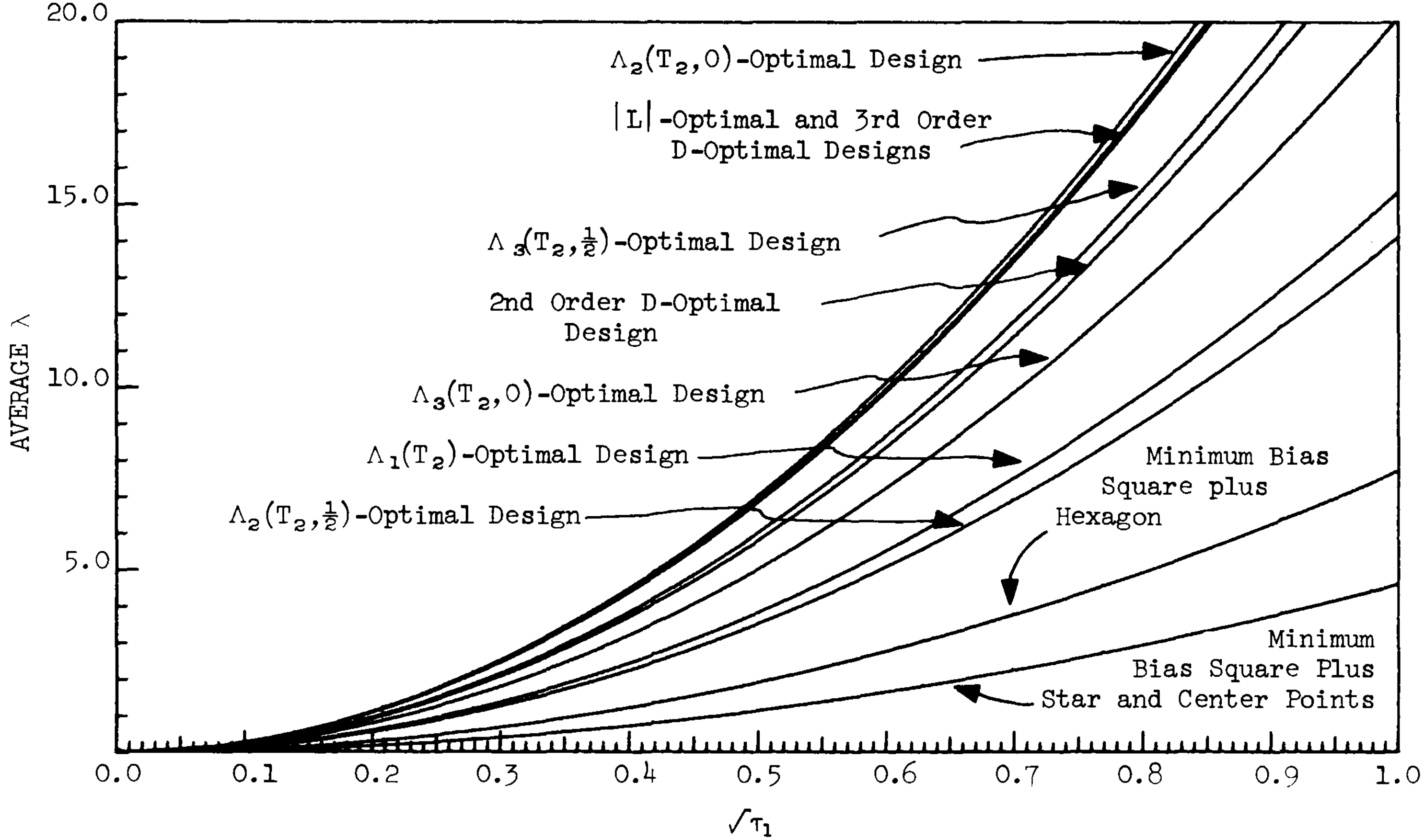


Figure 5.16. The Average Value of the Non-Centrality Parameter for Two-Factor $\Lambda(T_2)$-Optimal Designs for Second Order vs. Third Order Models and n = 10

$\Lambda_1(T_2)$-optimal design are nearly identical to those noted for the two-factor, n = 6, $\Lambda_1(T_2)$-optimal design for first order vs. second order polynomial models. The n = 10, $\Lambda_1(T_2)$-optimal design has only fair variance properties, but good bias properties relative to most of the other designs. However, again, the $\Lambda_3(T_2,0)$-optimal design appears to be superior to the $\Lambda_1(T_2)$-optimal design.

5.3.2.2. The $\Lambda_2(T_2,c)$-Optimal Designs.--Again, the use of c with this criterion seems to have a large effect upon the properties of a $\Lambda_2(T_2,c)$-optimal design. Both of these designs are singular for the higher order model. The c = 0 design has very good average properties for λ, but poor bias properties. On the other hand, the $c = \frac{1}{2}$ design is nearly minimum bias, but has somewhat poor power properties.

5.3.2.2. The $\Lambda_3(T_2,c)$-Optimal Designs.--The use of c with this criterion seems to have a small effect upon the properties of a $\Lambda_3(T_2,c)$-optimal design. It appears that, as c is increased the average value of λ seems to improve slightly, but this improvement appears to be at the expense of an increase in fitted bias. The variance properties for these designs are very good, especially for the higher order model. Again, it is somewhat surprising that the value of V_2 for these designs is smaller than the V_2 values of the third order D-optimal and $|L|$-optimal designs. On the whole, the $\Lambda_3(T_2,c)$-optimal designs appear to have achieved a favorable combination of variance, bias and power properties, although their bias properties are still somewhat weak relative to the minimum bias designs.

5.4. Summary

In this chapter, we have attempted to examine the $\Lambda(T)$ criteria for τ_2 by comparing the variance, bias and power properties of $\Lambda(T_2)$-optimal designs with D-optimal designs for both the lower order and higher order models, minimum bias designs and designs that maximize $|L|$.

5.4.1. One-Factor $\Lambda(T_2)$-Optimal Designs.

As far as the one-factor cases considered in this chapter are concerned, there appears to be little difference between $\Lambda_1(T_2)$-optimal, $\Lambda_2(T_2,c)$-optimal, and $\Lambda_3(T_2,c)$-optimal designs. For the cases considered, the one-factor $\Lambda(T_2)$-optimal designs appear to have exceptionally good properties. For one-factor, first order vs. second order polynomials models and n = 5, 9, they selected the designs that maximize the power of the lack of fit test. These designs were also nearly minimum bias, and their V_2 values were smaller then the value of V_2 for the second order D-optimal design. For one-factor, second order vs. third order models, the $\Lambda(T_2)$-optimal designs have similar properties.

5.4.2. Two-Factor $\Lambda(T_2)$-Optimal Designs.

5.4.2.1. Two-Factor $\Lambda_1(T_2)$-Optimal Designs.--The bias properties for these designs, as well as their properties for the average value of λ, were very similar to those of the $\Lambda_3(T_2,0)$-optimal designs. However, the properties of the $\Lambda_3(T_2,0)$-optimal designs for the minimum value of λ and for the average variance of $\hat{\eta}_1(\underset{\sim}{x})$ and $\hat{\eta}(\underset{\sim}{x})$ (V_1 and V_2) were clearly superior to those of the $\Lambda_1(T_2)$-optimal designs. On the whole, the $\Lambda_3(T_2,0)$-optimal designs appear to be slightly better than the $\Lambda_1(T_2)$-optimal designs.

5.4.2.2. Two-Factor $\Lambda_2(T_2,c)$-Optimal Designs.--The use of c for this criterion appears to have a large effect upon the properties of a $\Lambda_2(T_2,c)$-optimal design. The c = 0 design had very good properties for the average value of λ but poor bias properties. On the other hand, the $c = \frac{1}{2}$ design was nearly minimum bias, but its power properties were somewhat poor. However, it should be emphasized that, although the $c = \frac{1}{2}$ design was nearly minimum bias, it was clearly superior to the minimum bias designs examined. For all of the two-factor cases examined, the $\Lambda_2(T_2,c)$-optimal designs were singular for the higher order model.

5.4.2.1. Two-Factor $\Lambda_3(T_2,c)$-optimal Designs.--The effect of changing c from 0 to $\frac{1}{2}$ is not as marked for the $\Lambda_3(T_2,c)$-criterion as it is for the $\Lambda_2(T_2,c)$ criterion. The bias properties of the c = 0 design were slightly better than the bias properties of the $c = \frac{1}{2}$ design, but the $c = \frac{1}{2}$ design had slightly better properties for V_2 and the average value of λ. On the whole, the $\Lambda_3(T_2,c)$-optimal designs seem to have achieved a very good compromise with respect to variance, bias and power. Although the bias properties of the $\Lambda_3(T_2,c)$-optimal designs are weak compared with the minimum bias designs, they occupy a respectable position in the whole spectrum of designs considered in this comparison. Moreover, their power and variance properties rank high.

VI. $\Lambda_2(T_2,\frac{1}{2})$-OPTIMAL DESIGNS FOR CUBOIDAL AND SPHERICAL REGIONS OF INTEREST

6.1. Introduction

In the previous chapter, we compared $\Lambda_1(T_2)$, $\Lambda_2(T_2,c)$, and $\Lambda_3(T_2,c)$-optimal designs for $c = 0$ and $c = \frac{1}{2}$ with D-optimal, $|L|$-optimal and minimum bias designs. We observed that the $\Lambda(T_2)$ criteria seem to provide a spectrum of optimal designs from maximum power to minimum bias. The $\Lambda_3(T_2,\frac{1}{2})$-optimal designs were nearly minimum variance for the higher order model and maximum power for the lack of fit test while the $\Lambda_2(T_2,\frac{1}{2})$-optimal designs were nearly minimum bias.

In this chapter, we will further examine the $\Lambda_2(T_2,\frac{1}{2})$ criterion. This criterion was selected for further study because:

1. it discriminates between designs with a singular lack of fit matrix,

and 2. the results of the previous chapter indicate that the $\Lambda_2(T_2,\frac{1}{2})$ criterion selects nearly minimum bias designs, which are useful for some experiments.

It should be emphasized that $\Lambda_2(T_2,\frac{1}{2})$-optimality is not being selected for further examination because it seems to be applicable for most experiments. On the contrary, this criterion appears to select "good" minimum bias designs, and consequently, it seems most applicable for experiments in which a minimum bias design is needed.

6.2. One-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs

In this section, we will obtain some one-factor $\Lambda_2(T_2,\frac{1}{2})$-optimal designs for the region of interest defined by

$$-1 \leq x \leq 1. \tag{6.2.1}$$

However, because of the invariance results of Section 2.2, these designs can be scaled for any region of interest defined by

$$a \leq x \leq b,$$

for any $a < b$.

In addition, for the one-factor cases considered in this section, it is easily shown that the transformation $z = -x$ is a "moment preserving transformation" (see Section 2.3), Thus, by Theorems 2.11 and 2.12, it follows that for the one-factor cases considered in Sections 6.2.1 and 6.2.2, if D is a $\Lambda_2(T_2,\frac{1}{2})$-optimal design then $-D$ is also a $\Lambda_2(T_2,\frac{1}{2})$-optimal design.

6.2.1. One-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for First Order vs. Second Order Polynomial Models

Table 6.1 contains the one-factor $\Lambda_2(T_2,\frac{1}{2})$-optimal designs, and some of their properties, for $n = 3$--20, first order vs. second order polynomial models and a region of interest defined by (6.2.1). The $n = 5$ and $n = 9$ designs were examined in Section 3.2.1 (these designs are also $\Lambda(T_1)$-optimal). Except for the $n = 3$ and $n = 4$ designs, the ranges of the properties given in Table 6.1 are:

V_1 1.7500--2.1667,

V_2 2.1600--2.6133,

$n^{-1}L$ 0.21702--0.24000,

TABLE 6.1. One-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for First Order vs. Second Order Models

n	Design	$n^{-1}L$	T_2	$\Lambda_2(T_2,\frac{1}{2})$	Standardized Average Variances V_1	V_2
3	[± .855027, 0.0]	.11877	.11262	3.14258	1.6839	2.6321
4	[± .987230, 0.0 (2)]	.23747	.11260	6.28516	1.6840	2.1582

Design: n_1 at -1.0, n_2 at a, n_3 at 1.0

n	n_1	n_2	n_3	a	$n^{-1}L$	T_2	$\Lambda_2(T_2,\frac{1}{2})$	V_1	V_2
5	1	3	1	.000000	.24000	.09333	8.41698	1.8333	2.2222
6	1	4	1	.000000	.22222	.08889	8.38525	2.0000	2.4000
7	1	5	1	.000000	.20408	.09116	7.41520	2.1667	2.6133
8	1	5	2	.169316	.21702	.09409	7.51983	2.1383	2.5718
9	2	5	2	.000000	.24691	.10123	7.66570	1.7500	2.1600
10	2	6	2	.000000	.24000	.09333	8.41698	1.8333	2.2222
11	2	7	2	.000000	.23140	.08981	8.59817	1.9167	2.3048
12	2	8	2	.000000	.22222	.08889	8.38525	2.0000	2.4000
13	2	8	3	.091495	.23100	.09269	8.18578	1.9437	2.3450
14	2	9	3	.106702	.22309	.09065	8.17354	2.0234	2.4298
15	3	9	3	.000000	.24000	.09333	8.41698	1.8333	2.2222
16	3	10	3	.000000	.23438	.09063	8.59091	1.8889	2.2756
17	3	11	3	.000000	.22837	.08927	8.56176	1.9444	2.3354
18	3	12	3	.000000	.22222	.08889	8.38525	2.0000	2.4000
19	3	12	4	.070536	.22960	.09074	8.40004	1.9466	2.3418
20	4	12	4	.000000	.24000	.09333	8.41698	1.8333	2.2222

and T_2 0.08889--0.10123.

For this case, the minimum value of T_2 (achieved by minimum bias designs) is .08889. From Table 6.1, it is apparent that these designs are nearly minimum bias, and in fact, the n = 6, n = 12, and n = 18 designs are minimum bias designs. In addition, we observed in Section 3.2.1 that the n = 5 and n = 9 designs have very good variance properties, especially for the higher order model.

The power of the lack of fit test for these designs is illustrated in Figures 6.1--6.4 for α = .01, .05, .10 and .25. These figures are based upon an F-test in which the residual mean square for the higher order model is used in the denominator. They are provided for selecting the sample size and α-level needed to detect specified departures with a given probability.

6.2.2. One-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for Second Order vs. Third Order Polynomial Models

Table 6.2 contains the one-factor $\Lambda_2(T_2,\frac{1}{2})$-optimal designs, and some of their properties, for n = 4--20, second order vs. third order polynomial models and the region of interest defined by (6.2.1). The n = 6 and n = 10 designs were examined in Section 5.2.2. Except for the n = 4--7 designs, the ranges of the properties given in Table 6.2 are:

V_1 2.7641--3.1168,

V_2 3.1774--3.5663,

$n^{-1}L$ 0.05135--0.05974,

and T_2 0.02308--0.02558.

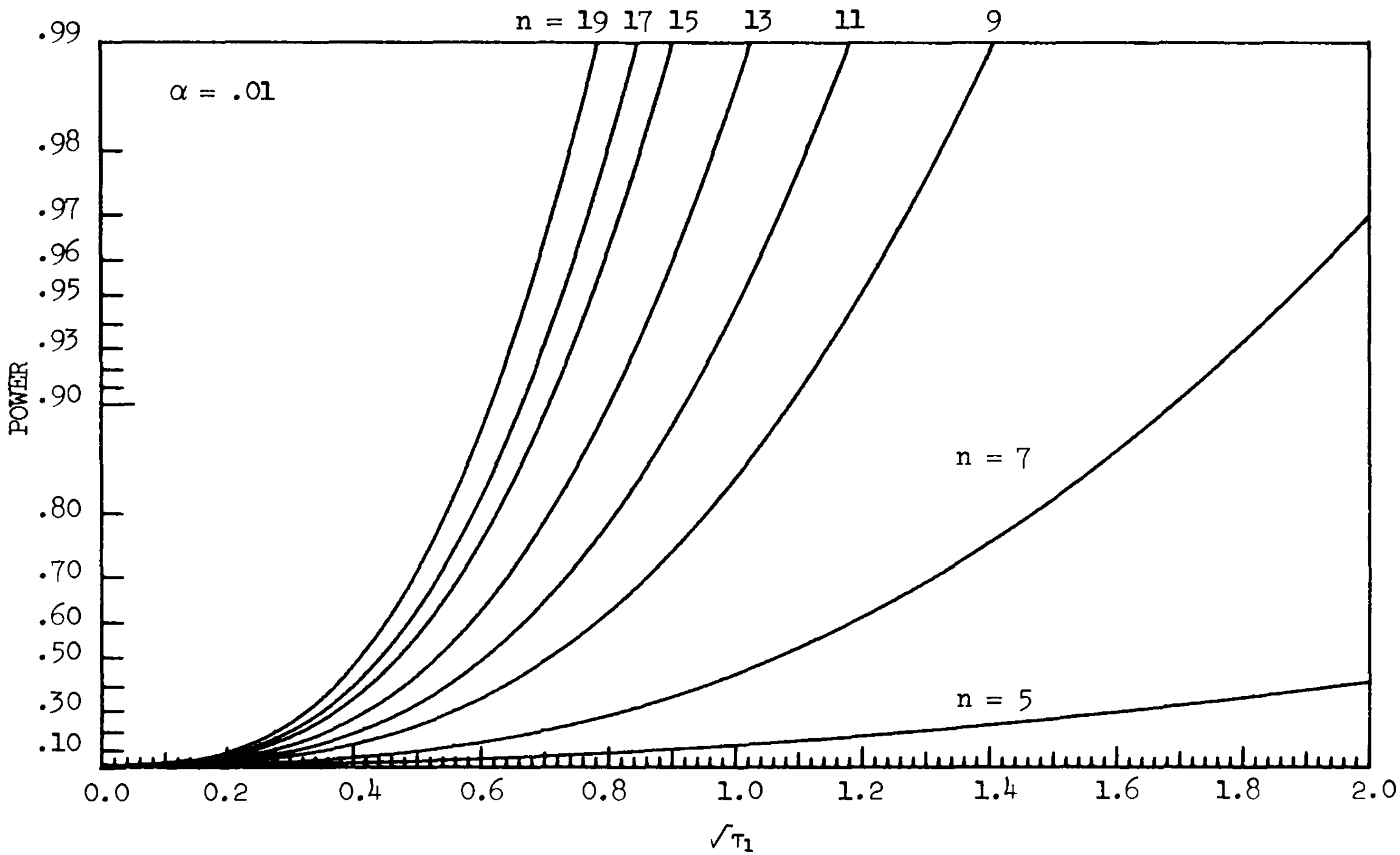


Figure 6.1. Power Functions for One-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for First Order vs. Second Order Models and $\alpha = .01$

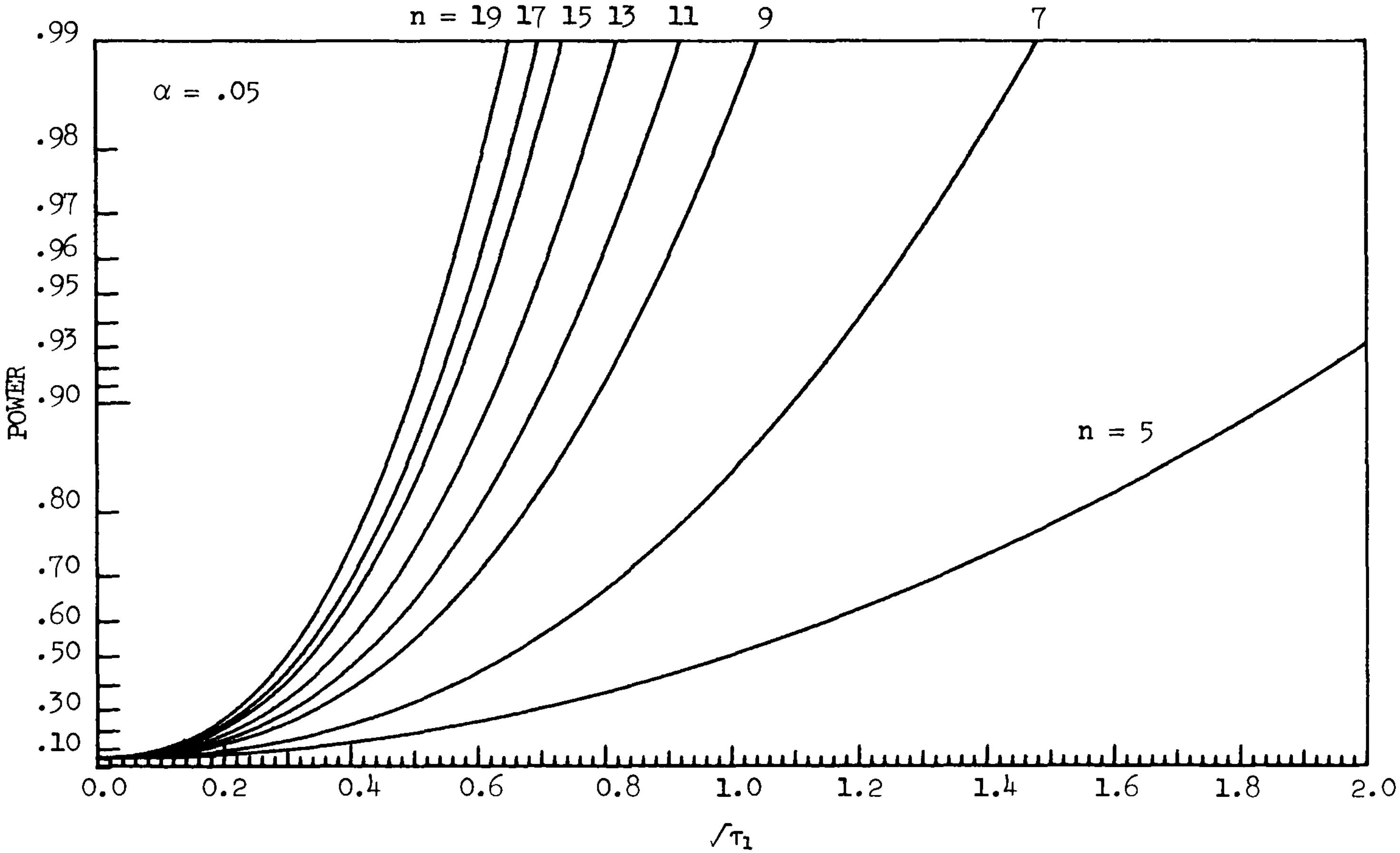


Figure 6.2. Power Functions for One-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for First Order vs. Second Order Models and $\alpha = .05$

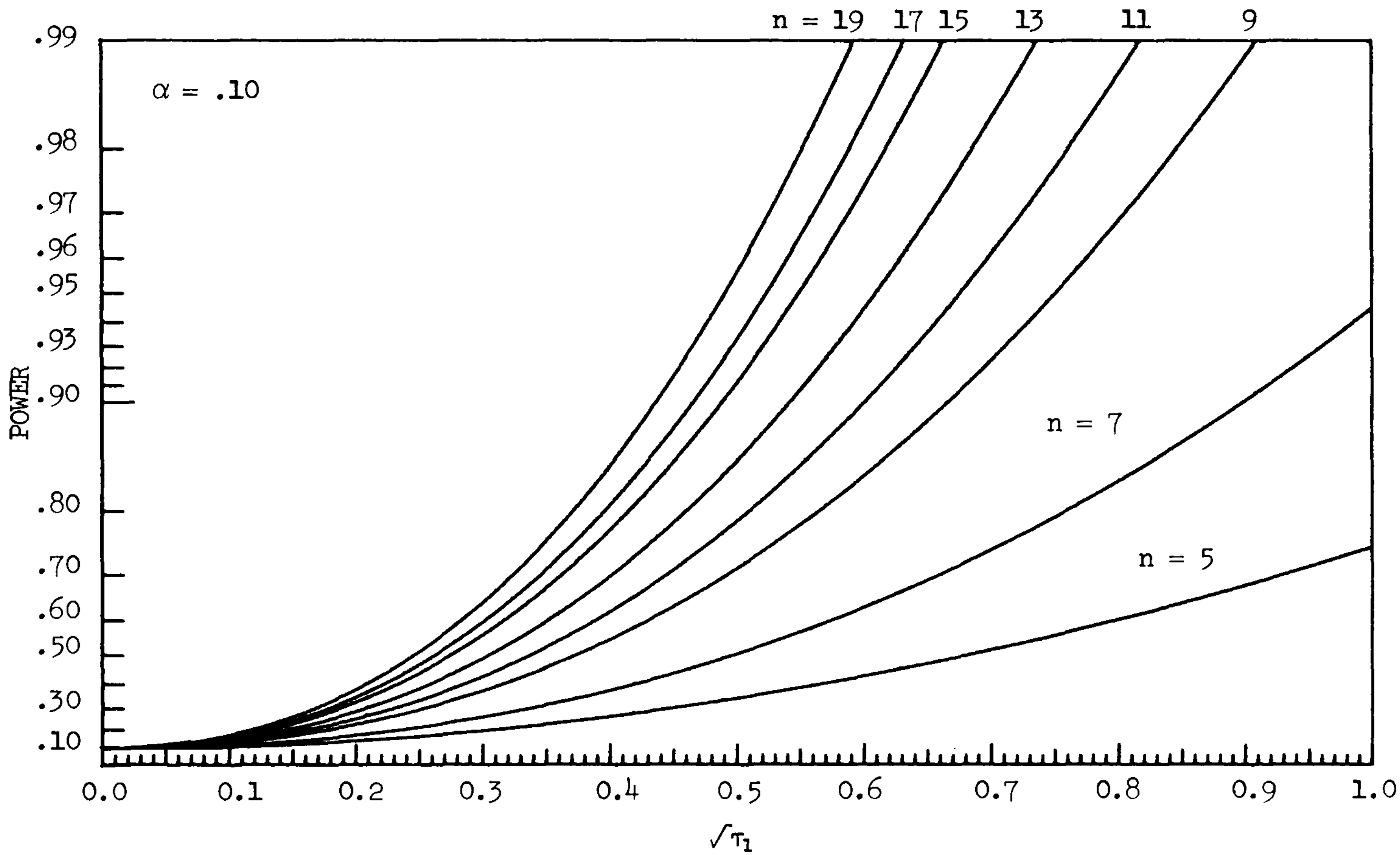


Figure 6.3. Power Functions for One-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for First Order vs. Second Order Models and α = .10

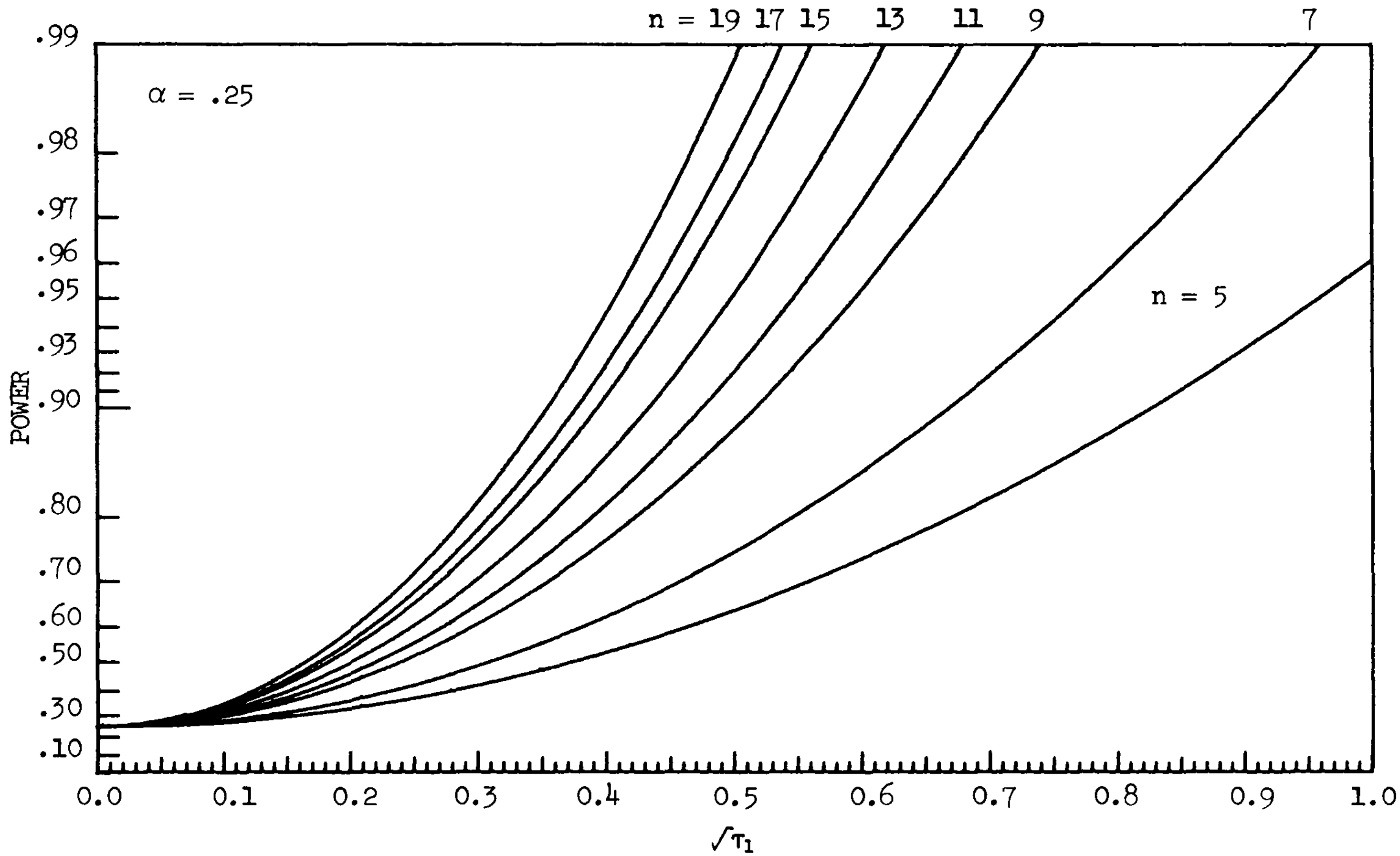


Figure 6.4. Power Functions for One-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for First Order vs. Second Order Models and α = .25

TABLE 6.2. One-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for Second Order vs. Third Order Models

n	Design	$n^{-1}L$	T_2	$\Lambda_2(T_2,\frac{1}{2})$	Standardized Average Variances V_1	V_2
4	[± .924632, ± .521277]	.035067	.027211	7.8125	3.2592	4.0351
5	[-.930182, .966647, -.464998, .643000 (2)]	.038306	.027744	8.2891	3.4906	4.2149
6	[± .983792, ± .536212 (2)]	.055652	.027211	12.3985	2.8308	3.3197
7	[-1.0, -.598058 (3), .498873 (2), .988385]	.056115	.026554	12.9687	2.9251	3.3983

n_1 n_2 n_3 n_4

-1.0 -a b 1.0

n	n_1	n_2	n_3	n_4	a	b	$n^{-1}L$	T_2	$\Lambda_2(T_2,\frac{1}{2})$	V_1	V_2
8	1	3	3	1	.518394	.518394	.059672	.024663	15.4066	2.7641	3.1774
9	1	3	4	1	.487852	.535878	.057111	.024070	15.2937	2.8503	3.2718
10	1	4	4	1	.484603	.484603	.056716	.023145	16.1074	2.8400	3.2481
11	1	4	5	1	.457876	.488015	.054588	.023169	15.4790	2.9331	3.3575
12	1	5	5	1	.447214	.447214	.053333	.022857	15.4336	3.0000	3.4286
13	1	5	6	1	.424544	.438631	.051347	.023079	14.6451	3.1168	3.5663
14	1	5	6	2	.415072	.552206	.055144	.023876	14.9474	3.0056	3.4386
15	2	5	6	2	.512828	.546597	.059742	.025582	14.6008	2.7891	3.2173
16	2	6	6	2	.518394	.518394	.059672	.024663	15.4066	2.7641	3.1774
17	2	6	7	2	.499758	.526386	.058650	.024219	15.5606	2.7921	3.2050
18	2	7	7	2	.501988	.501988	.058270	.023672	15.9986	2.7907	3.1970
19	2	7	8	2	.485097	.506309	.057279	.023453	15.9476	2.8242	3.2336
20	2	8	8	2	.484603	.484603	.056716	.023145	16.1074	2.8503	3.2718

For this case, the minimum value of T_2 is 0.022857. Hence, the designs in Table 6.2 are nearly minimum bias.

The power of the lack of fit test for these designs is illustrated in Figures 6.5--6.8 for α = .01, .05, .10 and .25. These figures are provided for selecting the sample size and α-level needed to detect specified alternatives with a given probability.

6.3. Two-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for Square Regions of Interest

In this section, we will obtain some two-factor $\Lambda_2(T_2,\frac{1}{2})$-optimal designs for a region of interest defined by

$$-1 \leq x_i \leq 1, \ i = 1, 2. \tag{6.3.1}$$

However, because of the invariance results of Section 2.2, the designs given in this section can be scaled for any region of interest that can be express as a non-singular linear transformation of (6.3.1), such as

$$a_i \leq x_i \leq b_i, \ i = 1, 2.$$

Furthermore, because of Theorems 2.11 and 2.12, any 90°, 180° or 270° rotation of these designs is also optimal.

6.3.1. Two-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for First Order vs. Second Order Polynomial Models and Square Regions of Interest

Figures 6.9 and 6.10 contain the two-factor $\Lambda_2(T_2,\frac{1}{2})$-optimal designs for n = 4--10, first order vs. second order polynomial models and a region of interest defined by (6.3.1). Some of the properties of these designs are given in Table 6.3. All of these designs are singular for the higher order model. However, for the experiments in which these designs would be used, it is unlikely that the

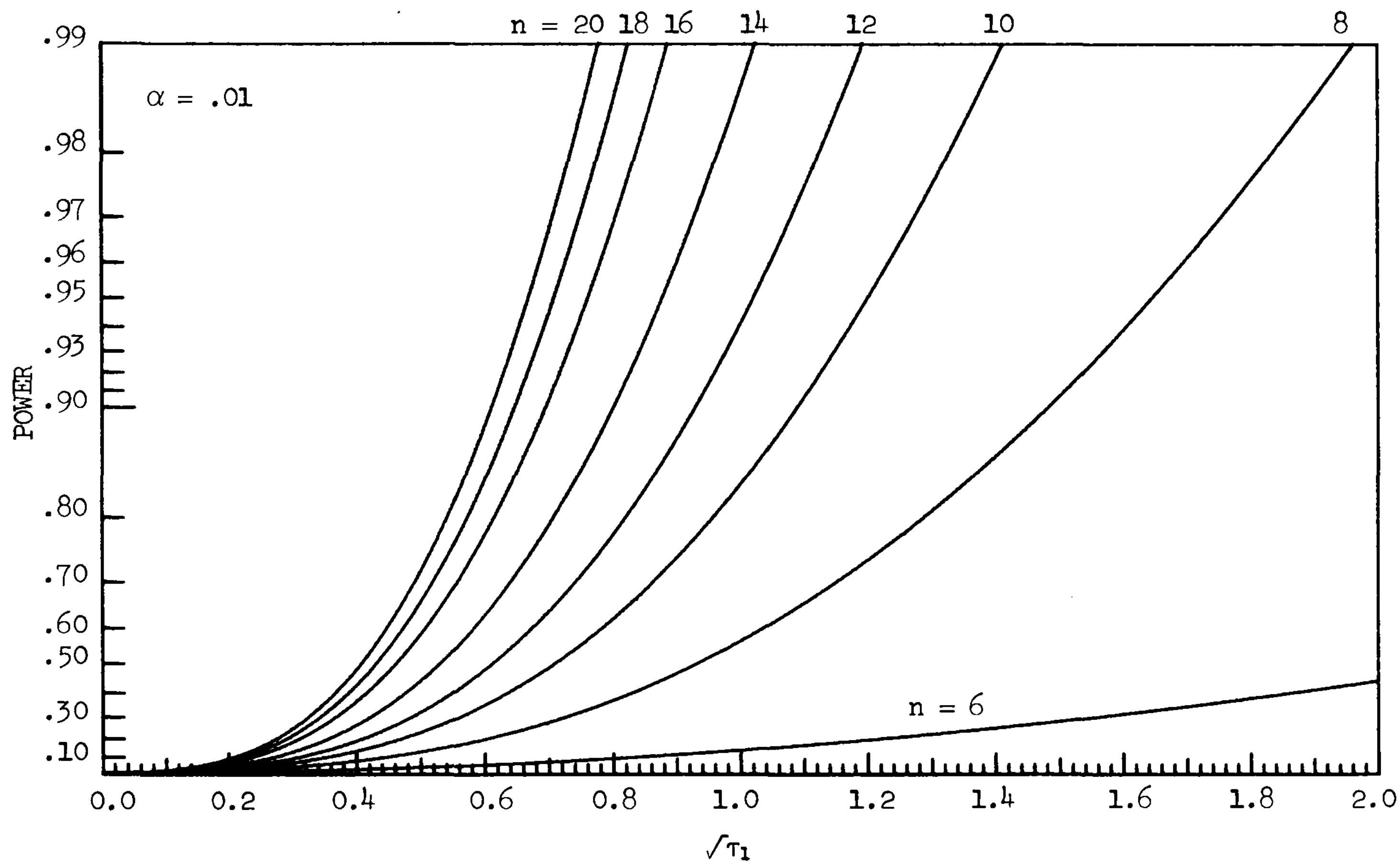


Figure 6.5. Power Functions for One-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for Second Order vs. Third Order Models and α = .01

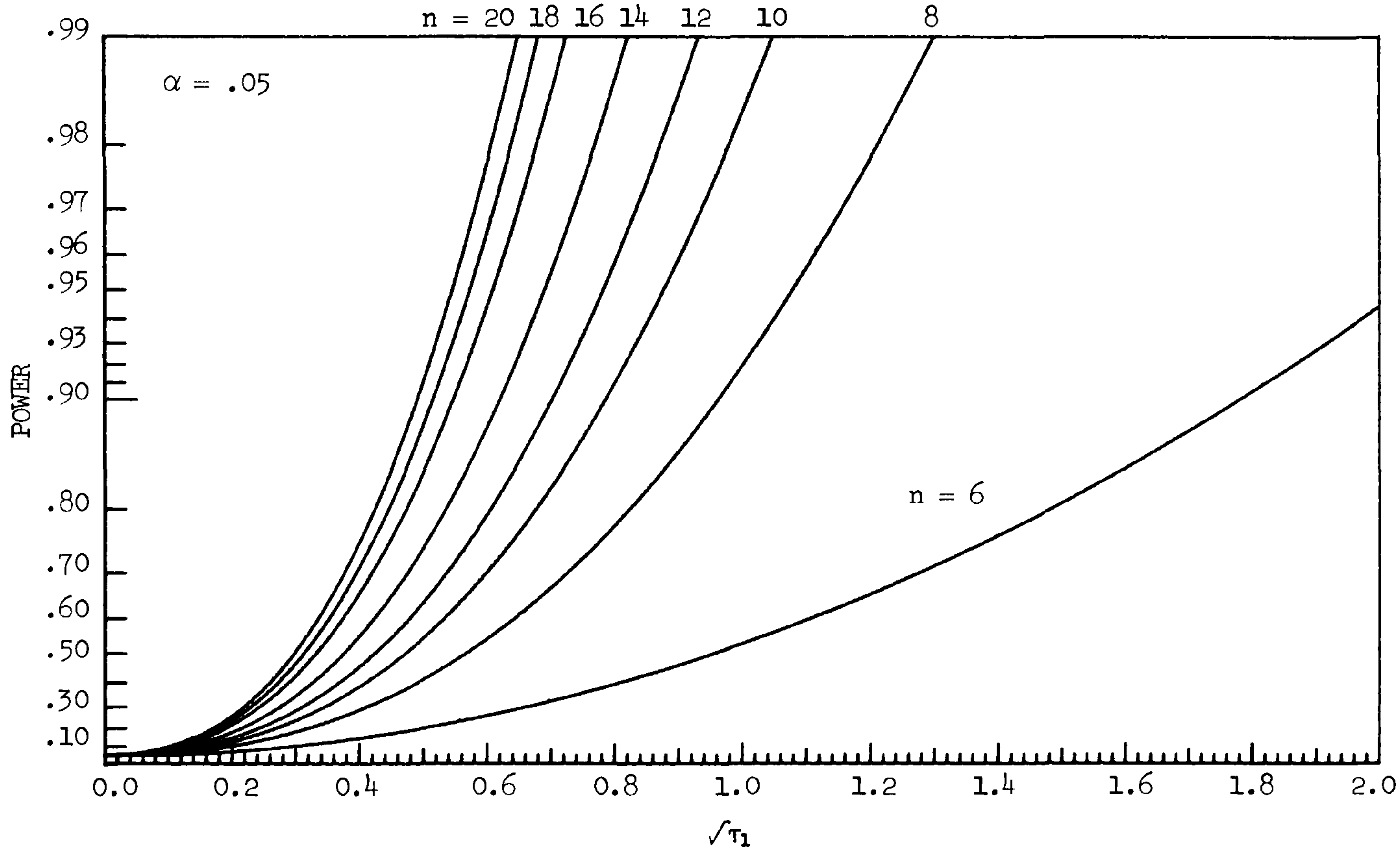


Figure 6.6. Power Functions for One-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for Second Order vs. Third Order Models and α = .05

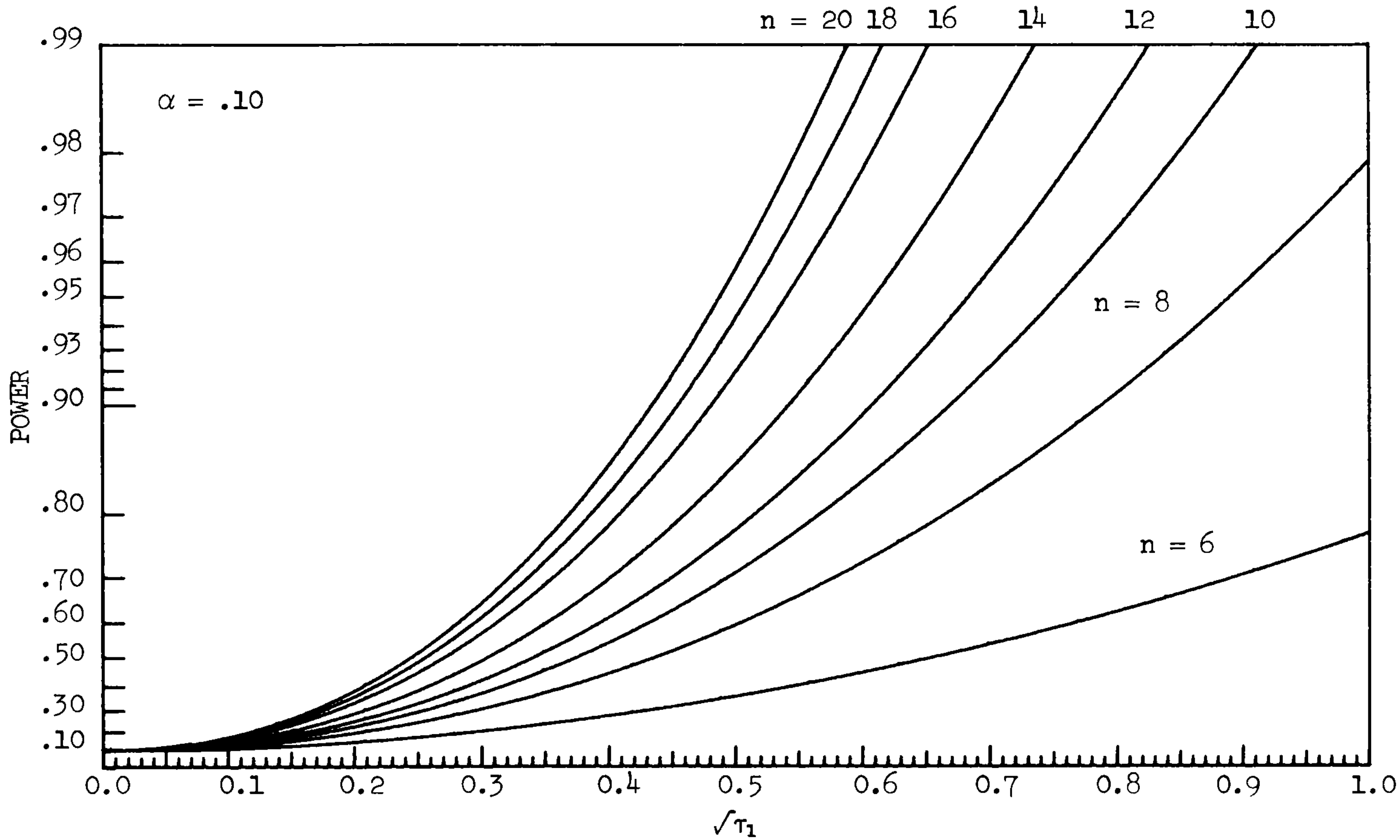


Figure 6.7. Power Functions for One-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for Second Order vs. Third Order Models and $\alpha = .10$

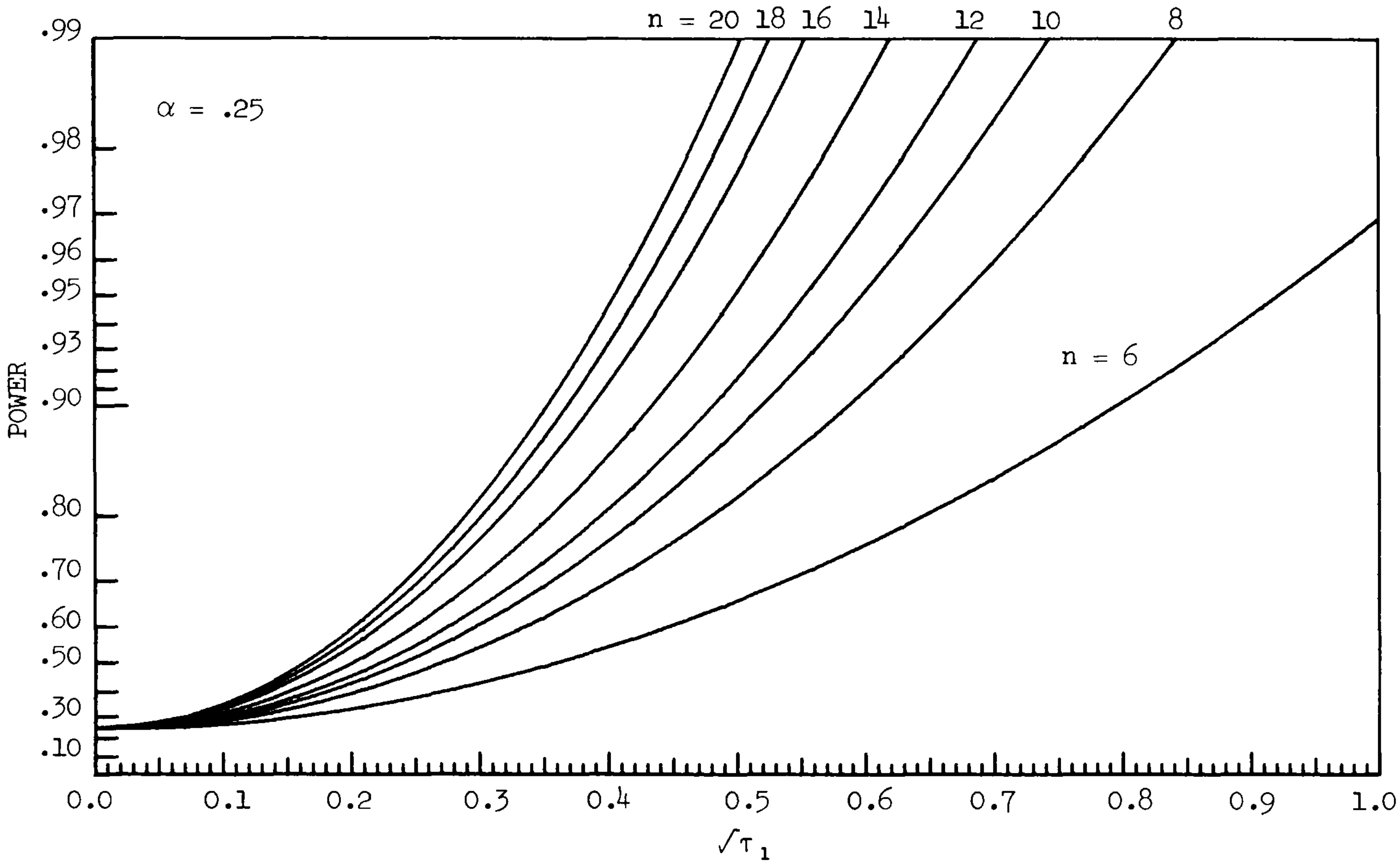
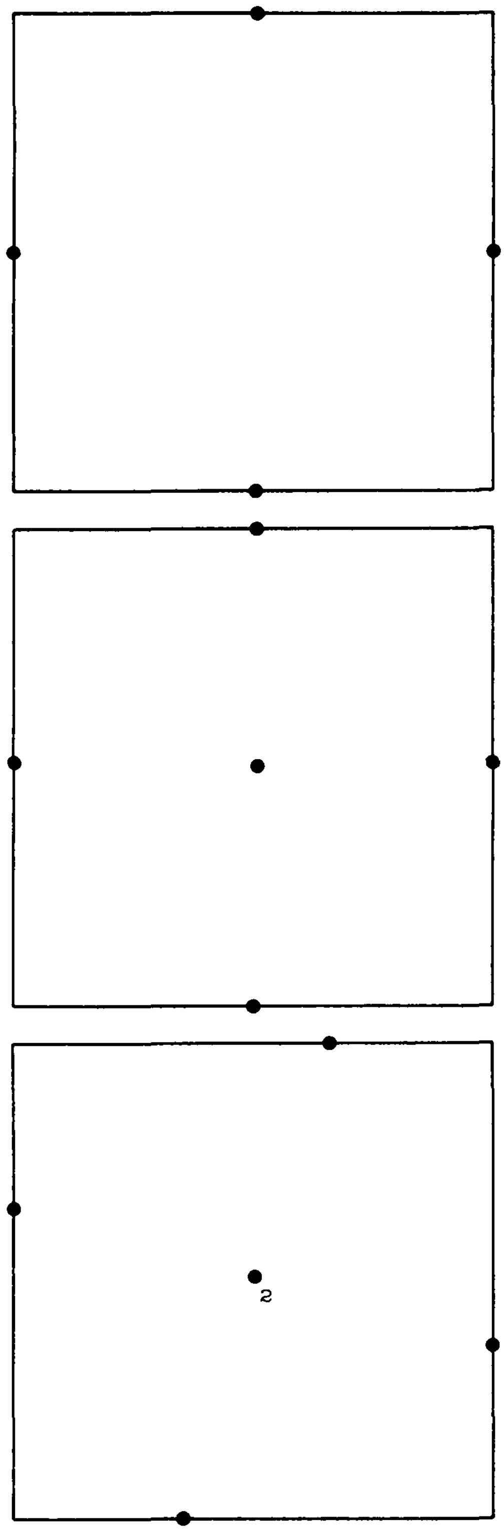


Figure 6.8. Power Functions for the One-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for Second Order vs. Third Order Polynomials and $\alpha = .25$



n = 4

1.000000	0.000000
-1.000000	0.000000
0.000000	1.000000
0.000000	-1.000000

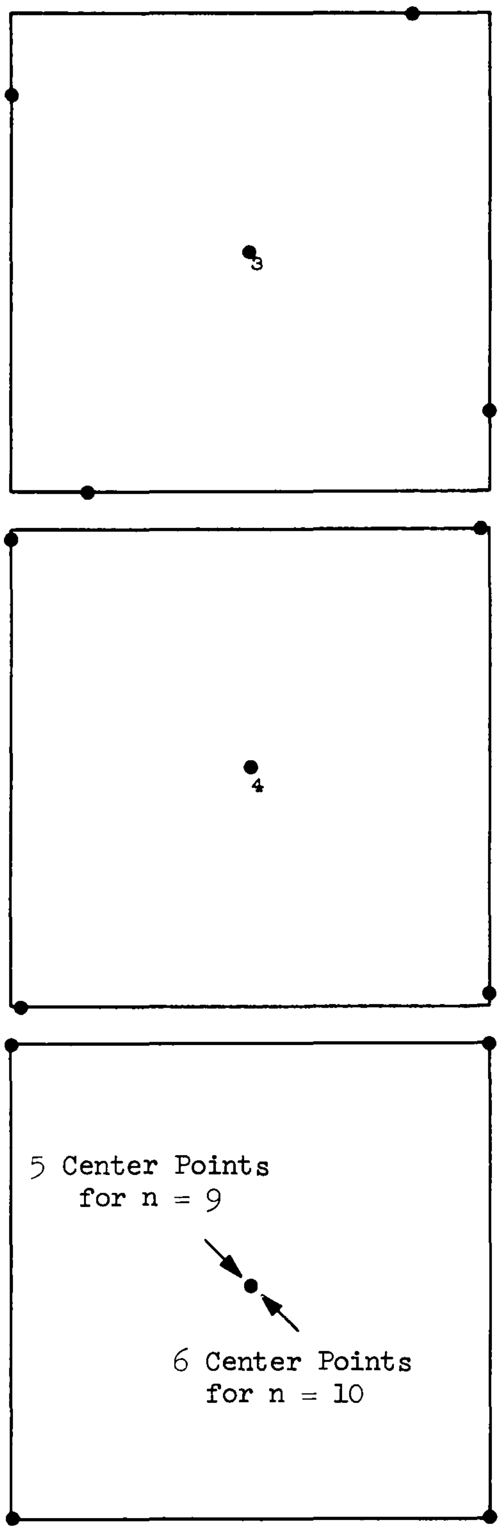
n = 5

1.000000	0.000000
-1.000000	0.000000
0.000000	1.000000
0.000000	-1.000000
0.000000	0.000000

n = 6

1.000000	-0.311446
-1.000000	0.311446
-0.311446	-1.000000
0.311446	1.000000
0.000000	0.000000
0.000000	0.000000

Figure 6.9. Two-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for First Order vs. Second Order Models, Square Region of Interest and n = 4-6



n = 7

3 Center Points plus

1.000000	-0.683725
-1.000000	0.683725
-0.683725	-1.000000
0.683725	1.000000

n = 8

4 Center Points Plus

1.000000	-0.905956
-1.000000	0.905956
-0.905956	-1.000000
0.905956	1.000000

n = 9

2^2 plus
5 Center Points

n = 10

2^2 plus
6 Center Points

Figure 6.10. Two-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for First Order vs. Second Order Models, Square Region of Interest and n = 7-10

TABLE 6.3

Characteristics of the Two-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for First Order vs. Second Order Models

n	$\Lambda_2(T_2,\frac{1}{2})$	$\|T_2\|$	$\|n^{-1} X_1' X_1\|$	V_1
4	148.93	.20276	.2500	2.3334
5	171.14	.17265	.1600	2.6667
6	170.45	.16889	.1337	2.8232
7	183.12	.17605	.1758	2.5900
8	212.67	.18523	.2072	2.4646
9	249.24	.18206	.1975	2.5000
10	273.82	.17265	.1600	2.6667

experimenter will want to fit the higher order model. Except for the n = 4 design, the ranges for the properties given in Table 6.3 are:

$$V_1 \quad 2.4646\text{--}2.8232,$$

$$\text{and} \quad \|T_2\| \quad 0.1689\text{--}0.1852.$$

The n = 6 design was examined in Section 5.3.1. We found that this design was nearly minimum bias, but its variance and power properties were superior to the minimum bias designs given by Lawrence (1964). For this case, the Euclidean norm of T_2 for the minimum bias designs is 0.16777. Consequently, it appears that the $\Lambda_2(T_2,\frac{1}{2})$-optimal designs given in Figures 6.9 and 6.10 are all nearly minimum bias designs.

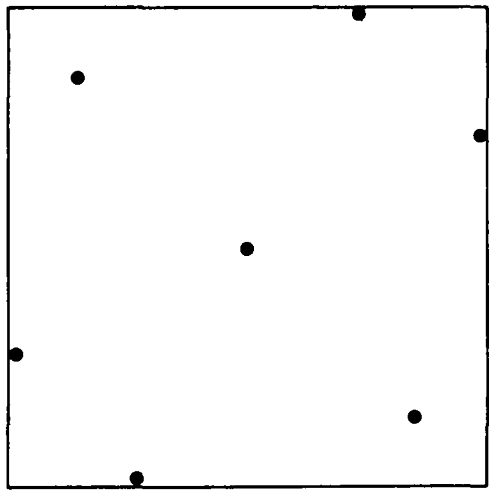
6.3.2. Two-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for Second Order vs. Third Order Polynomial Models and Square Regions of Interest

Figures 6.11--6.14 contain the two-factor $\Lambda_2(T_2,\frac{1}{2})$-optimal designs for n = 7--15, second order vs. third order polynomial models and a region of interest defined by (6.3.1). Some of the properties of these designs are given in Table 6.4. The n = 7--14 designs are singular for the third order model, and the n = 15 design does not have very good variance properties for the third order model. Except for the n = 7 and n = 15 designs, the ranges of the design properties given in Table 6.4 are:

$$V_1 \quad 5.2065\text{--}8.2975$$

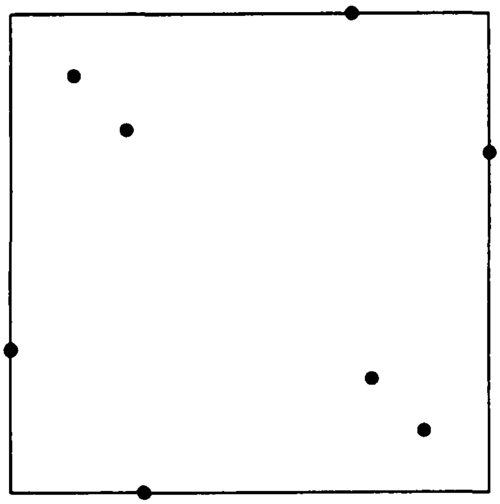
$$\text{and} \quad \|T_2\| \quad 0.0542\text{--}0.0596.$$

The n = 10 design was examined in Section 5.3.2. We observed



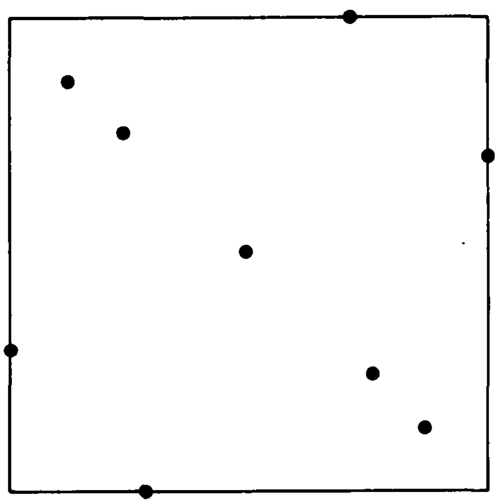
n = 7

0.729973	-0.729973
-0.729973	0.729973
0.961876	0.468310
0.468310	0.961876
-0.961876	-0.468310
-0.468310	-0.961876
0.000000	0.000000



n = 8

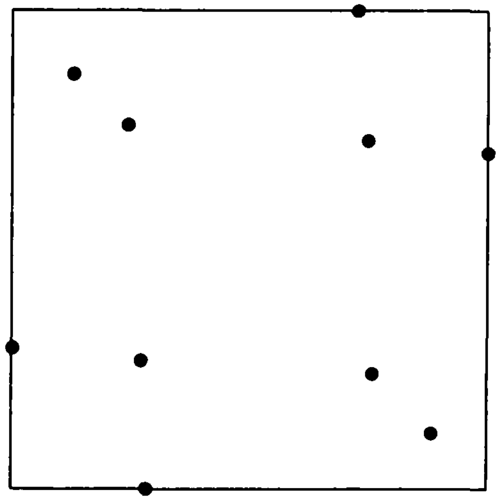
0.768293	-0.768293
-0.768293	0.768293
0.527703	-0.527703
-0.527703	0.527703
1.000000	0.429539
0.429539	1.000000
-1.000000	-0.429539
-0.429539	-1.000000



n = 9

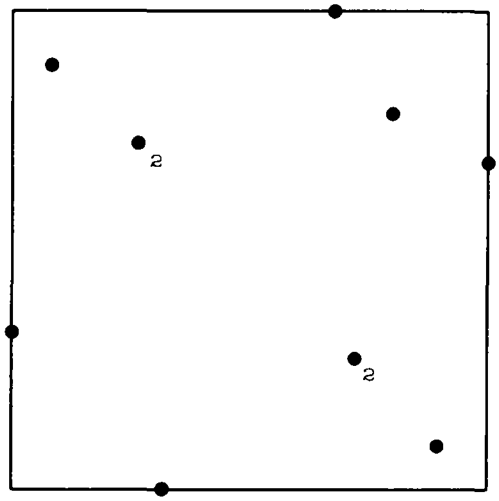
0.768293	-0.768293
-0.768293	0.768293
0.527703	-0.527703
-0.527703	0.527703
1.000000	0.429539
0.429539	1.000000
-1.000000	-0.429539
-0.429539	-1.000000
0.000000	0.000000

Figure 6.11. Two-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for Second Order vs. Third Order Models, Square Region of Interest and n = 7-9



n = 10

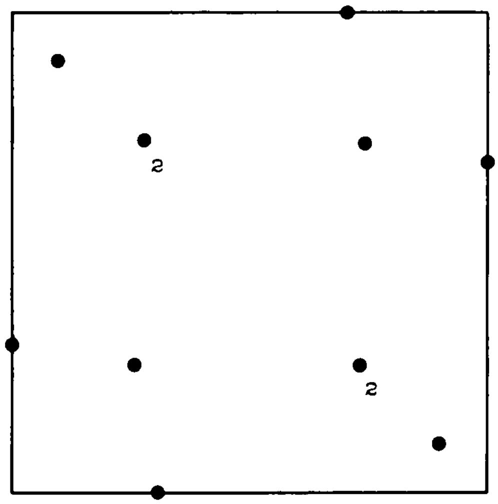
0.762200	-0.762200
-0.762200	0.762200
0.530722	-0.530722
-0.530722	0.530722
0.479968	0.479968
-0.479968	-0.479968
1.000000	0.430135
0.430135	1.000000
-1.000000	-0.430135
-0.430135	-1.000000



n = 11

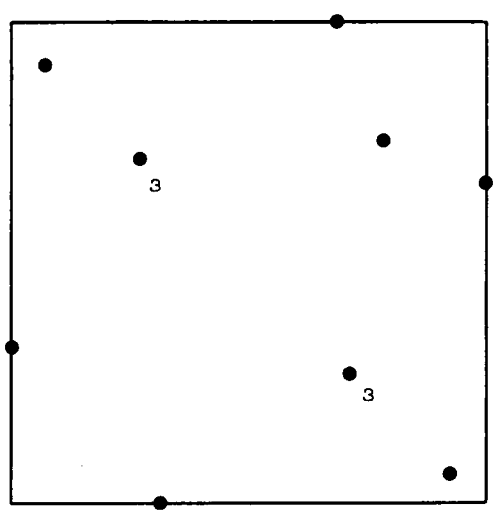
0.813458	-0.852933
-0.852933	0.813458
0.470393	-0.480962
0.470393	-0.480962
-0.480962	0.470393
-0.480962	0.470393
0.613371	0.613371
1.000000	0.374104
0.374104	1.000000
-1.000000	-0.388420
-0.388420	-1.000000

Figure 6.12. Two-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for Second Order vs. Third Order Models, Square Region of Interest and n = 10-11



n = 12

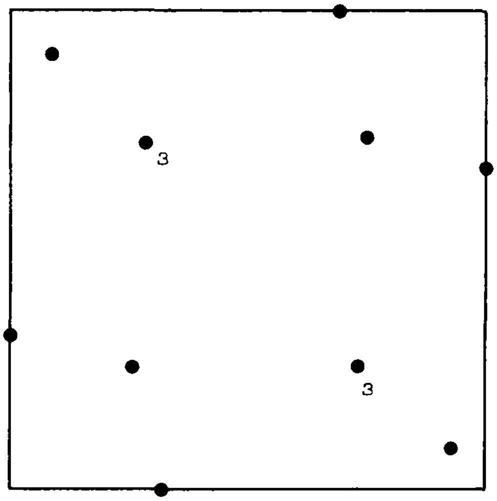
0.827229	-0.827229
-0.827229	0.827229
0.481063	-0.481063
0.481063	-0.481063
-0.481063	0.481063
-0.481063	0.481063
0.487374	0.487374
-0.487374	-0.487374
1.000000	0.389438
0.389438	1.000000
-1.000000	-0.389438
-0.389438	-1.000000



n = 13

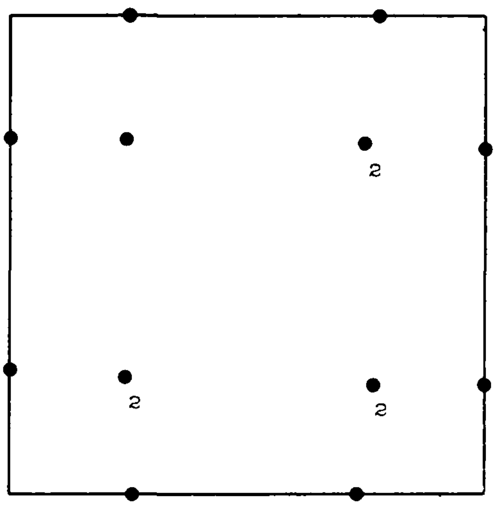
0.556060	0.556060
0.859586	-0.902330
-0.902330	0.859586
0.454403	-0.478285
0.454403	-0.478285
0.454403	-0.478285
-0.478285	0.454403
-0.478285	0.454403
-0.478285	0.454403
1.000000	0.369033
0.369033	1.000000
-1.000000	-0.372364
-0.372364	-1.000000

Figure 6.13. Two-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for Second Order vs. Third Order Models, Square Region of Interest and n = 12-13



n = 14

0.878587	-0.878587
-0.878587	0.878587
0.470128	-0.470128
0.470128	-0.470128
0.470128	-0.470128
-0.470128	0.470128
-0.470128	0.470128
-0.470128	0.470128
0.496904	0.496904
-0.496904	-0.496904
1.000000	0.368422
0.368422	1.000000
-1.000000	-0.368422
-0.368422	-1.000000



n = 15

0.496254	0.515918
0.496254	0.515918
-0.512918	-0.496254
-0.512918	-0.496254
0.571081	-0.571081
0.571081	-0.571081
1.000000	0.481446
-0.481446	-1.000000
1.000000	-0.569136
0.569136	-1.000000
-0.997470	0.494019
-0.494019	0.997470
1.000000	-0.509018
0.509018	-1.000000

Figure 6.14. Two-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for Second Order vs. Third Order Models, Square Region of Interest and n = 14-15

TABLE 6.4

Characteristics of the Two-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for Second Order vs. Third Order Models and n = 7-15

				Standardized Determinants		Standardized Average Variances	
n	$\Lambda_2(T_2,\frac{1}{2})$	$\|T_2\|$	$\lvert n^{-1} L\rvert$	$\lvert n^{-1} X_1' X_1\rvert$	$\lvert n^{-1} X' X\rvert$	V_1	V_2
7	4877.59	.059676	$.0000 \times 10^{0}$	$.1017 \times 10^{-3}$	$.0000 \times 10^{0}$	10.1706	∞
8	7387.70	.059560	$.0000 \times 10^{0}$	$.2779 \times 10^{-3}$	$.0000 \times 10^{0}$	8.2975	∞
9	6566.84	.059560	$.0000 \times 10^{0}$	$.4374 \times 10^{-3}$	$.0000 \times 10^{0}$	5.2065	∞
10	8112.34	.054694	$.0000 \times 10^{0}$	$.2392 \times 10^{-3}$	$.0000 \times 10^{0}$	6.0680	∞
11	7741.71	.056892	$.0000 \times\times 10^{0}$	$.3112 \times 10^{-3}$	$.0000 \times 10^{0}$	5.5527	∞
12	8542.34	.054236	$.0000 \times 10^{0}$	$.2464 \times 10^{-3}$	$.0000 \times 10^{0}$	5.4532	∞
13	8113.81	.057018	$.0000 \times 10^{0}$	$.2720 \times 10^{-3}$	$.0000 \times 10^{0}$	5.3533	∞
14	8753.72	.054753	$.0000 \times 10^{0}$	$.2213 \times 10^{-3}$	$.0000 \times 10^{0}$	5.4240	∞
15	8827.26	.092696	$.1471 \times 10^{-6}$	$.1592 \times 10^{-3}$	$.2342 \times 10^{-10}$	6.8936	23.8691

that this design was nearly minimum bias. In addition, we found that its variance and power properties were poor, although better than the minimum bias designs that we examined.

For this case, the Euclidean norm of T_2 for the minimum bias designs is 0.052922, and hence, it appears that all of these designs are nearly minimum bias designs. However, it should be noted that although the variance properties of these designs do not appear to be good, the n = 10 designs seems to be the worst with this respect.

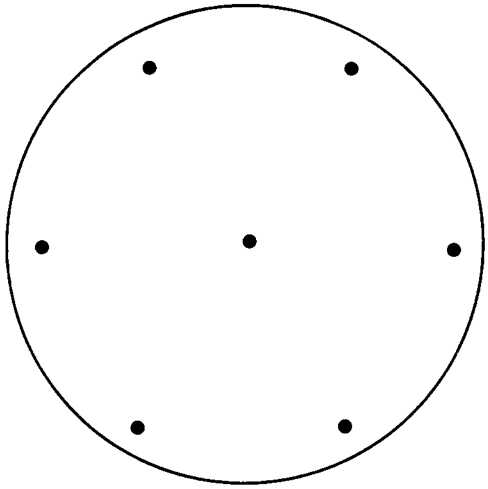
6.4. Two-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for Second Order vs. Third Order Polynomial Models and Circular Regions of Interest

In this section, we will obtain some of the two-factor $\Lambda_2(T_2,\frac{1}{2})$-optimal designs for second order vs. third order polynomial models and a region of interest defined by

$$\sum_{i=1}^{2} x_i^2 \leq 1. \tag{6.4.1}$$

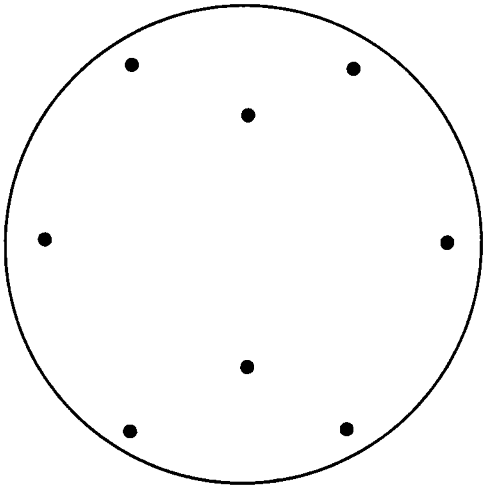
However, because of the invariance results of Section 2.2, the designs given in this section can be scaled for any region of interest that can be expressed as a non-singular linear transformation of (6.4.1). Furthermore, since any orthogonal rotation preserves the region moments of a circle, by Theorems 2.11 and 2.12, it follows that any othogonal rotation of the designs given in this section will also be optimal.

Figures 6.15--6.17 contain the $\Lambda_2(T_2,\frac{1}{2})$-optimal designs for $n = 7$--10, 12--14. The $n = 11$ design was omitted because the optimization algorithm described in Appendix A was slow in converging



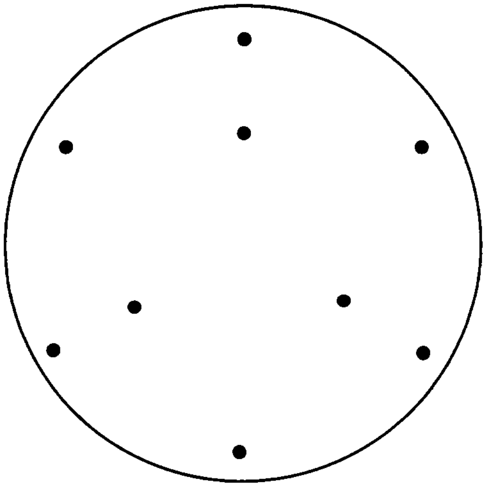
n = 7

0.897935	0.000000
-0.897935	0.000000
0.448968	0.777634
-0.448968	0.777634
0.448968	-0.777634
-0.448968	-0.777634
0.000000	0.000000



n = 8

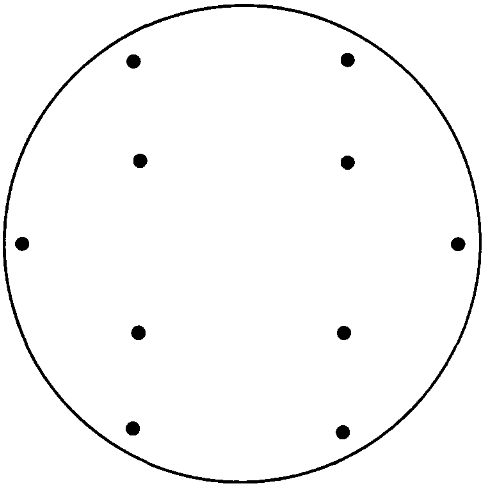
0.000000	0.551455
0.000000	-0.551455
0.900729	0.000000
-0.900729	0.000000
0.467020	0.794521
-0.467020	0.794521
0.467020	-0.794521
-0.467020	-0.794521



n = 9

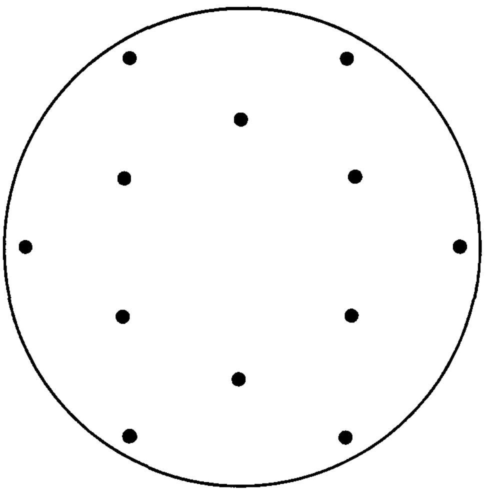
0.000000	0.933818
-0.808710	-0.466909
0.808710	-0.466909
0.000000	-0.893894
-0.774135	0.446947
0.774135	0.446947
0.000000	0.520959
-0.451163	-0.260479
0.451163	-0.260479

Figure 6.15. Two-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for Second Order vs. Third Order Models, Circular Region of Interest and n = 7-9



n = 10

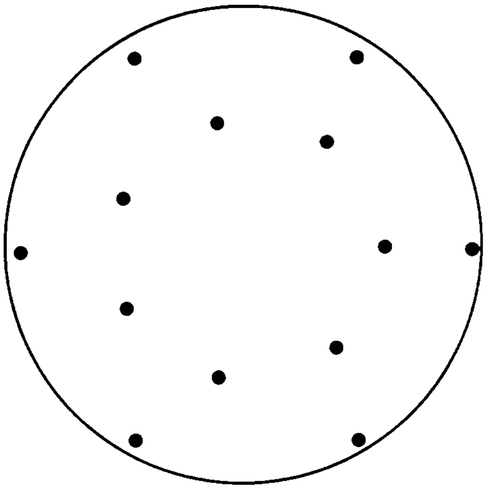
0.429401	0.379920
0.429401	-0.379920
-0.429401	0.379920
-0.429401	-0.379920
0.945738	0.000000
-0.945738	0.000000
0.446608	0.809342
-0.446608	-0.809342
0.446608	-0.809342
-0.446608	0.809342



n = 12

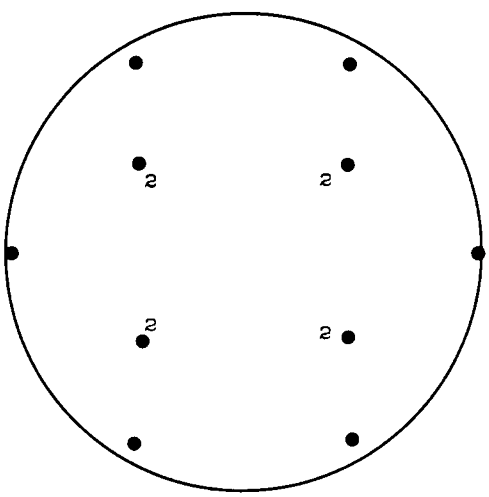
0.000000	0.572179
0.000000	-0.572179
0.495522	0.286090
0.495522	-0.286090
-0.495522	0.286090
-0.495522	-0.286090
0.952331	0.000000
-0.952331	0.000000
0.476165	0.824743
-0.476165	-0.824743
0.476165	-0.824743
-0.476165	0.824743

Figure 6.16. Two-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for Second Order vs. Third Order Models, Circular Region of Interest and n = 10,12



n = 13

0.962375	0.000000
-0.962375	0.000000
0.481187	0.833441
-0.481187	-0.833441
0.481187	-0.833441
-0.481187	0.833441
0.572802	0.013362
-0.510279	-0.260568
-0.140488	0.555467
0.367583	-0.439530
-0.114433	-0.561414
0.346689	0.456166
-0.521874	0.236490



n = 14

0.997544	0.000000
-0.997544	0.000000
0.448210	0.847876
-0.448210	-0.847876
0.448210	-0.847876
-0.448210	0.847876
0.432684	0.382608
0.432684	0.382608
-0.432684	-0.382608
-0.432684	-0.382608
0.432684	-0.382608
0.432684	-0.382608
-0.432684	0.382608
-0.432684	0.382608

Figure 6.17. Two-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for Second Order vs. Third Order Models, Circular Region of Interest and n = 13-14

to the optimal design. Some of the properties of these designs are given in Table 6.5. Except for the n = 12 and n = 13 designs, all of these designs are singular for the third order model. Excluding the n = 12 and n = 13 designs, the ranges of the design properties given in Table 6.5 are:

$$V_1 \quad 5.1490\text{--}6.1874,$$

$$\text{and} \quad \|T_2\| \quad 0.028195\text{--}0.030164.$$

Again, since for this case, the Euclidean norm of T_2 for the minimum bias designs is 0.027340, Table 6.5 indicates that these designs appear to be nearly minimum bias.

It is interesting to note the similarities between the designs of this section for a circular region of interest and those of the previous section for a square region of interest. For example, the n = 7 design illustrated in Figure 6.11 for a square region of interest appears to be a simple distortion of the n = 7 design illustrated in Figure 6.15 for a circular region of interest.

TABLE 6.5

Characteristics of the Two-Factor $\Lambda_2(T_2,\frac{1}{2})$-Optimal Designs for Second Order vs. Third Order Models and a Circular Region of Interest

				Standardized Determinants		Standardized Average Variances	
n	$\Lambda_2(T_2,\frac{1}{2})$	$\lVert T_2\rVert$	$\lvert n^{-1} L\rvert$	$\lvert n^{-1} X_1' X_1\rvert$	$\lvert n^{-1} X' X\rvert$	V_1	V_2
7	24520.8	.030164	$.0000 \times 10^{0}$	$.4612 \times 10^{-4}$	$.0000 \times 10^{0}$	5.1490	∞
8	34317.1	.029349	$.0000 \times 10^{0}$	$.2892 \times 10^{-4}$	$.0000 \times 10^{0}$	6.1874	∞
9	36086.7	.028921	$.0000 \times 10^{0}$	$.2711 \times 10^{-4}$	$.0000 \times 10^{0}$	5.4305	∞
10	41276.7	.028427	$.0000 \times 10^{0}$	$.2847 \times 10^{-4}$	$.0000 \times 10^{0}$	5.4035	∞
12	46186.6	.028381	$.1043 \times 10^{-7}$	$.2700 \times 10^{-4}$	$.2816 \times 10^{-12}$	5.2104	14.2305
13	48473.3	.028333	$.6992 \times 10^{-8}$	$.2611 \times 10^{-4}$	$.1825 \times 10^{-12}$	5.1840	20.0427
14	50927.0	.028195	$.0000 \times 10^{0}$	$.2538 \times 10^{-4}$	$.0000 \times 10^{0}$	5.1804	∞

VII. SUMMARY

7.1. The $\Lambda(T)$ Criteria

7.1.1. The Assumptions

In this investigation, we have concentrated on the development and examination of several criteria for the selection of an experimental design. These criteria (referred to as the $\Lambda(T)$ criteria) were primarily motivated by the following assumptions:

1. the true response surface has the form

$$\eta(\underset{\sim}{x}) = \underset{\sim}{x}_1' \underset{\sim}{\beta}_1 + \underset{\sim}{x}_2' \underset{\sim}{\beta}_2, \tag{7.1.1}$$

2. the proposed model has the form

$$\eta_1(\underset{\sim}{x}) = \underset{\sim}{x}_1' \underset{\sim}{\beta}_1, \tag{7.1.2}$$

3. a lack of fit test will be used to test the adequacy of the proposed model, (7.1.3)

and 4. the seriousness associated with $\underset{\sim}{\beta}_2$ is a monotone increasing function of the positive definite quadratic form

$$\tau = \sigma^{-2} \underset{\sim}{\beta}_2' T \underset{\sim}{\beta}_2, \tag{7.1.4}$$

where T is a specified matrix.

Essentially, the lack of fit test referred to in (7.1.3) is any test whose power is a monotone increasing function of the non-centrality parameter

$$\lambda = \sigma^{-2} \underset{\sim}{\beta}_2' L \underset{\sim}{\beta}_2$$

$$\text{where} \quad L = X_2' [I_n - X_1 (X_1' X_1)^{-1} X_1'] X_2 .$$

These tests include the usual F-tests for:

$$H_0: \underset{\sim}{\beta}_2 = \underset{\sim}{0}$$
$$\text{vs. } H_1: \underset{\sim}{\beta}_2 \neq \underset{\sim}{0}$$

and

$$H_0: E[\underset{\sim}{y}] = X_1 \underset{\sim}{\beta}_1$$
$$\text{vs. } H_1: E[\underset{\sim}{y}] \neq X_1 \underset{\sim}{\beta}_1,$$

where the vector $\underset{\sim}{y}$ contains n observations each assumed to be independent and identically distributed as a Gaussian random variable with expectation $\eta(\underset{\sim}{x})$ and variance σ^2.

7.1.2. Choices for τ

In Section 1.2.2, we proposed the use of two definitions for τ. τ_1 was proposed as a measure of the inherent departure of the true response surface $\eta(\underset{\sim}{x})$ from some assumed class of models $\mathcal{M}$, such as the class of all first order polynomials. Specifically, $\sigma^2\tau_1$ is the average squared deviation over the region of interest of the true response surface from the best model $\eta_1^*(\underset{\sim}{x})$ in the assumed class of models, i.e.,

$$\tau_1 = \sigma^{-2}\,\Omega \int_R \{\eta_1^*(\underset{\sim}{x}) - \eta(\underset{\sim}{x})\}^2\, dx_1 \cdot dx_2 \cdots dx_k$$

where Ω^{-1} is the volume of the region of interest R and $\eta_1^*(\underset{\sim}{x})$ is the response evaluated at $\underset{\sim}{x}$ of the model in $\mathcal{M}$ that minimizes τ_1.

Now for some experiments, the experimenter is only indirectly interested in the deviation of the true response surface from a class of models; he is more directly interested in the deviation of the true response surface from his fitted model. For these experiments, we have proposed the use of the average squared bias as a measure of the departure of the true response surface from the fitted model, i.e.,

$$\tau_2 = \sigma^{-2}\,\Omega \int_R \{E[\hat{\eta}_1(\underset{\sim}{x})] - \eta(\underset{\sim}{x})\}^2\, dx_1 \cdot dx_2 \cdots dx_k$$

where $\hat{\eta}_1(\underset{\sim}{x})$ is the least squares estimate of $\eta_1(\underset{\sim}{x})$.

We noted that both τ_1 and τ_2 can be expressed in the form given in (7.1.4). Specifically,

$$\tau_1 = \sigma^{-2}\,\underset{\sim}{\beta}_2'\, T_1\, \underset{\sim}{\beta}_2$$

where $T_1 = [M_{22} - M_{21}\, M_{11}^{-1}\, M_{12}]$;

and $\tau_2 = \sigma^{-2}\,\underset{\sim}{\beta}_2'\, T_2\, \underset{\sim}{\beta}_2$

where $T_2 = [A'M_{11}\, A - A'M_{12} - M_{21}\, A + M_{22}]$.

T_1 depends solely upon the region moment matrices

$$M_{ij} = \Omega \int_R \underset{\sim}{x}_i\, \underset{\sim}{x}_j'\; dx_1 \cdot dx_2 \cdots dx_k \,.$$

Consequently, τ_1 is not influenced by the experimental design. This is consistent with the definition of τ_1 as a measure of the inherent departure of the true response surface from an assumed class of models. On the other hand, τ_2 depends not only upon the region moment matrices but also upon the alias matrix

$$A = (X_1'\, X_1)^{-1}\, X_1'\, X_2.$$

Consequently, τ_2 is influenced by the experimental design. This is consistent with the use of τ_2 as a measure of the expected departure of the true response surface from the fitted model, since the expectation of the fitted model depends upon the experimental design, i.e.,

$$E[\hat{\eta}_1(\underset{\sim}{x})] = \underset{\sim}{x}_1' \underset{\sim}{\beta}_1 + \underset{\sim}{x}_1' A \underset{\sim}{\beta}_2.$$

7.1.3. The Criteria

In Section 2.1, we used assumptions (7.1.1)--(7.1.4) to motivate the development of the $\Lambda(T)$ criteria. We gave specific consideration to the following criteria:

1. maximize the minimum value of λ for $\tau = \delta$, (7.1.5)

2. minimize the maximum value of τ for $\lambda = \rho$, (7.1.6)

3. maximize the average value of λ for $\tau = \delta$, (7.1.7)

and 4. minimize the average value of τ for $\lambda = \rho$, (7.1.8)

for $\delta > 0$ and $\rho > 0$. We found that none of these criteria depend upon the experimenter's specification for δ or ρ.

7.1.3.1. $\Lambda_1(T)$-Optimality.--By using Theorem 2.1, we observed that criteria (7.1.5) and (7.1.6) were both equivalent to selecting designs that maximize the minimum characteristic root of $[T^{-1} L]$. We have referred to criteria (7.1.5) and (7.1.6) as $\Lambda_1(T)$-optimality.

7.1.3.2. $\Lambda_2(T,c)$-Optimality.--By using Theorem 2.2, we were able to characterize criteria (7.1.7) and (7.1.8). We found that criterion (7.1.7) is equivalent to selecting designs that maximize $Tr[T^{-1} L]$. In general, since τ can depend upon the design, the contour in the $\underset{\sim}{\beta}_2$-space defined by $\tau = \delta$ is not the same from one design to another. Consequently, if τ does depend upon the design, we may want to ensure that the $\tau = \delta$ contour is not "tight" about the origin. Hence, we modified criterion (7.1.7) to allow the experimenter to favor designs that minimize τ in the sense of maximizing the volume of the hyperellipsoid in the $\underset{\sim}{\beta}_2$-space defined by $\tau \leq \delta$. Specifically, we refer to a design as $\Lambda_2(T,c)$-optimal if it maximizes

$$\Lambda_2(T,c) \;=\; n^{-1}\,|T|^{-c}\,\mathrm{Tr}[T^{-1}\,L]$$

where c is some non-negative constant specified by the experimenter. The factor "n^{-1}" was included to standardize $\Lambda_2(T,c)$ by the sample size. If τ is not influenced by the design, $|T|$ is a constant and the use of c has no effect upon the selection of a $\Lambda_2(T,c)$-optimal design.

7.1.3.3. $\Lambda_3(T,c)$-Optimality.--In a similar spirit, we found that criterion (7.1.8) is equivalent to selecting designs that minimize $\mathrm{Tr}[L^{-1}\,T]$; and again, since the contour in the $\underset{\sim}{\beta}_2$-space defined by $\lambda = \rho$ is dependent upon the design, we modified this criterion to allow the experimenter to favor designs with "tight" λ-contours. Specifically, a design is $\Lambda_3(T,c)$-optimal if it minimizes

$$\Lambda_3(T,c) \;=\; |n^{-1}\,L|^{-c}\,n\,\mathrm{Tr}[L^{-1}\,T]$$

where c is some non-negative constant specified by the experimenter. The constant c is increased to favor designs that maximize λ, in the sense of minimizing the volume of the hyperellipsoid in the $\underset{\sim}{\beta}_2$-space defined by $\lambda \leq \rho$, by maximizing $|L|$. In fact, as c is increased, we would expect the $\Lambda_3(T,c)$-optimal designs to approach the $|L|$-optimal designs.

7.1.4. Some Analytical Properties of the $\Lambda(T)$ Criteria

Later in Chapter II, we were able to prove several useful results for the $\Lambda(T)$ criteria. In Section 2.2, we found that all of the $\Lambda(T)$ criteria are invariant under non-singular linear transformations of the independent variables, $\underset{\sim}{x}$, provided that τ is invariant under such transformations; and we were able to show that τ_1 and τ_2 are invariant under non-singular linear transformations of the independent variables.

In Section 2.3, we examined the effect of orthogonal rotations upon the criteria considered in this investigation when the underlying models are polynomials. For D-optimality and $|L|$-optimality, we showed that if the design D_0 is an optimal design and Q is an orthogonal matrix then

$$D_1 = D_0 Q$$

is also an optimal design provided that D_1 is a permissible design. For the $\Lambda(T)$ criteria using either τ_1 or τ_2, we proved that the same property holds provided that Q is a "moment preserving" non-singular linear transformation.

Finally, in Section 2.4, we examined the effect upon the $\Lambda(T)$ criteria and $|L|$-optimality of augmenting a design with one additional observation. These results could be used to develop an "exchange" algorithm similar to the algorithms developed for D-optimality by Wynn (1970), Dykstra (1971), and Mitchell (1972, 1974).

7.2. The Empirical Examination of $\Lambda(T)$-Optimal Designs for τ_1 and τ_2

In Chapters III and V, $\Lambda(T)$-optimal designs for τ_1 and τ_2 respectively were compared with D-optimal designs for the lower and higher order models, minimum bias designs and designs that maximize $|L|$. The primary purpose of these comparisons was to investigate the variance, bias and power properties of $\Lambda(T)$-optimal designs. The approach used for these comparisons was empirical. We examined $\Lambda(T)$-optimal designs for a cuboidal region of interest and the following cases:

1. one-factor, first order vs. second order polynomial models and $n = 5, 9$,
2. one-factor, second order vs. third order polynomial models and $n = 6, 10$,
3. two-factor, first order vs. second order polynomial models and $n = 6$,

and 4. two-factor, second order vs. third order polynomial models and $n = 10$.

For each of these cases, we examined the following designs:

1. $\Lambda_1(T)$-optimal, $\Lambda_2(T,c)$-optimal and $\Lambda_3(T,c)$-optimal designs for $c = 0$ and $c = \frac{1}{2}$,
2. D-optimal designs for both the lower and higher order models,
3. $|L|$-optimal designs,

and 4. minimum bias designs.

With the exception of the minimum bias designs and the two-factor, second order D-optimal design for $n = 6$ (which was given by Hartley and Ruud (1969) and also by Box and Draper (1971)), all of the designs in these comparisons were obtained using the computational algorithm described in Appendix A.

Summaries of these comparisons were given at the end of Chapters III and V. These comparisons suggest that $\Lambda(T)$-optimal designs generally have much better variance properties than the minimum bias designs, lower bias than D-optimal or $|L|$-optimal designs, and greater power than either for detecting lack of fit.

7.3. The Choice of $\Lambda(T)$ Criterion

The comparisons conducted in Chapters III and V suggest that, by a proper selection of $\Lambda(T)$ criteria, τ and possibly c, experimenters can obtain designs with a specified balance of variance, bias and power properties.

7.3.1. The Selection of a Design with Optimum Power Characteristics

Among all of the criteria considered in this investigation, the designs that seem to have the best power properties are: (1) $\Lambda(T_1)$-optimal designs, (2) $|L|$-optimal designs, and (3) D-optimal designs for the higher order model. The comparisons conducted in Chapter III indicate that the power properties of $\Lambda(T_1)$-optimal designs are as good as or better than those of D-optimal or $|L|$-optimal designs. Furthermore, these comparisons indicate that $\Lambda(T_1)$-optimal designs have better bias properties than either D-optimal or $|L|$-optimal designs, and somewhat surprising is the fact that $\Lambda_1(T_1)$-optimal and $\Lambda_3(T_1,c)$-optimal designs seem to have better average variance properties for prediction of the higher order model (V_2) than either D-optimal or $|L|$-optimal designs. Consequently, as far as the selection of a design with excellent power properties is concerned, we recommend the use of a $\Lambda(T_1)$ criterion.

There are several factors that can influence the particular choice of $\Lambda(T_1)$ criterion. If an experimenter is unable to conduct an experiment large enough to estimate the higher order model, $\Lambda_2(T_1)$-optimality is the only $\Lambda(T_1)$ criteria applicable. However, if he is able to conduct an experiment large enough to estimate the higher order model then $\Lambda_1(T_1)$-optimality would be preferred if an experimenter is concerned about the minimum power properties of his design, and $\Lambda_2(T_1)$-optimality would be preferred if he is concerned about the average power properties of his design.

Unfortunately, the $\Lambda_1(T_1)$ criterion has proven to be difficult to apply. The computational algorithm described in Appendix A converges very slowly for the $\Lambda_1(T_1)$ criterion. However, in all of the comparisons of Chapter III, the properties of the $\Lambda_1(T_1)$-optimal design were nearly identical to those noted for the $\Lambda_3(T_1,0)$-optimal design. Consequently, at this time, $\Lambda_3(T_1,0)$-optimality is recommended as a substitute for $\Lambda_1(T_1)$-optimality.

Chapter IV contains the following $\Lambda_2(T_1)$-optimal designs for a cuboidal region of interest:

1. one-factor, first order vs. second order polynomial models and n = 3--20,
2. one-factor, second order vs. third order polynomial models and n = 4--20,
3. two-factor, first order vs. second order polynomial models and n = 4--10,

and 4. two-factor, second order vs. third order polynomial models and n = 8--15.

In addition, Chapter IV contains graphs of the power of the lack of fit test for one-factor $\Lambda_2(T_1)$-optimal designs. These can be used to select an α-level and sample size for the lack of fit test.

7.3.2. The Selection of a Minimum Bias Design

The selection of a minimum bias design has been given a good deal of attention (e.g., Box and Draper (1959, 1963), Draper and Lawrence (1965) and Thompson (1973)). The usual approach has been to obtain minimum bias designs that follow some specified pattern, such as

$$D = \begin{bmatrix} -a & -a \\ a & -a \\ -a & a \\ a & a \\ b & 0 \\ -b & 0 \\ 0 & b \\ 0 & -b \end{bmatrix}$$

where $-1 \leq a \leq 1$ and $-1 \leq b \leq 1$. Requiring an experimental design to follow such a pattern generally makes it easier to specify a minimum bias design. However, it seems that not enough attention has been given to whether the specified pattern is rich enough to contain minimum bias designs that also have reasonably good variance and power properties. The two-factor minimum bias designs that were examined in Chapters III and V were obtained by this procedure, and we found that their variance and power properties are poor. In fact, the minimum bias square plus hexagon for second order vs. third order polynomial models (see Figure 3.18) is nearly singular for the lower order model.

In Chapters V and VI, we found that $\Lambda_2(T_2,\frac{1}{2})$-optimality selects designs that are essentially minimum bias. However, for all of the cases considered in Chapter V, $\Lambda_2(T_2,\frac{1}{2})$-optimal designs had considerably better properties for the average variance of $\hat{\eta}_1(\underset{\sim}{x})$ and the average value of λ than any of the minimum bias designs examined. Furthermore, to date, we have been unable to find a minimum bias design with better properties for the average value of λ and the average variance of $\hat{\eta}_1(\underset{\sim}{x})$. Consequently, we recommend the use of $\Lambda_2(T_2,\frac{1}{2})$-optimality to obtain designs that have near minimum bias.

In Chapter VI, these designs were given for the following cases:

1. one-factor, first order vs. second order polynomial models and $n = 3$--20,
2. one-factor, second order vs. third order polynomial models and $n = 4$--20,
3. two-factor, first order vs. second order polynomial models, $n = 5$--10 and a square region of interest,
4. two-factor, second order vs. third order polynomial models, $n = 7$--10 and a square region of interest,
5. two-factor, second order vs. third order polynomial models, $n = 7$--10, 12--14 and a circular region of interest.

In addition, Chapter VI contains graphs of the power of the lack of fit test for one-factor $\Lambda_2(T_2,\frac{1}{2})$-optimal designs.

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APPENDIX A

The Computational Algorithm

Interactive computer programs were used to obtain most of the optimal designs given in this investigation. Zangwill's modified Powell algorithm was used as the basic search algorithm. The details of this algorithm are described in Zangwill (1967) and Powell (1964).

The Powell algorithm is an unconstrained function minimization procedure. In this investigation, designs were constrained to either a hypercube or a hypersphere. Thus, in order to use the Powell algorithm, it was necessary to transform the design variables x_i into new unconstrained variables, a_i. This technique for optimizing a constrained function is discussed in Box (1965) and Atkinson (1969). For the hypercube

$$R = \{\underset{\sim}{x} : -1 \le x_i \le 1,\ i = 1, 2, \ldots, k\}$$

the transformation given by Box (1965) was used. Specifically, the transformation used was:

$$a_i = \text{Sin}^{-1}[x_i],\ i = 1, 2, \ldots, k.$$

For the hypersphere

$$R = \{\underset{\sim}{x} : \underset{\sim}{x}'\ \underset{\sim}{x} \le 1\}$$

the following transformation was used:

$$a_1 = \text{Sin}^{-1}[x_1]$$

$$a_2 = \text{Sin}^{-1}[x_2 \ /\ (1 - x_1^2)^{\frac{1}{2}}]$$

$$\vdots$$

$$\vdots$$

$$a_k = \text{Sin}^{-1}[x_k \;/\; (1 - x_1^2 - x_2^2 - \cdots - x_{k-1}^2)^{\frac{1}{2}}].$$

Of course, it should be recognized that this algorithm can only guarantee convergence to a locally optimal design. Thus it is necessary to execute this algorithm several times with different starting designs, and even then, we cannot be certain that the best design obtained is truly optimal. To ensure that the designs presented in this investigation were optimal, or at least nearly optimal, at least ten randomly chosen initial designs were used as input to the search algorithm. This number of initial designs was increased when it became evident that an optimality criterion had numerous (approximately more than 3) locally optimal designs.

APPENDIX B

A Summary of the Variance, Bias and Power Properties Used to Examine the $\Lambda(T)$-Optimal Designs

Variance Properties

$$E_1 = \left[|X_1' X_1|_{D_o} \Big/ \underset{D \,\varepsilon\, \Delta}{\text{Max}} |X_1' X_1|_D \right]^{p_1^{-1}}$$

$$E_2 = \left[|X' X|_{D_o} \Big/ \underset{D \,\varepsilon\, \Delta}{\text{Max}} |X' X|_D \right]^{(p_1+p_2)^{-1}}$$

$$V_1 = (n/\sigma^2)\, \Omega \int_R \text{Var}[\hat{\eta}_1(\underset{\sim}{x})] \quad dx_1 \cdot dx_2 \cdots dx_k$$

$$V_2 = (n/\sigma^2)\, \Omega \int_R \text{Var}[\hat{\eta}(\underset{\sim}{x})] \quad dx_1 \cdot dx_2 \cdots dx_k$$

Bias Properties

$$B = \Omega \int_R \{E[\hat{\eta}_1(\underset{\sim}{x})] - \eta(\underset{\sim}{x})\}^2 \quad dx_1 \cdot dx_2 \cdots dx_k$$

$$\|T_2\| = \left[\sum_{i,j} t_{ij}^2 \right]^{\frac{1}{2}}$$

Power Properties

$$\lambda = \sigma^{-2}\, \underset{\sim}{\beta}_2'\, L\, \underset{\sim}{\beta}_2$$

$$|n^{-1} L| = |n^{-1} X_2' [I_n - X_1 (X_1' X_1)^{-1} X_1'] X_2|$$

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RESPONSE SURFACE DESIGNS FOR THE
DETECTION OF MODEL INADEQUACY

by

Edward R. Jones

(ABSTRACT)

In many experiments, it is tentatively assumed that the experimental response is related to some independent variables, $\underset{\sim}{x}$, by $\eta_1(\underset{\sim}{x}) = \underset{\sim}{x}_1' \underset{\sim}{\beta}_1$. However, there is frequently some doubt whether this model adequately approximates the true response function, so a lack of fit test is used as part of the analysis. We suppose that the true response function is $\eta(\underset{\sim}{x}) = \underset{\sim}{x}_1' \underset{\sim}{\beta}_1 + \underset{\sim}{x}_2' \underset{\sim}{\beta}_2$. The power of the usual lack of fit test is a monotone increasing function of the non-centrality parameter $\lambda = \sigma^{-2} \underset{\sim}{\beta}_2' L \underset{\sim}{\beta}_2$, where the positive semi-definite matrix L is determined by the experimental design. We use λ as a measure of a design's ability to detect the higher order parameters, $\underset{\sim}{\beta}_2$.

This investigation has concentrated on the development and evaluation of criteria for the selection of experimental designs that have good properties for the detection of model inadequacy. We suppose that the inadequacy of our proposed model is measured by the positive definite quadratic form $\tau = \sigma^{-2} \underset{\sim}{\beta}_2' T \underset{\sim}{\beta}_2$, where T is specified by the experimenter according to his own interests. Two choices for τ are proposed. τ_1 is proposed as a measure of the inherent departure of a response surface from an assumed class of models. Another choice for

τ, τ_2, is the ratio of the average squared bias to the sampling variance, σ^2. Whereas τ_1 measures the inherent departure of a response surface, τ_2 measures the departure of the fitted model from the response surface. As a result, τ_1 is independent of the design, whereas τ_2 depends upon the experimental design.

We examine the following criteria:

(1) maximize the minimum value of λ for $\tau = \delta$,

(2) maximize the average value of λ for $\tau = \delta$,

(3) minimize the maximum value of τ for $\lambda = \rho$,

and (4) minimize the average value of τ for $\lambda = \rho$,

where δ and ρ are any positive constants. We show that criteria (1) and (3) are equivalent. They select designs that maximize the minimum characteristic root of $[T^{-1} L]$. We also show that criterion (2) selects designs that maximize $Tr[T^{-1} L]$, and that criterion (4) selects designs that minimize $Tr[L^{-1} T]$. In addition, we propose a modification of (2) to allow the experimenter to favor designs that afford greater "protection" in the sense of minimizing τ, and a modification of (4) to allow the experimenter to favor designs that afford greater "detection" in the sense of maximizing λ. We show that all of these criteria, referred to as the $\Lambda(T)$ criteria, are invariant under non-singular linear transformations of the independent variables provided that τ is invariant to such transformations, and we show that τ_1 and τ_2 are invariant to such transformations. In addition, we obtain several results for rotations of D-optimal and $\Lambda(T)$-optimal designs.

Optimal designs for all of these criteria are obtained and evaluated for a variety of cases. Primary consideration is given to the use of τ_1 and τ_2 for one and two factor, first order vs. second order and second order vs. third order, polynomial models. We have found that the $\Lambda(T)$-optimal designs generally have much better variance properties than minimum bias designs, lower bias than D-optimal designs, and greater power than either for detecting lack of fit.

Criterion (2) was also selected and used as the basis for a more extensive investigation of the types of designs generated by our approach.