LOCALLY OPTIMAL DESIGNS FOR BINARY AND WEIGHTED REGRESSION MODELS

by

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SUMMARY

The main aim of this thesis is to review and augment the theory and methods of optimal experimental designs for non-linear problems with a single variable using geometric and other arguments. It represents a continuation of the work on locally optimal designs for binary response experiments, which has been studied by Ford, Torsney, and Wu (1992) among others.

Chapter 1 serves as an introduction to the non-linear design problem. The main point of difference between the non-linear case is emphasised and contrasted with the linear case.

Chapter 2 presents a review of the general theory and the appropriate notation needed for the development of this thesis. Also the canonical transformation of a design problem is discussed. A necessary and sufficient condition for D-optimality of a design measure is given.

Chapters 3 and 4 are devoted to the problem of constructing locally D-optimal and c-optimal designs for two parameter models respectively. In addition, the geometrical characterisation of designs optimising these criteria is discussed. Explicit solutions to compute the optimal weights of such designs are derived. Several examples of optimal designs which may be found analytically are given in chapter 3.

In chapter 5 attention is focused on the problem of determining D-optimal designs for three parameter models, including those for weighted quadratic regression and generalised linear models.

Chapter 6, considering the situations and problems for future work, gives a list of possible ways in which the work of this thesis may be extended.

CONTENTS

CHAPTER ONE

INTRODUCTION

The problem of optimal experimental design has paid more attention to linear experimental design (LED) than to non-linear experimental design (NLED) in the statistical literature. In their review work Steinberg and Hunter (1985) devoted only one paragraph to non-linear models. John and Draper (1975) did the same seventeen years earlier.

Work on linear models led to the development of a powerful body of theory and methodology. Ford (1976) provided a critical review of optimal static and sequential design. Titterington (1980) reviewed the geometric approach to (LED). Pazman (1980) contributed on a theoretical level. Pukelshiem and Titterington (1983) offered a general approach to optimal (LED) and Torsney (1981,1983,1988) viewed the optimum linear design problem as a more general optimisation problem. Fedorov (1972) and Silvey (1980) contributed excellent monographs on linear experimental design. Recently Wynn and Logothetis (1989) published a comprehensive book on linear experimental design.

Non-linear problems, including non-linear regression, quantal response models and linear problems where interest is in a non-linear function of the parameters have the feature that either the information matrix or some concave function of the information matrix is a function of the unknown parameters. In order to emphasise this fact the design is called locally optimal. It is the dependence of the design on the unknown parameters which leads to the term **"Locally Optimal"**.

This dependence on the unknown parameters is the main point of difference between linear experimental design, which originated in Smith (1918) and the non-linear case, originating in Fisher (1922). What is also very important, and we would like to put special emphasis on it, is that linear experimental design is usually concerned with design for a normal linear model, where as non-linear experimental design techniques are needed in the case of a non-linear model.

In contrast the linear problem is, relatively speaking, straightforward because the information matrix does not depend on any unknown parameters in the model, it depends proportionately on σ^2 and the choice of design can usually be reduced to the mathematical problem of finding a design to maximize some concave function of the Fisher information matrix.

The aim of this thesis is to consider locally optimal designs for binary response experiments, namely experiments of which the outcomes are either '**occurrence**' or '**non-occurrence**' of some event of interest.

This type of problem has been studied by several authors. See Abdelbasit and Plackett (1983) and its references. Wu (1985,1988) has worked on binary response problems. Salomin Minkin (1987) obtained some results on optimal designs for the binary data, including those on likelihood-based regions and global D-optimality. Ford, Torsney, and Wu (1992) study D-optimal and c-optimal designs for generalised linear models, including models for binary responses. We propose to extend the results of the latter authors.

CHAPTER TWO

MOTIVATION

2.1 MODELS UNDER CONSIDERATION

Consider the non-linear experimental design in which the scalar response variable, y , say, is distributed as a member of the exponential family $p(y,\eta)$.

In particular assume that

$$E(y/x)=\eta(x,\underline{\theta}). \qquad (2.1.1)$$

Where x is a scalar variable called the explanatory, independent, or control variable because it can be chosen by the experimenter, $x\in\chi\subseteq R^{l}$ and $\underline{\theta}\in\Theta\subseteq R^{m}$. The set χ is the design space and the set Θ is the parameter space, the set where the m-vector of unknown parameters of interest $\underline{\theta}=(\theta_1,\theta_2,\ldots,\theta_m)'$ takes their values.

Let us assume that we have obtained a set of N independent observations $\underline{y}=(y_1,y_2,\ldots,y_N)'$ from the probability distribution $p(y/x,\underline{\theta})$, where these have been obtained only at the distinct points $x_1,x_2,\ldots,x_r$ in χ. Suppose that $N=\sum_{i=1}^{r}n_i$, where n_i denotes the number of observations which were taken at the point x_i , so that $p_i={}^{n_i}\!/_{N}$ is the proportion of observations taken at x_i , and r is the number of distinct x_i's which were chosen.

Definition (2.1.1): We shall call the set of points $Supp(p^{*})=\{x_i;i=1,2,\ldots,r\}$ the support of the experimental design.

Definition (2.1.2): The pair $\xi = \left\{ \begin{bmatrix} x_i \\ p_i \end{bmatrix} ; i = 1,2,\ldots,r \right\}$ will be called the design measure, where the variables p_i can take any value between and including 0 and 1. i.e.

$$\sum_{i=1}^{r} p_i = 1 \quad , \quad 0 \le p_i \le 1. \tag{2.1.2}$$

More generally, a design will be characterized by some probability measure $\xi(x)$, given on the design space χ and satisfying the conditions

$$\int_{x \in \chi} d\xi(x) = 1 \quad , \quad \xi(\mathrm{x}) \ge 0, \quad x \in \chi. \tag{2.1.3}$$

For the response variable, y, we further assume that $y \in \{0,1\}$, namely we have a binary response experiment. In this case the outcome is either **'occurrence'** or **'non-occurrence'** of some event and is linked with the explanatory variables and the parameters through a distribution function $'F'$ with

$$p(y_j = 1) = F\left[u(x_j, \underline{\theta})\right] \ , \ p(y_j = 0) = 1 - F\left[u(x_j, \underline{\theta})\right]. \tag{2.1.4}$$

Where x_j is the value of x at which the observation y_j is obtained.

Hence

$$E(y_j) = F(u^*).$$

$$Var(y_j) = F(u^*)\left[1 - F(u^*)\right].$$

2.2 EXISTENCE OF ESTIMATORS

After collection of the data the question arises as to whether it is possible to get estimates for the unknown parameters of interest. For the binary response problem Silvapulle (1981) provided conditions under which the likelihood function L, where

$$L \propto \prod \left[F(u_i)\right]^{y_i} \left[1-F(u_i)\right]^{1-y_i} \quad , \qquad (2.2.1)$$

can provide maximum likelihood estimators (Appendix AI.3). Roughly speaking that occurs when the intersection of the sets of values taken by the explanatory variables corresponding to 1's and to 0's is not a null set. This happens to be a necessary and sufficient condition for the logit and probit models.

Now, having ensured that the likelihood equation can provide MLE's $\hat{\underline{\theta}}$ of $\underline{\theta}$, and denoting by $\ell(\underline{\theta})$ the log-likelihood, then for N large enough a log-likelihood confidence region for $\underline{\theta}$ is given by

$$R(\hat{\underline{\theta}}) = \left\{\underline{\theta}: \ell(\hat{\underline{\theta}}) - \ell(\underline{\theta}) \leq \text{constant}\right\}. \qquad (2.2.2)$$

Next, we define the matrix

$$s(\underline{\theta}) = -\left[\frac{\partial^2}{\partial\theta_i \partial\theta_j} \ \ell(\underline{\theta})\right]_{\underline{\theta}=\hat{\underline{\theta}}},$$

to be called the sample information matrix.

2.3 FISHER INFORMATION MATRIX

For the exponential family of models the Fisher information matrix for $\underline{\theta}$, given an observation at design point x, is defined to be

$$I(\underline{\theta},x) = [a(\underline{\theta},x)]^{-1}\ \eta_\theta\ \eta_\theta^t \quad . \tag{2.3.1}$$

Where η_θ denotes the vector of partial derivatives

$$\eta_\theta = \left(\frac{\partial\eta}{\partial\theta_1}, \frac{\partial\eta}{\partial\theta_2}, \ldots, \frac{\partial\eta}{\partial\theta_m} \right)^t . \tag{2.3.2}$$

And $a(\underline{\theta},x) = \text{var}(y/x)$ for the exponential family.

Consider the case of non-linear problems in which the explanatory variable x and the parameter $\underline{\theta}$ appear together linearly as follows

$$\eta = \eta(\underline{\theta}^t \underline{s}) = \eta(z) \quad , \quad \underline{s}^t = (1, \underline{x}^t) \quad , \quad z = \underline{\theta}^t \underline{s} \quad . \tag{2.3.3}$$

Then

$$\eta_\theta = \frac{\partial\eta}{\partial z} \frac{\partial z}{\partial \underline{\theta}} = \frac{\partial\eta}{\partial z}\ \underline{s} . \tag{2.3.4}$$

Hence

$$\eta_\theta\ \eta_\theta^t = \left(\frac{\partial\eta}{\partial z} \right)^2 \underline{s}\underline{s}^t \ . \tag{2.3.5}$$

Therefore, the Fisher information matrix is equal to

$$I(\underline{\theta},x) = \ \text{w}(z)\ \left[\underline{s}\underline{s}^t \right]. \tag{2.3.6}$$

Where $w(z)=\left(\frac{\partial\eta}{\partial z}\right)^2 / \operatorname{var}(y/x)$, and for the binary data problems $w(z)=\frac{f^2}{F(1-F)}$. We will further assume that the weight function $w(\cdot)$ is measurable.

The concept of the expected information matrix per-observation will play an important role in our setting for the non-linear experimental design problem. For the design of definition 2.1.2 it is defined to be

$$M(\underline{\theta},\xi)=\sum_{i=1}^{r} p_i\, I(\underline{\theta},x_i). \tag{2.3.7}$$

For the continuous case

$$M(\underline{\theta},\xi)=\int_{x\in\chi} I(\underline{\theta},x)\ \xi\ (dx). \tag{2.3.8}$$

We now define the basic properties of the Fisher information matrix, as has been noted by Fedorov (1972), in the following theorem.

<u>Theorem :</u> (Fedorov 1972, p 66)

1- For any design ξ the information matrix $M(\xi,\underline{\theta})$ is a symmetric positive-semidefinite matrix.

2- The matrix $M(\xi,\underline{\theta})$ is singular $\left[i.e\ |\mathrm{M}(\xi,\underline{\theta})|=0\right]$, if the support points of the design ξ contains less than m points (m is the number of unknown parameters).

3- The family of matrices $M(\xi,\underline{\theta})$, corresponding to all possible normalised designs is convex.

4- Given 2.3.6 the matrix $M(\xi,\underline{\theta})$ can be represented in the form of

$$M(\xi,\underline{\theta}) = \sum_{i=1}^{n} p_i\, w_i\, s_i\, s_i^t \ ,$$

Where $\quad n \leq \dfrac{m(m+1)}{2}+1 \quad , \quad 0 \leq p_i \leq 1 \quad , \quad \sum_{i=1}^{n} p_i = 1.$

2.4 THE CANONICAL PROBLEM

Let χ be the design space to which we are constrained in selecting design points x.

Let ξ be a design measure on χ, hence

$$M(\xi,\underline{\theta}) = \int_{x\in\chi} w(\underline{\theta}^t \underline{s})\ \underline{ss^t}\ \xi\, d(x). \tag{2.4.1}$$

The design problem usually involves seeking a design which maximises some concave criterion, ϕ, say of the expected information matrix $M = M(\xi,\underline{\theta})$. Since M depends on $\underline{\theta}$ so will the optimal design. We cope with this as follows.

Suppose the criterion is invariant under transformations of the form $\underline{s} \rightarrow \underline{t} = B\underline{s}$, where B is a non-singular $m \times m$. If further B is chosen such that its first row is $(1,0,\ldots,0)^t$ and its last row is $\underline{\theta}^t$, (so that $t_1 = 1$, $t_m = \underline{\theta}^t \underline{s}$) we shall see that this can lead to a canonical version of the design problem, which can be solved independently of $\underline{\theta}$ and for which

i) the design variables are images of $\underline{x}$ under the mapping namely $\underline{z}$, where $\underline{t} = (1, \underline{z}^t)^t$;

ii) the design space Z is the image of χ under the mapping;

iii) the expected information matrix is

$$M_z = \int_{z \in Z} w(t_m)\ \underline{t}\,\underline{t}^t\ \xi\,(dz)$$

$$= \int_{z \in Z} w(z_{m-1})\ \underline{t}\,\underline{t}^t\ \xi\,(dz).$$

The importance of the transformation from x to z is that the dependence of the optimal design on the true value $\underline{\theta}$ for given design space χ is replaced, in the transformed problem, by a design space which varies with $\underline{\theta}$. Hence, if we can solve the transformed problem for arbitrary Z, we have implicitly solved the optimal design problem for arbitrary χ and $\underline{\theta}$.

We note that for the above to be useful we have to be able to construct the optimal design for any canonical design space Z which might arise from the canonical transformation. A further induced design space, which is given below by the set G, plays a role in constructing optimal designs.

$$G = \left\{ \underline{g} \in R^m : \underline{g} = \left[w(t_m)\right]^{1/2} \underline{t},\ \underline{t} = (1, \underline{z}^t)^t,\ \underline{z} \in \mathrm{Z} \right\}. \qquad (2.4.2)$$

It has been established (Silvey (1980), chapter 6) that the structure of optimal designs, in particular their supports, depends critically on the geometry of this space.

2.5 DESIGN CRITERIA

In the previous section we have formulated a very general experimental design problem, namely to optimise some concave function of $M(\xi,\underline{\theta})$, $M(\xi,\underline{\theta}) \in \mu_\theta$, where μ_θ represents the set of all Fisher information matrices that experimental conditions permit. We now consider possible candidates for the function ϕ.

2.5.1

In this paragraph we shall assume that the experimenter is interested in all of the parameters jointly or in some linear combination of them. We shall consider two optimality criteria.

i) $\phi_1 = \log \ \det[M(\xi,\underline{\theta})]$

Suppose that $\hat{\underline{\theta}}$ is the M.L estimator of $\underline{\theta}$ obtained from data arising under a design ξ chosen on the provisional assumption that $\underline{\theta} = \tilde{\underline{\theta}}$. Then from equation (2.2.2) log-likelihood confidence regions for $\underline{\theta}$ can be closely approximated by ellipsoids of the form

$$\left\{\underline{\theta} : (\underline{\theta} - \hat{\underline{\theta}})' \ \mathrm{M}(\xi,\tilde{\underline{\theta}}) \ (\underline{\theta} - \hat{\underline{\theta}}) \ \le \text{constant}\right\}.$$

The contents of these ellipsoids will represent regions of equal **'confidence'.** The volume of the above ellipsoids is proportional to $\left\{\det\left(M(\xi,\tilde{\underline{\theta}})\right)\right\}^{-1/2}$, so maximising $\log\det\left[M(\xi,\tilde{\underline{\theta}})\right]$ would be equivalent to minimising the volume of all confidence ellipsoids for $\underline{\theta}$ of the above form. That is, we are making our confidence regions, in some sense, as small as possible. We take ϕ_1 as log det for nice mathematical ease later on. The criterion ϕ_1 is the celebrated **D-optimality,** the most intensively studied of all design criteria, and has by far dominated the literature of optimal designs (See Fedorov (1972) ; Silvey (1980)).

Properties of ϕ_1

a) ϕ_1 is an increasing function of the positive definite symmetric matrices.

That is, for M_1 positive definite symmetric and M_2 positive semi-definite symmetric matrices

$$\phi_1\{M_1 + M_2\} \geq \phi_1\{M_1\}.$$

b) ϕ_1 is a strictly concave function of the positive definite symmetric matrices. That is, for M_1, M_2 positive definite symmetric matrices

$$\phi_1\{\alpha M_1 + (1-\alpha)M_2\} > \alpha\phi_1\{M_1\} + (1-\alpha)\phi_1\{M_2\} \qquad , \; 0 < \alpha < 1$$

c) ϕ_1 remains ' invariant ' under non-singular linear transformations of the design variable x, and thus we can transform to a canonical problem as outlined in section 2.4.

Let $\underline{t} = B\underline{s}$, where first row of B equals e^t , and last row equals $\underline{\theta}^t$, so that $x \to z$ where $\underline{s} = (1, \underline{x}^t)^t$, $\underline{t} = (1, \underline{z}^t)^t$, $t_m = z_{m-1} = \underline{\theta}^t \underline{s}$. Then the expected information matrix in terms of the induced design variable Z is

$$M_z = E\{w(t_m)\, \underline{t}\, \underline{t}^t\}$$

$$= E\{w(\underline{\theta}^t \underline{s}) B\, \underline{s}\, \underline{s}^t B^t\}$$

$$= B\, E\{w(\underline{\theta}^t \underline{s})\, \underline{s}\, \underline{s}^t\} B^t$$

$$= B\, M_x\, B^t \qquad , \text{ say}$$

Thus, criterion ϕ_1 can be written as follows

$$\phi_1 = \log\det M_z = \log[\det B]^2 + \log\det M_x$$

Where $\log[\det B]^2$ is constant for linear transformation. Hence maximizing, $\log\det M_z$ is the same as that of maximizing $\log\det M_x$.

ii) $\phi_2 = -\, \underline{c}' M(\xi, \underline{\theta})^{-1} \underline{c}$

Typically, this criterion deals with the case where the interest of the experimenter is centred upon some linear combination of the unknown parameter $\underline{\theta}$, say $\underline{c}'\underline{\theta}$. Arguments similar to those motivating ϕ_1 confirm that maximising ϕ_2 is proportional to minus the asymptotic variance of $\underline{c}'\hat{\underline{\theta}}$. The criterion ϕ_2 has been termed **c-optimality**, see for instance, Elfving (1952).

<u>Properties of</u> ϕ_2

a) ϕ_2 is an increasing function over the set of positive definite symmetric matrices.

b) ϕ_2 is a concave function over the set of positive definite symmetric matrices.

c) ϕ_2 is ' invariant ' under linear transformations of the design variable x, and thus we can transform to a canonical version of the problem.

For the matrix B as above we have

$$M_z = B\, M_x B^t$$

$$\therefore\; M_x = B^{-1} M_z \left(B^{-1}\right)^t$$

$$\therefore\ M_x^{-1} = B^t M_z^{-1} B$$

Therefore, criterion ϕ_2 can be written as

$$-\underline{c}^t M_x^{-1}\underline{c} = -\underline{c}^t\left[\sum w(\cdot)\underline{s}_i\underline{s}_i^{\ t}\right]^{-1}\underline{c}$$

$$= -\underline{c}^t B^t\left[B^t\right]^{-1}\left[\sum w(\cdot)\underline{s}_i\underline{s}_i^{\ t}\right]^{-1} B^{-1}B\underline{c}$$

$$= -(B\underline{c})^t\left\{w(\cdot)\left[B\underline{s}_i\right]\left[B\underline{s}_i\right]^t\right\}^{-1}(B\underline{c})$$

$$= -\underline{c}_z^t M_z^{-1}\underline{c}_z \quad , \quad \text{with} \quad \underline{c}_z = B\underline{c}.$$

Thus the original c-optimality criterion is transformed to another but with terms depending on the unknown parameters.

2.6 EQUIVALENCE THEOREM

The equivalence of various types of optimality criteria has been investigated and proved by several authors. Define the mean of the response surface by

$$E(y/z^*) = \sqrt{w(z^*)}\,\underline{f}^t(z^*)\underline{\theta}. \tag{2.6.1}$$

And the variance of the estimated response surface by

$$d(z^*,\xi) = Var\left[y(z^*)\right] = w(z^*)\underline{f}^t(z^*)M_z^{-1}\underline{f}(z^*). \tag{2.6.2}$$

Where M_z is equal's to particular design matrix.

Kiefer and Wolfowitz (1960) establish the equivalence of the following three conditions.

i) ξ^* maximizes $|M(\xi,\underline{\theta})|$ $\left[\text{minimizes } |M^{-1}(\xi,\underline{\theta})|\right]$;

ii) ξ^* *minimizes* $\max_{z^* \in Z} d(z^*,\xi)$;

iii) $\max_{z^* \in Z} d(z^*,\xi^*) = m$ [m is the number of unknown parameters in the model].

Thus the theorem establishes a characterisation of D-optimal designs. In particular it is sufficient to verify that the estimated variance $d(z^*,\xi)$ does not exceed m. In this case it is very useful to obtain the following corollary of the theorem.

Corollary (1):

At the support points of the optimal design ξ^* the estimated variance of the response surface $d(z^*,\xi^*)$ takes its maximum value m.

Corollary (1) is particularly useful in that it gives us a test to verify the D-optimality of a design on a given support; namely we must have

$$d(z^*,\xi^*) = m \ , \tag{2.6.3}$$

for all the support points z_i^* of the design.

We note that equality (2.6.3) holds at the support points of the D-optimal design is a necessary condition but is not sufficient. A design measure ξ^* is D-optimal if and only if the inequality

$$d(z^*,\xi^*) \le m, \tag{2.6.4}$$

holds for all $z^* \in Z$.

CHAPTER THREE

LOCALLY D-OPTIMAL DESIGNS

3.1 INTRODUCTION

In this chapter we concentrate on two parameter models and assume that there is interest in estimating both parameters, so that we consider the D-optimal criterion.

3.2 MODEL

Specifically we consider the case

i) $\eta = \eta(\alpha + \beta x)$.

ii) The design variable x is a scalar.

iii) The design space χ is a line segment , say $\chi = [c,d]$.

Hence $$\underline{\theta} = (\alpha, \beta)',$$

and the matrix B of chapter 2 is

$$B = \begin{pmatrix} 1 & 0 \\ \alpha & \beta \end{pmatrix},$$

leading to canonical problem for which

iv) The design variable $z = \alpha + \beta x$.

v) The design space Z is a line segment $Z = [a,b]$.

vi) The expected information matrix is

$$M_z = E\left\{ w(z) \begin{pmatrix} 1 \\ z \end{pmatrix} (1 \quad z) \right\}.$$

We aim to solve this problem for all line segments Z. A two-step approach is used. Firstly we identify or characterise the support points of an optimal design, that is z-values with positive weight. Then we determine these optimal weights. First we consider some results on the calculation of weights.

3.3 SOME RESULTS ON OPTIMAL WEIGHTS

We consider the case of the widest choice of Z for the binary models, namely $Z_w = (-\infty, \infty)$. In the two parameter case a result of caratheodory's theorem is that there exists a D-optimal design with a support of two or three points (Appendix AI.2). When the support consists of two points, the optimal weights are $\frac{1}{2}, \frac{1}{2}$. We show this below. Also in our examples we encounter two symmetric models with symmetric D-optimal designs on $Z_w = (-\infty, \infty)$ supported on three points $(-z, 0, z)$ with weights $(p, 1-2p, p)$, namely the double exponential and the double reciprocal models. The optimal value of p can be determined explicitly. We consider each case in turn.

Firstly, suppose that a design ξ assigns weights p_1, p_2 to two points z_1, z_2 such that $\underline{g}(z_1)$, $\underline{g}(z_2) \in R^2$ are linearly independent. Then the information matrix of this design ,M_z, is given by

$$M = M_z = \left\{ p_1 \underline{g}(z_1) \underline{g}(z_1)' + p_2 \underline{g}(z_2) \underline{g}(z_2)' \right\}$$

$$= \begin{bmatrix} p_1 w(z_1) + p_2 w(z_2) & p_1 z_1 w(z_1) + p_2 z_2 w(z_2) \\ p_1 z_1 w(z_1) + p_2 z_2 w(z_2) & p_1 z_1^2 w(z_1) + p_2 z_2^2 w(z_2) \end{bmatrix} \qquad (3.3.1)$$

The determinant of M is equal to

$$|M| = p_1 p_2 w(z_1) w(z_2) (z_1 - z_2)^2$$

$$= p_1(1-p_1) w(z_1) w(z_2)(z_1 - z_2)^2 \qquad (3.3.2)$$

since $p_1 + p_2 = 1$, which implies that $p_2 = 1 - p_1$.

The determinant above is proportional to the simple function $f(p_1) = p_1(1-p_1)$ of p_1. Thus an elementary one variable optimisation technique shows that (3.3.2) is maximised at $\hat{p}_1 = \hat{p}_2 = \frac{1}{2}$ (which verifies a standard result).

Secondly, consider the case of symmetric three point design $(-z, 0, z)$ with weights $(p, 1-2p, p)$ and p subject to $0 \le p \le \frac{1}{2}$. Then the information matrix for this design is given by

$$M = \left\{ p\underline{g}(-z)\underline{g}(-z)^t + (1-2p)\underline{g}(0)\underline{g}(0)^t + p\underline{g}(z)\underline{g}(z)^t \right\} \qquad (3.3.3)$$

$$= p\begin{bmatrix} w(-z) & 0 \\ 0 & (-z)^2 w(-z) \end{bmatrix} + (1-2p)\begin{bmatrix} w(0) & 0 \\ 0 & 0 \end{bmatrix} + p\begin{bmatrix} w(z) & 0 \\ 0 & z^2 w(z) \end{bmatrix} \qquad (3.3.4)$$

$$= \begin{bmatrix} 2pw(z) + (1-2p)w(0) & 0 \\ 0 & 2pz^2 w(z) \end{bmatrix} \qquad (3.3.5)$$

since for symmetric models w(-z)=w(z). The determinant of M is equal to

$$|M| = \left\{ 2z^2 w(z) \right\} \left\{ 2p^2 w(z) - 2p^2 w(0) + pw(0) \right\}, \qquad (3.3.6)$$

and the criterion ϕ_1 is

$$\phi_1 = \ln\{2z^2 w(z)\} + \ln\{2p^2 w(z) - 2p^2 w(0) + pw(0)\}. \tag{3.3.7}$$

If the optimal p lies strictly within $\left[0, \frac{1}{2}\right]$ it will be a stationary value of ϕ_1.

Hence

$$\frac{\partial \phi_1}{\partial \hat{p}} = 0 \ , \ i.e \ \ 4\hat{p}w(z) - 4\hat{p}w(0) + w(0) = 0. \tag{3.3.8}$$

Which implies that $$\hat{p}\{4[w(0) - w(z)]\} = w(0). \tag{3.3.9}$$

$$\therefore \quad \hat{p} = \frac{w(0)}{4[w(0) - w(z)]}. \tag{3.3.10}$$

Substituting the value of $\hat{p}$ in equation (3.3.6), yields

$$|M| = 2z^2 w(z)\left[-2\{w(0) - w(z)\}\left\{\frac{w(0)}{4[w(0) - w(z)]}\right\}^2 + w(0)\left\{\frac{w(0)}{4[w(0) - w(z)]}\right\}\right] \tag{3.3.11}$$

$$= 2z^2 w(z)\left[\frac{-w(0)^2}{8[w(0) - w(z)]} + \frac{w(0)^2}{4[w(0) - w(z)]}\right] \tag{3.3.12}$$

$$= 2z^2 w(z)\left[\frac{w(0)^2}{8[w(0) - w(z)]}\right]. \tag{3.3.13}$$

If w(0)=1 as is the case for the double exponential and the double reciprocal models, then the determinant of the matrix becomes

$$|M| = \frac{z^2 w(z)}{4[1 - w(z)]}. \tag{3.3.14}$$

Allowing for the possibility that (3.3.10) is outside $\left[0, \frac{1}{2}\right]$ the complete solution is

$$\hat{p} = \min\left\{\frac{1}{2}, \frac{1}{4[1-w(z)]}\right\}. \tag{3.3.15}$$

With $|M|$ given by (3.3.2) or (3.3.14) as appropriate.

We note in conclusion that explicit formulae like these are the exception. Numerical techniques are usually needed to determine optimal weights, if, in a two parameter model, a D-optimal design has three support points.

3.4 GEOMETRIC APPROACH

The set G introduced in section 2.4 is given here by

$$G = G(z) = \left\{\underline{g}(z) = (g_1, g_2)^t : g_1 = \{w(z)\}^{1/2}, g_2 = zg_1, z \in Z = [a,b]\right\}. \tag{3.4.1}$$

A geometrical procedure for potentially identifying the support points of a D-optimal design is available. These are the points of contact between G and the smallest ellipsoid centred on the origin containing G. See Sibson (1972); Silvey and Titterington (1973) ; Silvey (1980) . This is the reason for considering G. It's shape is crucial.

We are primarily interested in the case $w(z) = \dfrac{f^2(z)}{F(z)[1-F(z)]}$. For given w(z) the G corresponding to any Z of interest will be a contiguous section of a trajectory in R^2. Note $\eta = F(z)$, the probability of a response at z, is nondecreasing, $F(-\infty)=0$ and $F(\infty)=1$, and f(z) is the associated density function.

For most choices of f, F the widest choice of Z is $Z_w=(-\infty,\infty)$ and the set G is a closed convex curve beginning and ending at the origin as z ranges from $-\infty$ to ∞.

For the sake of completeness we consider three other weight functions from the literature on weighted linear regression, since their induced G's are also of this form, though their widest choice Z_w can differ from $(-\infty,\infty)$. They also yield explicit solutions, see Fedorov (1972); Karlin and Studden (1966).

Plots of G are similar in all nine binary models (see Table 3.1) and the three weight functions, except that G is asymmetric when F is asymmetric (which includes the skewed logistic distributions and the complementary log-log distribution and $w_1(z)$ ($\alpha\neq\beta$) and $w_2(z)$). Also G is non differentiable at $z=0$ in the symmetric two binary models, namely the double exponential and the double reciprocal. See figures (3.1) to (3.9) for the plots of G for all models mentioned above.

3.5 EXPLICIT SOLUTIONS

We will find explicit formulae for the D-optimal designs for the three following weight functions in turn, namely

i) $w_1(z)=(1-z)^{\alpha+1}(1+z)^{\beta+1}$, $Z\subseteq Z_w=(-1,1)$, $\alpha,\beta>-1$

ii) $w_2(z)=z^{\alpha+1}e^{-z}$, $Z\subseteq Z_w=(0,\infty)$, $\alpha>-1$

iii) $w_3(z)=e^{-z^2}$, $Z\in Z_w=(-\infty,\infty)$

Fedorov (1972), Karlin and Studden (1966) prove that there are only two D-optimal support points on Z_w. Denote these by, say z_1 and z_2. As already shown in section 3.3 the optimal design ξ assigns weights of $\frac{1}{2}$ *and* $\frac{1}{2}$. Thus the determinant of the information matrix M from (3.3.2) is given by

$$|M| = \frac{1}{4} w(z_1) w(z_2)(z_1 - z_2)^2. \tag{3.5.1}$$

The optimal pair (z_1, z_2) must maximise (3.5.1).

A check that these two-point designs are globally D-optimal is provided by the equivalence theorem of section 2.6; namely we must have

$$\underline{g}(z)^t M_z^{-1} \underline{g}(z) \begin{cases} = 2 & for\ z = z_1\ and\ z_2 \\ \leq 2 & for \quad z \in Z \end{cases} \tag{3.5.2}$$

If for an arbitrary $w(\cdot)$ equation (3.5.2) is violated by the best two-point design, then the implication is that three points are needed. We now proceed to determine the values of z_1 and z_2 for $Z = Z_w$ and other choices of Z for both $w_1(z)$ and $w_2(z)$. The problem of identifying the support of optimal designs for $w_3(z)$ will be considered later.

<u>1- a) Case</u> $w(z) = w_1(z)$, $Z = Z_w = (-1,1)$:

The best two-point designs for all α and β are achieved by maximizing the determinant in (3.5.1) with respect to both variables z_1 and z_2; that is maximise

$$\phi_1 = \ln w(z_1) + \ln w(z_2) + 2\ln(z_1 - z_2).$$

Note that neither z_1 nor z_2 can assume the values 1 or -1, since w(-1)=w(1)=0, so z_1 and z_2 are given by first order conditions, namely

$$\frac{\partial \phi_1}{\partial z_1} = \frac{w'(z_1)}{w(z_1)} + \frac{2}{z_1 - z_2} = 0 \qquad (1)$$

$$\frac{\partial \phi_1}{\partial z_2} = \frac{w'(z_2)}{w(z_2)} - \frac{2}{z_1 - z_2} = 0 \qquad (2)$$

Which implies that

$$z_2 = z_1 + \frac{2w(z_1)}{w'(z_1)} \qquad (1)$$

$$z_1 = z_2 + \frac{2w(z_2)}{w'(z_2)} \qquad (2)$$

Equations (1) and (2) simplify to

$$z_2 = \frac{2 + (\beta - \alpha)z_1 - (\alpha + \beta + 4)z_1^2}{(\beta - \alpha) - (\alpha + \beta + 2)z_1} \qquad (1)'$$

$$z_1 = \frac{2 + (\beta - \alpha)z_2 - (\alpha + \beta + 4)z_2^2}{(\beta - \alpha) - (\alpha + \beta + 2)z_2} \qquad (2)'$$

Substituting the value of z_2 in equation $(2)'$, a tedious algebraic manipulation reveals that , as a function of z, equations $(1)'$ *and* $(2)'$ reduce to

$$f(z) = az^4 - 2bz^3 - 4cz^2 + 2dz - e = 0.$$

Where

$$a = (\alpha + \beta + 3)(\alpha + \beta + 4).$$

$b = (\beta - \alpha)(\alpha + \beta + 3)$.

$c = (\alpha\beta + 2\alpha + 2\beta + 4)$.

$d = (\beta - \alpha)(\alpha + \beta + 3)$.

$e = (\alpha^2 + \beta^2 - 2\alpha\beta - \alpha - \beta - 4)$.

Two of the roots are $z = \pm 1$, hence

$$f(z) = (z^2 - 1)(az^2 - 2bz + e) = 0.$$

Therefore, the support points (i.e. the other two roots) of the best two-point designs are given by

$$z = \frac{(\beta - \alpha)(\alpha + \beta + 3) \pm 2\sqrt{(\alpha + 2)(\beta + 2)(\alpha + \beta + 3)}}{(\alpha + \beta + 3)(\alpha + \beta + 4)}. \tag{3.5.3}$$

For example, if we let $\alpha = 1$ and $\beta = 2$ in (3.5.3), then the support of the best two-point design on $Z_w = (-1,1)$ are $\left\{\frac{1 - 2\sqrt{2}}{7}, \frac{1 + 2\sqrt{2}}{7}\right\}$ with optimal weights $\left(\frac{1}{2}, \frac{1}{2}\right)$. These are globally D-optimal because they satisfy the necessary and sufficient condition of the equivalence theorem; that is they satisfy equation (3.5.2). Fedorov (1972), Karlin and Studden (1966) proved this; see figure (3.10). Note if $(\alpha = \beta = \gamma)$, then the weight function $w_1(z)$ is symmetric about the origin, which implies symmetry of the best two-point designs, and equation (3.5.3) simplifies to

$$z = \pm \frac{1}{\sqrt{2\gamma + 3}}. \tag{3.5.4}$$

For instance, if we let $\gamma = 3$ in equation (3.5.4), then the support of the best two-point design on $Z_w = (-1,1)$ are $\left\{\frac{-1}{3}, \frac{1}{3}\right\}$ with optimal weights $\left(\frac{1}{2}, \frac{1}{2}\right)$. These symmetric best two-points design are globally D-optimal as well for the same reason, namely they satisfy equation (3.5.2), see figure (3.11).

1-b) Case $w(z) = w_2(z)$, $Z = Z_w = (0,\infty)$:

In the case of $w_2(z)$, let

$$u = z - z_{\max} \qquad , \quad u \geq -(\alpha+1)$$

where $z_{\max} = (\alpha+1)$ is the value of z which maximizes $w_2(z)$. Then

$$w(u) = [u + (\alpha+1)]^{\alpha+1} e^{-[u+(\alpha+1)]} \qquad , \qquad \text{(i.e. w(u) maximized at u=0).}$$

Now, the best two-point designs for all α, can be determined by maximizing the criterion function ϕ_1 for both variables u_1 and u_2, where

$$\phi_1 = 2\ln(u_2 - u_1) + (\alpha+1)\ln[u_1 + (\alpha+1)] + (\alpha+1)\ln[u_2 + (\alpha+1)] - (u_1 + u_2).$$

Again u_1 and u_2 must be internal to U_w and are given by

$$\frac{\partial \phi_1}{\partial u_1} = \frac{(\alpha+1)}{u_1 + (\alpha+1)} - \frac{2}{u_2 - u_1} - 1 = 0 \qquad (1)$$

$$\frac{\partial \phi_1}{u_2} = \frac{(\alpha+1)}{u_2 + (\alpha+1)} + \frac{2}{u_2 - u_1} - 1 = 0 \qquad (2)$$

Equations (1) and (2) simplify to

$$u_2 = \frac{u_1^2 - 2u_1 - 2(\alpha+1)}{u_1} \qquad (1)'$$

$$u_1 = \frac{u_2^2 - 2u_2 - 2(\alpha+1)}{u_2} \qquad (2)'$$

Substituting the value of u_2 in equation $(2)'$, a little algebraic manipulation reveals that, as a function of u, equations $(1)'$ and $(2)'$ reduce to

$$f(u) = u^3 + u^2(\alpha-1) - 3u(\alpha+1) - (\alpha+1)^2 = 0.$$

One root of the equation is $u = -(\alpha+1)$, hence

$$f(u) = [u + (\alpha+1)][u^2 - 2u - (\alpha+1)] = 0.$$

Therefore, the support points (i.e. the other two roots) of the best two-point design are given by

$$u = 1 \pm \sqrt{(\alpha+2)} \qquad , \quad \alpha > -1$$

Transforming back to the variable z, we get

$$z = (\alpha+2) \pm \sqrt{(\alpha+2)}. \qquad (3.5.5)$$

For instance, if we let $\alpha = 2$ in equation (3.5.5), the resulting support is $\{2,6\}$ with optimal weight $\left(\frac{1}{2},\frac{1}{2}\right)$. Again the necessary and sufficient condition of the equivalence theorem in equation (3.5.2) is satisfied on $Z_w = (0,\infty)$ by this design. Thus it is globally D-optimal; see figure (3.12).

2) Arbitrary Z:

It is also of interest to find D-optimal designs on arbitrary intervals Z=[d,c] for any particular weight function $w(\cdot)$. If Z contains the support points of the optimal design onZ_w then that design is still optimal. Otherwise inspection of the plot of G suggests that the optimal support consists of two points at least one of which is an end point of Z. Assuming that is c, the other point, say z, can be identified by maximizing the determinant, namely

$$|M| = (z-c)^2 \, w(\cdot), \tag{3.5.6}$$

over Z. This follows easily from (3.5.1). We can now cover two cases simultaneously; namely Z=[d,c] and Z=[c,e] ,d<c<e.

Assuming the conjecture to be true, supports of D-optimal designs on these sets are respectively $\{\ell,c\}$ and {c,u} where ℓ denotes the value of z which maximizes the determinant over Z=[d,c], and u denotes the value of z which maximizes the determinant over Z=[c,e]. Note the solutions on Z=[d,c] and on Z=[c,e] may be internal to Z=[d,c] or to Z=[c,e] or may be z=d or z=e.

Such designs do appear to be D-optimal designs. Plots suggest that the equivalence theorem is satisfied. We proceed to determine the values of ℓ and u for both weight functions $w_1(z)$ and $w_2(z)$.

2-a) case $w(z) = w_1(z)$, $Z = [-1,c]$ and $Z = [c,1]$:

For the weight function $w_1(z)$ the criterion function ϕ_1 from (3.5.6) is

$$\phi_1 = 2\ln(z-c) + (\alpha+1)\ln(1-z) + (\beta+1)\ln(1+z).$$

Since -1 and 1 can't ever be support points, ℓ and u must satisfy first order conditions and are given by the roots of the following equation

$$f(z) = z^2(\alpha + \beta + 4) - z(\beta - \alpha + \alpha c + \beta c + 2c) - (\alpha c - \beta c + 2) = 0.$$

Thus

$$z = \frac{(\beta - \alpha + \alpha c + \beta c + 2c) \pm \sqrt{(\beta - \alpha + \alpha c + \beta c + 2c)^2 + 4(\alpha + \beta + 4)(\alpha c - \beta c + 2)}}{2(\alpha + \beta + 4)} \quad (3.5.7)$$

In particular, if $c = z_{\max}$ where $z_{\max}$ is the value of z which maximizes the weight function $w_1(z)$, namely

$$z_{\max} = \frac{(\beta - \alpha)}{(\alpha + \beta + 2)}, \quad (3.5.8)$$

then the support on $Z = [-1, z_{\max}]$ and on $Z = [-1, z_{\max}]$ can be identified by setting $c = z_{\max}$ in equation (3.5.7) to get

$$z = \frac{(\beta - \alpha) \pm 2\sqrt{\dfrac{(3\alpha + 3\beta + 2\alpha\beta + 4)}{(\alpha + \beta + 2)}}}{(\alpha + \beta + 4)}. \quad (3.5.9)$$

Note that if $(\alpha = \beta = \gamma)$, then $z_{\max} = 0$, and the support on Z=[-1,0] and on Z=[0,1] can be determined from equation (3.5.7) by setting c=0 to get

$$z = \pm \frac{1}{\sqrt{\gamma + 2}}. \quad (3.5.10)$$

For instance, if we let $\gamma = 2$, then the conjectured optimal support on Z=[- 1,0]

is $\left\{-\frac{1}{2},0\right\}$ and on Z=[0,1] is $\left\{0,\frac{1}{2}\right\}$ with optimal weights $\left\{\frac{1}{2},\frac{1}{2}\right\}$. These two designs satisfy the necessary and sufficient condition of the equivalence theorem. Thus they are globally D-optimal , see figure (3.13) and (3.14).

2-b) case $w(z)=w_2(z)$, $Z=[0,c]$ and $Z=[c,\infty)$:

For the weight function $w_2(z)$ the criterion function ϕ_1 from (3.5.6) is given by

$$\phi_1 = 2\ln(z-c)+(\alpha+1)\ln z - z \quad .$$

Again for the above choices of z, ℓ and u must satisfy first order conditions. An elementary one variable optimisation technique for z shows that the values of ℓ and u are the solutions of the following equation, namely

$$f(z)=z^2-z(\alpha+3+c)+c(\alpha+1)=0 .$$

Thus

$$z=\frac{(\alpha+3+c)\pm\sqrt{(\alpha+3+c)^2-4c(\alpha+1)}}{2} \quad . \tag{3.5.11}$$

In particular, if $c=z_{\max}$ where $z_{\max}$ is the value of z which maximises the weight function $w_2(z)$, that is

$$z_{\max}=(\alpha+1), \tag{3.5.12}$$

then the support on $Z=[0,z_{\max}]$ and on $Z=[z_{\max},\infty)$ can be identified by setting $c=z_{\max}$ in equation (3.5.11) to get

$$z=(\alpha+2)\pm\sqrt{(2\alpha+3)} \quad , \quad \alpha>-1 \tag{3.5.13}$$

For example, if we let $\alpha = 3$, then $z_{\max} = 4$ and the support on Z=[0,4] is {2,4} and on $Z = [4,\infty)$ is {4,8} with optimal weights $\left(\frac{1}{2},\frac{1}{2}\right)$.

3) case $w(z) = w_3(z)$, $Z = Z_w = (-\infty,\infty)$, $Z = (-\infty,c]$, $Z = [c,\infty)$:

Fedorov (1972), Karlin and Studden (1966) show that the D-optimal design on $Z_w = (-\infty,\infty)$ has two supports which must be say $\pm z^*$ since $w_3(z)$ is symmetric about zero. In fact in view of (3.5.1) z^* solves the following problem for d=0, k=1; namely for fixed d, k

$$\max_{z \in Z} \ (z-d)^k w_3(z). \tag{3.5.14}$$

Suppose that $Z = (-\infty,c]$ or $Z = [c,\infty)$ excludes at least one of the support points of this latter design. Then inspection of G suggests that their respective D-optimal design have two support points one of which is c. The other say z^* solves (3.5.14) for d=c, k=2. That is, the two supports are $\{\ell,c\}$ and {c,u} where ℓ, u are 'lower' and 'upper' solutions to (3.5.14); they maximize (3.5.14) over $Z = (-\infty,c]$ and over $Z = [c,\infty)$ respectively. The values of ℓ and u must be internal to their respective Z's , since $w(-\infty) = w(\infty) = 0$. Thus they satisfy first order conditions. Hence

$$f(z) = 2z^2 - 2dz - k = 0.$$

$$z^* = \frac{d \pm \sqrt{d^2 + 2k}}{2}. \tag{3.5.15}$$

In particular, if we set d=0, k=1 in equation (3.5.15), then the support of the best two-point design on the widest choice $Z_w = (-\infty,\infty)$ is $\left\{\frac{-1}{\sqrt{2}},\frac{1}{\sqrt{2}}\right\}$ with optimal weight $\left(\frac{1}{2},\frac{1}{2}\right)$.The necessary and sufficient condition of the equivalence theorem as stated earlier is satisfied by this best symmetric two point design. Thus it is globally D-optimal, see figure (3.15).

Taking d=0, k=2 in (3.5.15) suggest a support on $Z=(-\infty,0]$ of $\{-1,0\}$ and a support on $Z=[0,\infty)$ of $\{0,1\}$ with optimal weights $\left(\frac{1}{2},\frac{1}{2}\right)$. Since these designs satisfy equation (3.5.2) as well, they are D-optimal designs, see figure (3.16).

3.6 BINARY MODELS SOME NUMERICAL RESULTS

3.6.1: Consider the problem of finding the support points of the D-optimal designs for the binary response models, with weight functions of the form $w(z) = \frac{f^2(z)}{F(z)[1-F(z)]}$. In general when $Z_w = (-\infty,\infty)$, i.e. the widest choice of Z, it is not possible to identify support points for a given F from visual inspection of G and the smallest ellipsoid containing it.

To find the best two-point design we must maximise the determinant in (3.5.1) with respect to both variables z_1 and z_2. This exercise simplifies when F is symmetric, that is F(-z)=1-F(z), which in turn guarantees symmetry of $w(\cdot)$ and symmetry of D-optimal designs about the origin. Thus $z_1 = -z_2$, $z_2 > 0$, and z_2 must, from (3.5.1) , maximise $z^2 w(z)^2$ over $Z = (0,\infty)$.

We list the z_1 and z_2 values of the nine choices of F in Table (3.1) as reported by Ford, Torsney, and Wu (1992). For seven of them the necessary and sufficient condition of the equivalence theorem in (3.5.2) is satisfied and therefore the D-optimal two-point designs are globally D-optimal. However for the double exponential and the double reciprocal models, (3.5.2) is violated.

The global D-optimal design on $Z_w = (-\infty,\infty)$ for both these symmetric models, namely the double exponential and the double reciprocal, must be symmetric about the origin by the same arguments mentioned above. So if it is a three-point design, its support must be of the form $\{-z^*, 0, z^*\}$ with optimal weights $(\hat{p}, 1-2\hat{p}, \hat{p})$. z^* and $\hat{p}$ must maximize the determinant of the information matrix. In fact the optimal weight $\hat{p}$ can be determined explicitly for given z^* from equation (3.3.10), and z^* must maximize the determinant of equation (3.3.14).

We now list the support points and the optimal weights for both models in Table (3.2).

Table (3.2); Global D-optimal designs on $Z_w = (-\infty, \infty)$.

Model	***Support points***	***Optimal Weights***
1) Double Exponential.	(-1.5936,0,1.5936)	(0.2819,0.4362,0.2819)
2) Double Reciprocal.	$(-\sqrt{2}, 0, \sqrt{2})$	(0.2617,0.4766,0.2617)

In both models the necessary and sufficient condition of the equivalence theorem (see section 2.6), namely equation (3.5.2) is satisfied and therefore these designs are globally D-optimal, see figures (3.17) and (3.18).

3.6.2 :

In this section the support points of the D-optimal designs on symmetric intervals $Z_k = [-k, k]\ \forall$k, for four symmetric binary models, and the weight functions $w_1(z)$ $(with\ \alpha = \beta)$ and $w_3(z)$ of section 3.5, will be determined and characterized.

For the logistic and the probit models and the weight functions $w_1(z)$ and $w_3(z)$, denote the global support points by $\pm z^*$ $(z^* > 0)$ (See Table 3.1 and equation 3.5.15 with d=0 , k=1). Then for $k \le z^*$, the D-optimal designs are supported on {-k,k} with equal optimal weights $\left(\frac{1}{2}, \frac{1}{2}\right)$, and for k > z*, the D-optimal design is that for Z_w.

For the double exponential and the double reciprocal, when $Z_k = [-k,k]$ in general, there exists a critical value k^* such that $\forall k \leq k^*$, the D-optimal designs are supported on {-k,k} with equal optimal weights $\left(\frac{1}{2},\frac{1}{2}\right)$. The value of k^* can be determined by solving the equation

$$\frac{1}{4[1-w(k^*)]} = \frac{1}{2}. \tag{3.6.1}$$

For $k^* < k < z^*$, the D-optimal designs are three-point designs supported on {-k,0,k} with optimal weights $(p^*, 1-2p^*, p^*)$, where the optimal value of p^* can be obtained for given k from

$$p^* = \frac{1}{4[1-w(k)]}. \tag{3.6.2}$$

For $k > k^*$, the optimal design is that for Z_w.

We now record the values of k^* for both models.

1) For the double exponential model the exact value of k^* is determined by solving equation (3.6.1) algebraically, to get

$$k^* = -\ln(2/3).$$

2) For the double reciprocal model a numerical value for k^* is $k^* = 0.1974$.

3.6.3 :

Now consider the two cases $Z = (-\infty, c]$ and $Z = [c, \infty)$. Reiterating the arguments of section 3.5, if these contain global supports then that design is still optimal. Otherwise inspection of the graphs of G of our nine distributions suggests, with some possible restrictions on c in the case of the double exponential and the double reciprocal models, that for both choices of Z the optimal support consists of two-points one of which is c. Thus the respective conjectured supports are $\{\ell,c\}$ and {u,c} where as in section 3.5 ℓ and u maximise the determinant

$$|M| = (z-c)^2\ w(\cdot),$$

over $Z = (-\infty,c]$ and over $Z = [c,\infty)$ respectively.

For the binary weight functions $w(z) = \dfrac{f^2(z)}{F(z)[1-F(z)]}$, ℓ and u must be calculated numerically. We tabulate such values of ℓ and u.

Table (3.3) gives values of ℓ and u for the asymmetric complementary log-log distribution for c ranging from -1.3 to 0.9, which are approximately the two global support points; see Table (3.1).

Table (3.4) gives the value $z_{\max}$ and ℓ , u for $c = z_{\max}$ for nine choices of the weight function w(z), where $z_{\max}$ is the value of z which maximises w(z). The first four are symmetric, so that $z_{\max} = 0$ and $\ell = $ -u .

3.6.4 :

Consider the problem of finding D-optimal designs for general Z=[a,b]. For the seven choices of the distribution function F in Table (3.1), excluding the double exponential and the double reciprocal distributions, and for the three weight functions considered in section 3.5 the D-optimal designs (appear to) have two support points which are categorised by a common form of solution.

Denote the support points of the best two-point design on the widest choice of Z, i.e. Z_w, by a^* and b^* and on Z by z_1, z_2, where $a^* < b^*$, $z_1 < z_2$.

1) case $b \geq b^*$ *and* $a \leq a^*$:

If the two-point design on a^* and b^* is D-optimal for $Z_w = (-\infty,\infty)$, then it is D-optimal for Z=[a,b]. Otherwise, it is only guaranteed to be D-optimal among two-point designs. We conclude that this design is globally D-optimal for seven of the nine choices of F in Table (3.1), and the three weight functions studied in section 3.5, see Ford, Torsney, and Wu (1992).

2) Case $Z = [-b,b]$, $b \leq b^*$:

For a symmetric distribution function F, if the function w(z)z is non decreasing over Z=[0,b], then $z_1 = -b$ and $z_2 = b$. This follows from the discussion of D-optimal designs in section (3.6.1). The first two symmetric distributions in Table (3.1), and in addition the symmetric weight functions of section 3.5, namely $w_1(z)$ [*for* $\alpha = \beta$], $w_3(z)$ satisfy this condition on w(z).

3) Case $b \leq b^*$:

If the function $w(z)(z-\ell_1)^2$ is non-decreasing in z over $Z = [\ell_1, b]$ for any $\ell_1 \geq a$, then $z_2 = b$ and $z_1 = z_b(a)$, where $z_b(a) = \max\{a, \ell(b)\}$, $\ell(b)$ being the value which maximises $w(z)(z-b)^2$ over Z=[a,b]. For any F such that w(z) is log concave and differentiable over $Z = [a^*, b^*]$, $w(z)(z-\ell_1)^2$ is non-decreasing over $Z = [\ell_1, b^*]$ for any $\ell_1 \geq a^*$. Wu (1988) shows such log concavity in respect of the logistic and skewed logistic distributions and the complementary log-log distribution. The property is also enjoyed by the three weight functions of section 3.5.

4) Case $a \geq a^*$:

If the function $w(z)(z-u_2)^2$ is non-increasing in z over $Z=[a,u_2]$ for any $u_2 \leq b$, then $z_1 = a$ and $z_2 = z_a(b)$, where $z_a(b) = \min\{b,u(a)\}$, $u(a)$ being the value which maximises $w(z)(z-a)^2$ over Z=[a,b]. It can be shown that for the examples cited in case 3, $w(z)(z-u_2)^2$ is non-increasing over $Z=[a^*,u_2]$ for any $u_2 \leq b^*$.

5) case $a \geq a^*$, $b \leq b^*$:

If w(z) is log-concave and differentiable over $Z=[a^*,b^*]$, then $z_1 = a$ and $z_2 = b$. This follows from combining the results in cases (3) and (4) above.

We summarise the above statements in Table (3.5). The values z_1, z_2 are only guaranteed to be D-optimal among two-point designs on the appropriate Z. However extensive numerical and empirical results show that for all w(z) considered except those corresponding to the double exponential and the double reciprocal models these best two point designs satisfy the necessary and sufficient condition of the equivalence theorem. Thus they are globally D-optimal. See figures (3.19) and (3.20).

3.7 DEXP AND DREC MODELS

This section will be devoted to the problem of finding D-optimal designs for an arbitrary interval Z=[a,b], for two symmetric binary models, namely the double exponential and the double reciprocal. In some cases the designs have three support points. However in a two parameter context an explicit solution is available for the weights given three support points. We now derive this.

So, suppose that a design ξ assigns weights p_1, p_2, p_3 to three points z_1, z_2, z_3 such that any two of $\underline{g}(z_1), \underline{g}(z_2), \underline{g}(z_3) \in R^2$ are linearly independent of each other. Then the information matrix of this design is given by

$$M = \left\{ p_1 \underline{g}(z_1)\underline{g}(z_1)^t + p_2 \underline{g}(z_2)\underline{g}(z_2)^t + p_3 \underline{g}(z_3)\underline{g}(z_3)^t \right\}$$

$$= \sum_{i=1}^{3} p_i \, \underline{v_i} \, \underline{v_i^t} \quad , \; \underline{v_i} = \underline{g_i} \; . \tag{3.7.1}$$

Let $V_{ij} = (\underline{v_i} \vdots \underline{v_j})$, so that V_{ij} is a 2×2 matrix, and denote its determinant by $D_{ij} = |V_{ij}|$. Then the determinant of M is given by

$$\varphi = |M| = p_1 p_2 D_{12}^2 + p_1 p_3 D_{13}^2 + p_2 p_3 D_{23}^2 \; , \tag{3.7.2}$$

where

$$D_{12}^2 = w(z_1) w(z_2) (z_1 - z_2)^2,$$

$$D_{13}^2 = w(z_1) w(z_3) (z_1 - z_3)^2,$$

$$D_{23}^2 = w(z_2) w(z_3) (z_2 - z_3)^2.$$

To find the optimal weights we must maximise (3.7.2) with respect to the variables p_1, p_2, p_3 subject to $\sum p_j = 1$. First order conditions are

$$\frac{\partial\varphi}{\partial p_j} = \sum p_i \frac{\partial\varphi}{\partial p_i} = 2\varphi\ , \tag{3.7.3}$$

which yield three linear equations in p_1, p_2, p_3. Solving this linear system by the well established elimination method gives the optimal value of p_i as

$$\hat{p}_i = \frac{D_i}{\sum_{j=1}^{3} D_j}\ , \tag{3.7.4}$$

where

$$D_1 = D_{23}^2 (D_{12}^2 + D_{13}^2 - D_{23}^2),$$

$$D_2 = D_{13}^2 (D_{12}^2 + D_{23}^2 - D_{13}^2),$$

$$D_3 = D_{12}^2 (D_{13}^2 + D_{23}^2 - D_{12}^2).$$

Substituting the optimal value of $\hat{p}_i$ in equation (3.7.2), we get

$$\varphi = |M| = \frac{D_{12}^2 D_{13}^2 D_{23}^2}{\sum_{i=1}^{3} D_i}. \tag{3.7.5}$$

Consider the case when the interval Z=[a,b] does not contain zero. In this case we believe that the D-optimal designs have two support points at least one of which is an end point of Z (a if a > 0 , b if b < 0). That is

$$Supp(p^*) = \begin{Bmatrix} \{a, \min\} \ , \ a > 0 \\ \{\max, b\} \ , \ b < 0 \end{Bmatrix},$$

where $\min = \min\{b, b^*(a)\}, b^*(a)$ being the value which maximises $w(z)(z-a)^2$ over $Z = [a, \infty)$ for any a > 0, and $\max = \max\{a, a^*(b)\}, a^*(b)$ being the value which maximises $w(z)(z-b)^2$ over $Z = (-\infty, b]$ for any b < 0.

In particular, if $Z = [0, \infty)$ then the D-optimal design is a two-point design supported on $\{0, u_1\}$ with optimal equal weights $\left(\frac{1}{2}, \frac{1}{2}\right)$ where u_1 must, from (3.5.1), maximise $z^2 w(z)$ over $Z = [0, \infty)$. By symmetry $\{-u_1, 0\}$ are the support points of the D-optimal design on $Z = (-\infty, 0]$.

We now consider the case when the interval Z=[a,b] contains zero , i.e. a < 0 and b > 0. In this case the D-optimal designs are supported on either two points with optimal equal weights $\left(\frac{1}{2}, \frac{1}{2}\right)$ or three-points with optimal weights given by equation (3.7.4). These designs are categorised by a general form of solution. Define the following terms

i) Let $-u_1$ denote the negative support point of the global D-optimal design on $Z = (-\infty, 0]$. Thus $-u_1 = -1.841$ for the double exponential distribution and $-u_1 = -1.618$ for the double reciprocal distribution.

ii) Let $-u_2$ denote the negative support point of the global D-optimal design on the widest choice of Z , i.e. $Z_w = (-\infty, \infty)$. Thus $-u_2 = -1.5936$ for the double exponential distribution and $-u_2 = -\sqrt{2}$ for the double reciprocal distribution.

iii) Let $-u_3$ be the smallest value of a^* such that the D-optimal design on the set $\{a^*,0\}$ is optimal on $Z=[a^*,0]$ but it is not optimal on $Z=[a^*,y]$ for any positive y. (We note that $-u_3$ is obtained by solving the equation $F'(0)=0$) and that the function F denotes the variance function. Thus $-u_3=-1$ for the double exponential distribution and $-u_3=-0.5$ for the double reciprocal distribution.

iv) Let $-u_4$ denote the critical value of $-k$ at which the D-optimal design on $Z_k=[-k,k]\ \forall\ k$ changes from a 3-point to a 2-point design (see section 3.6.2). Thus $-u_4=-0.4055$ for the double exponential distribution and $-u_4=-0.1974$ for the double reciprocal distribution.

v) Consider the D-optimal design on $Z=(-\infty,0]$ with support points $\{-u_1,0\}$ (see(i)). Let $\tilde{z}(u_1)$ be the smallest positive value of z such that $F[z]=2$. Thus $\tilde{z}(u_1)=0.3528$ for the double exponential distribution and $\tilde{z}(u_1)=0.5062$ for the double reciprocal distribution.

1) Case $a<-u_2$ *and* $b>u_2$:

Obviously, from section 3.6.1, the D-optimal design for both models in this case is that for Z_w. So it is a three-point design supported on

$$Supp(p^*)=\{-u_2,0,u_2\},$$

with optimal weights $(\hat{p},1-2\hat{p},\hat{p})$, see Table (3.2).

We now assume $b<u_2$ and $b\le|a|$, then

2) Case $a<-u_1$:

Here the support points of the D-optimal design are classified as follows

$$Supp(p^*) = \begin{Bmatrix} \{-u_1, 0\} & , \ b < \tilde{z}(u_1) \\ \{a^*(b), 0, b\} & , \ \tilde{z}(u_1) < b < u_2 \end{Bmatrix},$$

where $a^*(b)$ is the value of a^* which maximises the determinant of M, where M is the design matrix under the design $\{a^*, 0, b\}$ with optimal weights given by equation (3.7.4). We note that always $a^*(b) > u_1$ as empirical results suggest.

3) Case $-u_1 < a < -u_2$:

The support points of the D-optimal design in this case are either two points or three points classified as follows

$$Supp(p^*) = \begin{Bmatrix} \{a, 0\} & , \ b < \tilde{z}(a) \\ \{a, 0, b\} & , \ \tilde{z}(a) < b < \tilde{z}(u_1) \\ \{\max, 0, b\} & , \ \tilde{z}(u_1) < b < u_2 \end{Bmatrix},$$

where

(i) $\max = \max\{a, a^*(b)\}, a^*(b)$ being the value of a^* which maximises the determinant of M, where$M$ is as in case 2.

(ii) and $\tilde{z}(a)$ is the value of z such that $F[z] = 2$ under the design on $\{a, 0\}$.

4) Case $-u_2 < a < -u_3$:

The support points of the D-optimal design in this case are classified as follows

$$Supp(p^*) = \begin{Bmatrix} \{a, 0\} & , \ b < \tilde{z}(a) \\ \{a, 0, b\} & , \ \tilde{z}(a) < b < |a| \end{Bmatrix},$$

where $\tilde{z}(a)$ is as in case (3) above.

<u>***5) Case***</u> $-u_3 < a < -u_4$:

The support points of the D-optimal designs in this case are classified as follows

$$Supp(p^*) = \begin{cases} \{a,b\} & , \quad b < z^+(a) \\ \{a,0,b\} & , \quad z^+(a) < b < |a| \end{cases},$$

where $z^+(a)$ is the (unique) value of b such that $F(0) = 2$ under the D-optimal design on the set {a,b}.

<u>***6) Case***</u> $a > -u_4$:

Finally, the D-optimal designs in this case are supported on two points. Namely

$$Supp(p^*) = \{a, b\} \text{ , } b < |a|$$

Table (3.1); Supports z_1, z_2 of two-point D-optimal designs on $Z_w = (-\infty, \infty)$. (Note s=sign(z)).

Name	$f_i(z)$	$F_i(z)$	z_1	z_2
1) Logit	$e^{-z}(1+e^{-z})^{-2}$	$(1+e^{-z})^{-1}$	-1.543	1.543
2) Probit	$\frac{1}{\sqrt{2\pi}} e^{(-z^2/2)}$	$\Phi(z)$	-1.138	1.138
3) Double Exponential	$\frac{1}{2} e^{-\lvert z\rvert}$	$\frac{(1+s)}{2} - \frac{s}{2} e^{-\lvert z\rvert}$	-0.768	0.768
4) Double Reciprocal	$\frac{1}{2}(1+\lvert z\rvert)^{-2}$	$\frac{(1+s)}{2} - \frac{s}{2}(1+\lvert z\rvert)^{-1}$	-0.390	0.390
5) Complementary Log-Log	$Exp(z-e^z)$	$1-Exp(-e^z)$	-1.338	0.980
6-9) Skewed Logit	$m[F_1(z)]^{m-1} f_1(z)$	$(1+e^{-z})^{-m}$	-------	-------
6) $m=1/3$	...	...	-4.409	0.552
7) $m=2/3$	...	...	-2.284	1.191
8) $m=3/2$	...	...	-0.939	1.898
9) $m=3$	...	...	-0.060	2.525

Table (3.3); Supports of two-point D-optimal designs for the asymmetric complementary log-log model on $Z=(-\infty,c]$ $(\{\ell,c\})$ and on $Z=[c,\infty)$ $(\{c,u\})$.

The value of c	*The value of ℓ*	*The value of u*	*The value of c*	*The value of ℓ*	*The value of u*
-1.3	-3.337	0.985	-0.1	-2.127	1.222
-1.2	-3.240	0.999	0.0	-2.129	1.250
-1.1	-3.144	1.015	0.1	-2.042	1.279
-1.0	-3.049	1.031	0.2	-1.956	1.310
-0.9	-2.954	1.048	0.3	-1.871	1.343
-0.8	-2.860	1.066	0.4	-1.788	1.378
-0.7	-2.766	1.085	0.5	-1.706	1.415
-0.6	-2.672	1.105	0.6	-1.626	1.454
-0.5	-2.580	1.126	0.7	-1.548	1.496
-0.4	-2.488	1.148	0.8	-1.471	1.539
-0.3	-2.397	1.171	0.9	-1.396	1.585
-0.2	-2.307	1.196	------	------	------

Table (3.4); Supports of two-point D-optimal designs on $Z=(-\infty, z_{\max}]\left(\{\ell, z_{\max}\}\right)$ and on $Z=[z_{\max}, \infty)\left(\{z_{\max}, u\}\right)$. (Note s=sign(z)).

Name	$f_i(z)$	$F_i(z)$	$z_{\max}$	ℓ	u
1) logit	$e^{-z}(1+e^{-z})^{-2}$	$(1+e^{-z})^{-1}$	0.0	-2.399	2.399
2) Probit	$\frac{1}{\sqrt{2\pi}}\, e^{(-z^2/2)}$	$\Phi(z)$	0.0	-1.575	1.575
3) Double Exponential	$\frac{1}{2}\, e^{-\lvert z\rvert}$	$\frac{(1+s)}{2}-\frac{s}{2}\, e^{-\lvert z\rvert}$	0.0	-1.841	1.841
4) Double Reciprocal	$\frac{1}{2}\,(1+\lvert z\rvert)^{-2}$	$\frac{(1+s)}{2}-\frac{s}{2}\,(1+\lvert z\rvert)^{-1}$	0.0	-1.618	1.618
5)Complementary Log-Log	$Exp(z-e^z)$	$1-Exp(-e^z)$	0.466	-1.734	1.402
6-9) Skewed Logit	$m[F_1(z)]^{m-1}f_1(z)$	$(1+e^{-z})^{-m}$	------	------	------
6) $m=1/3$	• • •	• • •	-0.519	-5.736	1.983
7) $m=2/3$	• • •	• • •	-0.228	-3.305	2.212
8) $m=3/2$	• • •	• • •	0.269	-1.671	2.628
9) $m=3$	• • •	• • •	0.807	-0.653	3.105

Table (3.5); Supports of two-point D-optimal designs on a general Z=[a,b].

$Z=[a,b]$	z_1	z_2
1) $a \le a^*$, $b \ge b^*$	a^*	b^*
2) $a = -b$, $b \le b^*$	$-b$	b
3) $a > -\infty$, $b \le b^*$	$z_b(a) = \max\{a, \ell(b)\}$	b
4) $a \ge a^*$, $b < \infty$	a	$z_a(b) = \min\{b, u(a)\}$
5) $a \ge a^*$, $b \le b^*$	a	b

Notes on Table (3.5) :

i) The designs with a support consisting of the two points z_1 and z_2 (and equal weights of 1/2) are only guaranteed to be D-optimal among two-point designs in cases 1 to 5. However they are globally D-optimal in case 1 for seven of the nine choices of F in Table (3.1) and the three weight functions considered in section 3.5.

ii) a^* , b^* are such that $z_1 = a^*$, $z_2 = b^*$ when $Z_w = (-\infty, \infty)$; see Table (3.1).

iii) $\ell(b)$ maximises $w(z)(z-b)^2$ over Z=[a,b] and $u(a)$ maximises $w(z)(z-a)^2$ over Z=[a,b].

Figure (3.1)

Plot of the set $G=\{(g_1,g_2)':g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\}$, for the symmetric logistic distribution.

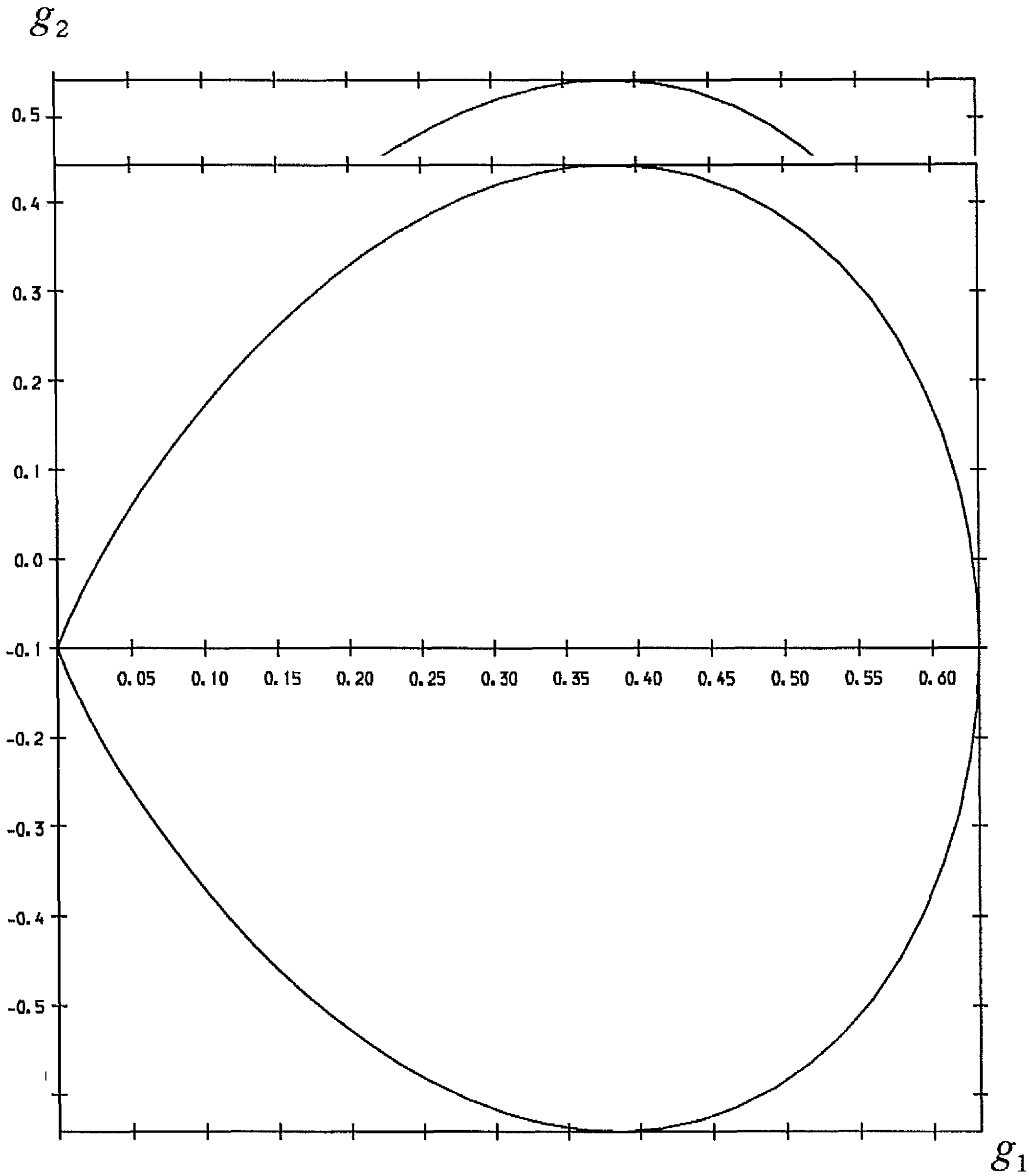


Figure (3.2)

Plot of the set $G=\{(g_1,g_2)^t : g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\}$, for the symmetric probit distribution.

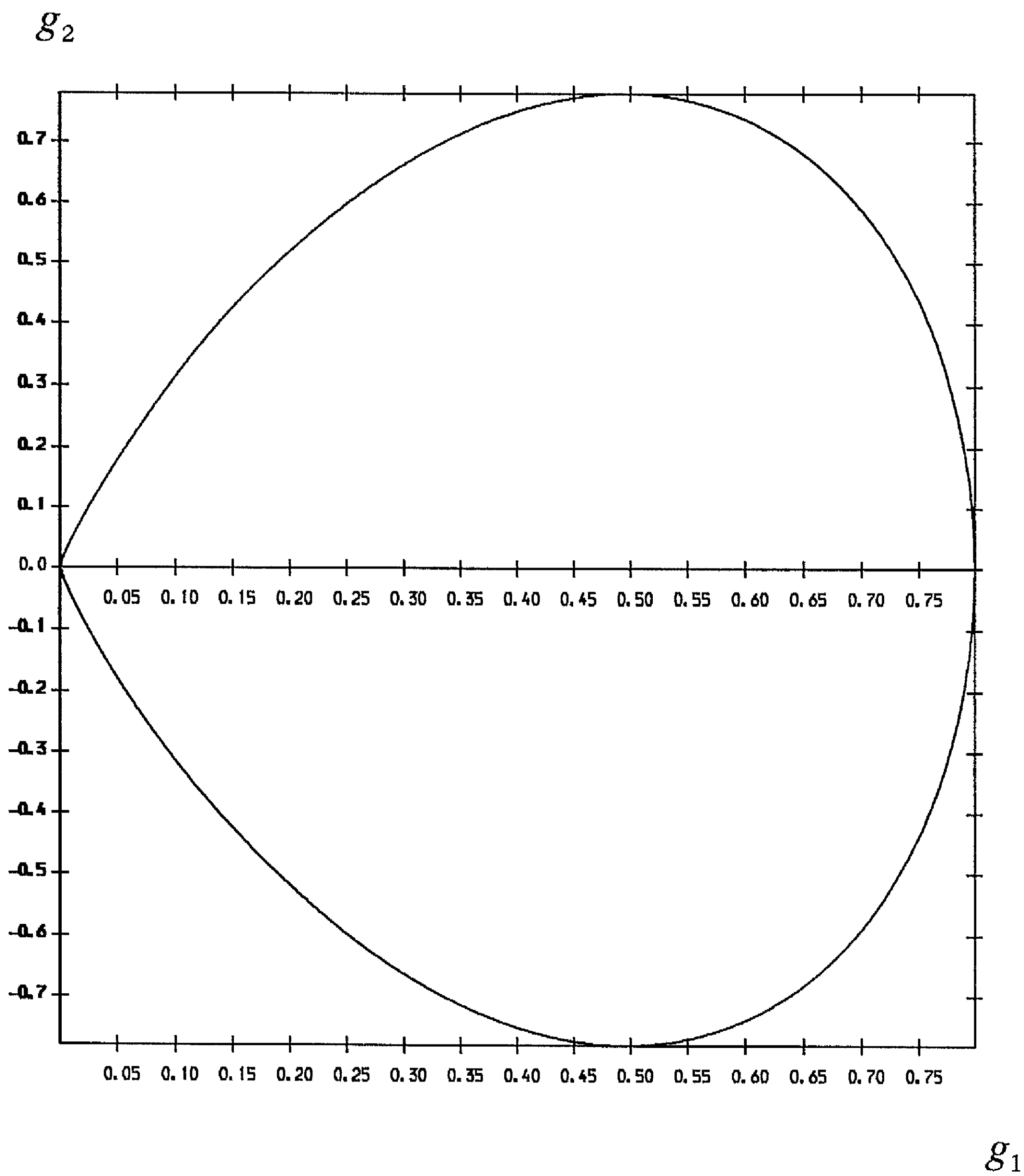


Figure (3.3)

Plot of the set $G=\left\{(g_1,g_2)^t : g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\right\}$, for the symmetric double exponential distribution.

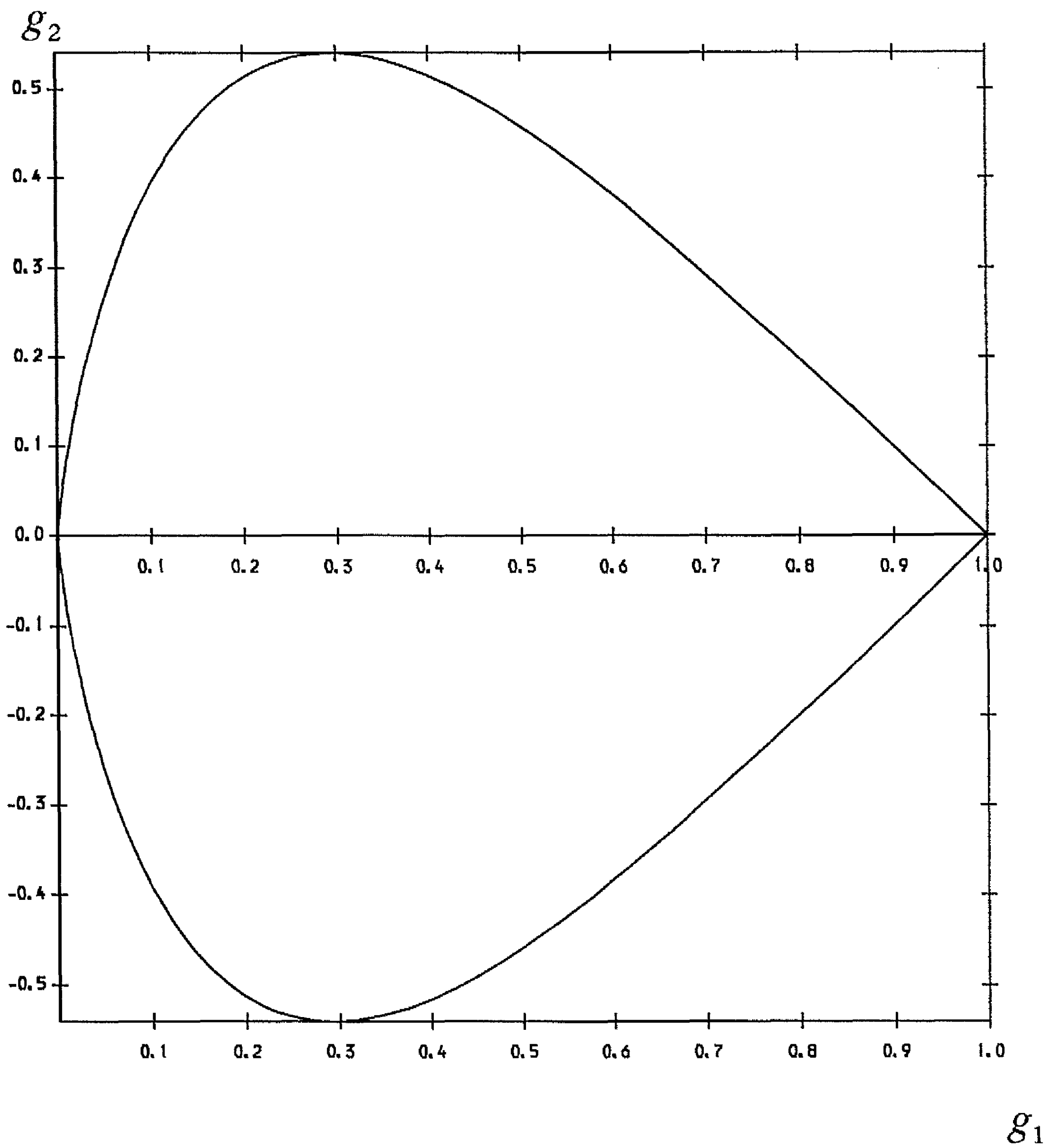


Figure (3.4)

Plot of the set $G=\left\{(g_1,g_2)':g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\right\}$, for the symmetric double reciprocal distribution.

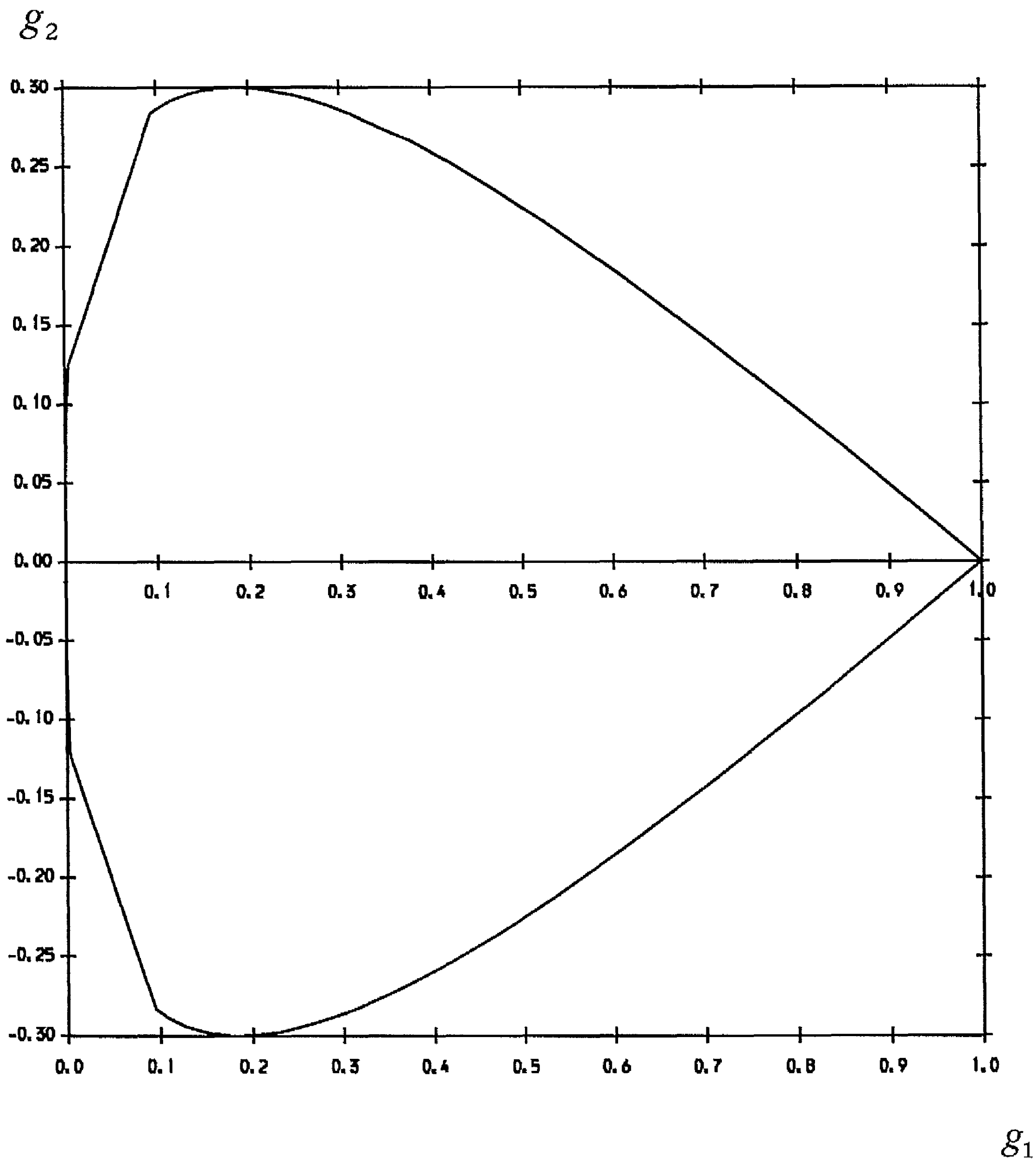


Figure (3.5)

Plot of the set $G = \{(g_1, g_2)' : g_1 = \sqrt{w(z)},\ g_2 = z g_1,\ z \in R\}$, for the asymmetric complementary log-log distribution.

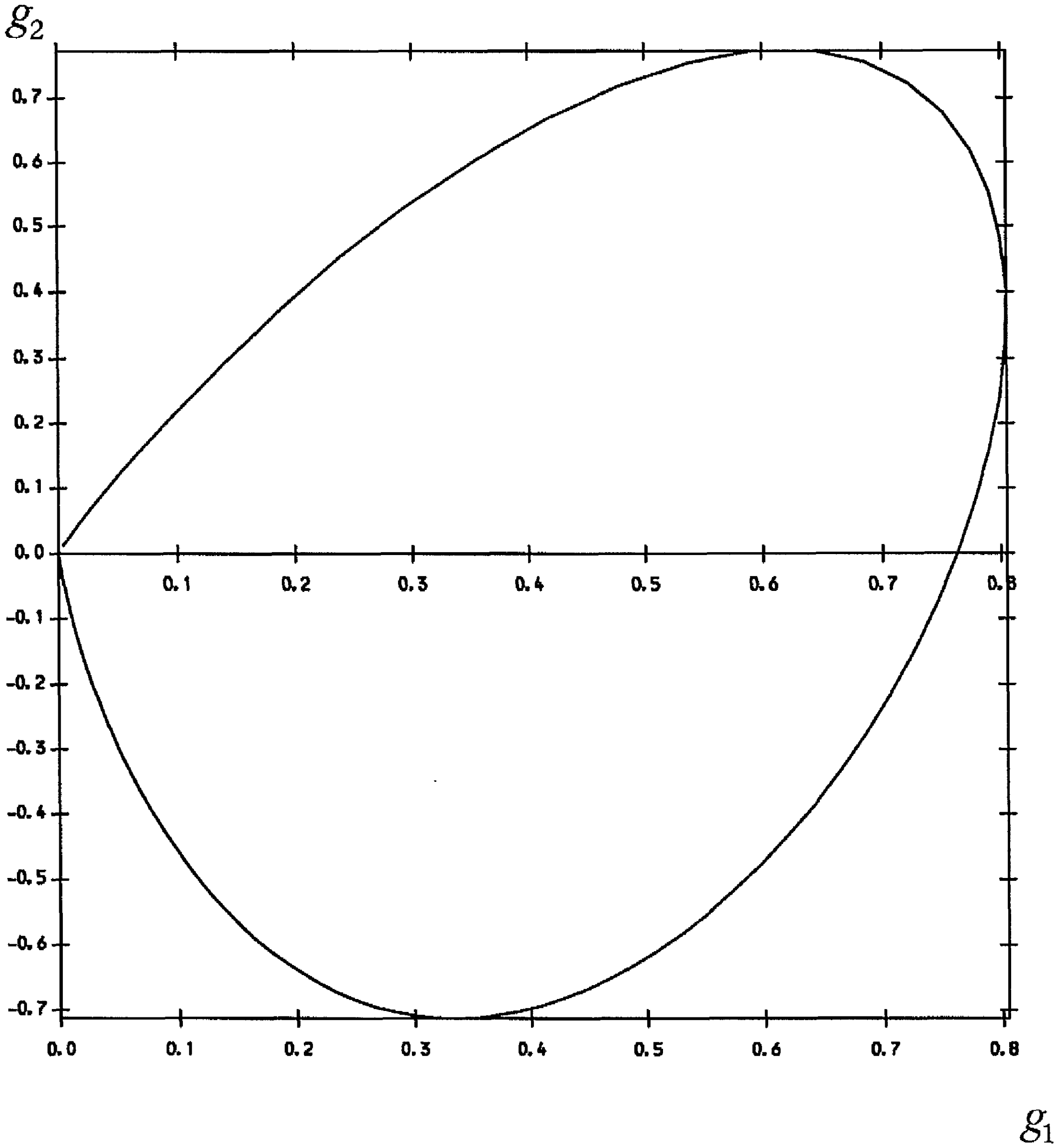


Figure (3.6)

Plot of the set $G=\left\{(g_1,g_2)':g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\right\}$, for the asymmetric skewed logistic distribution with m=3.

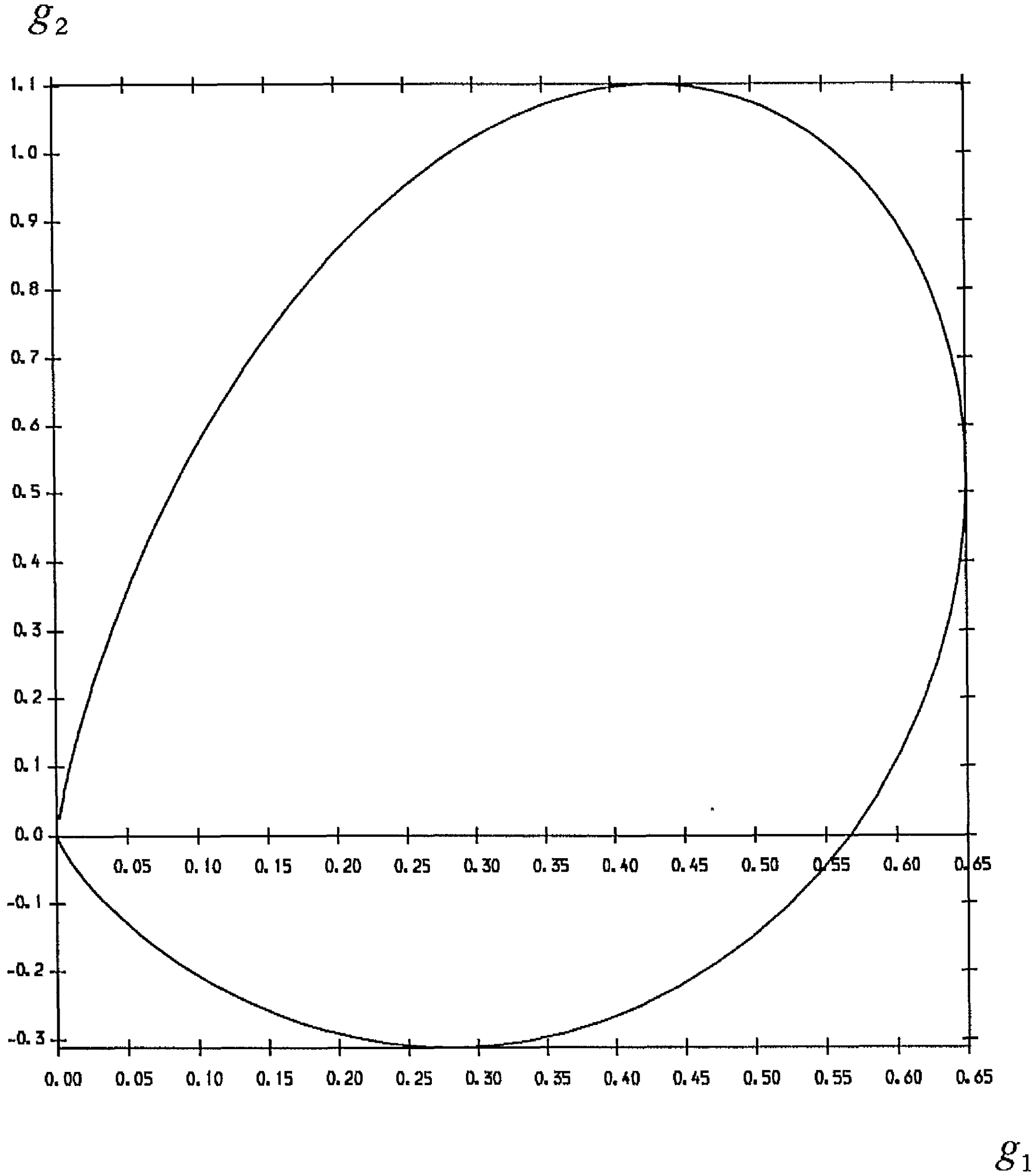


Figure (3.7)

Plot of the set $G=\left\{(g_1,g_2)^t : g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\subseteq Z_w=(-1,1)\right\}$, for the asymmetric weight function $w_1(z)$ with $(\alpha=1,\beta=2)$.

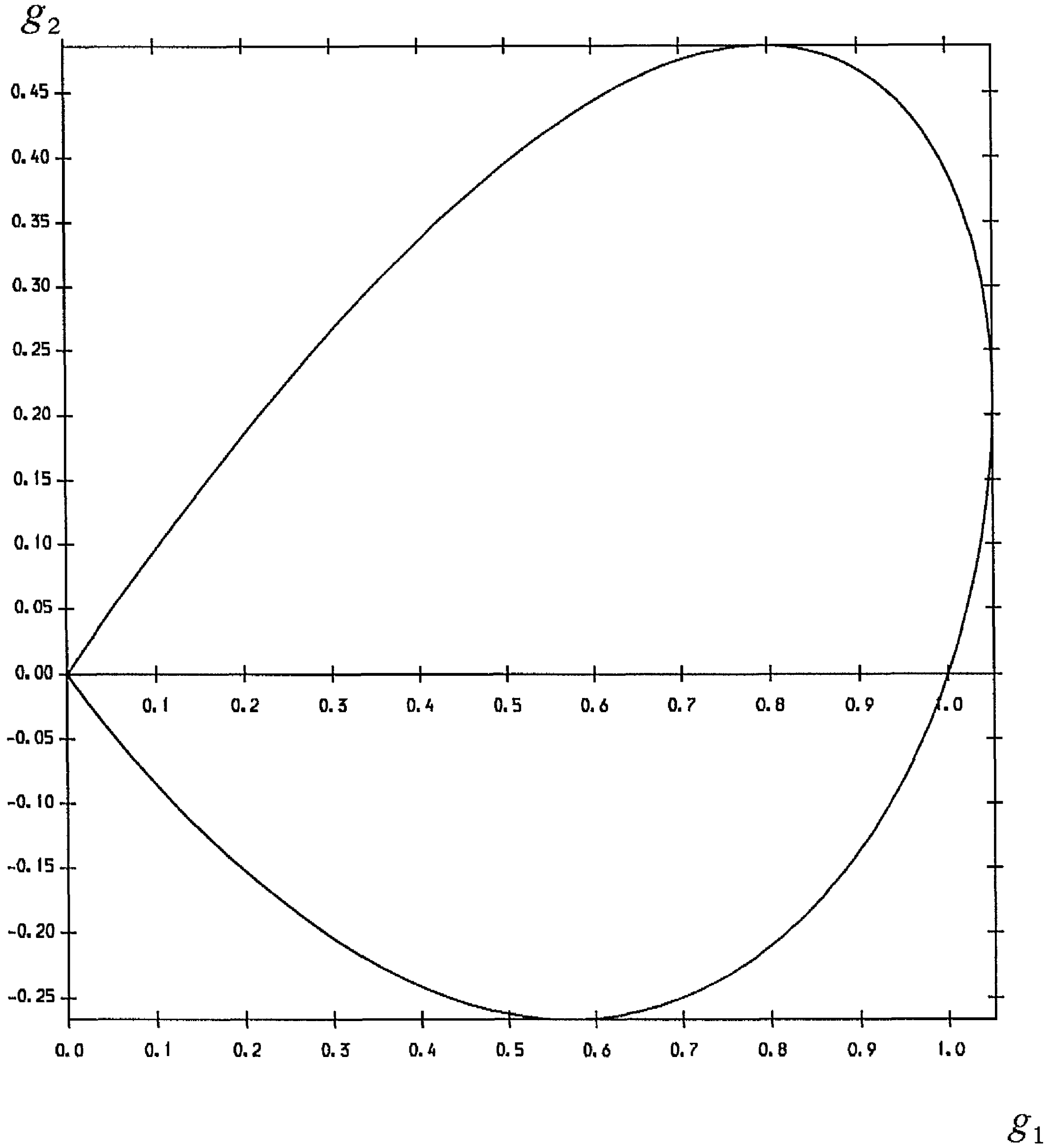


Figure (3.8)

Plot of the set $G=\left\{(g_1,g_2)':g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\subseteq Z_w=(0,\infty)\right\}$, for the asymmetric weight function $w_2(z)$ with $(\alpha=2)$.

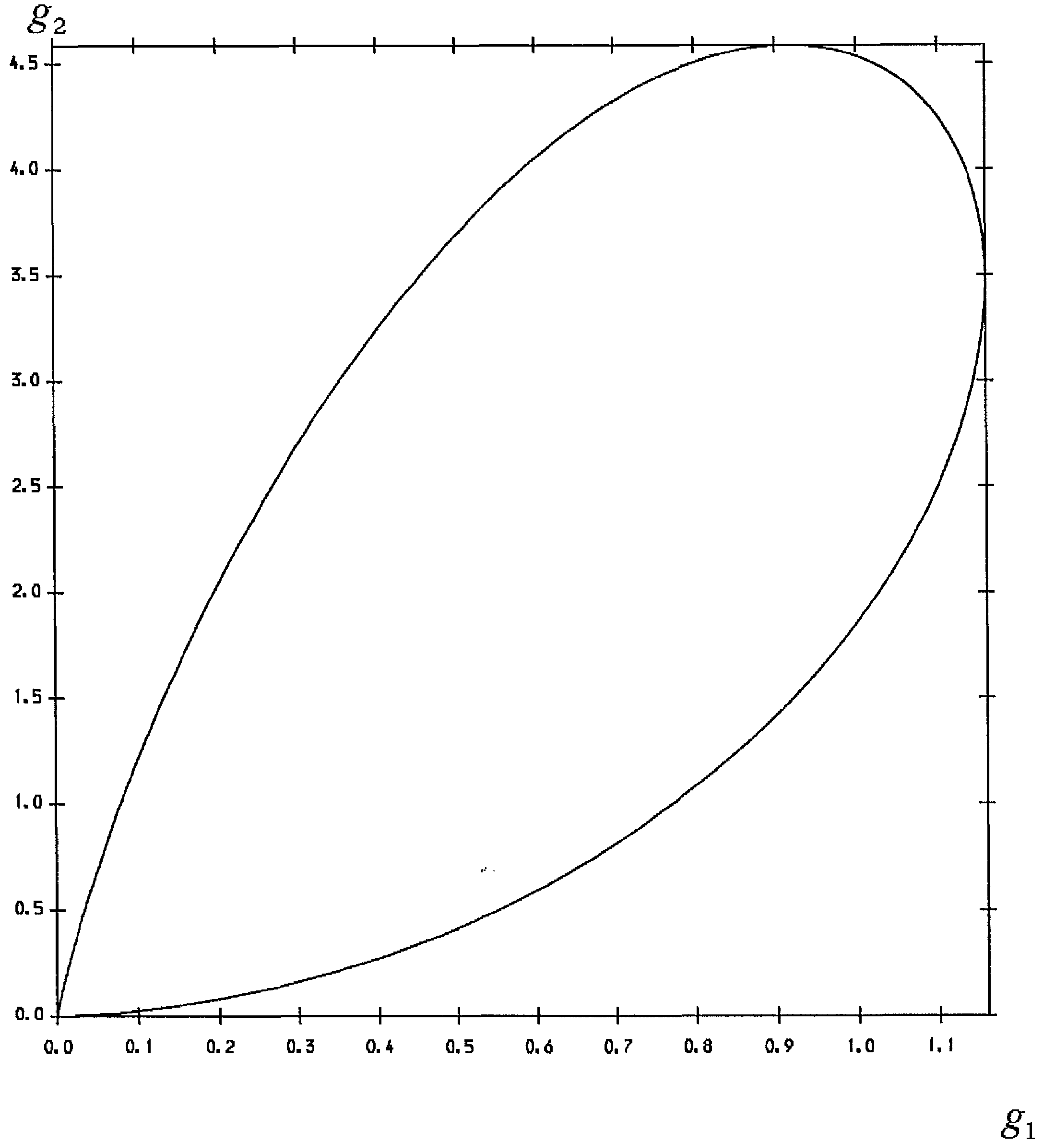


Figure (3.9)

Plot of the set $G=\{(g_1,g_2)':g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\}$, for the symmetric weight function $w_3(z)$.

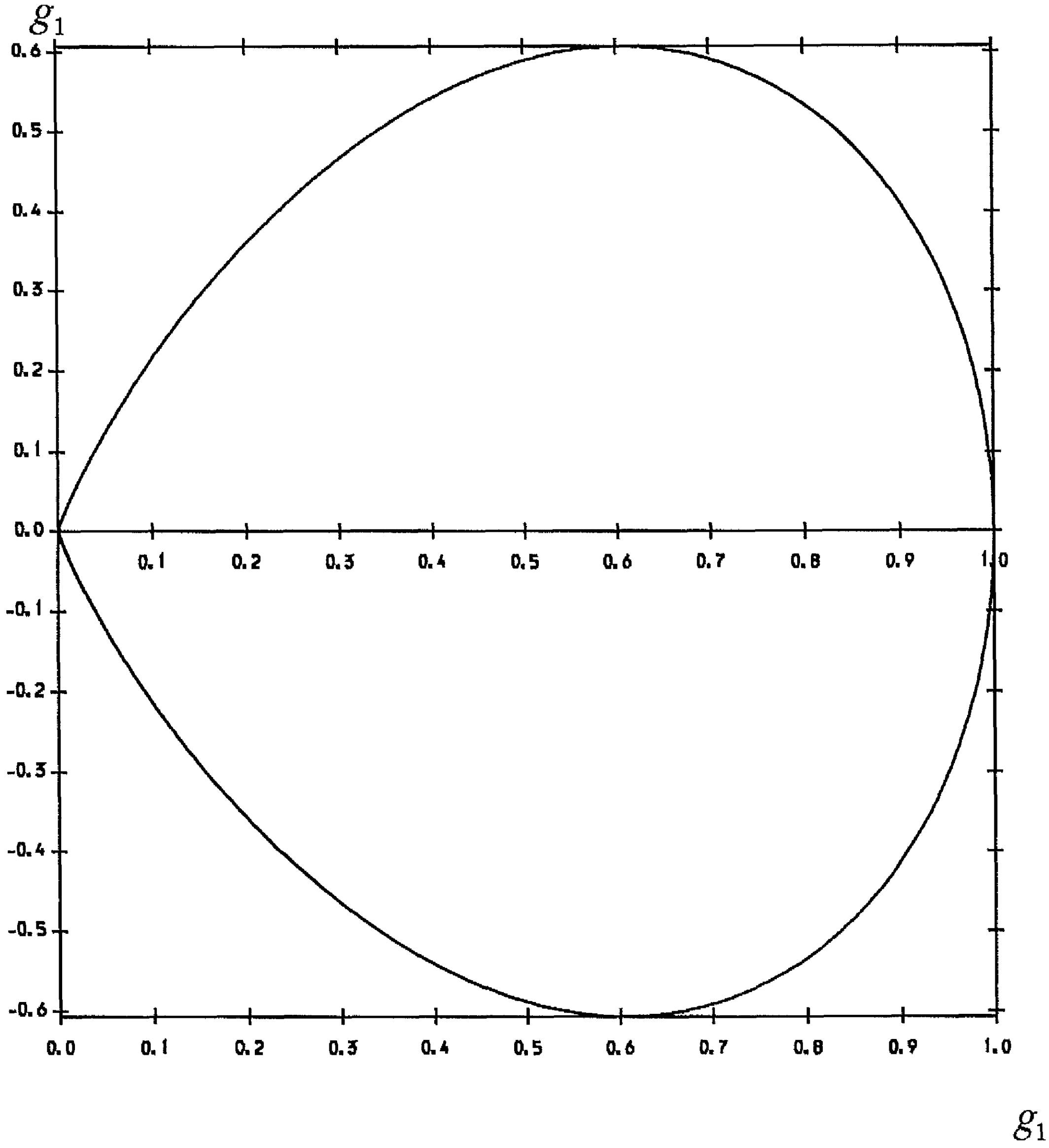


Figure (3.10)

Plot of the variance function for the global D-optimal two-point design on Z_w for the weight function $w_1(z)$ with $(\alpha = 1,\ \beta = 2)$.

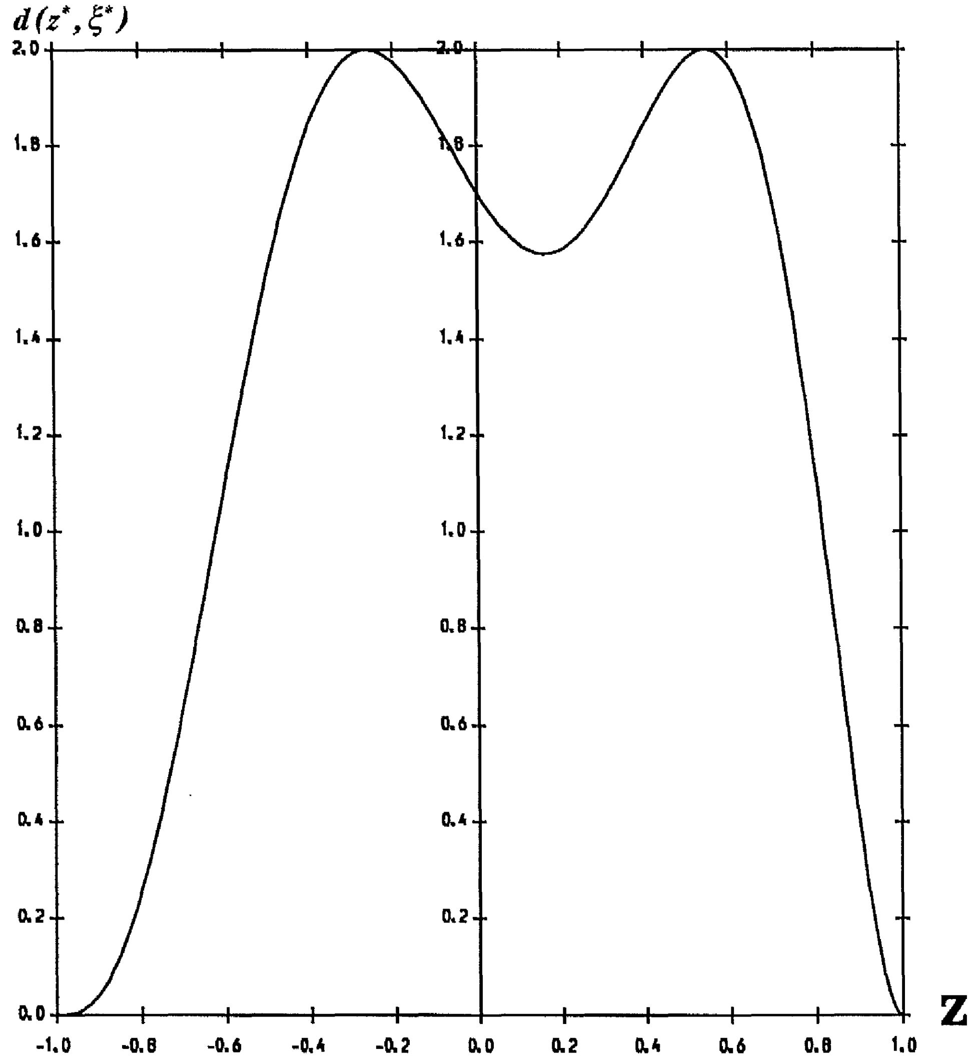


Figure (3.11)

Plot of the variance function for the global symmetric D-optimal two-point design on Z_w for the weight function $w_1(z)$ with $(\alpha = \beta = 3)$.

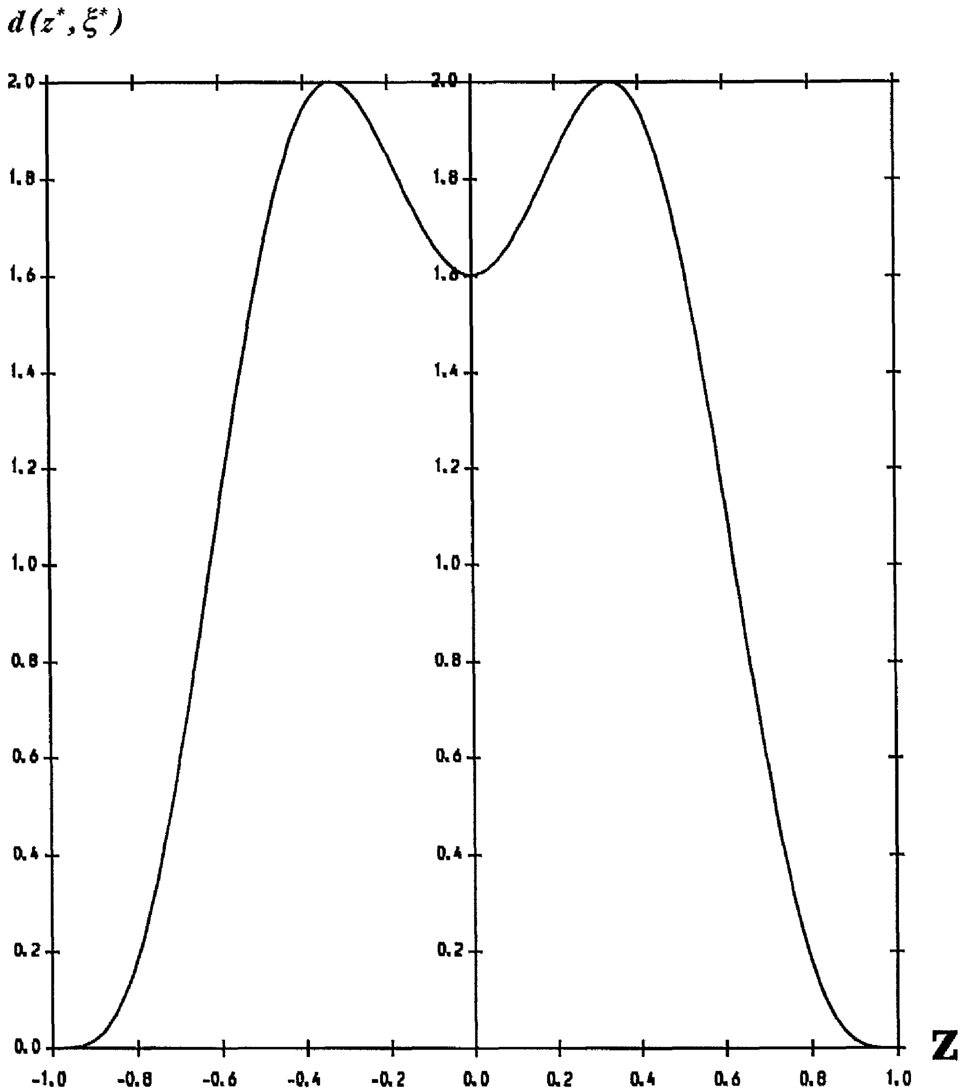


Figure (3.12)

Plot of the variance function for the global D-optimal two-point design on Z_w for the weight function $w_2(z)$ with $(\alpha = 2)$.

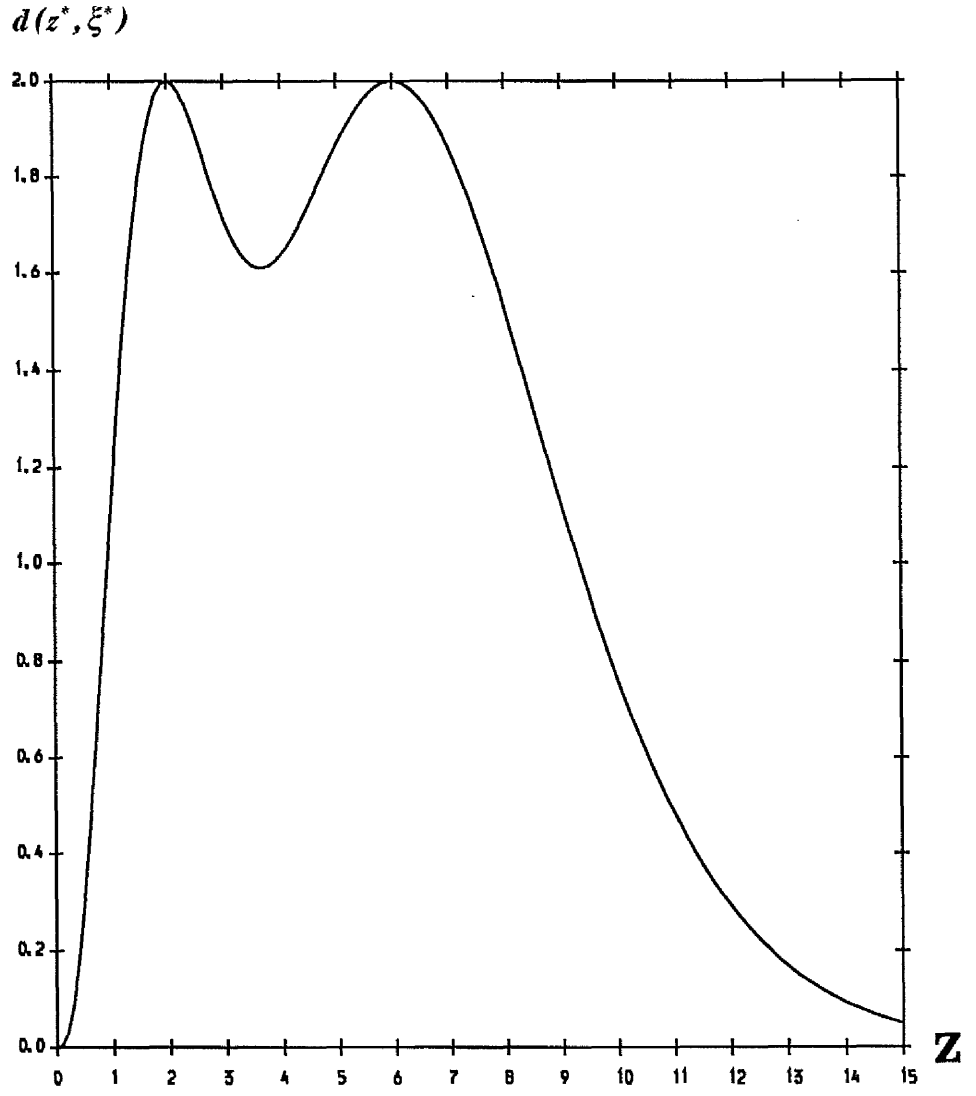


Figure (3.13)

Plot of the variance function for the global D-optimal two-point design on Z=[-1,0] for the weight function $w_1(z)$ with $(\alpha = \beta = 2)$.

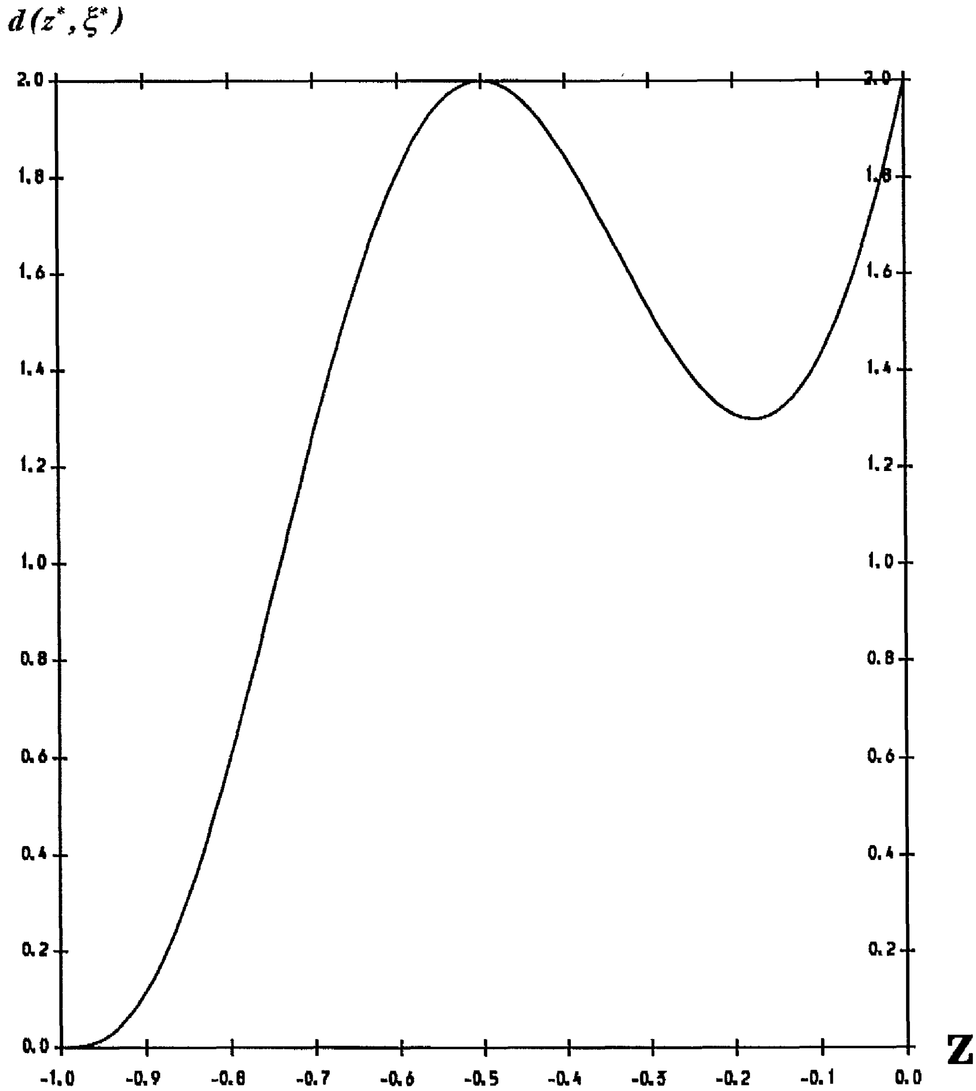


Figure (3.14)

Plot of the variance function for the global D-optimal two-piont design on Z=[0,1] for the weight function $w_1(z)$ with $(\alpha = \beta = 2)$.

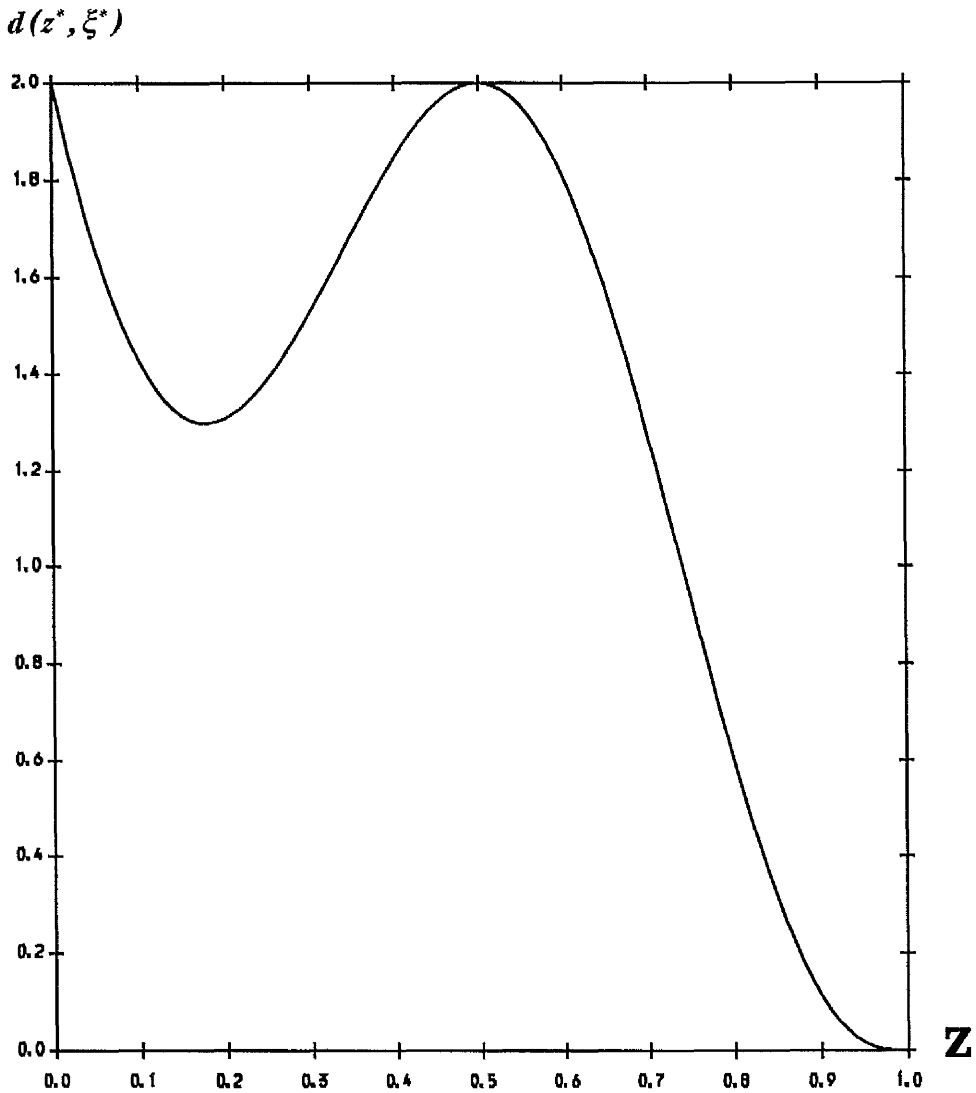


Figure (3.15)

Plot of the variance function for the global symmetric D-optimal two-point design on Z_w for the weight function $w_3(z)$.

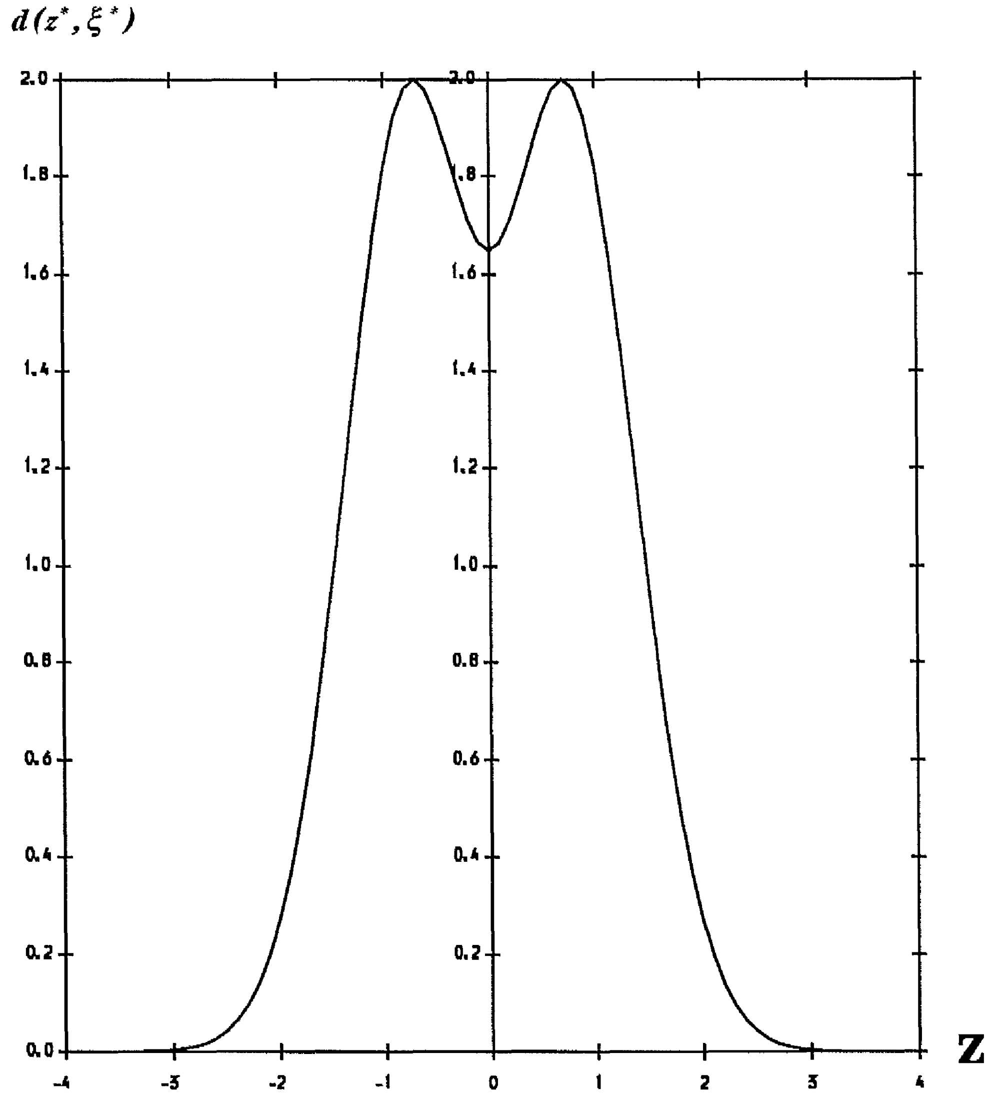


Figure (3.16)

Plot of the variance function for the global D-optimal two-point design on $Z = [0, \infty)$ for the weight function $w_3(z)$.

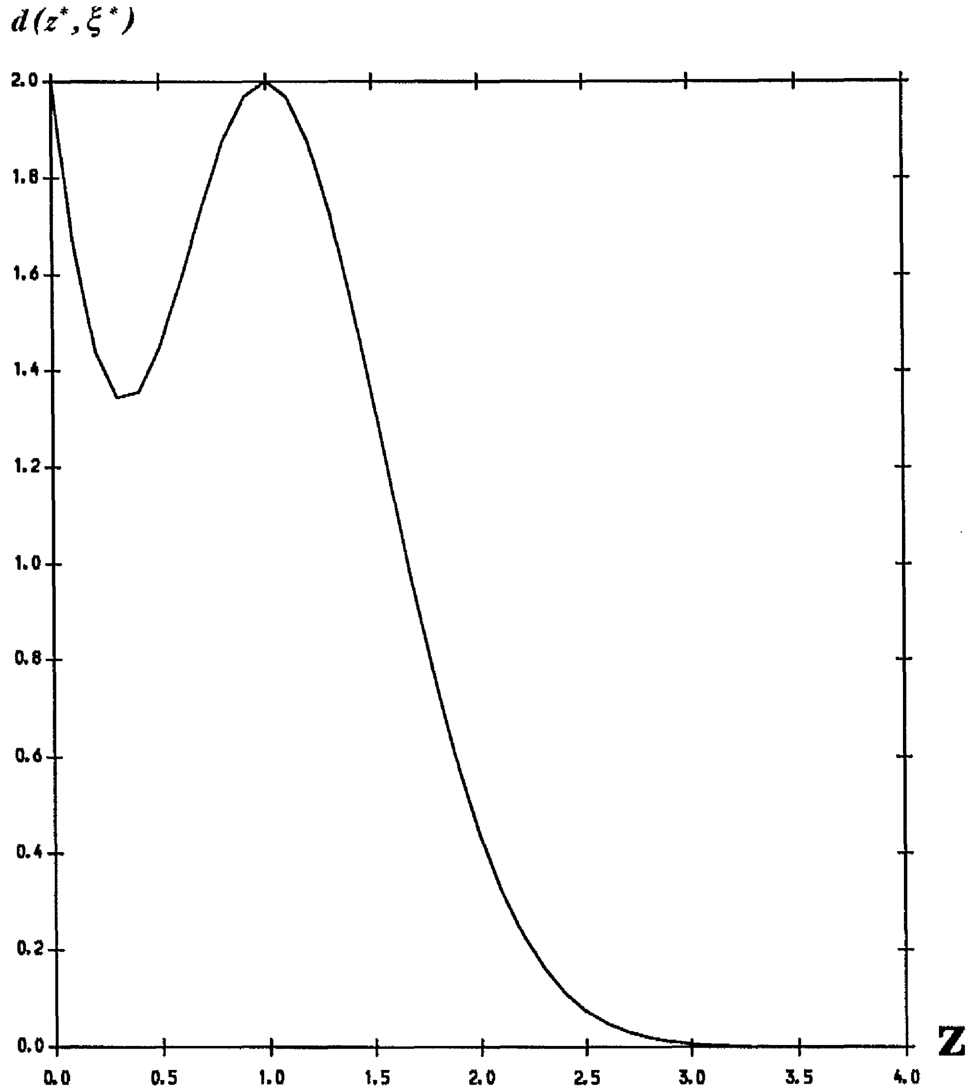


Figure (3.17)

Plot of the variance function for the Global symmetric D-optimal three-point design on Z_w for the double exponential distribution.

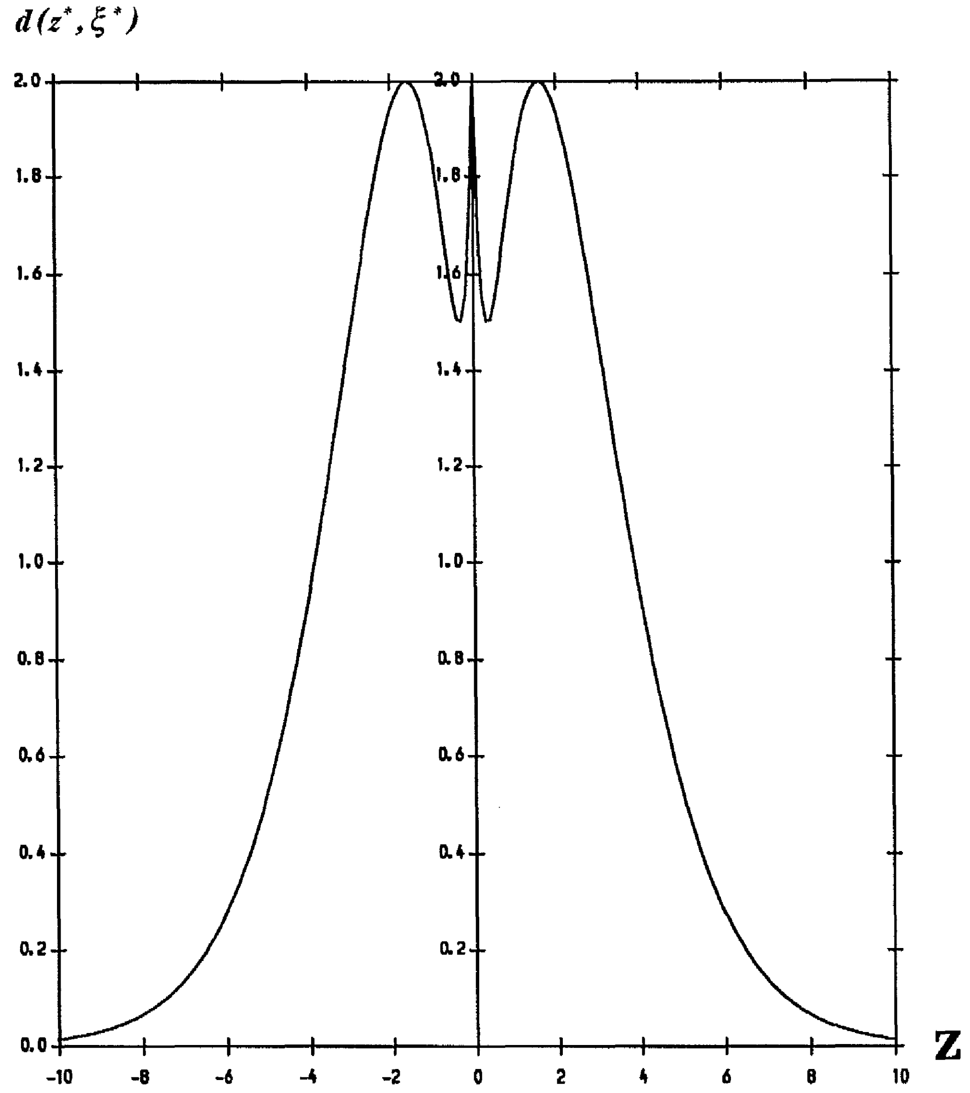


Figure (3.18)

Plot of the variance function for the Global symmetric D-optimal three-point design on Z_w for the double reciprocal distribution.

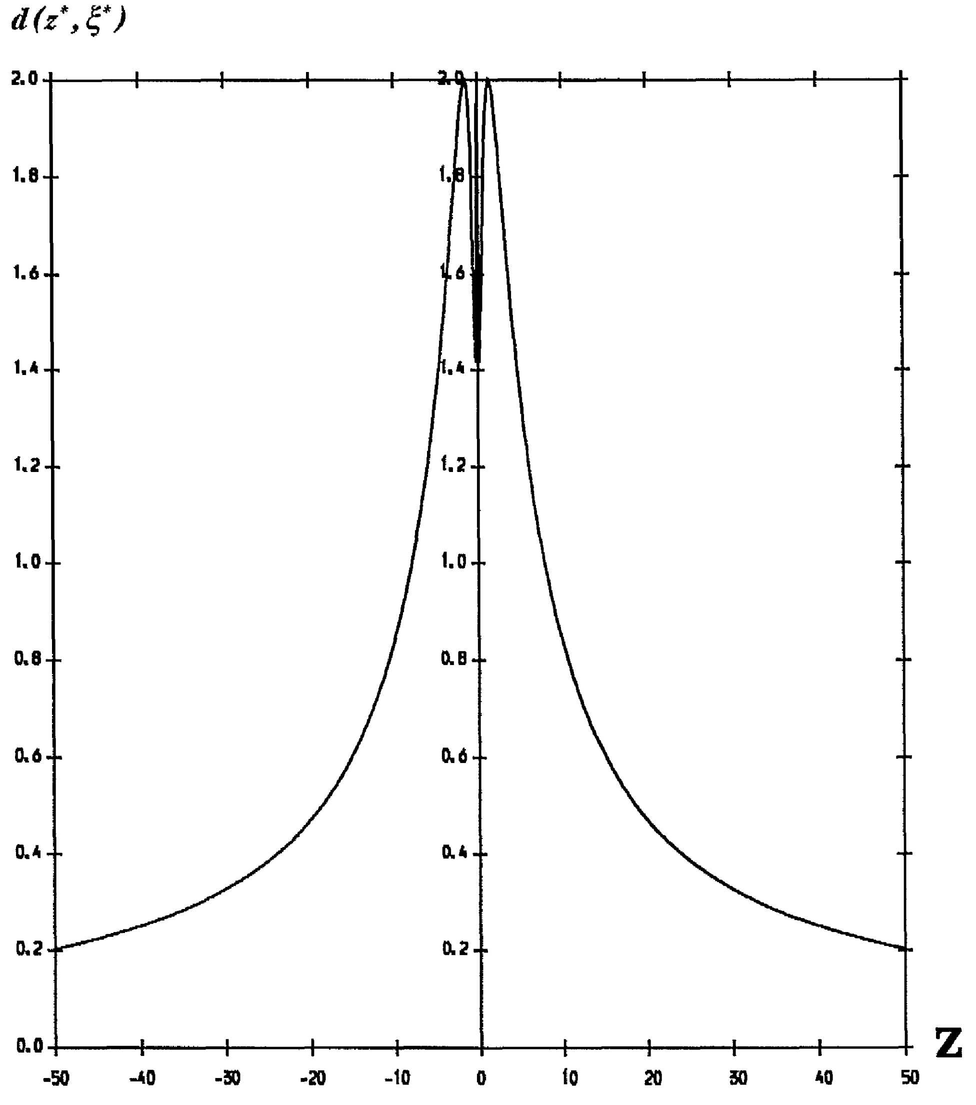


Figure (3.19)

Plot of the variance function for the D-optimal two-point design on Z=[-1.3,0.9] for the case (3) of section 3.6.4 for the complementary log-log distribution.

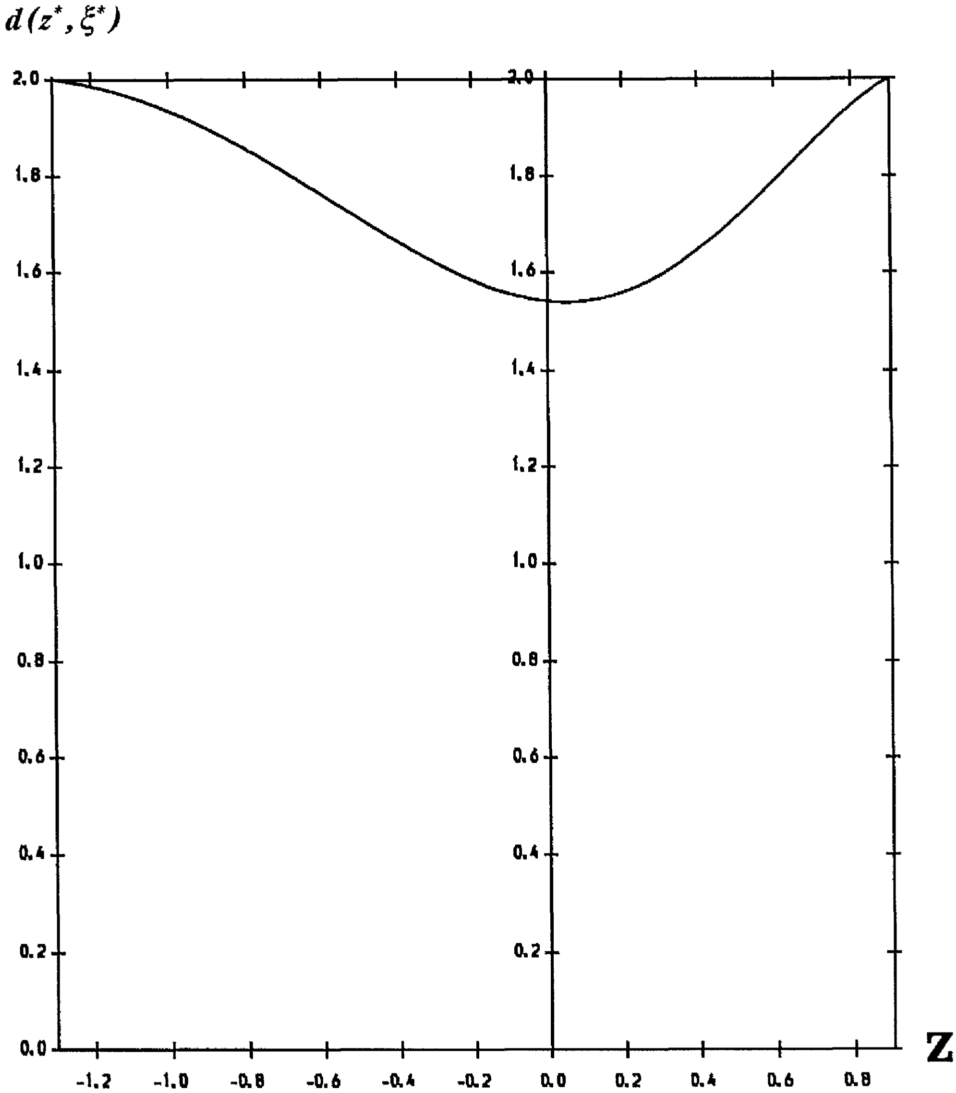


Figure (3.20)

Plot of the variance function for the D-optimal two-point design on Z=[-4,0.5] for the case (4) of section 3.6.4 for the skewed logistic distribution with $(m = 1/3)$.

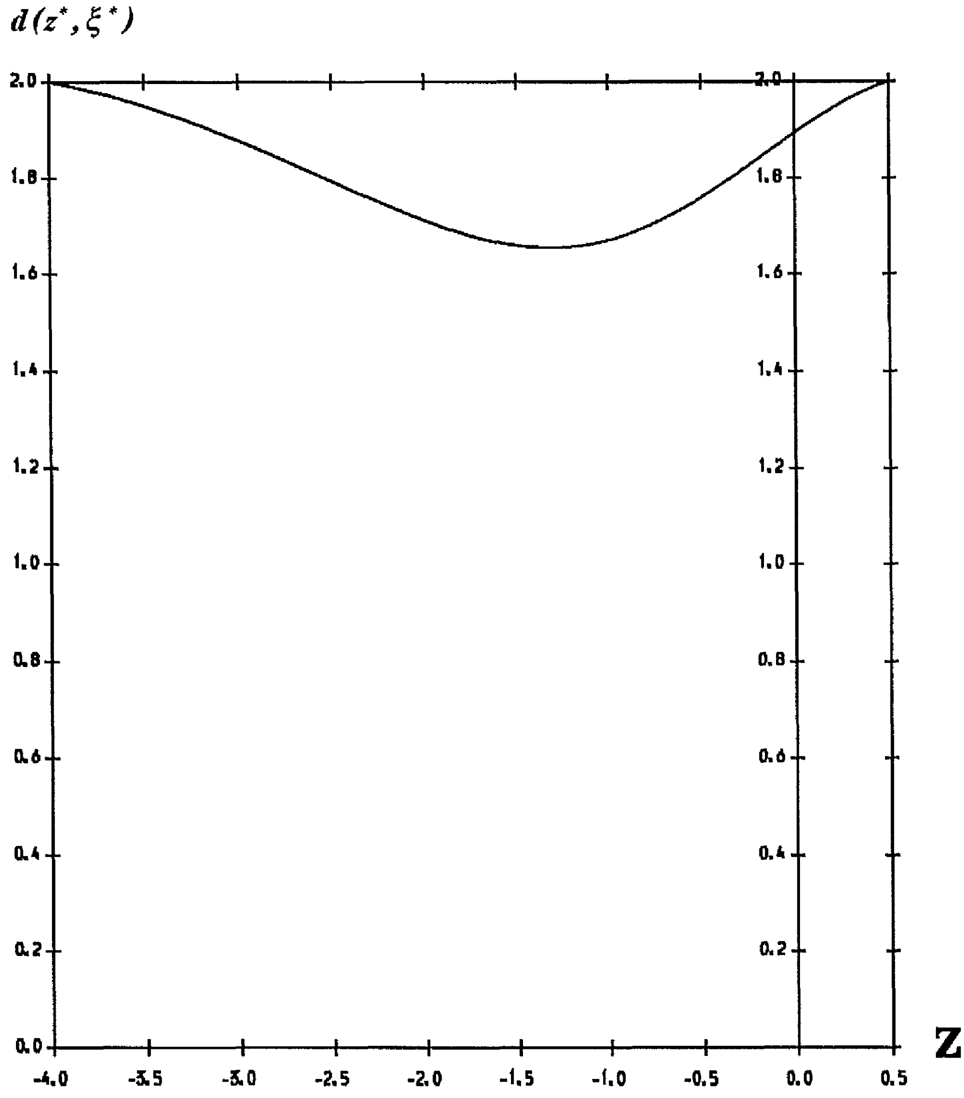


Figure (3.21)

Combined plots of the set $G=\{(g_1,g_2)^t : g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\}$ and the ellipsoid $Q=\left\{(g_1,g_2)^t : (g_1,g_2)^t M^{*^{-1}}\begin{pmatrix} g_1 \\ g_2 \end{pmatrix}=2\right\}$ for the double exponential distribution and the case $a<-u_2$ and $b>u_2$, where M^* is the global D-optimal design matrix on $Z_w=(-\infty,\infty)$, whose support points are $\{-u_2,0,u_2\}$ (u_2=1.5936) and weights {0.2819,0.4362,0.2819}.

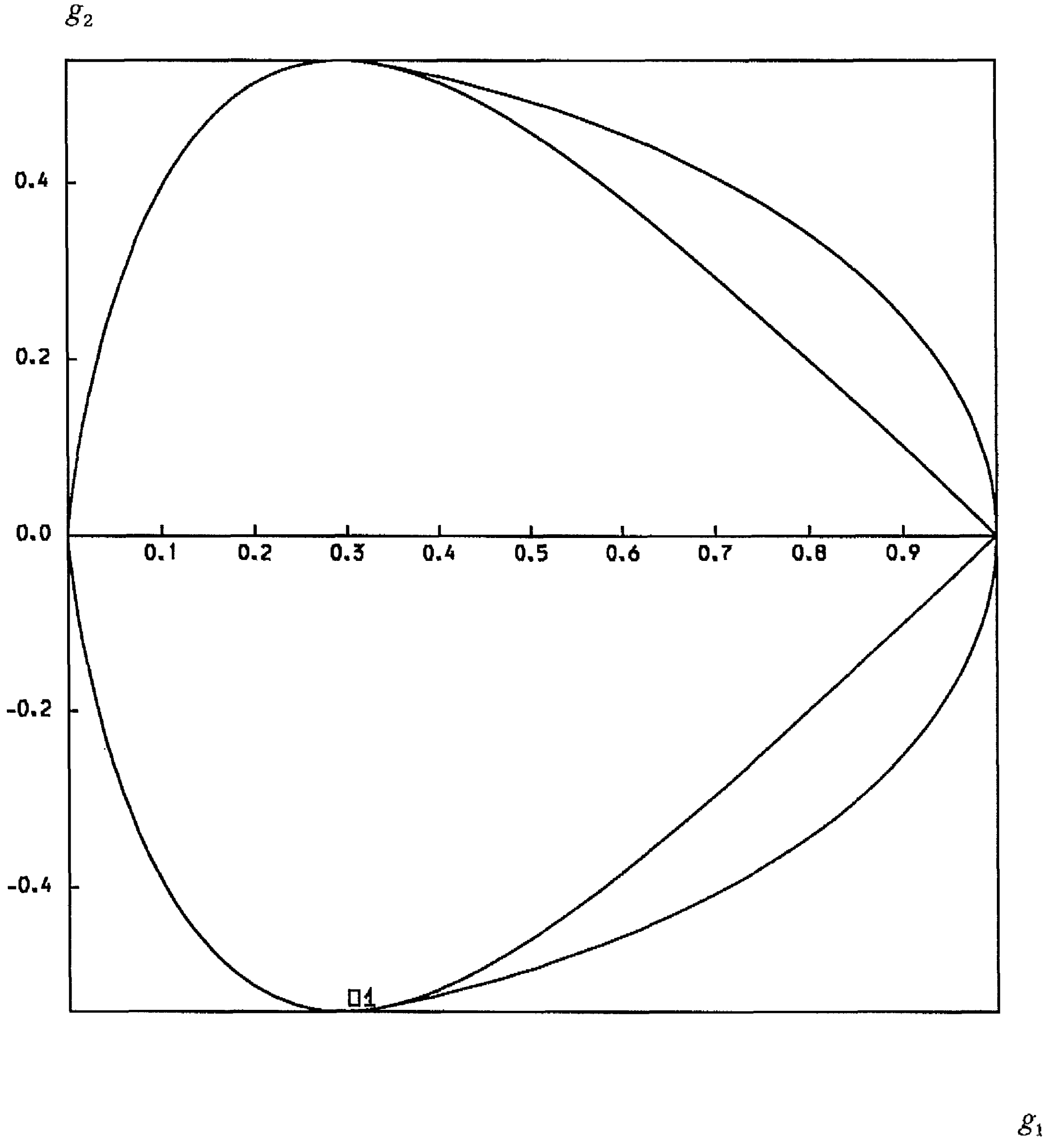


Figure (3.22)

Combined plots of the set $G=\{(g_1,g_2)^t : g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\}$ and the ellipsoid $Q=\left\{(g_1,g_2)^t : (g_1,g_2)^t M^{*^{-1}}\begin{pmatrix} g_1 \\ g_2 \end{pmatrix}=2\right\}$ for the double exponential distribution and the case $a<-u_1$, where M^* is the global D-optimal design matrix on $Z=(-\infty,0]$, whose support points are $\{-u_1,0\}$, $b<\tilde{z}(u_1)$ (u_1=1.841).

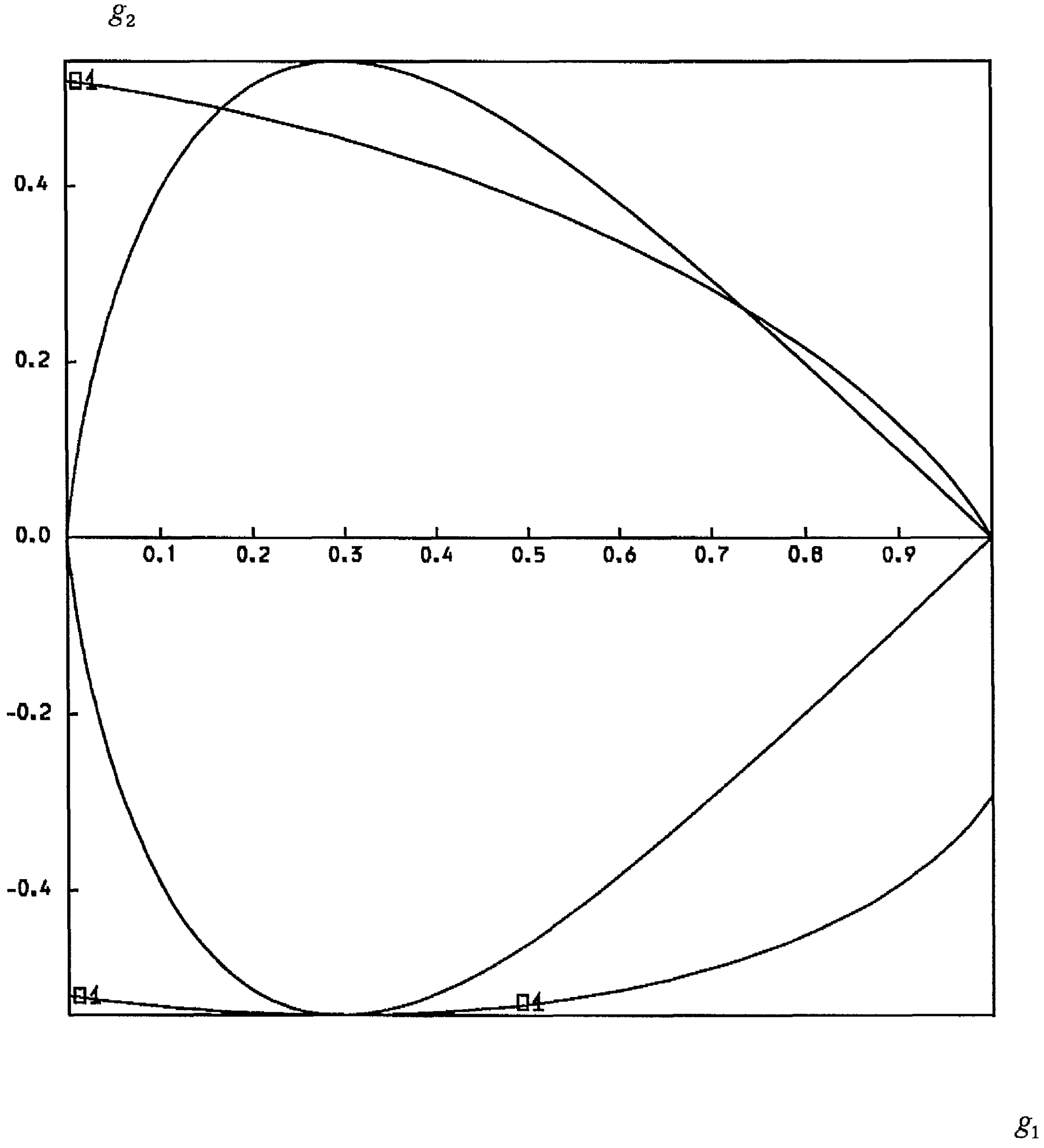


Figure (3.23)

Combined plots of the set $G=\{(g_1,g_2)':g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\}$ and the ellipsoid $Q=\left\{(g_1,g_2)':(g_1,g_2)'M^{*^{-1}}\begin{pmatrix}g_1\\g_2\end{pmatrix}=2\right\}$ for the double exponential distribution and the case $a<-u_1$, where M^* is the global D-optimal design matrix on Z=[a,b], whose support points are $\{a^*(b),0,b\}$, $\tilde{z}(u_1)<b<u_2$ with b=0.5, and $a^*(b)$=-1.7862

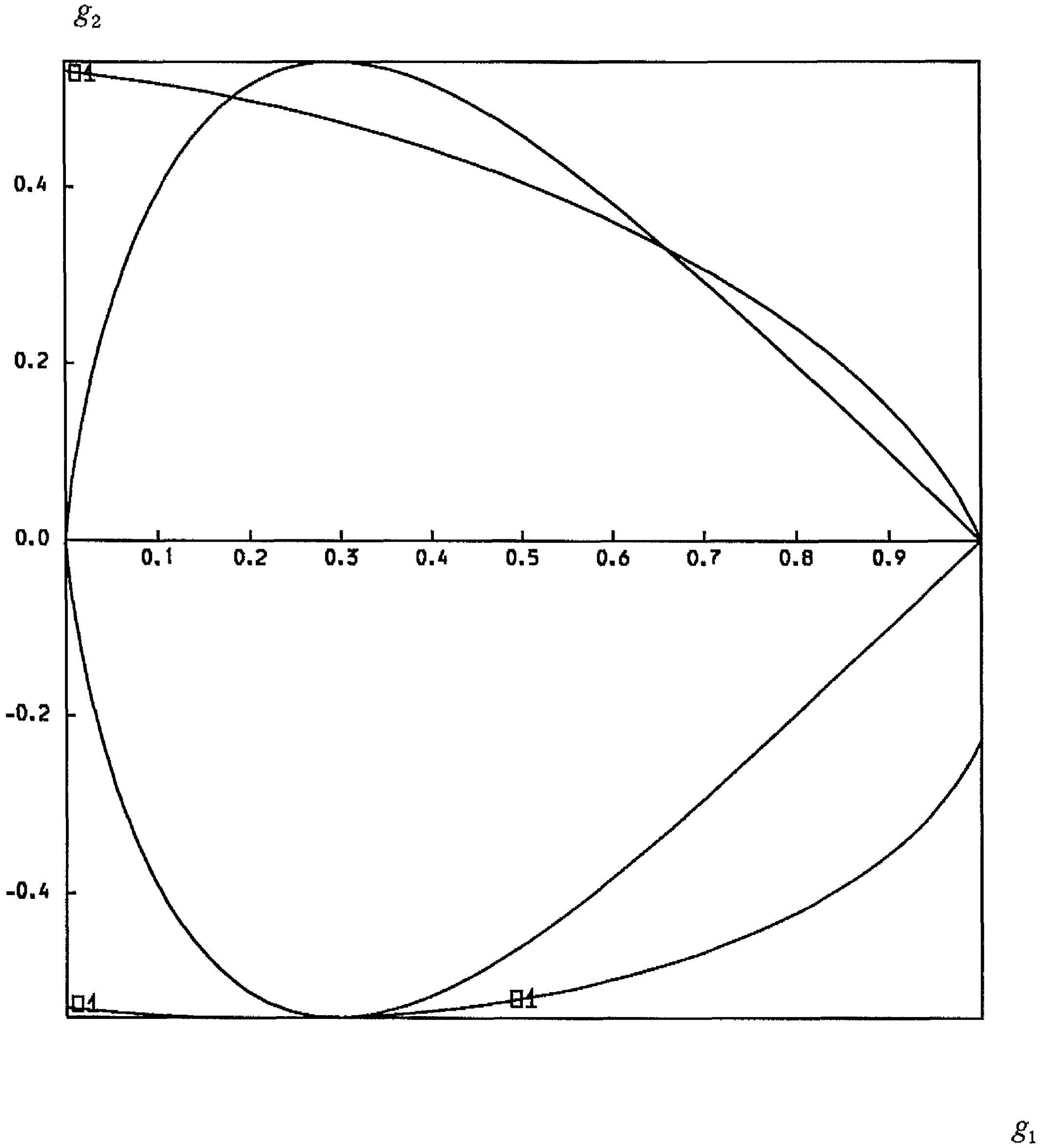


Figure (2.24)

Combined plots of the set $G=\left\{(g_1,g_2)':g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\right\}$ and the ellipsoid $Q=\left\{(g_1,g_2)':(g_1,g_2)'M^{*^{-1}}\begin{pmatrix}g_1\\g_2\end{pmatrix}=2\right\}$ for the double exponential distribution and the case $-u_1<a<-u_2$, where M^* is the global D-optimal design matrix on Z=[a,b], whose support points are {a,0}, $b<\tilde{z}(a)$, with a=-1.7211.

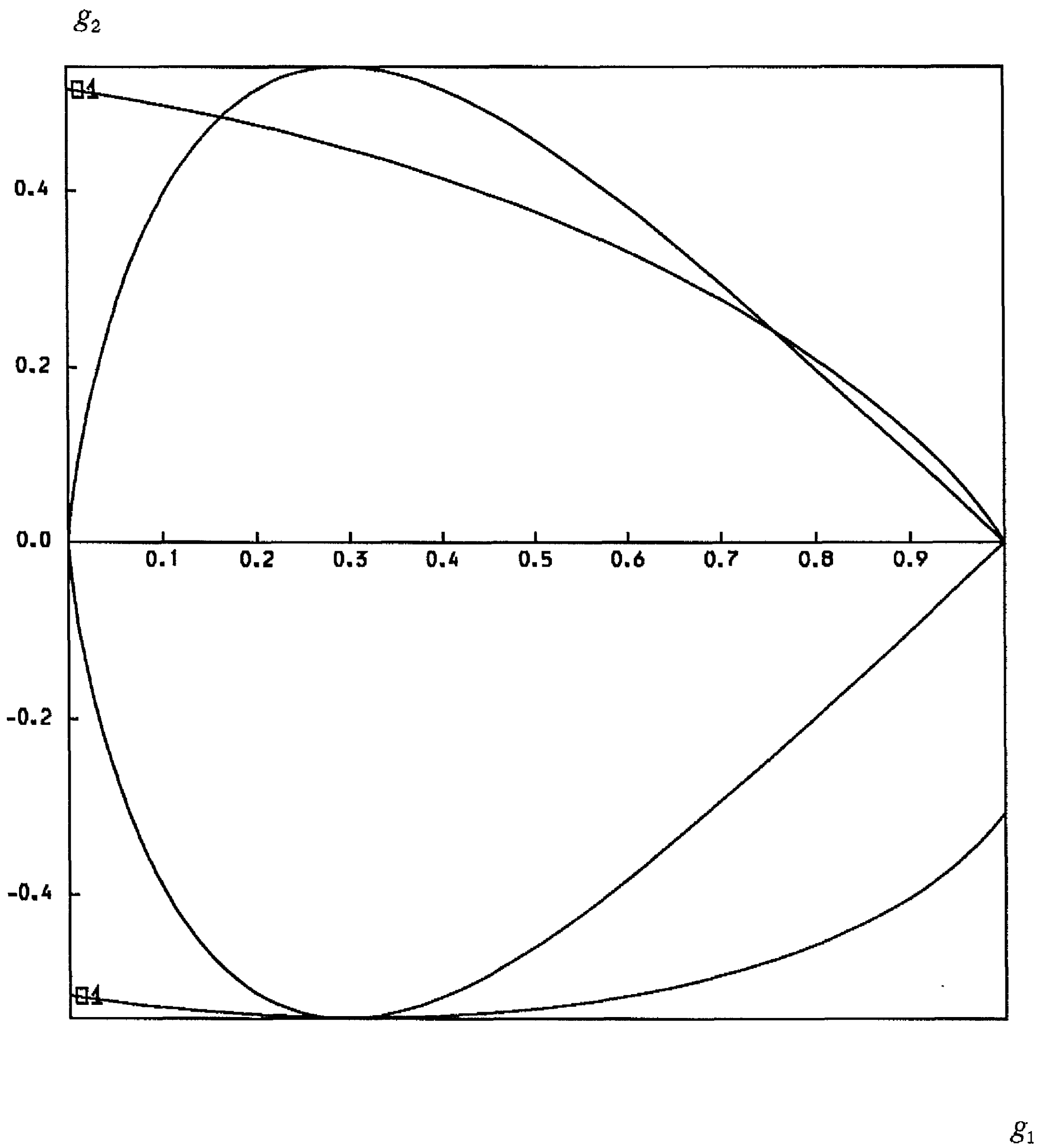


Figure (3.25)

Combined plots of the set $G = \left\{(g_1, g_2)^t : g_1 = \sqrt{w(z)},\ g_2 = zg_1,\ z \in R\right\}$ and the ellipsoid $Q = \left\{(g_1, g_2)^t : (g_1, g_2)^t M^{*^{-1}} \begin{pmatrix} g_1 \\ g_2 \end{pmatrix} = 2\right\}$ for the double exponential distribution and the case $-u_1 < a < -u_2$, where M^* is the global D-optimal design matrix on Z=[a,b], whose support points are {a,0,b}, $\tilde{z}(a) < b < \tilde{z}(u_1)$ with a=-1.25, $\tilde{z}(a)$=0.1167 and b=0.2.

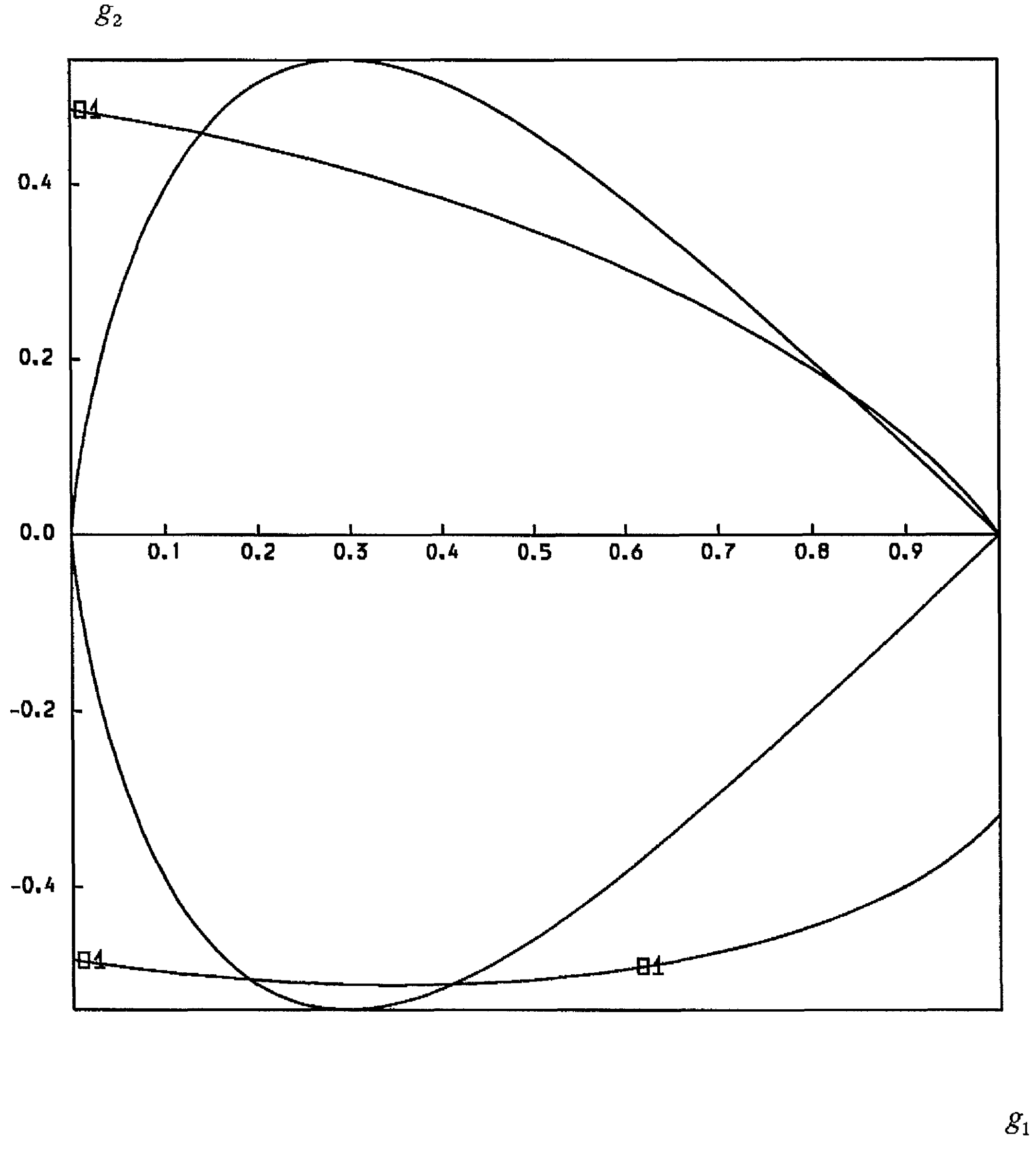


Figure (3.26)

Combined plots of the set $G=\left\{(g_1,g_2)':g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\right\}$ and the ellipsoid $Q=\left\{(g_1,g_2)':(g_1,g_2)'M^{*^{-1}}\begin{pmatrix}g_1\\g_2\end{pmatrix}=2\right\}$ for the double exponential distribution and the case $-u_1<a<-u_2$, where M^* is the global D-optimal design matrix on Z=[a,b], whose support points are {max,0,b}, $\tilde{z}(u_1)<b<u_2$ where $\max=\max\{a,a^*(b)\}$={-1.7,-1.6708} and b=0.9.

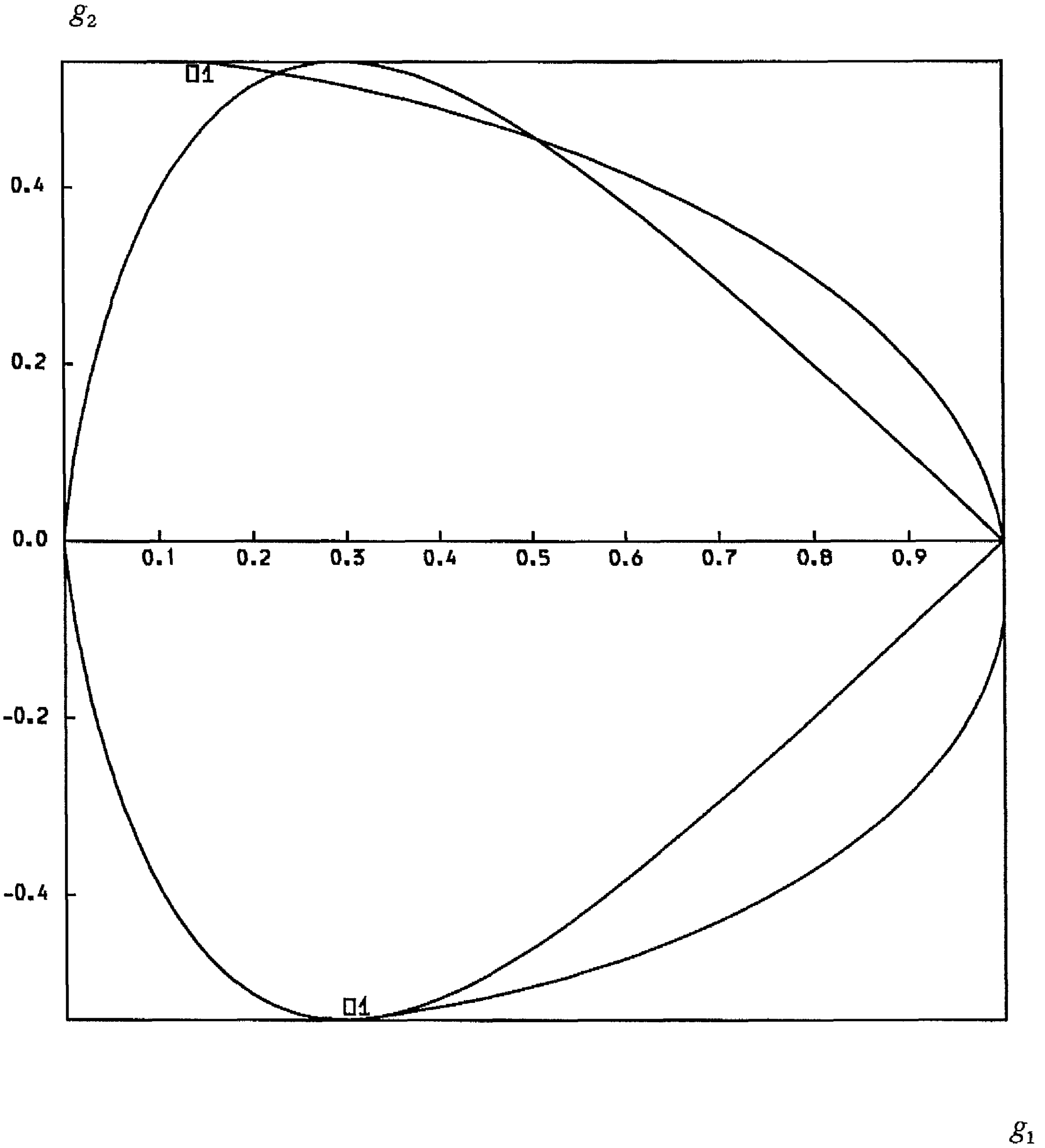


Figure (3.27)

Combined plots of the set $G=\left\{(g_1,g_2)^t : g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\right\}$ and the ellipsoid $Q=\left\{(g_1,g_2)^t : (g_1,g_2)^t M^{*^{-1}}\begin{pmatrix} g_1 \\ g_2 \end{pmatrix}=2\right\}$ for the double exponential distribution and the case $-u_2<a<-u_3$, where M^* is the global D-optimal design matrix on Z=[a,b], whose support points are {a,0}, $b<\tilde{z}(a)$ with a=-1.25 and $\tilde{z}(a)$=0.1167.

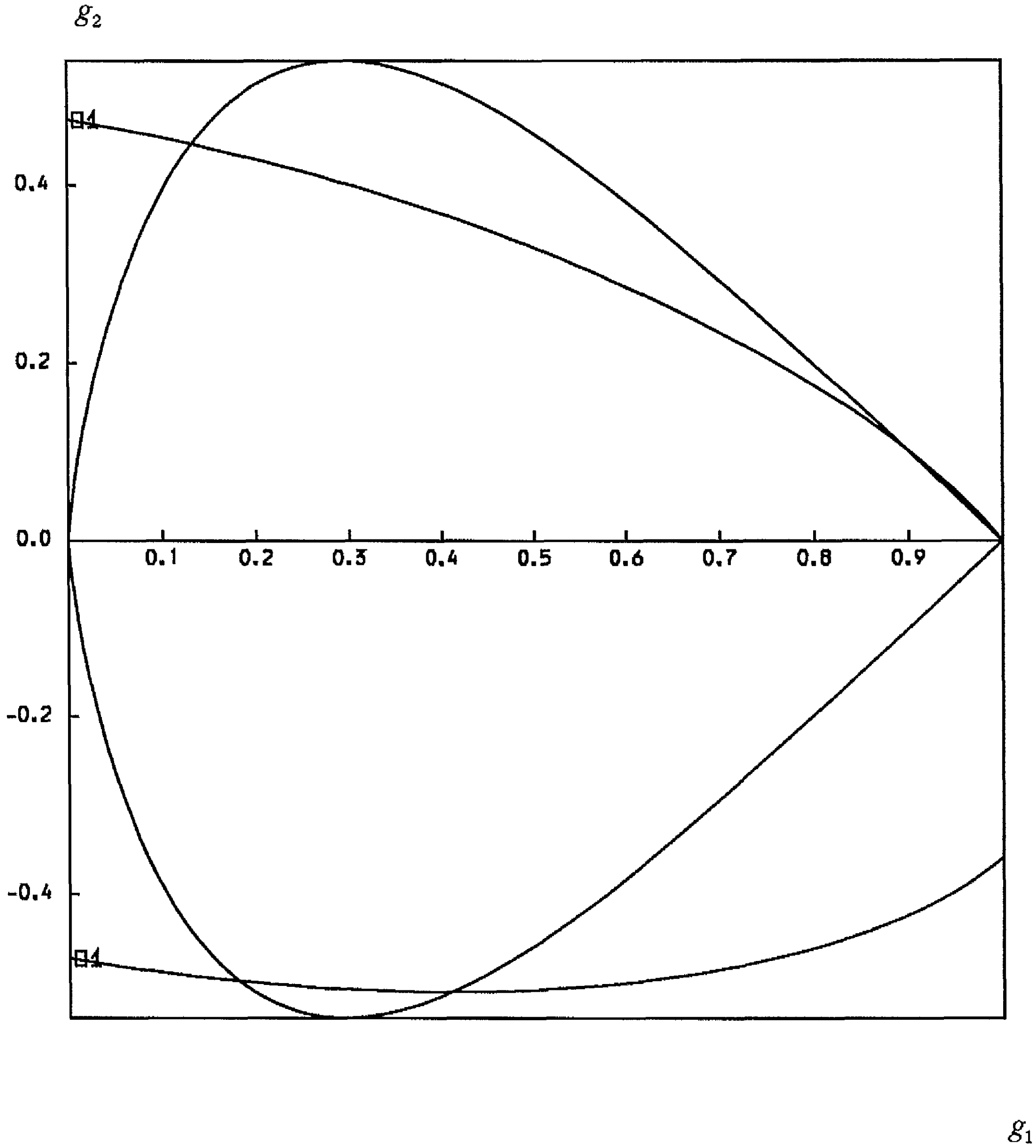


Figure (3.28)

Combined plots of the set $G=\left\{(g_1,g_2)^t : g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\right\}$ and the ellipsoid $Q=\left\{(g_1,g_2)^t : (g_1,g_2)^t M^{*^{-1}}\begin{pmatrix} g_1 \\ g_2 \end{pmatrix}=2\right\}$ for the double exponential distribution and the case $-u_2<a<-u_3$, where M^* is the global D-optimal design matrix on Z=[a,b], whose support points are {a,0,b}, $\tilde{z}(a)<b<|a|$ with a=-1.5, $\tilde{z}(a)$=0.2297 and b=0.2.

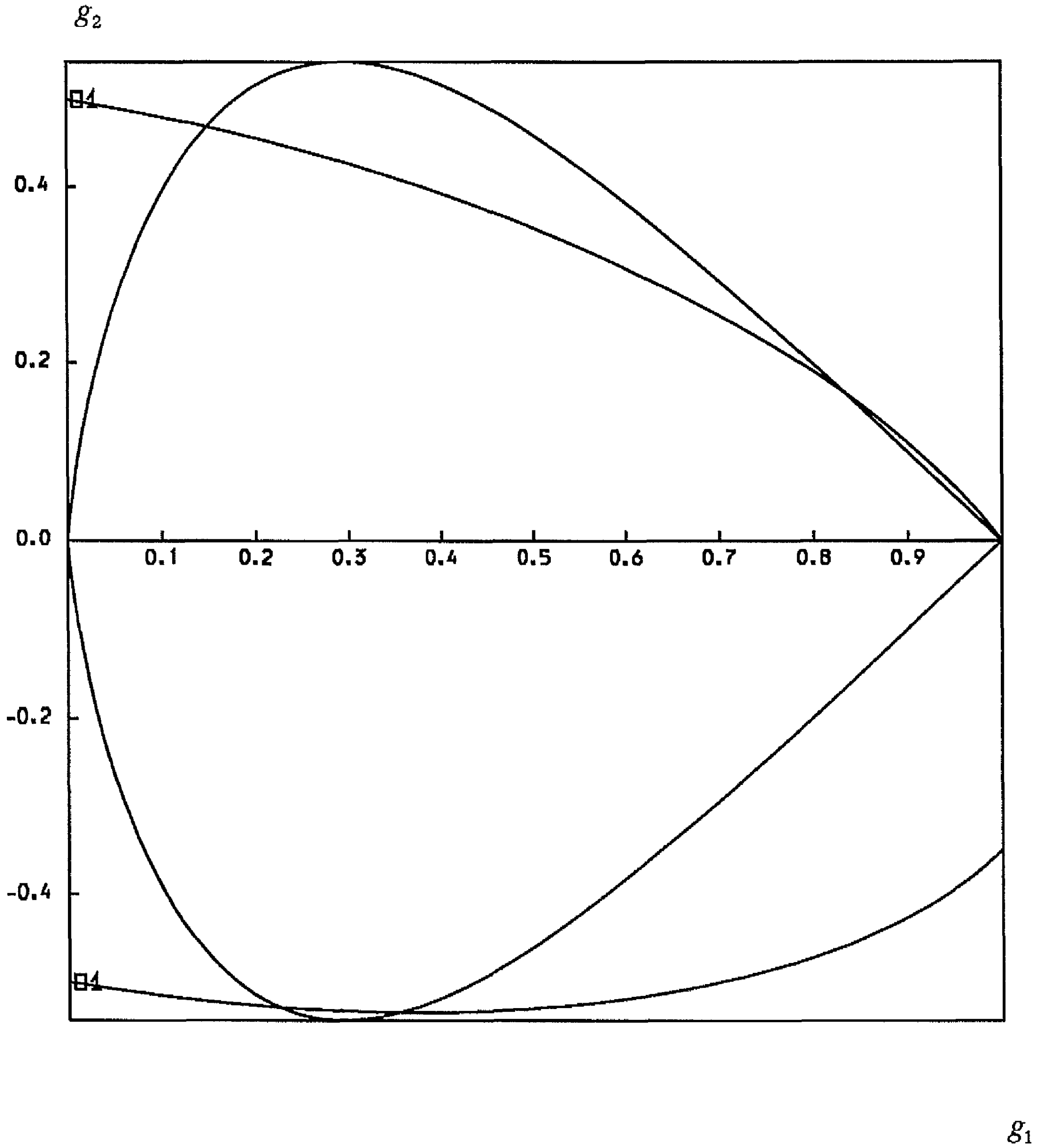


Figure (3.29)

Combined plots of the set $G=\{(g_1,g_2)':g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\}$ and the ellipsoid $Q=\left\{(g_1,g_2)':(g_1,g_2)'M^{*^{-1}}\begin{pmatrix}g_1\\g_2\end{pmatrix}=2\right\}$ for the double exponential distribution and the case $-u_3<a<-u_4$, where M^* is the global D-optimal design matrix on Z=[a,b], whose support points are {a,b}, $b<z^+(a)$ with a=-0.6, $z^+(a)$=0.24 and b=0.2.

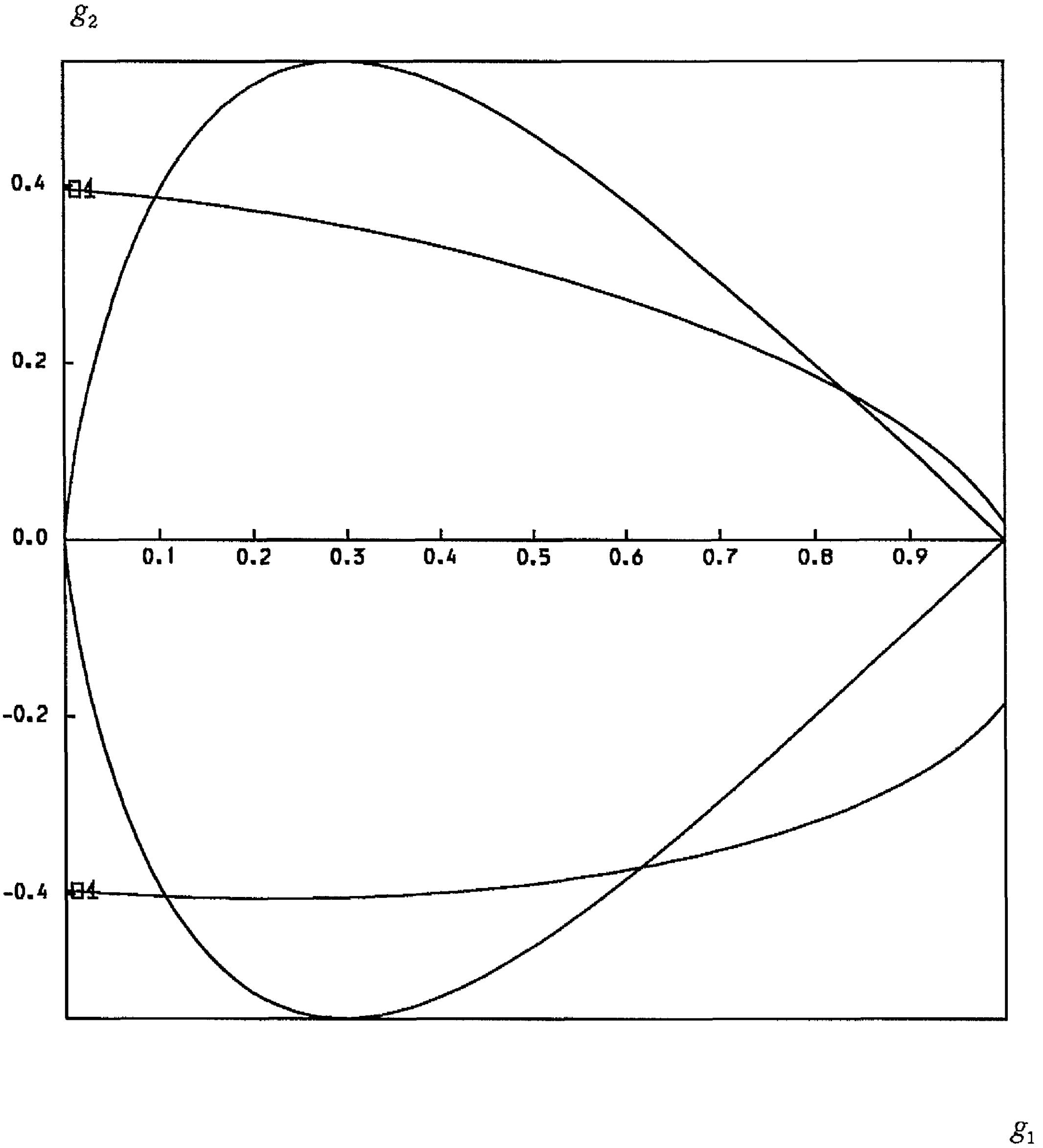


Figure (3.30)

Combined plots of the set $G=\{(g_1,g_2)':g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\}$ and the ellipsoid $Q=\left\{(g_1,g_2)':(g_1,g_2)'M^{*^{-1}}\begin{pmatrix}g_1\\g_2\end{pmatrix}=2\right\}$ for the double exponential distribution and the case $-u_3<a<-u_4$, where M^* is the global D-optimal design matrix on Z=[a,b], whose support points are {a,0,b}, $z^+(a)<b<|a|$ with a=-0.6, $z^+(a)$=0.24 and b=0.3.

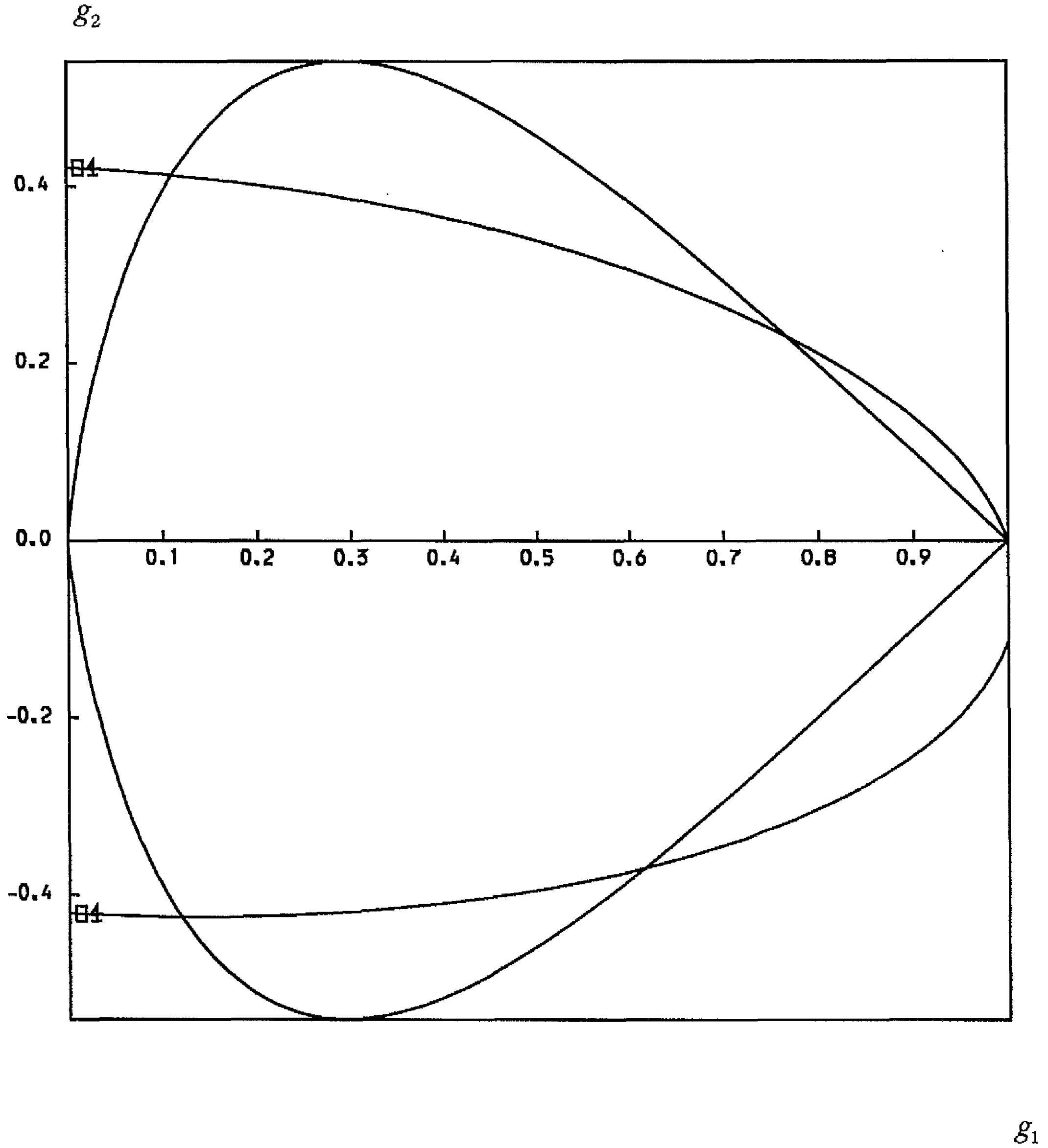


Figure (3.31)

Combined plots of the set $G=\left\{(g_1,g_2)^t : g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\right\}$ and the ellipsoid $Q=\left\{(g_1,g_2)^t : (g_1,g_2)^t M^{*^{-1}}\begin{pmatrix} g_1 \\ g_2 \end{pmatrix}=2\right\}$ for the double exponential distribution and the case $a>-u_4$, where M^* is the global D-optimal design matrix on Z=[a,b], whose support points are {a,b}, $b<|a|$ with a=-0.4 and b=0.2.

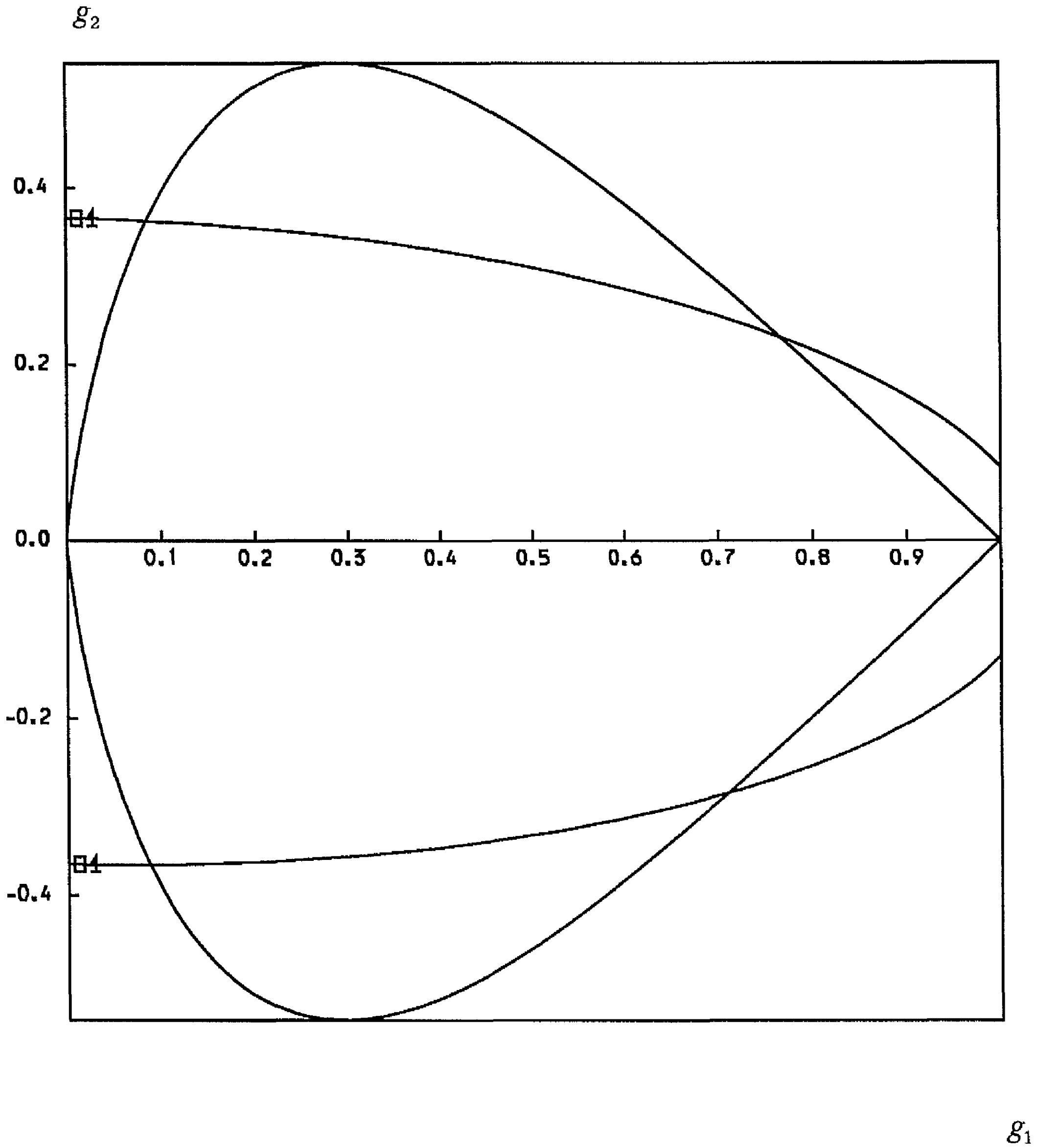


Figure (3.32)

Combined plots of the set $G=\left\{(g_1,g_2)^t : g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\right\}$ and the ellipsoid $Q=\left\{(g_1,g_2)^t : (g_1,g_2)^t M^{*^{-1}}\begin{pmatrix} g_1 \\ g_2 \end{pmatrix}=2\right\}$ for the double reciprocal distribution and the case $a<-u_2$ and $b>u_2$, where M^* is the global D-optimal design matrix on $Z_w=(-\infty,\infty)$, whose support points are $\{-u_2,0,u_2\}$ $(u_2=\sqrt{2})$ and weights $\{0.2617,0.4766,0.2617\}$.

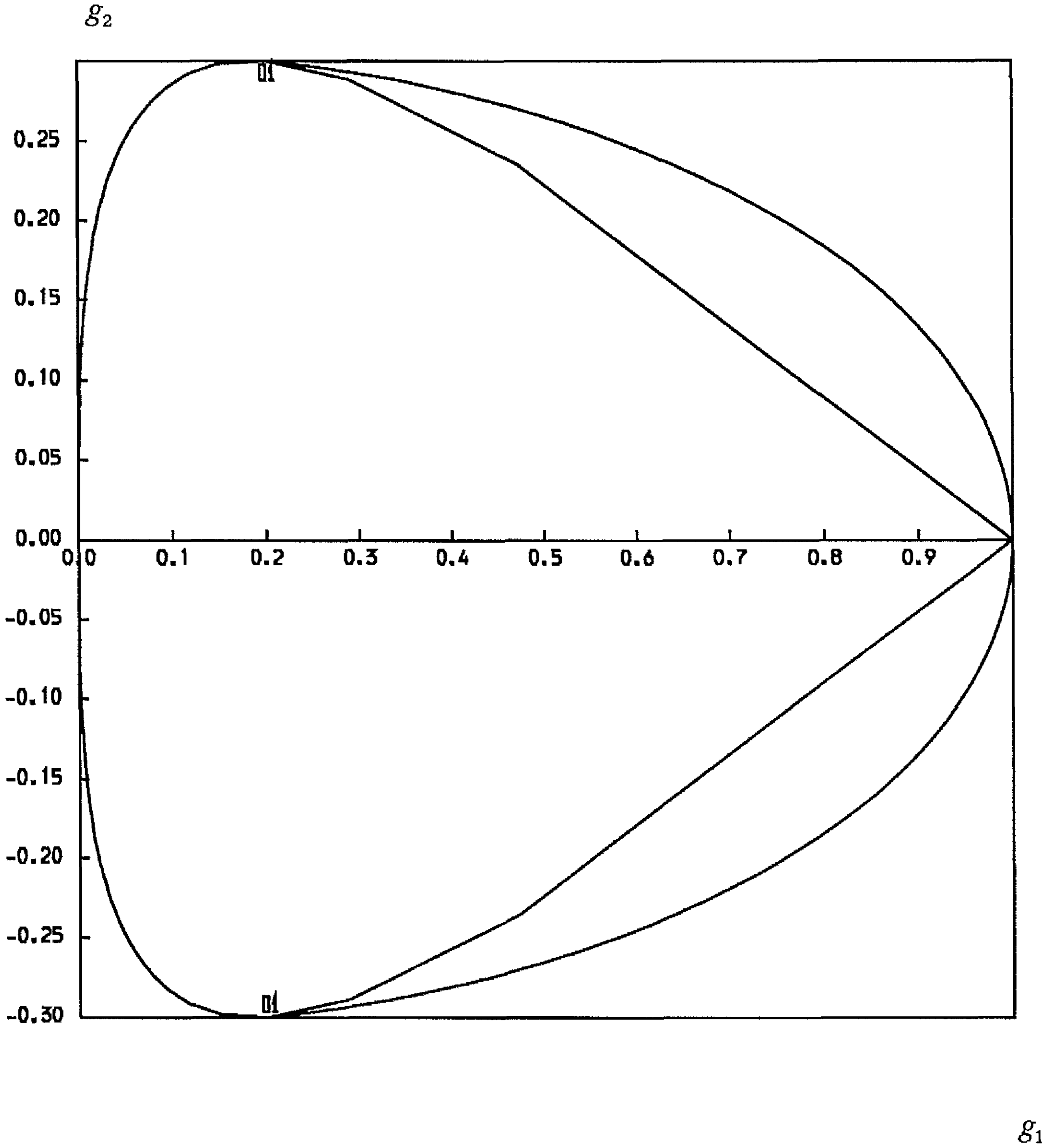


Figure (3.33)

Combined plots of the set $G=\{(g_1,g_2)^t : g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\}$ and the ellipsoid $Q=\left\{(g_1,g_2)^t : (g_1,g_2)^t M^{*^{-1}}\begin{pmatrix} g_1 \\ g_2 \end{pmatrix}=2\right\}$ for the double reciprocal distribution and the case $a<-u_1$, where M^* is the global D-optimal design matrix on $Z=(-\infty,0]$, whose support points are $\{-u_1,0\}$, $b<\tilde{z}(u_1)$ (u_1=1.618).

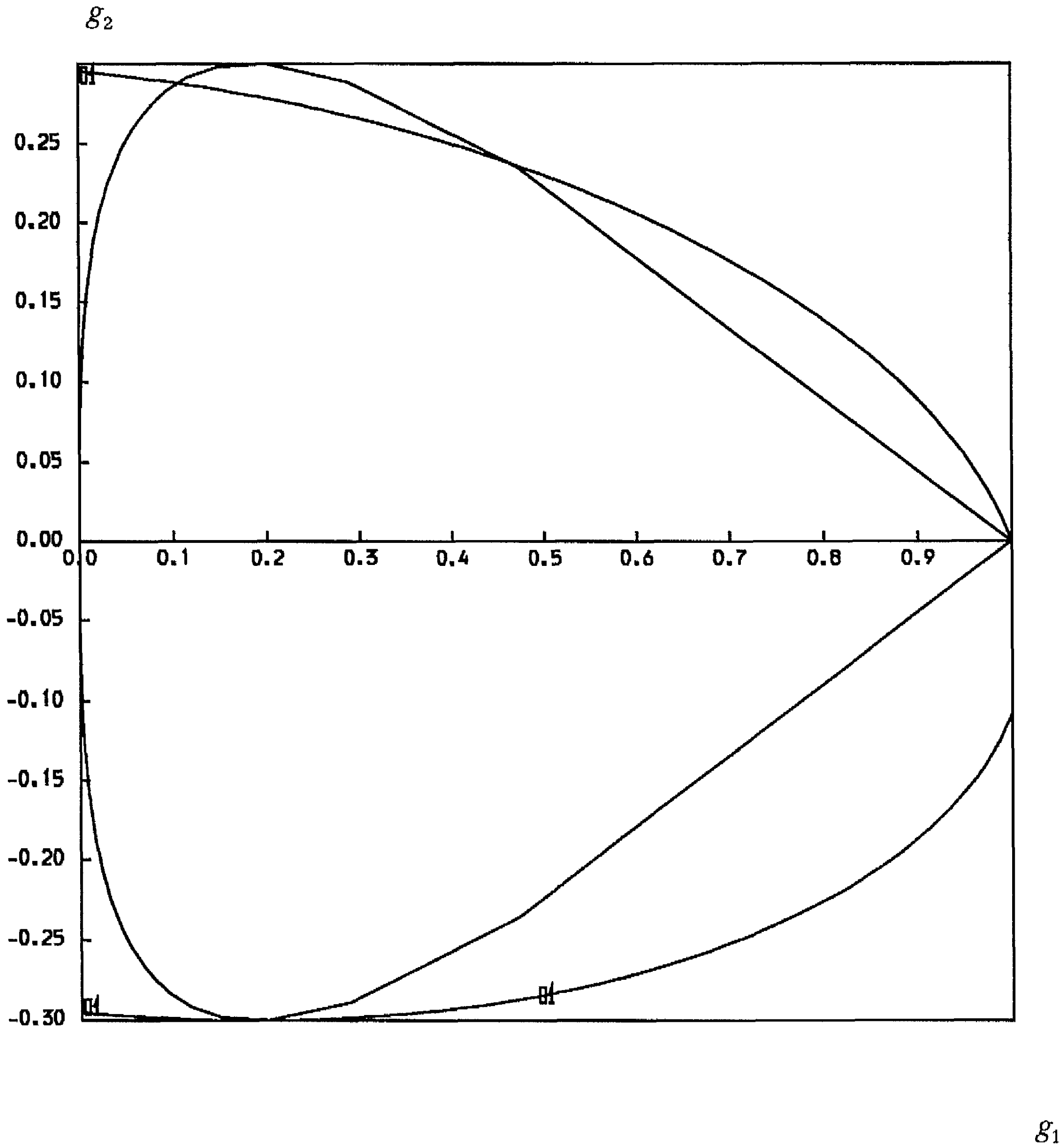


Figure (3.34)

Combined plots of the set $G=\{(g_1,g_2)^t : g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\}$ and the ellipsoid $Q=\left\{(g_1,g_2)^t : (g_1,g_2)^t M^{*^{-1}}\begin{pmatrix} g_1 \\ g_2 \end{pmatrix}=2\right\}$ for the double reciprocal distribution and the case $a<-u_1$, where M^* is the global D-optimal design matrix on Z=[a,b], whose support points are $\{a^*(b),0,b\}$,$\tilde{z}(u_1)<b<u_2$, with b=0.8, and $a^*(b)$=-1.4978.

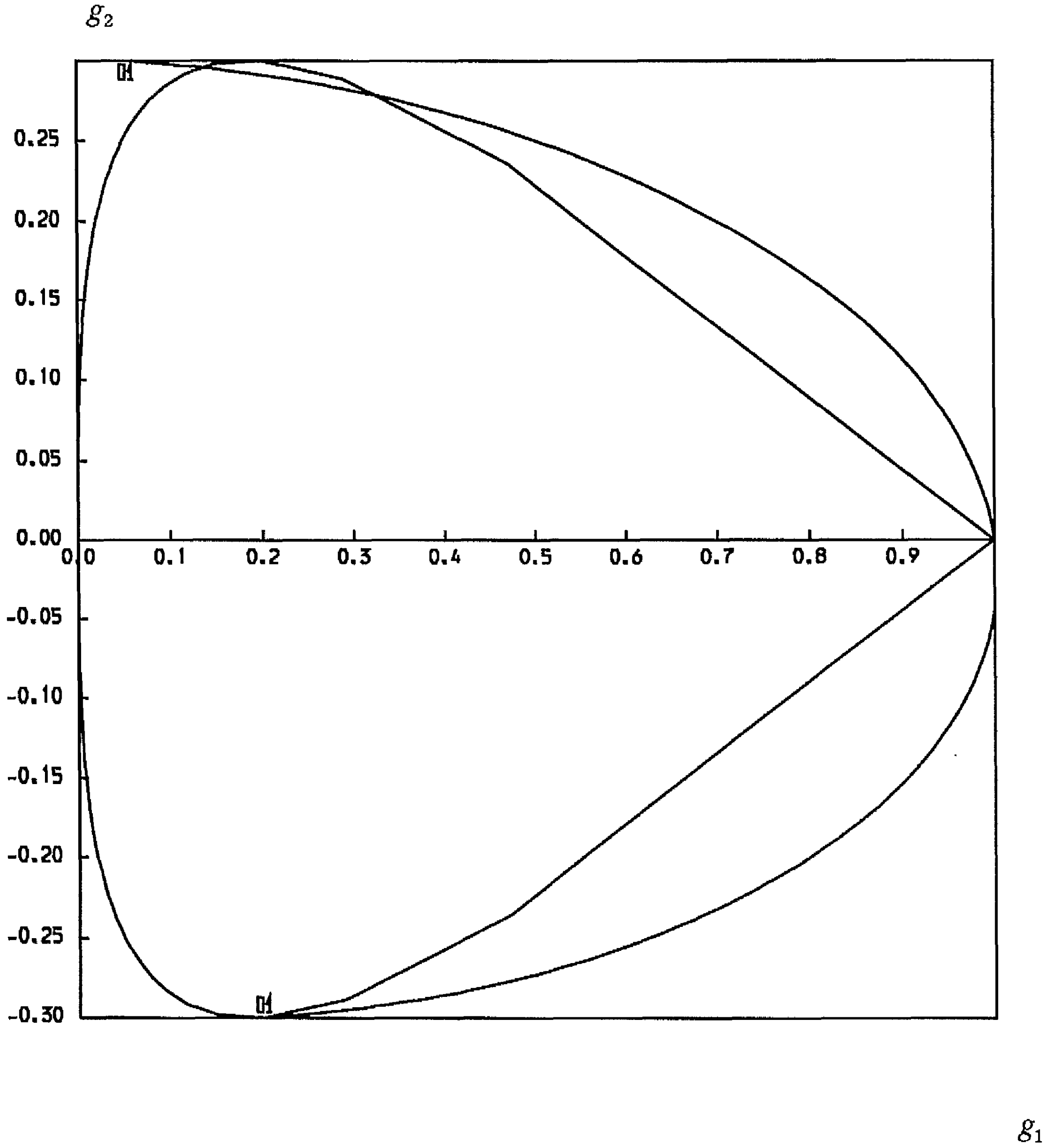


Figure (3.35)

Combined plots of the set $G=\{(g_1,g_2)^t : g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\}$ and the ellipsoid $Q=\left\{(g_1,g_2)^t : (g_1,g_2)^t M^{*^{-1}}\begin{pmatrix} g_1 \\ g_2 \end{pmatrix}=2\right\}$ for the double reciprocal distribution and the case $-u_1<a<-u_2$, where M^* is the global D-optimal design matrix on Z=[a,b], whose support points are {a,0}, $b<\tilde{z}(a)$, with a=-1.5.

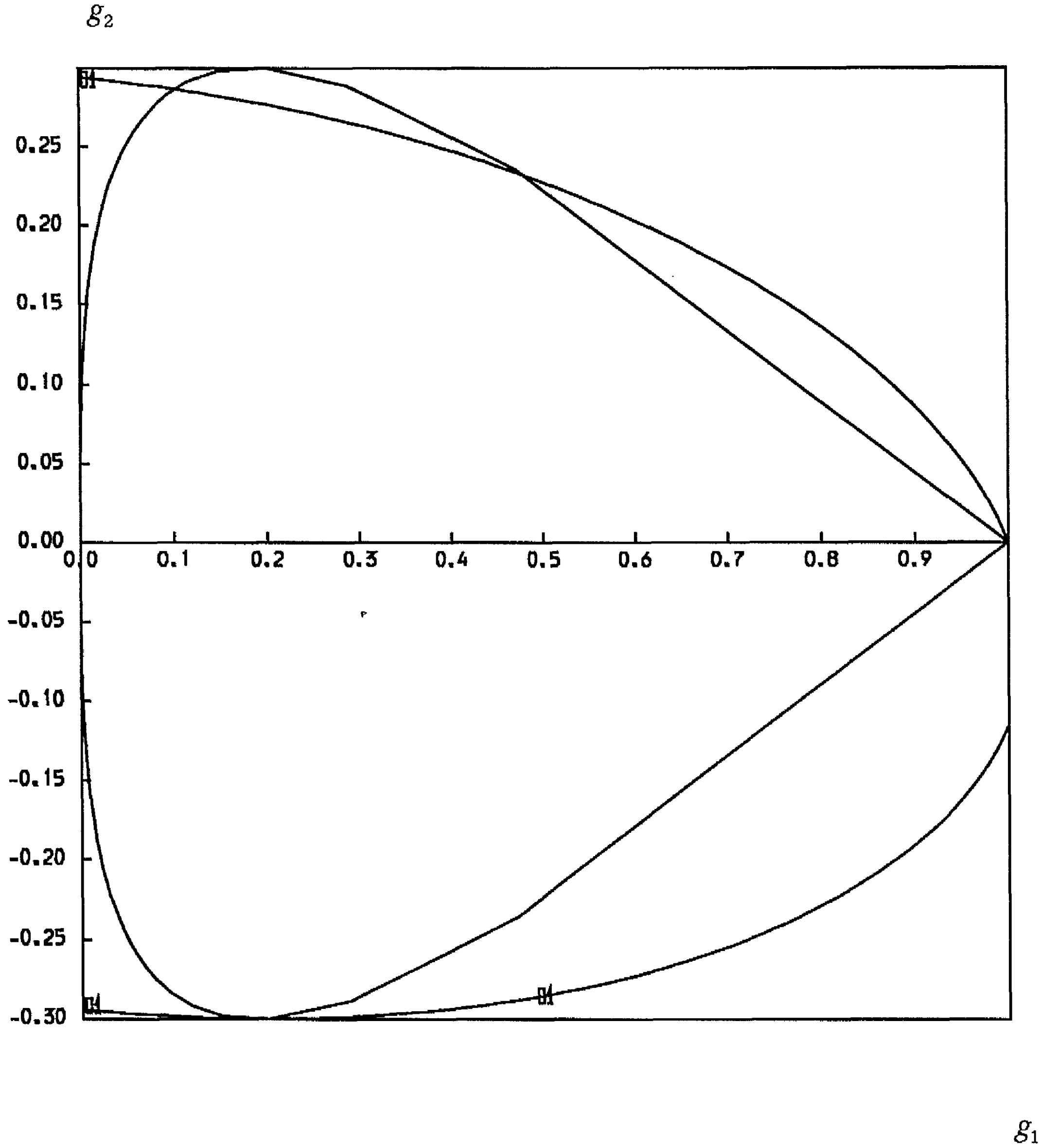


Figure (3.36)

Combined plots of the set $G=\left\{(g_1,g_2)^t : g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\right\}$ and the ellipsoid $Q=\left\{(g_1,g_2)^t : (g_1,g_2)^t M^{*^{-1}}\begin{pmatrix} g_1 \\ g_2 \end{pmatrix}=2\right\}$ for the double reciprocal distribution and the case $-u_1 < a < -u_2$, where M^* is the global D-optimal design matrix on Z=[a,b], whose support points are {a,0,b}, $\tilde{z}(a) < b < \tilde{z}(u_1)$, with a=-1.3105, $\tilde{z}(a)$=0.4113 and b=0.4.

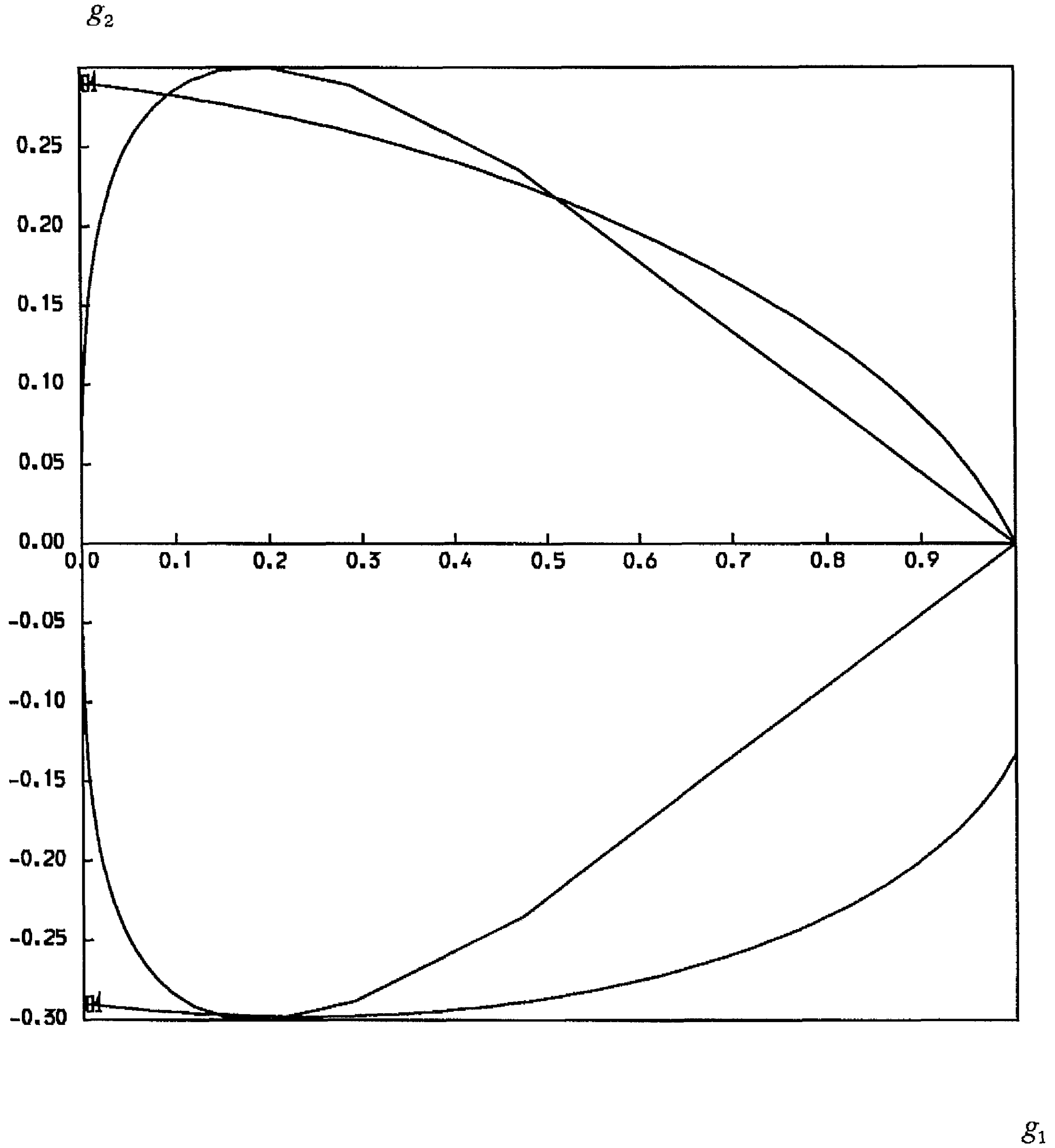


Figure (3.37)

Combined plots of the set $G=\left\{(g_1,g_2)^t : g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\right\}$ and the ellipsoid $Q=\left\{(g_1,g_2)^t : (g_1,g_2)^t M^{*^{-1}}\begin{pmatrix} g_1 \\ g_2 \end{pmatrix}=2\right\}$ for the double reciprocal distribution and the case $-u_1 < a < -u_2$, where M^* is the global D-optimal design matrix on Z=[a,b], whose support points are {max,0,b}, $\tilde{z}(u_1) < b < u_2$ where $\max=\max\{a,a^*(b)\}$={-1.2,-1.5316} and b=0.7.

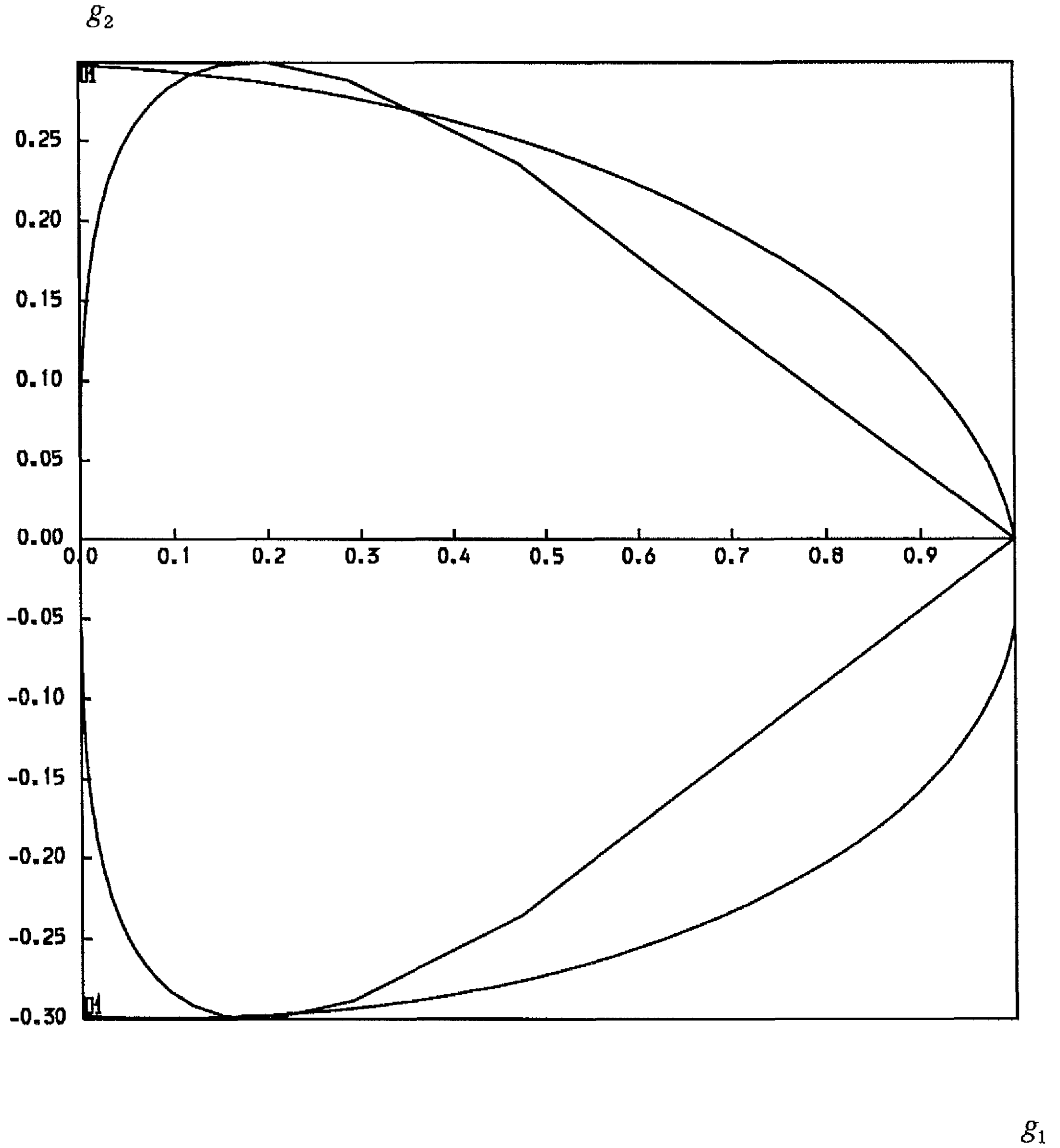


Figure (3.38)

Combined plots of the set $G=\{(g_1,g_2)':g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\}$ and the ellipsoid $Q=\left\{(g_1,g_2)':(g_1,g_2)'M^{*^{-1}}\begin{pmatrix}g_1\\ g_2\end{pmatrix}=2\right\}$ for the double reciprocal distribution and the case $-u_2<a<-u_3$, where M^* is the global D-optimal design matrix on Z=[a,b], whose support points are {a,0}, $b<\tilde{z}(a)$ with a=-0.9 and $\tilde{z}(a)$=0.2146.

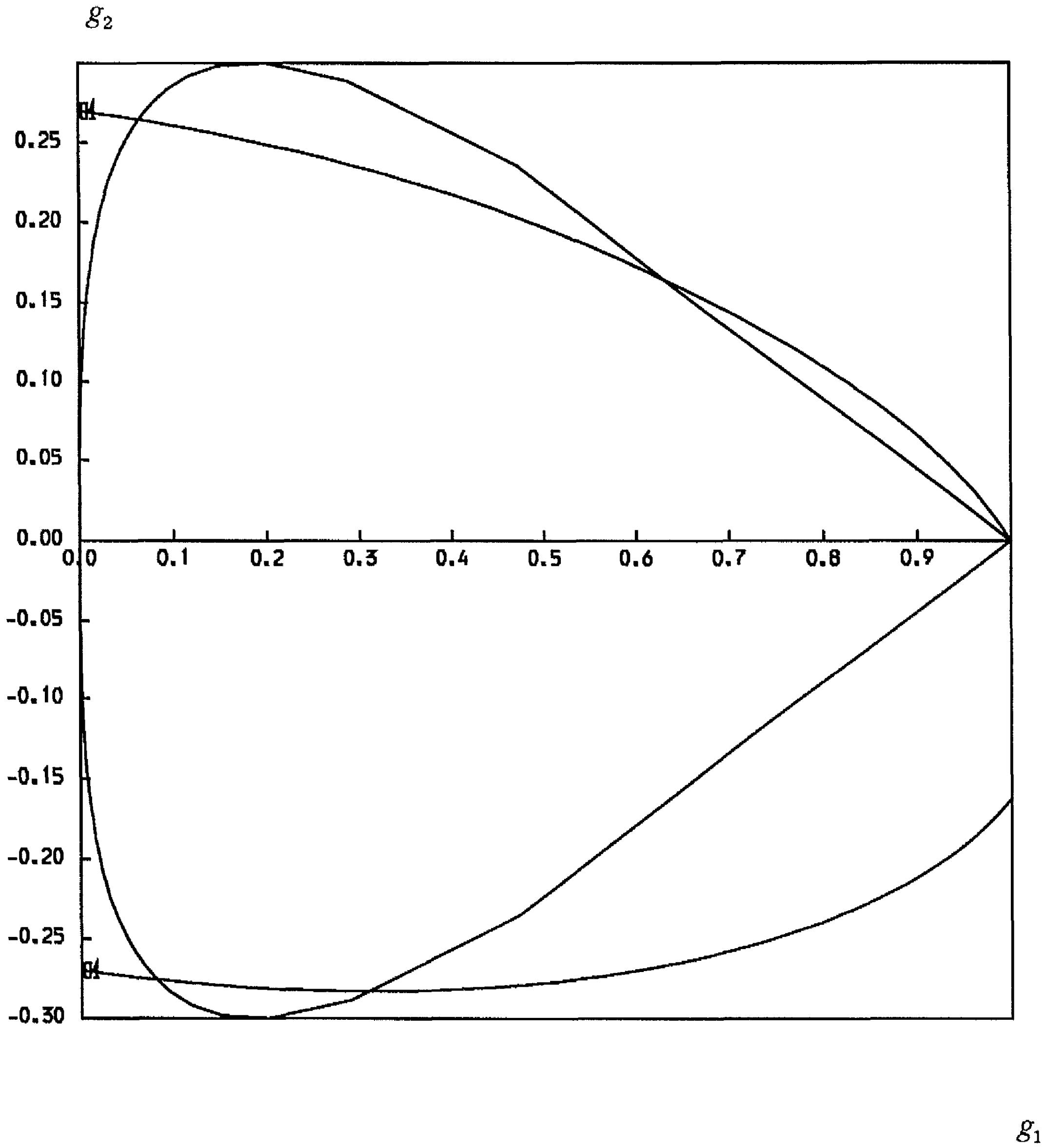


Figure (3.39)

Combined plots of the set $G=\left\{(g_1,g_2)':g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\right\}$ and the ellipsoid $Q=\left\{(g_1,g_2)':(g_1,g_2)'M^{*^{-1}}\begin{pmatrix}g_1\\g_2\end{pmatrix}=2\right\}$ for the double reciprocal distribution and the case $-u_2<a<-u_3$, where M^* is the global D-optimal design matrix on Z=[a,b], whose support points are {a,0,b}, $\tilde{z}(a)<b<|a|$ with a=-0.7, $\tilde{z}(a)$=0.1040 and b=0.3.

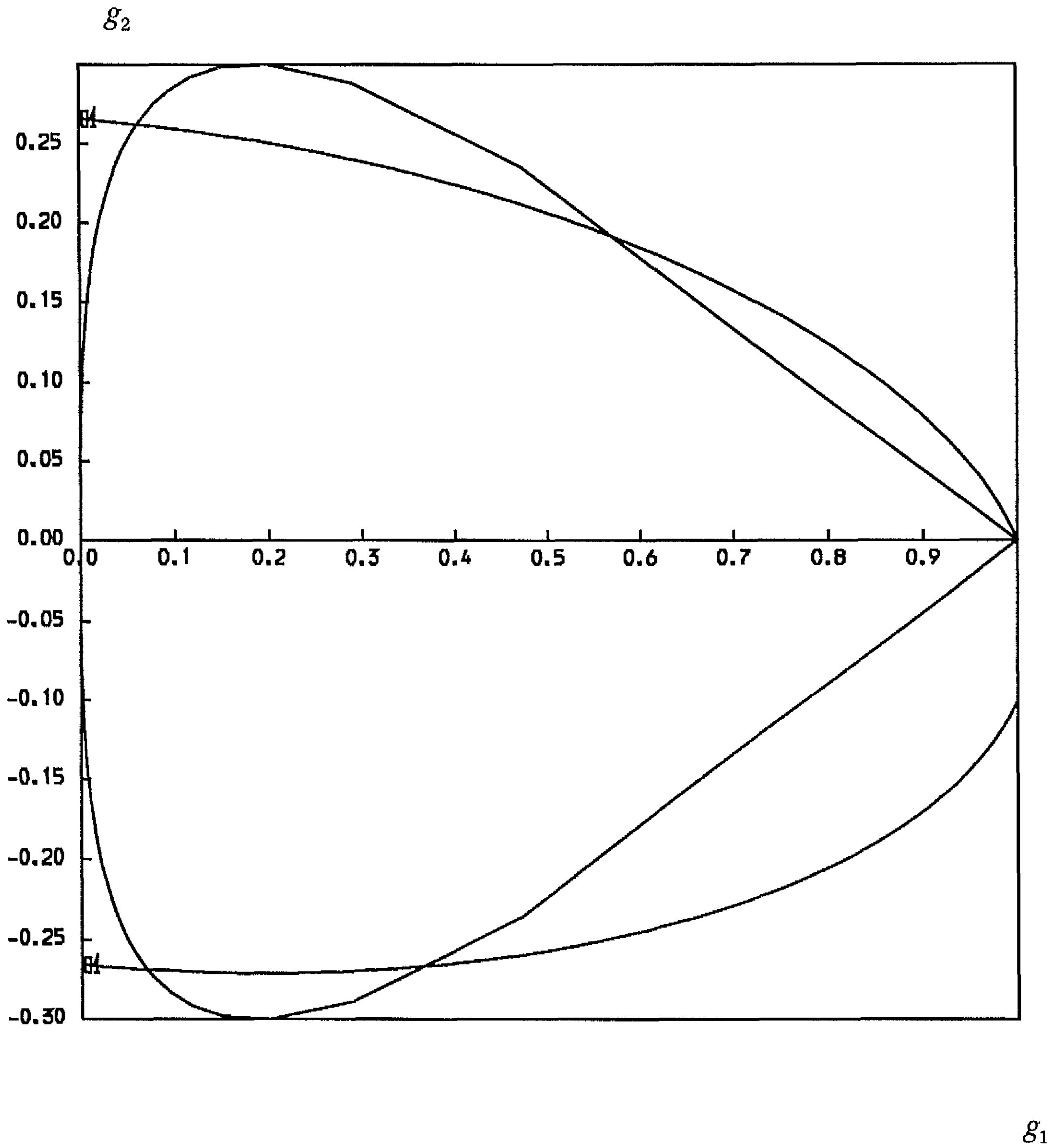


Figure (3.40)

Combined plots of the set $G=\{(g_1,g_2)^t: g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\}$ and the ellipsoid $Q=\left\{(g_1,g_2)^t:(g_1,g_2)^t M^{*^{-1}}\begin{pmatrix}g_1\\ g_2\end{pmatrix}=2\right\}$ for the double reciprocal distribution and the case $-u_3<a<-u_4$, where M^* is the global D-optimal design matrix on Z=[a,b], whose support points are {a,b}, $b<z^+(a)$ with a=-0.3, $z^+(a)$=0.12, and b=0.1.

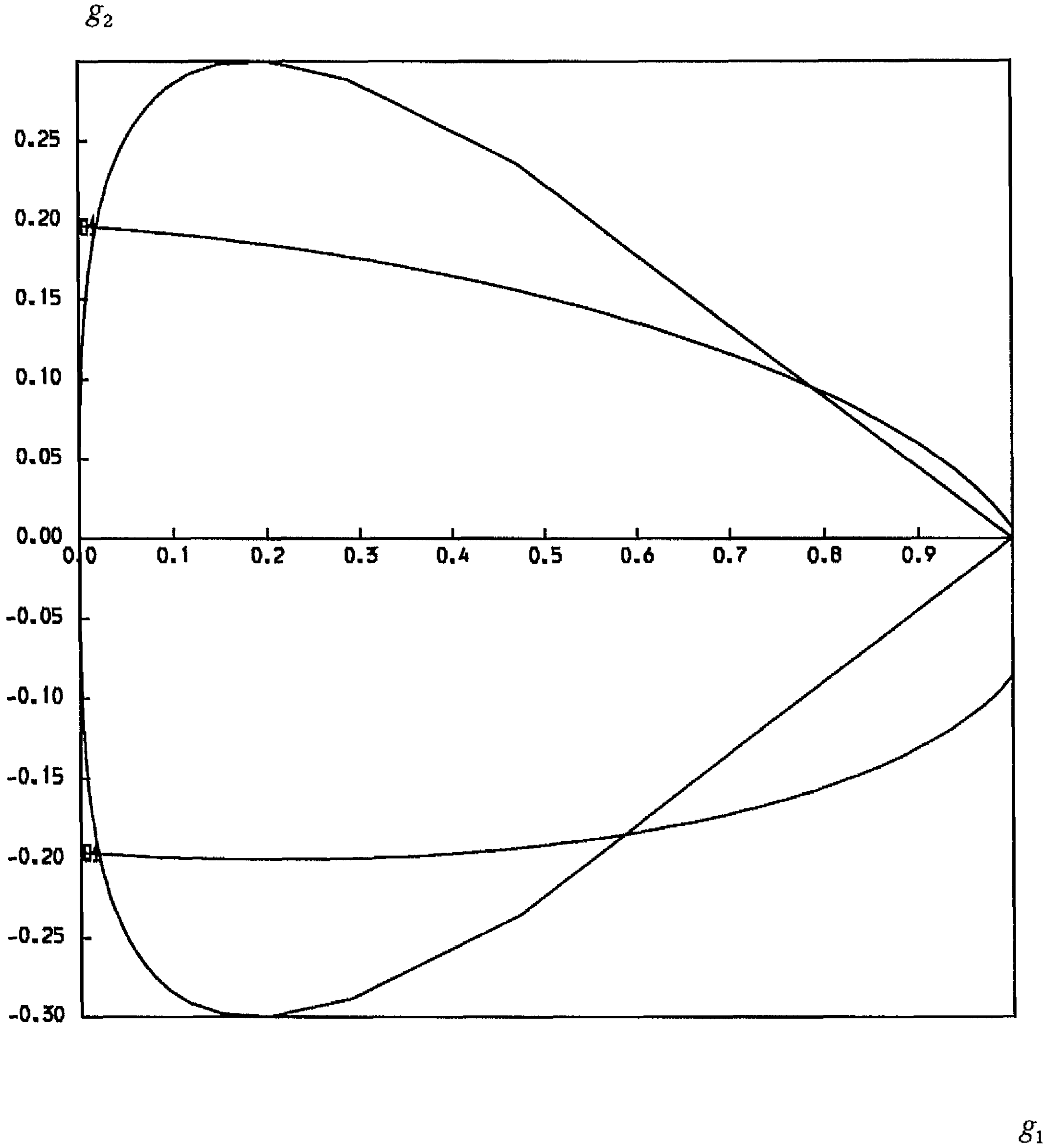


Figure (3.41)

Combined plots of the set $G=\left\{(g_1,g_2)':g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\right\}$ and the ellipsoid $Q=\left\{(g_1,g_2)':(g_1,g_2)'M^{*^{-1}}\begin{pmatrix}g_1\\g_2\end{pmatrix}=2\right\}$ for the double reciprocal distribution and the case $-u_3<a<-u_4$, where M^* is the global D-optimal design matrix on Z=[a,b], whose support points are {a,0,b}, $z^+(a)<b<|a|$ with a=-0.4, $z^+(a)$=0.05, and b=0.3.

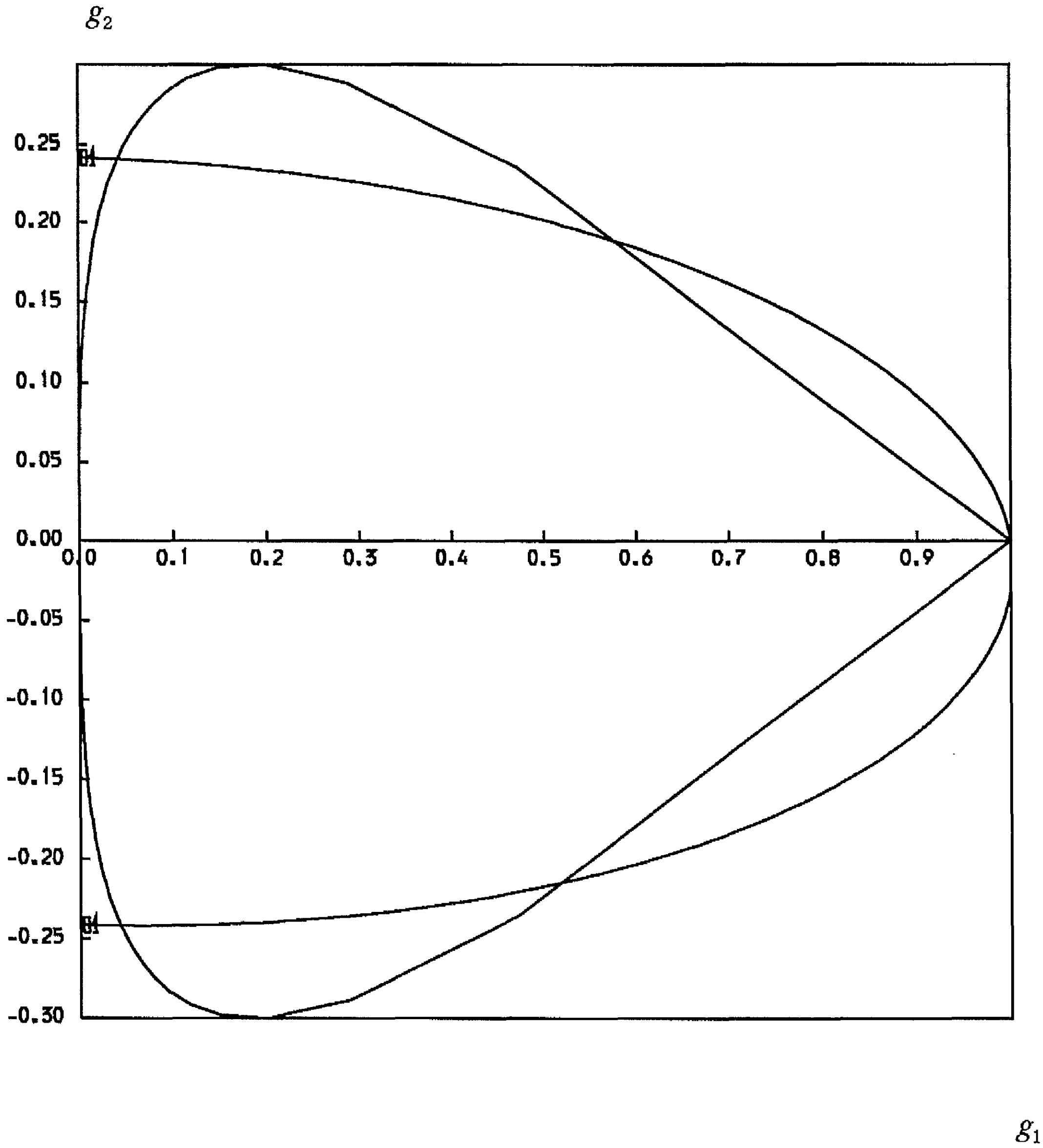
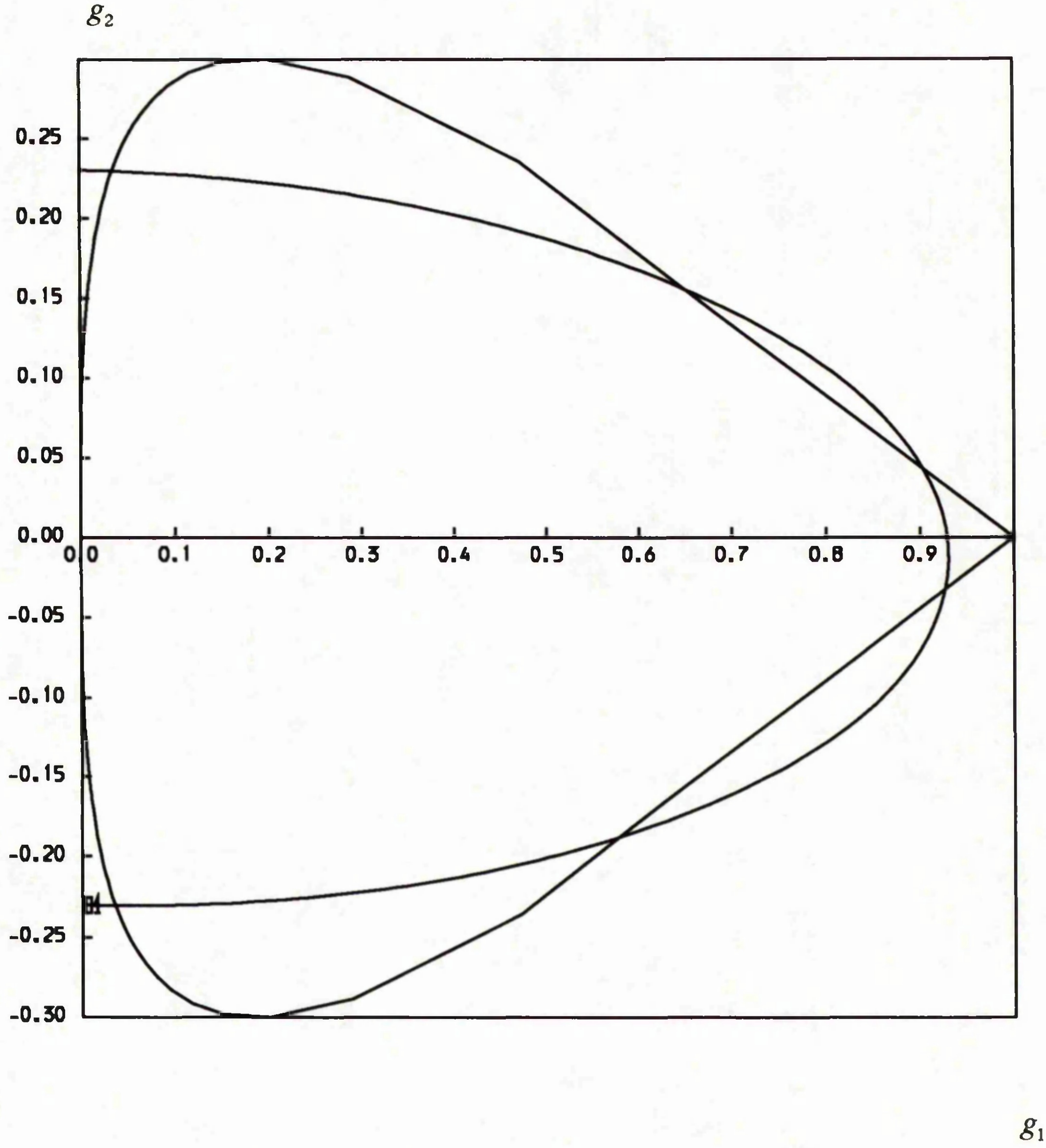


Figure (3.42)

Combined plots of the set $G=\{(g_1,g_2)':g_1=\sqrt{w(z)},\ g_2=zg_1,\ z\in R\}$ and the ellipsoid $Q=\left\{(g_1,g_2)':(g_1,g_2)'M^{*^{-1}}\begin{pmatrix}g_1\\g_2\end{pmatrix}=2\right\}$ for the double reciprocal distribution and the case $a>-u_4$, where M^* is the global D-optimal design matrix on Z=[a,b], whose support points are {a,b}, $b<|a|$ with a=-0.3, and b=0.2.



CHAPTER FOUR

LOCALLY c-OPTIMAL DESIGNS

4.1 INTRODUCTION

As in the previous chapter we will continue to focus on two parameter models and assume that there is interest in estimating a particular linear combination of both parameters, so that we consider the **c**-optimal criterion.

4.2 MODEL

Recall the model employed in section 3.2. Using the same notation, we specifically consider the following case in which

1) $\eta = \eta(\alpha + \beta x)$.

2) The design variable x is a scalar.

3) The design space χ is a line segment, say $\chi = [c,d]$.

That is $$\underline{\theta} = (\alpha,\beta)^t \ ,$$

and the matrix B of section 2.4 is

$$B = \begin{pmatrix} 1 & 0 \\ \alpha & \beta \end{pmatrix},$$

leading to a canonical version of the design problem for which

4) The design variable $z = \alpha + \beta x$, and hence the dependence of the solution on α and β is only through the transformation z to $x = (z - \alpha)/\beta$.

5) The design space Z is also a line segment, say $Z = [a,b]$.

6) The expected information matrix is

$$M_z = E\left\{ w(z)\begin{pmatrix}1\\ z\end{pmatrix}(1 \quad z)\right\}.$$

7) As noted in section 2.5, $\underline{c} \rightarrow \underline{c}_z$, with $\underline{c}_z = B\underline{c}$.

In this case we try to solve this problem for all possible line segments. A two-stage approach is employed. Firstly we identify or distinguish the support points of an optimal design, that is z-values with positive weight. Then we determine these optimal weights. First we derive an explicit formula to calculate the **c**-optimal weights.

4.3 c-OPTIMAL WEIGHTS

Recently Kitsos, Titterington and Torsney (1988, section 6.1) established an explicit formula to compute **c**-optimal design weights provided the regression vectors that support the design are linearly independent, but the result first appeared in Torsney (1981). We consider the two parameter context. A consequence of caratheodory's theorem is that there exists a **c**-optimal design with a support of at most two points, say z_1 , z_2 with positive weights p_1, p_2 (Appendix AI.2). We now derive an explicit expression to calculate these optimal weights.

Let us suppose that a design ξ assigns weights p_1, p_2 to two points z_1 , z_2 such that $\underline{g}(z_1)$, $\underline{g}(z_2) \in R^2$ are linearly independent. Then the information matrix of this design from section 3.3 is given by

$$M = \begin{bmatrix} p_1 w(z_1) + (1-p_1) w(z_2) & p_1 z_1 w(z_1) + (1-p_1) z_2 w(z_2) \\ p_1 z_1 w(z_1) + (1-p_1) z_2 w(z_2) & p_1 z_1^2 w(z_1) + (1-p_1) z_2^2 w(z_2) \end{bmatrix},$$

since $p_1 + p_2 = 1$, which implies that $p_2 = 1 - p_1$.

The criterion function ϕ_2 with $\underset{\sim}{c} = (c_1, c_2)^t$ can be written in a more general form, namely

$$\phi_2 = -\underset{\sim}{c}^t M^- \underset{\sim}{c},$$

where M^- is any generalised inverse (g-inverse) of the information matrix M, that is any matrix such that $M M^- M = M$ (Appendix AII.1). We permit M to be singular because, as it turns out, the optimal design is often a one-point design with a singular M. Thus

$$\phi_2 = -\left\{ \frac{h_{z_1}^2}{p_1} + \frac{h_{z_2}^2}{(1-p_1)} \right\}, \tag{4.3.1}$$

where $h_{z_1} = \dfrac{(c_1 z_2 - c_2)}{(z_2 - z_1) v(z_1)}$, $h_{z_2} = \dfrac{(c_1 z_1 - c_2)}{(z_2 - z_1) v(z_2)}$ and $v(z) = \{w(z)\}^{1/2}$.

Straightforward differentiation of equation (4.3.1) shows that the optimal value of p_1 is given by

$$p_1^* = \frac{|h_{z_1}|}{|h_{z_1}| + |h_{z_2}|}. \tag{4.3.2}$$

Which is equivalent to

$$p_1^* = \frac{(c_1 z_2 - c_2) v(z_2)}{(c_1 z_2 - c_2) v(z_2) + (c_1 z_1 - c_2) v(z_1)}.$$

Substituting the value of p_1^* in equation (4.3.1), yields

$$\phi_2 = -\left(h_{z_1} + h_{z_2}\right)^2. \tag{4.3.3}$$

4.4 GEOMETRICAL CONSTRUCTION

We rely on a construction of Elfving (1952) to deduce the **c**-optimal designs, which can be obtained by the following remarkable method; see also Chernoff (1979).

Let us assume that the induced design space G is closed and bounded, i.e. the set G defined in equation (3.4.1) is compact. Let G^- be the reflection of G about the origin and G^* be the boundary of the convex hull generated by G and G^-. Consider the vector $\underline{c}$. Let this define a ray from the origin and let it stretch out, if necessary, to intersect G^*. When $G \in R^2$ this intersection can be expressed as a convex combination of at most two points taken from G and/or G^-. If it is a one point design then the support point is z_c where $\underline{c} \propto \underline{g}(z_c)$. In the case of two points let z_1^* and z_2^* be the related points in Z. Then the **c**-optimal design has support at z_1^* and z_2^* with optimal weights p_1^* and $p_2^*=1-p_1^*$, where p_1^* given by equation (4.3.2).

We now use Elfving's method, to derive **c**-optimal designs for all induced design spaces G's considered in chapter 3, including those gleaned from the literature on weighted linear regression.

4.4.1 Determination of G^*

(a) $a=-\infty, b=\infty$:

For binary weight functions $w(z)=\dfrac{f^2(z)}{F(z)[1-F(z)]}$, G depends on the distribution function F. Realistically we must impose some restrictions on the latter. A key assumption is that $F\in\Im_c$, where $\Im_c$ denotes the set of F such that the curve $G=\{v(z)(1,z),-\infty<z<\infty\}$ satisfies

i) G is closed and bounded,

ii) G is convex. (4.4.1)

Let the slope of the curve G at z be denoted by $r(z)$ or by $s(z_1,z_2)$, namely

$$r(z)=\left[\frac{d}{dz}\{v(z)z\}\right]\left[\frac{d}{dz}\{v(z)\}\right]^{-1}$$

$$=z+\frac{v(z)}{v'(z)}. \tag{4.4.2}$$

While

$$s(z_1,z_2)=\left[v(z_1)z_1+v(z_2)z_2\right]\left[v(z_1)+v(z_2)\right]^{-1}. \tag{4.4.3}$$

The condition (4.4.1) on G is crucial for the previous development of c-optimal designs. The convexity of G can be established by showing that the slope $r(z)$ of G, is nondecreasing over each of the two intervals $Z=(-\infty,z_{\max}]$ and $Z=[z_{\max},\infty)$, where $z_{\max}$ is the value of z which maximises $v(z)$ over the widest choice $Z_w=(-\infty,\infty)$. If $v(z)$ is symmetric about the origin (so that $z_{\max}=0$), this property needs to be verified only for one of the two intervals

$Z = (-\infty, 0]$ or $Z = [0, \infty)$. A sufficient condition for this is that $\frac{d}{dz}[\log v(z)]$ is non increasing, i.e. $v(z)$ is log-concave. See Ford, Torsney and Wu (1992) for the proof.

The second method has the additional advantage that it automatically ensures condition (4.4.1) (ii). This follows because $w(z)$ is assumed to be measurable and $v(z)$ is integrable as the following confirms.

$$\int_{-\infty}^{\infty} v(z)dz,$$

$$= \int_{-\infty}^{\infty} \{F(z)[1-F(z)]\}^{\frac{-1}{2}} f(z)dz$$

$$= \int_{0}^{1} \{u(1-u)\}^{\frac{-1}{2}} du = B(\tfrac{1}{2}, \ \tfrac{1}{2}) = \pi < \infty,$$

where $u = F(z)$ and $B(a,b)$ denote the beta function with parameters a,b.

When the condition (4.4.1) is satisfied, G^* decomposes into two arcs and two line segments. Thus there exists two values z_1, z_2, such that the boundary G^* consists of the arc $A = \{v(z)(1,z), z_1 < z < z_2\}$, its reflection A^- about the origin, the line segment L which connects $-v(z_1)(1,z_1)$ and $v(z_2)(1,z_2)$ and its reflection L^- about the origin. For the widest choice $Z_w = (-\infty, \infty)$, z_1, z_2 are the solutions to

$$r(z_1) = s(z_1, z_2), \tag{4.4.4a}$$

and

$$r(z_2) = s(z_1, z_2), \tag{4.4.4b}$$

where $r(z)$ and $s(z_1, z_2)$ are given in equations (4.4.2) and (4.4.3).

The problem is simplified when F is symmetric, that is $F(-z)=1-F(z)$, $F(z)>0$. The solution of (4.4.4) is $z_1=-z_2$, $z_2>0$ satisfying $r(z_2)=0$. Ford, Torsney and Wu (1992) list the values of z_1 ,z_2 for all the binary models.

(b) $a \geq -\infty, b \leq \infty$:

Here G^* again consists of two arcs and two line segments, but with potentially different z_1, z_2. Denote the z_1 and z_2 values for the widest choice Z_w by a^*, b^* respectively. There are four cases which depend on the relationship of a,b to a^*, b^*. The following results are direct consequences of Elfving's approach.

(i) $a \leq a^*$ and $b \geq b^*$: $z_1 = a^*$ and $z_2 = b^*$;

(ii) $a \geq a^*$ and $b \leq b^*$: $z_1 = a$ and $z_2 = b$;

(iii) $a \leq a^*$ and $b < b^*$: $z_1 = \max(a, z_b)$ and $z_2 = b$,

where z_b solves (4.4.4a), with $z_2 = b$. It is clear that $z_b < a^*$;

(iv) $a > a^*$ and $b \geq b^*$: $z_1 = a$ and $z_2 = \min(b, z_a)$,

where z_a solves (4.4.4b), with $z_1 = a$. obviously $z_a > b^*$.

We summarise the above statements in Table (4.1) and report calculations in Table (4.2) for $Z = Z_1 = (-\infty, z_{\max}]$ and $Z = Z_2 = [z_{\max}, \infty)$, where $z_{\max}$ is the value of z which maximises $v(z)$.

We note that if two supports are needed on these spaces then one of them is $z_{\max}$, i.e. if $Z = Z_1, z_2 = z_{\max}$; if $Z = Z_2$,$z_1 = z_{\max}$. Denote by u_1 the value of z_1 on Z_1 and by u_2 the value of z_2 on Z_2. The values of $u_1, z_{\max}, u_2$ are listed in Table (4.2).

(c) $\boldsymbol{G} = \boldsymbol{G}_i$ $(i = 1,2,3)$:

Under (4.4.1), the previous decomposition of G^* for all the binary models, into two arcs and two line segments, holds with one major difference. Here $z_1 < z_2$ are in $Z_w = (-1,1)$ and in $Z_w = (0,\infty)$ for the asymmetric weight functions $w_1(z)$ and $w_2(z)$ (symmetric if $(\alpha = \beta)$) of chapter 3 respectively, and are the solutions to equation (4.4.4). The widest choice Z_w of the symmetric weight function $w_3(z)$ is the same as that for the binary models. We tabulate the values of z_1 and z_2 for the three weight functions considered in chapter 3 in particular cases in Table (4.3).

Table (4.4) records for these weight functions the same information as is recorded in Table (4.2) for the binary models.

4.4.2 Determination of optimal designs:

For all G's satisfying (4.4.1) we may summarise the results in the following two main steps.

(i) If $\underline{c}$ is proportional to $g(z_c)$, where z_c is such that $z_1 \le z_c \le z_2$, then the **c**-optimal design is a one point design concentrated at z_c;

(ii) for other $\underline{c}$, the **c**-optimal design is a two point-design concentrating on z_1 with weight p_1 and on z_2 with weight $(1-p_1)$, where z_1 and z_2 are determined by (4.4.4a) and (4.4.4b) and the optimal value of p_1 can be obtained explicitly from equation (4.3.2).

Finally we note, in respect of the binary models, that optimal designs for estimating percentiles are **c**-optimal designs. Wu (1988) shows that for given p the optimal design for estimating L_p, where $F(L_p) = p$, is the **c**-optimal design for

$\underline{c} = (1, L_p)^t$. It follows that the c-optimal design for any $\underline{c}$ with $c_1 \neq 0$ is equivalent to the optimal design for estimating $L_p = {}^{c_2}/_{c_1}$ for some p when the distribution function $F(z) > 0$ for all $z \in R$. Wu (1988) derives L_p-optimal designs for a range of values of p for all the binary models considered in the previous chapter.

Table (4.1); Supports of two-point **c**-optimal designs on a general interval Z=[a,b] .

$Z=[a,b]$	z_1	z_2
1) $a \le a^*$, $b \ge b^*$	a^*	b^*
2) $a \ge a^*$, $b \le b^*$	a	b
3) $a \le a^*$, $b < b^*$	$\max\{a,z_b\}$	b
4) $a > a^*$, $b \ge b^*$	a	$\min\{b,z_a\}$

Notes on Table (4.2) :

i) a^*,b^* are such that $z_1=a^*$ and $z_2=b^*$ when $Z_w=(-\infty,\infty)$; see Table (4.2) for particular cases.

ii) z_a solves equation (4.4.4b) with $z_1=a$ while z_b solves equation (4.4.4a) with$z_2=b$.

Table (4.2); Support of two-point **c**-optimal designs on $Z_1 = \{z : z \le z_{\max}\}$ ($\{u_1, z_{\max}\}$) and on $Z_2 = \{z : z \ge z_{\max}\}$ ($\{z_{\max}, u_2\}$). (Note s=sign(z)).

Name	$f_i(z)$	$F_i(z)$	u_1	$z_{\max}$	u_2
1) Logit	$e^{-z}\,(1+e^{-z})^{-2}$	$(1+e^{-z})^{-1}$	-3.087	0.0	3.087
2) Probit	$\frac{1}{\sqrt{2\pi}}\,e^{(-z^2/2)}$	$\Phi(z)$	-1.895	0.0	1.895
3) Double Exponential	$\frac{1}{2}\,e^{-\lvert z\rvert}$	$\frac{(1+s)}{2} - \frac{s}{2}e^{-\lvert z\rvert}$	-2.333	0.0	2.333
4) Double Reciprocal	$\frac{1}{2}(1+\lvert z\rvert)^{-2}$	$\frac{(1+s)}{2} - \frac{s}{2}(1+\lvert z\rvert)^{-1}$	-2.414	0.0	2.414
5) Complementary Log-Log	$Exp(z-e^z)$	$1-Exp(-e^z)$	-2.398	0.466	1.564
6-9) Skewed Logit	$m[F_1(z)]^{m-1}f_1(z)$	$(1+e^{-z})^{-m}$	-------	-------	-------
6) $m=1/3$	...	...	-7.672	-.519	2.677
7) $m=2/3$	...	...	-4.306	-.228	2.903
8) $m=3/2$	...	...	-2.166	0.269	3.311
9) $m=3$	...	...	-0.971	0.807	3.783

Table (4.3); Supports z_1, z_2 of two-point **c**-optimal designs of the three weight functions of chapter 3 on Z_w.

Weight function	α	β	z_1	z_2
$w_1(z) = (1-z)^{\alpha+1}(1+z)^{\beta+1}$	0.0	0.0	-0.707	0.707
" "	0.0	1.0	-0.447	0.789
" "	1.0	0.0	-0.789	0.447
" "	1.0	1.0	-0.577	0.577
" "	1.0	2.0	-0.400	0.657
" "	1.0	3.0	-0.255	0.711
" "	2.0	3.0	-0.366	0.571
$w_2(z) = z^{\alpha+1}e^{-z}$	0.0	----	0.386	4.255
" "	1.0	----	0.926	5.725
" "	2.0	----	1.542	7.114
" "	3.0	----	2.204	8.454
" "	4.0	----	2.899	9.760
" "	5.0	----	3.620	11.04
$w_3(z) = e^{-z^2}, Z_w = (-\infty, \infty)$	----	----	-1.0	1.0

Table(4.4); Supports of two-point **c**-optimal designs on $Z_1 = \{z : z \le z_{\max}\}$ $(\{u_1, z_{\max}\})$ and on $Z_2 = \{z : z \ge z_{\max}\}$ $(\{z_{\max}, u_2\})$ for the three weight functions of chapter 3.

Weight function	α	β	u_1	$z_{\max}$	u_2
$w_1(z) = (1-z)^{\alpha+1}(1+z)^{\beta+1}$	----	----	$u_1 \in (-1, z_{\max}]$	$(\beta-\alpha)/(\alpha+\beta+2)$	$u_2 \in [z_{\max}, 1)$
" "	0.0	0.0	-0.786	0.0	0.786
" "	0.0	1.0	-0.527	1/3	0.862
" "	1.0	1.0	-0.662	0.0	0.662
" "	1.0	2.0	-0.483	1/5	0.737
" "	2.0	1.0	-0.737	-1/5	0.483
" "	2.0	2.0	-0.582	0.0	0.582
" "	3.0	1.0	-0.784	-1/3	0.333
$w_2(z) = z^{\alpha+1}e^{-z}$	----	----	$u_1 \in (0, z_{\max}]$	$(\alpha+1)$	$u_2 \in [z_{\max}, \infty)$
" "	0.0	----	0.195	1.0	4.512
" "	1.0	----	0.605	2.0	6.126
" "	2.0	----	1.118	3.0	7.622
$w_3(z) = e^{-z^2}, Z_w = (-\infty, \infty)$	----	----	-1.216	0.0	1.216

CHAPTER FIVE

WEIGHTED REGRESSION MODELS

5.1 INTRODUCTION

The preceding two chapters have been concerned with the development and the establishment of the D-optimal and the c-optimal designs for two parameter models. In the present chapter we turn our attention to the problem of constructing D-optimal designs for three parameter models, including those for weighted quadratic regression and generalised linear models. We assume that there is interest in estimating all parameters.

5.2 OPTIMAL WEIGHTS

In the three parameter case a result of caratheodory's theorem is that there exists a D-optimal design with a support of between three and six points (Appendix AI.2). If the support has three points, then the optimal weights are $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$. We now derive this.

Suppose that a design ξ assigns weights p_1, p_2, p_3 to three points z_1, z_2, z_3 such that any two of $\underline{g}(z_1), \underline{g}(z_2), \underline{g}(z_3) \in R^3$ are linearly independent of each other. Then the information matrix of this design is given by

$$M = \left\{p_1 \underline{g}(z_1)\underline{g}(z_1)^t + p_2 \underline{g}(z_2)\underline{g}(z_2)^t + p_3 \underline{g}(z_3)\underline{g}(z_3)^t\right\}.$$

Let
$$V = \begin{pmatrix} 1 & 1 & 1 \\ z_1 & z_2 & z_3 \\ z_1^2 & z_2^2 & z_3^2 \end{pmatrix},$$

so that V is a 3×3 matrix, and denote its determinant by det(V). Then the determinant of M is given by

$$\varphi = |M| = p_1p_2(1-p_1-p_2)w(z_1)w(z_2)w(z_3)[\det(V)]^2, \qquad (5.2.1)$$

where $\det(V) = (z_3-z_1)(z_3-z_2)(z_2-z_1)$ and $p_1+p_2+p_3=1$, which implies that $p_3 = 1-p_1-p_2$.

To find the optimal weights we must maximise (5.2.1) with respect to both variables p_1, p_2. Thus p_1 and p_2 are given by first order conditions, namely

$$\frac{\partial\varphi}{\partial p_1} = \frac{1}{p_1} - \frac{1}{1-p_1-p_2} = 0 \qquad (1)$$

$$\frac{\partial\varphi}{\partial p_2} = \frac{1}{p_2} - \frac{1}{1-p_1-p_2} = 0 \qquad (2)$$

Equations (1) and (2) simplify to

$$p_1 = \tfrac{1}{2}(1-p_2) \qquad (1)$$

$$p_2 = \tfrac{1}{2}(1-p_1) \qquad (2)$$

Substituting the value of p_2 in equation (1) yields

$$\hat{p}_1 = \hat{p}_2 = \hat{p}_3 = 1/3. \qquad (5.2.2)$$

We note that as far as the supports of the D-optimal designs are concerned, numerical techniques are usually needed to determine the optimal weights, if, in a three parameter model, a D-optimal design has more than three support points; see Torsney (1983,1988), Torsney and Alahmadi (1992).

5.3 WEIGHTED QUADRATIC REGRESSION

In this section we consider models which we simply view as weighted quadratic regressions using the same weight functions as in chapter 3. Namely

$$E(y) = \alpha + \beta z + \gamma z^2,$$

$$Var(y) = \sigma^2 / w(z),$$

with information matrix M of the form

$$M = \sum p_i \underline{g}_i \underline{g}_i^t .$$

We note that $\underline{g}_i$ belongs to the induced design space

$$G = \left\{ \underline{g} = (g_1, g_2, g_3)^t, g_1 = \{w(z)\}^{1/2}, g_2 = z g_1, g_3 = z^2 g_1, z \in Z \right\}.$$

We also note that for all our weight functions except the double reciprocal, the case of G corresponding to the widest choice Z_w of Z is bounded. In the case of the double reciprocal as $z \to \pm\infty$ $g_1, g_2 \to 0$ but $g_3 \to +\infty$. So we need to restrict attention to bounded intervals Z. e.g. $Z_k = [-k, k]$ $k < \infty$.

<u>**5.3.1:**</u>

Here we consider the problem of finding the support points of the D-optimal designs on the widest choice Z_w for all the weight functions excluding the double reciprocal one which will be considered later in subsection 5.3.2. In general when $Z = Z_w$, it is not possible to identify support points for any given weight function $w(\cdot)$ from visual inspection of G and the smallest ellipsoid containing it.

The best three-point design must be obtained by maximising the determinant of the information matrix in (5.2.1) with respect to all variables z_1, z_2 and z_3. This problem simplifies when the weight function is symmetric about the origin, that is $w(z) = w(-z)$, which in turn implies symmetry of D-optimal designs about the origin. Thus $z_1 = -z_3$, $z_2 = 0$ and $z_3 > 0$, and $z_3 = z$, say, must, from (5.2.1), maximise the resultant determinant $z^6 w(z)^2$ over $Z = (0, \infty)$.

The main tool for checking if these best three-point designs are globally D-optimal is provided by the necessary and sufficient condition of the variance function of the equivalence theorem of chapter 2; that is we must have

$$d(z^*, \xi^*) = \underline{g}(z)^t M_z^{-1} \underline{g}(z) \begin{cases} = 3 & \text{for } z = z_1, z_2 \text{ and } z_3 \\ \leq 3 & \text{for } z \in Z \end{cases} \tag{5.3.1}$$

If for an arbitrary weight function equation (5.3.1) is violated by the best three-point design; then the implication is that more than three support points are needed.

For all the binary weight functions except the double reciprocal, the D-optimal designs on Z_w are three point ones. We report the values of z_1, z_2 and z_3 in Table (5.1). These best three point designs satisfy the necessary and sufficient condition of the variance function as stated in (5.3.1). Thus they are globally D-optimal. See figures (5.1) to (5.5).

We note that Fedorov (1972), Karlin and Studden (1966) proved that the D-optimal designs on Z_w had minimal supports of three points for the weight functions $w_1(z), w_2(z)$ and $w_3(z)$ as is confirmed by figures (5.5) to (5.8). We tabulate such values of z_1, z_2 and z_3 in Tables (5.2) and (5.3).

5.3.2:

Now the support points of the D-optimal designs on symmetric intervals $Z_k = [-k,k]$ $\forall$k, for the four symmetric binary weight functions, and in addition for the symmetric weight functions $w_1(z)$ $(\alpha = \beta = \mu)$ and $w_3(z)$ will be discussed and determined.

For the logistic and the probit and the double exponential models and the weight functions $w_1(z)$ and $w_3(z)$, denote the global support points by $(-z^*, 0, z^*)$ $(z^* > 0)$ (see Tables 5.1, 5.2 and 5.3). Then for $k \le z^*$, the D-optimal designs are supported on three-points $\{-k, 0, k\}$ (i.e. the two end points and zero) with equal optimal weights $(⅓, ⅓, ⅓)$, and for $k > z^*$, the D-optimal design is the same as that for the global one Z_w.

For the double reciprocal we noted that we must restrict attention to bounded Z. Extensive numerical calculations suggest that, the support points of the D-optimal designs on the bounded symmetric design space $Z_k = [-k,k]$ k $< \infty$, consists of either three points (i.e. the two end points and zero), or five points (i.e. the two end points and two other symmetric points within the interval and zero), depending on some critical value k^* and are classified as follows

$$Supp(p^*) = \left\{ \begin{array}{ll} \{-k, 0, k\} & , k \le k^* \\ \{-k, -\tilde{k}, 0, \tilde{k}, k\} & , k > k^* \end{array} \right\},$$

where

(i) $k^* = 7.4819$ on the basis of a numerical search;

(ii) the optimal weights in the case of three-points are $(\frac{1}{3},\frac{1}{3},\frac{1}{3})$, and in the case of five-points are (p_2,p_1,p_0,p_1,p_2) $\{p_0=1-2(p_1+p_2)\}$, where the optimal values of p_1,p_2 and of $\tilde{k}$ must be calculated numerically for given k.

We list the support points and the optimal weights of the D-optimal designs for some particular intervals in Table (5.4).

5.3.3:

Consider now the problem of determining the support points of the D-optimal designs on arbitrary intervals Z=[d,c] and Z=[c,e], d<c<e for all the weight functions except the double reciprocal one. If these contain the support points of the D-optimal design on the widest choice Z_w (i.e. the global design), then that design is still optimal. Otherwise numerical studies suggest that for both choices of Z, the optimal support consists of three points one of which is an end point of Z. Assuming that $c=z_1$, say, the other two points, say, z_2 and z_3 must for given c maximise the determinant

$$|M|=w(c)w(z_2)w(z_3)\left[(z_3-c)(z_2-c)(z_3-z_2)\right]^2 \tag{5.3.2}$$

over $z_2,z_3\in Z$ $(z_2<z_3)$. Denote the optimising values by z_2^*,z_3^*. Assuming the conjecture to be true, supports of D-optimal designs on the interval Z=[d,c] are $\{z_2^*,z_3^*,c\}$ and the supports on the interval Z=[c,e] are $\{c,z_2^*,z_3^*\}$ with equal optimal weights of $(\frac{1}{3},\frac{1}{3},\frac{1}{3})$.

In Table (5.5) we list the points which emerge as the support of the D-optimal designs on the two particular intervals $Z=(-\infty,0]$ and $Z=[0,\infty)$ for all the binary models and the weight function $w_3(z)$ excluding the double reciprocal model.

Table (5.6) gives the support points of D-optimal designs on the two intervals Z=(-1,0] and Z=[0,1) for the weight function $w_1(z)$.

Such designs do appear to be D-optimal designs. Plots suggest that the necessary and sufficient condition of the variance function in (5.3.1) is satisfied. For example see figures (5.9) and (5.10) for both the double exponential and the complementary log-log models respectively on $Z=[0,\infty)$.

5.3.4:

Finally we consider the problem of identifying the support points of D-optimal designs on the bounded interval $Z=[0,k]$ $k<\infty$, for the double reciprocal model. Numerical calculations suggest that these supports consist of three-points, namely the two end points 0 and k and one other point z^*, say, where z^* is the value of z which, from (5.2.1), maximises the resultant determinant

$$|M| = z^2 w(z)(z-k)^2,$$

over Z=[0,k] for given k.

We report the support points $\{0,z^*,k\}$ of the D-optimal designs for some particular intervals in Table (5.7).

5.4 GENERALISED LINEAR MODELS

This section is more properly the generalisation of the previous section 5.3. We consider generalised linear models with a quadratic deterministic function. i.e.

$$E(y/x) = \eta(\alpha + \beta x + \gamma x^2),$$

where x is a scalar to be selected from a design space $\chi = [d,e]$, and $\underline{\theta} = (\alpha, \beta, \gamma)' \in R^3$. Taking the matrix B of chapter 2 to be

$$B = \begin{bmatrix} 1 & 0 & 0 \\ {}^{s\beta}\!/_{2\sqrt{|\gamma|}} & \sqrt{|\gamma|} & 0 \\ {}^{\beta^2}\!/_{4\gamma} & s\beta & s\gamma \end{bmatrix},$$

this transforms to a canonical design problem with the following ingredients

$\eta = \eta(sz^2 + c)$, s=sign(γ).

$z = x\sqrt{|\gamma|} + \dfrac{s\beta}{2\sqrt{|\gamma|}}$, $z \in Z = [a,b]$.

$c = \alpha - \dfrac{s\beta^2}{4\gamma}$.

$M_z = E\left\{ w^*(z) \begin{pmatrix} 1 \\ z \\ z^2 \end{pmatrix} \begin{pmatrix} 1 & z & z^2 \end{pmatrix} \right\}$, where $w^*(z) = w(sz^2 + c)$, and in general the weight function $w^*(z)$ is symmetric even for asymmetric $w(z)$.

Our goal is to find optimal designs for particular line segments Z=[a,b] for all given values of $c \in \boldsymbol{R}$.

5.4.1:

In this subsection we consider the problem of finding the support points of the D-optimal designs on the widest choice $Z_w = (-\infty, \infty)$ for all the binary weight functions of the form $w^*(z) = w(sz^2 + c) = \dfrac{f^2(sz^2+c)}{F(sz^2+c)[1-F(sz^2+c)]}$. Since $w^*(z)$ and Z_w are symmetric about zero all D-optimal designs must be symmetric about zero. Further, if the original weight function $w(z)$ is symmetric, then the supports of D-optimal designs in the case of $w^*(z) = w(z^2+c)$, are equal to the supports when $w^*(z) = w(-z^2-c)$.

For all the binary weight functions except those corresponding to the double exponential and the double reciprocal models, the D-optimal designs on Z_w prove to have either three points or four points, depending on some critical value of c, say c^*, three points if $c \le c^*$. In view of the above symmetry a general result is that

$$Supp(p^*) = \left\{ \begin{array}{ll} \{-z^+, 0, z^+\} & , c \le c^* \\ \{-z_2^*, -z_1^*, z_1^*, z_2^*\} & , c > c^* \end{array} \right\},$$

where:

(i) z^+ is the optimal value of z which for given $c \in R$ maximises $\det(M)$ where M is the design matrix of the D-optimal design with support $\{-z^+, 0, z^+\}$; i.e. z^+ maximises $z^6 w^*(z)^2$ over $Z = (0, \infty)$.

(ii) The critical value c^* when the D-optimal designs change from three points to four points can be obtained by solving the following two equations simultaneously, namely

$$\frac{d}{dz}\ln\det(M) = 0 \qquad (1)$$

$$F''(0) = 0 \qquad (2)$$

where $\det(M)$ is as in (i) above, and $F(z) = \underline{g}(z)' M^{-1} \underline{g}(z)$, i.e. $F(z)$ is the variance function defined in (5.3.1).

(iii) z_1^* and z_2^* are the optimal values of z_1 and z_2 $(z_1 < z_2)$ which for

$$p = \frac{(2B-A)-\sqrt{A^2-AB+B^2}}{6(B-A)}\ , \quad 0 < \mathrm{p} < \tfrac{1}{2} \qquad (5.4.1)$$

maximise

$$\det(M) = 4p^2(1-2p)A + 2p(1-2p)^2 B, \qquad (5.4.2)$$

where $A = [z_1^6 w^*(z_1)^2 w^*(z_2) - 2z_1^4 z_2^2 w^*(z_1)^2 w^*(z_2) + z_1^2 z_2^4 w^*(z_1)^2 w^*(z_2)]$,

$$B = [z_2^6 w^*(z_1) w^*(z_2)^2 - 2z_1^2 z_2^4 w^*(z_1) w^*(z_2)^2 + z_1^4 z_2^2 w^*(z_1) w^*(z_2)^2].$$

This is because $\det(M)$ as given by (5.4.2) is the determinant of M the design matrix with support $\{-z_2, -z_1, z_1, z_2\}$ and respective weights $(p, \frac{1}{2}-p, \frac{1}{2}-p, p)$, which is symmetric as we require in its support points and in its weights. For given z_1, z_2 (5.4.2) can be maximised explicitly with respect to p the solution being given in (5.4.1).

For both the double exponential and the double reciprocal models, the D-optimal designs on the widest choice Z_w turn out to be three points for all positive values of c (i.e. three points if $c \geq 0$), and four points or five points or six points for all values of $c < 0$, relying on two critical negative values of c, say c_1^* and c_2^*. These designs are categorised by a common form of solution, namely

$$Supp(p^*) = \begin{Bmatrix} \{-z^+, 0, z^+\} & , c \geq 0 \\ \{-z^*, -\sqrt{|c|}, \sqrt{|c|}, z^*\} & , c_1^* \leq c < 0 \\ \{-z^\times, -\sqrt{|c|}, 0, \sqrt{|c|}, z^\times\} & , c_2^* \leq c \leq c_1^* \\ \{-z_2', -\sqrt{|c|}, -z_1', z_1', \sqrt{|c|}, z_2'\} & , c \leq c_2^* \end{Bmatrix},$$

where:

(1) z^+ is the value of z which maximises the determinant in (i) above for given $c \geq 0$.

(2) z^* is the value of z which maximises the determinant in (5.4.2) for given c and p under the design $\{-z, -\sqrt{|c|}, \sqrt{|c|}, z\}$ with optimal weights $(p, \frac{1}{2}-p, \frac{1}{2}-p, p)$. In fact the optimal value p is given explicitly by equation (5.4.1). Note that for both models $w^*\left(\sqrt{|c|}\right) = 1$, and that the quantities A and B appearing in (5.4.2) in this case are

$$A = [z^6 w^*(z)^2 - 2|c| z^4 w^*(z)^2 + |c|^2 z^2 w^*(z)^2],$$

$$B = [|c| z^4 w^*(z) - 2|c|^2 z^2 w^*(z) + |c|^3 w^*(z)].$$

The critical value c_1^* when the D-optimal designs change from four points to five points can be determined by solving the following two equations simultaneously with respect to z and c, that is

$$\frac{d}{dz}\ln\det(M)=0 \qquad (1)$$

$$F(0)=3 \qquad (2)$$

where as in (ii) above $F(z)=\underline{g}(z)'M^{-1}\underline{g}(z)$ is the variance function.

(3) In the case of five points $\{-z,-\sqrt{|c|},0,\sqrt{|c|},z\}$ with weights (p_2,p_1,p_0,p_1,p_2) $\{p_0=1-2(p_1+p_2)\}$, the determinant of M is given by

$$\det(M)=4(p_1p_2-2p_1^2p_2-2p_1p_2^2)w^*(0)w^*(z)A+4(p_1^2-2p_1^3-2p_1^2p_2)w^*(0)|c|^3$$

$$+4(p_2^2-2p_1p_2^2-2p_2^3)z^6w^*(0)w^*(z)^2+8p_1^2p_2w^*(z)B+8p_1p_2^2w^*(z)^2D\ ,$$

where $\qquad A=[|c|z^4+|c|^2z^2]$,

$B=[|c|z^4-2|c|^2z^2+|c|^3]$,

$D=[z^6-2|c|z^4+|c|^2z^2]$,

and the optimal value $z^{\times}$ of z and p_1^*,p_2^* of p_1,p_2 must be calculated numerically for given c.

The critical value of c_2^* when the D-optimal designs change from five points to six points can be obtained by solving the following four equations simultaneously with respect to all the variables z,p_1,p_2 and c, namely

$$\frac{\partial}{\partial u}\ln\det(M)=0,\ u=z,p_1,p_2 \quad (1\text{-}3)$$

$$F''(0)=0 \qquad (4)$$

where again $F(z)$ is as in (2) above.

(4) In the case of six points $\{-z_2, -\sqrt{|c|}, -z_1, z_1, \sqrt{|c|}, z_2\}$ $(z_1 < \sqrt{|c|} < z_2)$ with weights $(p_2, p_1, p_0, p_0, p_1, p_2)$ $\{p_0 = (\frac{1}{2} - p_1 - p_2)\}$, the determinant of M is given by $\det(M) = (AD - B^2)B$ with

$$A = [2p_1 w^*(z_1) + 2p_2 + (1 - 2p_1 - 2p_2) w^*(z_2)],$$
$$B = [2p_1 z_1^2 w^*(z_1) + 2p_2|c| + (1 - 2p_1 - 2p_2) z_2^2 w^*(z_2)],$$
$$D = [2p_1 z_1^4 w^*(z_1) + 2p_2|c|^2 + (1 - 2p_1 - 2p_2) z_2^4 w^*(z_2)].$$

The optimal values z_1', z_2' of z_1, z_2 and p_1^*, p_2^* of p_1, p_2 must be determined numerically for given c.

In Tables (5.8) to (5.20) we list the resultant support points and the optimal weights (i.e. in the case of five and six points) and the critical values of c's of the D-optimal designs on the widest choice Z_w for some particular values of c for all the binary models. These designs satisfy the necessary and the sufficient condition of the variance function of the equivalence theorem in (5.3.1). Thus they are globally D-optimal. See figures (5.11) to (5.20).

5.4.2:

Now the support points of the D-optimal designs on the two particular intervals $Z = (-\infty, 0]$ and $Z = [0, \infty)$ for all the binary models will be obtained and characterized. Reiterating the same arguments of subsection 5.3.3, if these contain global supports then that design is still optimal. Otherwise empirical results show that for both choices of Z, the optimal support consists of either three points or four points one of which is the end point zero.

For the logistic and the probit and the complementary log-log and the skewed logistic models, the D-optimal designs are supported only on the three points $\{0, \hat{z}_1, \hat{z}_2\}$ with equal optimal weights $(⅓,⅓,⅓)$ where $\hat{z}_1, \hat{z}_2$ denotes the optimal values of z_1, z_2 which for given c must maximise the following determinant

$$\det(M) = w^*(0)w^*(z_1)w^*(z_2)z_1^2 z_2^2 (z_2 - z_1)^2, \tag{5.4.3}$$

over $z_1, z_2 \in Z = [0, \infty)$ $(z_1 < z_2)$. This follows easily from (5.2.1).

For the double exponential and the double reciprocal models, the D-optimal designs on the two intervals prove to change at some critical negative value $\hat{c}_1$ from the three points $\{0, \hat{z}_1, \hat{z}_2\}$ to the three points $\{0, \sqrt{|c|}, \hat{z}\}$ and at a further critical negative value $\hat{c}_2$ $(\hat{c}_2 < \hat{c}_1)$ from the latter three points to the four points $\{0, \tilde{z}_1, \sqrt{|c|}, \tilde{z}_2\}$ with optimal weights $(p_1^*, p_2^*, p_3^*, p_4^*)$ $\{p_4^* = 1 - p_1^* - p_2^* - p_3^*\}$. Definitions and values are now outlined.

(1) The defining characteristic of $\hat{c}_1$ is that it is the value of c such that $\hat{z}_1 = \sqrt{|c|}$. Thus $\hat{c}_1 = -0.2540$ and $\hat{c}_2 = -0.1617$ for the double exponential and the double reciprocal respectively.

(2) The defining characteristic of $\hat{c}_2$ is it is the value of c such that $\tilde{z}_1 = \sqrt{|c|}$. Thus $\hat{c}_1 = -3.722$ for the double exponential model and $\hat{c}_2 = -9.310$ for the double reciprocal model. We note that $\hat{c}_1, \hat{c}_2$ have to be obtained by search methods as a calculus approach fails because the variance function $F(z)$ is not differentiable at $z = \sqrt{|c|}$ under any design.

(3) $\hat{z}_1, \hat{z}_2$ as defined above denote the optimal values of z_1 and z_2 $(z_1 < z_2)$ which maximise the determinant of M in (5.4.3).

(4) $\hat{z}$ is the optimal value of z which from (5.4.3), must maximise the resultant determinant for given c under the design with support $\{0,\sqrt{|c|},z\}$ and weights $(⅓,⅓,⅓)$; that is

$$\det(M) = w^*(0)w^*(\sqrt{|c|})w^*(z)|c|z^2\left[z-\sqrt{|c|}\right]^2.$$

(5) $\tilde{z}_1,\tilde{z}_2$ and p_1^*,p_2^*,p_3^* are the optimising values of z_1 and z_2 and of p_1,p_2,p_3 which must maximise the determinant of M under the four point design with support $\{0,z_1,\sqrt{|c|},z_2\}$ and respective weights (p_1,p_2,p_3,p_4) $(p_4 = 1-p_1-p_2-p_3)$; namely

$$\det(M) = A(DF-E^2)-B(BF-DE)+D(BE-D^2),$$

with $\quad A = [p_1w^*(0)+p_2w^*(z_1)+p_3+(1-p_1-p_2-p_3)w^*(z_2)]$,

$$B = [p_2z_1w^*(z_1)+p_3\sqrt{|c|}+(1-p_1-p_2-p_3)z_2w^*(z_2)],$$

$$D = [p_2z_1^2w^*(z_1)+p_3|c|+(1-p_1-p_2-p_3)z_2^2w^*(z_2)],$$

$$E = [p_2z_1^3w^*(z_1)+p_3|c|^{3/2}+(1-p_1-p_2-p_3)z_2^3w^*(z_2)],$$

$$F = [p_2z_1^4w^*(z_1)+p_3|c|^2+(1-p_1-p_2-p_3)z_2^4w^*(z_2)].$$

We report the support points and the optimal weights of the D-optimal designs for all the binary models on the interval $Z=[0,\infty)$ for all given values of c in Tables (5.21) to (5.32). Such designs do appear to D-optimal designs. Plots suggest that the necessary and the sufficient condition of the variance function is satisfied. For instance see figures (5.21) to (5.28).

Table (5.1); Supports z_1, z_2, z_3 of the best three-point D-optimal designs on the widest choice $Z_w = (-\infty, \infty)$. (Note s=sign(z)).

Name	$f_i(z)$	$F_i(z)$	z_1	z_2	z_3
1) Logit	$e^{-z}(1+e^{-z})^{-2}$	$(1+e^{-z})^{-1}$	-3.244	0.0	3.244
2) Probit	$\frac{1}{\sqrt{2\pi}} e^{(-z^2/2)}$	$\Phi(z)$	-1.898	0.0	1.898
3) Double Exponential	$\frac{1}{2} e^{-\lvert z\rvert}$	$\frac{(1+s)}{2} - \frac{s}{2} e^{-\lvert z\rvert}$	-2.919	0.0	2.919
4) Complementary Log-Log	$Exp(z-e^z)$	$1-Exp(-e^z)$	-3.776	-0.392	1.254
5-8) Skewed Logit	$m[F_1(z)]^{m-1} f_1(z)$	$(1+e^{-z})^{-m}$	-------	-------	-------
5) $m=1/3$	...	...	-12.42	-2.151	1.482
6) $m=2/3$	...	...	-5.437	-0.704	2.543
7) $m=3/2$	...	...	-1.966	0.580	3.858
8) $m=3$	...	...	-0.635	1.404	4.731

Table (5.2); Supports z_1, z_2, z_3 of the best three-point D-optimal designs for the asymmetric weight function $w_1(z)$ (symmetric if $\alpha = \beta = \mu$) of chapter 3 on the widest choice $Z_w = (-1,1)$.

Weight function	α	β	z_1	z_2	z_3
$w_1(z) = (1-z)^{\alpha+1}(1+z)^{\beta+1}$	μ	μ	$-\sqrt{3/(2\mu+5)}$	0.0	$+\sqrt{3/(2\mu+5)}$
" "	0.0	1.0	-0.575	0.181	0.823
" "	0.0	2.0	-0.410	0.306	0.854
" "	0.0	3.0	-0.273	0.398	0.876
" "	0.0	4.0	-0.160	0.468	0.892
" "	0.0	5.0	-0.064	0.523	0.904
" "	1.0	0.0	-0.823	-0.181	0.575
" "	1.0	2.0	-0.508	0.132	0.709
" "	1.0	3.0	-0.382	0.233	0.748
" "	1.0	4.0	-0.273	0.313	0.778
" "	1.0	5.0	-0.180	0.378	0.802
" "	2.0	3.0	-0.461	0.104	0.630
" "	2.0	4.0	-0.359	0.189	0.670

Table(5.3); Supports z_1,z_2,z_3 of the best three-point D-optimal designs on the widest choice Z_w for the asymmetric weight function $w_2(z)$ and the symmetric weight function $w_3(z)$ of chapter 3.

Weight function	α	z_1	z_2	z_3
$w_2(z)=z^{\alpha+1}e^{-z}, Z_w=(0,\infty)$	0.0	0.4158	2.2943	6.2899
" "	1.0	0.9358	3.3054	7.7588
" "	2.0	1.5174	4.3116	9.1710
" "	3.0	2.1412	5.3155	10.543
" "	4.0	2.7965	6.3182	11.885
" "	5.0	3.4764	7.3203	13.203
" "	6.0	4.1763	8.3218	14.502
" "	7.0	4.8928	9.3230	15.784
" "	8.0	5.6234	10.324	17.053
" "	9.0	6.3662	11.325	18.309
" "	10.0	7.1197	12.325	19.555
$w_3(z)=e^{-z^2}, Z_w=(-\infty,\infty)$	----	$-\sqrt{3/2}$	0.0	$+\sqrt{3/2}$

Table (5.4); Support points and optimal weights for the D-optimal designs on the bounded symmetric interval$Z_k = [-k,k] k < \infty$, for the double reciprocal model.

Interval	**Support points**					**Optimal weights**				
$Z_k = [-k,k]$	$-k$	$-\tilde{k}$	0	$\tilde{k}$	k	p_2	p_1	p_0	p_1	p_2
[-7.4819,7.4819] or less	The two end points and zero					Equal optimal weights i.e. $p_i = 1/3, \quad (i = 1,2,3)$				
[-8,8]	-8	-1.7	0	1.7	8	.318	.016	.332	.016	.318
[-10,10]	-10	-1.6	0	1.6	10	.278	.057	.330	.057	.278
[-15,15]	-15	-1.6	0	1.6	15	.233	.104	.326	.104	.233
[-20,20]	-20	-1.5	0	1.5	20	.214	.124	.324	.124	.214
[-25,25]	-25	-1.5	0	1.5	25	.204	.135	.322	.135	.204
[-30,30]	-30	1.5	0	1.5	30	.197	.142	.322	.142	.197
[-35,35]	-35	-1.45	0	1.45	35	.193	.147	.320	.147	.193
[-40,40]	-40	-1.45	0	1.45	40	.189	.151	.320	.151	.189
[-45,45]	-45	-1.45	0	1.45	45	.186	.154	.320	.154	.186
[-50,50]	-50	-1.45	0	1.45	50	.184	.156	.320	.156	.184

Table(5.5); Supports of D-optimal designs for all the binary models except the double reciprocal model and the weight function $w_3(z)$ on the appropriate intervals shown.

Model	**Interval** $Z=(-\infty,0]$			**Interval** $Z=[0,\infty)$		
1) Logit	-5.005	-1.599	0.0	0.0	1.599	5.005
2) Probit	-2.459	-0.965	0.0	0.0	0.965	2.459
3) Double exponential	-4.626	-1.134	0.0	0.0	1.134	4.626
4) Complementary log-log	-4.821	-1.379	0.0	0.0	0.764	1.678
5-8) Skewed logistic		...			...	
5) $m=1/3$	-13.78	-3.335	0.0	0.0	1.545	4.962
6) $m=2/3$	-7.207	-2.114	0.0	0.0	1.572	4.984
7) $m=3/2$	-3.554	-1.192	0.0	0.0	1.639	5.038
8) $m=3$	-2.059	-0.695	0.0	0.0	1.759	5.133
9) Weight function $w_3(z)$	-1.618	-0.618	0.0	0.0	0.618	1.618

Table (5.6); Supports of D-optimal designs for the weight function $w_1(z)$ on the two intervals Z=(-1,0] and Z=[0,1).

Weight function	α	β	**Interval** $Z=(-1,0]$			**Interval** $Z=[0,1)$		
$w_1(z)$	0.0	0.0	-0.859	-0.388	0.0	0.0	0.388	0.859
" "	0.0	1.0	-0.743	-0.302	0.0	0.0	0.421	0.872
" "	0.0	2.0	-0.652	-0.246	0.0	0.0	0.453	0.883
" "	0.0	3.0	-0.578	-0.208	0.0	0.0	0.484	0.892
" "	0.0	4.0	-0.519	-0.180	0.0	0.0	0.512	0.900
" "	0.0	5.0	-0.470	-0.158	0.0	0.0	0.539	0.907
" "	1.0	0.0	-0.872	-0.421	0.0	0.0	0.302	0.743
" "	1.0	1.0	-0.761	-0.328	0.0	0.0	0.328	0.761
" "	1.0	2.0	-0.671	-0.268	0.0	0.0	0.355	0.778
" "	1.0	3.0	-0.598	-0.225	0.0	0.0	0.383	0.792
" "	1.0	4.0	-0.538	-0.194	0.0	0.0	0.409	0.806
" "	1.0	5.0	-0.488	-0.169	0.0	0.0	0.435	0.818

Table (5.7);Supports $\{0, z^*, k\}$ of D-optimal designs for the double reciprocal model on the bounded interval $Z = [0, k]$ $k < \infty$.

0.0	z^*	k
0.0	0.3489	1.0
0.0	0.5525	2.0
0.0	0.6929	3.0
0.0	0.7975	4.0
0.0	0.8793	5.0
0.0	0.9453	6.0
0.0	1.000	7.0
0.0	1.046	8.0
0.0	1.086	9.0
0.0	1.120	10.0
0.0	1.313	20.0
0.0	1.397	30.0
0.0	1.445	40.0

Table (5.8); Supports $\{-z^+, 0, z^+\}$ of three point D-optimal designs on the widest choice $Z_w = (-\infty, \infty)$ for some particular values of c for the logistic model with $w^*(z) = w(z^2 + c)$.

c	z^+	c	z^+
0.0	1.4073	-0.1	1.4203
0.1	1.3948	-0.2	1.4338
0.2	1.3830	-0.3	1.4480
0.3	1.3717	-0.4	1.4626
0.4	1.3611	-0.5	1.4778
0.5	1.3510	-0.6	1.4935
0.6	1.3415	-0.7	1.5097
0.7	1.3325	-0.8	1.5263
0.8	1.3241	-0.9	1.5434
0.9	1.3162	-1.0	1.5608
1.0	1.3089	-2.0	1.7518

Table (5.9); Supports $\{-z^{+},0,z^{+}\}$ of three point D-optimal designs on the widest choice $Z_w = (-\infty,\infty)$ for some particular values of c for the probit model with $w^{*}(z) = w(z^2 + c)$.

c	z^{+}	c	z^{+}
0.0	1.1737	-0.1	1.1965
0.1	1.1512	-0.2	1.2196
0.2	1.1289	-0.3	1.2429
0.3	1.1070	-0.4	1.2664
0.4	1.0854	-0.5	1.2901
0.5	1.0643	-0.6	1.3139
0.6	1.0434	-0.7	1.3379
0.7	1.0230	-0.8	1.3620
0.8	1.0030	-0.9	1.3862
0.9	0.9835	-1.0	1.4105
1.0	0.9644	-2.0	1.6536

Table (5.10); Supports $\{-z^{+}, 0, z^{+}\}$ of three point D-optimal designs on the widest choice $Z_w = (-\infty, \infty)$ for some particular values of c for the complementary log-log model with $w^*(z) = w(z^2 + c)$.

c	z^{+}	c	z^{+}
0.0	1.0731	-0.1	1.1063
0.1	1.0397	-0.2	1.1393
0.2	1.0061	-0.3	1.1721
0.3	0.9725	-0.4	1.2045
0.4	0.9387	-0.5	1.2367
0.5	0.9051	-0.6	1.2686
0.6	0.8715	-0.7	1.3001
0.7	0.8381	-0.8	1.3313
0.8	0.8049	-0.9	1.3621
0.9	0.7721	-1.0	1.3927
1.0	0.7397	-2.0	1.6793

Table (5.11); Supports $\{-z^{+},0,z^{+}\}$ of three point D-optimal designs on the widest choice $Z_w = (-\infty,\infty)$ for some particular values of c for the complementary log-log model with $w^{*}(z) = w(-z^2 + c)$.

c	z^{+}	c	z^{+}
0.0	1.2894	-0.1	1.2836
0.1	1.2958	-0.2	1.2783
0.2	1.3027	-0.3	1.2734
0.3	1.3102	-0.4	1.2690
0.4	1.3183	-0.5	1.2649
0.5	1.3271	-0.6	1.2612
0.6	1.3366	-0.7	1.2578
0.7	1.3468	-0.8	1.2548
0.8	1.3578	-0.9	1.2520
0.9	1.3696	-1.0	1.2494
1.0	1.3821	-2.0	1.2339

Table (5.12); Supports $\{-z^+, 0, z^+\}$ of three point D-optimal designs on the widest choice $Z_w = (-\infty, \infty)$ for some particular values of c between -0.5 and 0.5 for the skewed logistic model with $w^*(z) = w(z^2 + c)$.

c	m	z^+	m	z^+	m	z^+	m	z^+
-0.5	**1/3**	1.4443	**2/3**	1.4614	**3/2**	1.5013	**3**	1.5636
-0.4	"	1.4307	"	1.4469	"	1.4851	"	1.5452
-0.3	"	1.4175	"	1.4330	"	1.4694	"	1.5273
-0.2	"	1.4050	"	1.4196	"	1.4543	"	1.5098
-0.1	"	1.3929	"	1.4068	"	1.4397	"	1.4929
0.0	"	1.3814	"	1.3945	"	1.4257	"	1.4765
0.1	"	1.3705	"	1.3828	"	1.4123	"	1.4606
0.2	"	1.3601	"	1.3717	"	1.3995	"	1.4454
0.3	"	1.3502	"	1.3611	"	1.3873	"	1.4307
0.4	"	1.3409	"	1.3511	"	1.3757	"	1.4167
0.5	"	1.3321	"	1.3416	"	1.3646	"	1.4033

Table (5.13); Supports $\{-z^{+},0,z^{+}\}$ of three point D-optimal designs on the widest choice $Z_w = (-\infty,\infty)$ for some particular values of c between -0.5 and 0.5 for the skewed logistic model with $w^{*}(z) = w(-z^{2}+c)$.

c	m	z^{+}	m	z^{+}	m	z^{+}	m	z^{+}
-0.5	**1/3**	1.9229	**2/3**	1.5441	**3/2**	1.1688	**3**	0.8808
-0.4	"	1.9202	"	1.5506	"	1.1814	"	0.8950
-0.3	"	1.9180	"	1.5577	"	1.1947	"	0.9101
-0.2	"	1.9162	"	1.5653	"	1.2085	"	0.9259
-0.1	"	1.9150	"	1.5734	"	1.2231	"	0.9426
0.0	"	1.9144	"	1.5822	"	1.2382	"	0.9600
0.1	"	1.9143	"	1.5915	"	1.2540	"	0.9783
0.2	"	1.9149	"	1.6014	"	1.2703	"	0.9973
0.3	"	1.9162	"	1.6119	"	1.2873	"	1.0170
0.4	"	1.9182	"	1.6230	"	1.3047	"	1.0374
0.5	"	1.9210	"	1.6346	"	1.3227	"	1.0585

Table (5.14); Critical values of $c^* \& z^+$ when the D-optimal designs on the widest choice Z_w changes from three points to four points for all the binary models except the double exponential and the double reciprocal.

Model	$w^*(z) = w(z^2 + c)$		$w^*(z) = w(-z^2 + c)$	
	c^*	z^+	c^*	z^+
1) Logistic	-1.3068	1.6166	1.3068	1.6166
2) Probit	-0.9920	1.4085	0.9920	1.4085
3) Comp Log-Log	-1.1925	1.4505	0.8266	1.3609
4-7) Skewed Logistic	• • •	• • •	• • •	• • •
4) $m = 1/3$	-4.0000	2.0948	0.1045	1.9143
5) $m = 2/3$	-2.0138	1.7288	0.9125	1.6881
6) $m = 3/2$	-0.7260	1.5396	1.6895	1.5665
7) $m = 3$	0.1263	1.4566	2.3456	1.5121

Table (5.15); Supports $\{-z^{+},0,z^{+}\}$ of three point D-optimal designs on the widest choice $Z_w=(-\infty,\infty)$ for some particular values of c>0 for the double exponential and the double reciprocal models with $w^{*}(z)=w(z^2+c)$.

The double exponential model		The double reciprocal model	
c	z^{+}	c	z^{+}
0.0	1.1378	0.0	0.8918
0.1	1.1482	0.1	0.9487
0.2	1.1572	0.2	1.0018
0.3	1.1649	0.3	1.0519
0.4	1.1716	0.4	1.0995
0.5	1.1774	0.5	1.1450
0.6	1.1825	0.6	1.1885
0.7	1.1870	0.7	1.2305
0.8	1.1910	0.8	1.2710
0.9	1.1945	0.9	1.3101
1.0	1.1976	1.0	1.3481

Table (5.16); Supports $\{-z^*, -\sqrt{|c|}, \sqrt{|c|}, z^*\}$ of four point D-optimal designs on the widest choice $Z_w = (-\infty, \infty)$ for some particular values of c<0 for the double exponential and the double reciprocal models with $w^*(z) = w(z^2 + c)$.

The double exponential model		**The double reciprocal model**	
c	z^*	c	z^*
-0.1	1.1994	-0.1	1.0367
-0.2	1.2682	-0.2	1.1748
-0.3	1.3322	-0.3	1.2594
-0.4	1.3875	-0.4	1.3206
-0.5	1.4358	-0.5	1.3711
-0.6	1.4792	-0.6	1.4156
-0.7	1.5192	-0.7	1.4565
-0.8	1.5567	-0.8	1.4948
-0.9	1.5923	-0.9	1.5312
-1.0	1.6265	-1.0	1.5661

Table (5.17); Supports $\{-z^{\times},-\sqrt{|c|},0,\sqrt{|c|},z^{\times}\}$ and optimal weights p_1^*,p_2^* of five point D-optimal designs on the widest choice $Z_w=(-\infty,\infty)$ for some particular values of c<0 for the double exponential and the double reciprocal models with $w^*(z)=w(z^2+c)$.

	The double exponential model			**The double reciprocal model**		
c	$z^{\times}$	p_1^*	p_2^*	$z^{\times}$	p_1^*	p_2^*
-1.1	1.6530	0.3073	0.1815	1.5918	0.3237	0.1591
-1.2	1.6788	0.3067	0.1707	1.6196	0.3238	0.1472
-1.3	1.7051	0.3068	0.1610	1.6482	0.3241	0.1380
-1.4	1.7319	0.3074	0.1527	1.6776	0.3245	0.1316
-1.5	1.7593	0.3083	0.1458	1.7075	0.3249	0.1279
-1.6	1.7871	0.3093	0.1407	1.7378	0.3253	0.1270

Table (5.18); Supports $\{-z_2',-z_1',-\sqrt{|c|},\sqrt{|c|},z_1',z_2'\}$ and optimal weights p_1^*,p_2^* of six point D-optimal designs on the widest choice $Z_w=(-\infty,\infty)$ for some particular values of c<0 for the double exponential model with $w^*(z)=w(z^2+c)$.

c	z_1'	z_2'	p_1^*	p_2^*
-1.7	0.3262	1.8148	0.1381	0.3096
-1.8	0.4543	1.8422	0.1357	0.3098
-1.9	0.5535	1.8691	0.1335	0.3101
-2.0	0.6375	1.8957	0.1316	0.3103
-2.1	0.7116	1.9219	0.1298	0.3104
-2.2	0.7787	1.9477	0.1282	0.3106
-2.3	0.8405	1.9732	0.1267	0.3107
-2.4	0.8980	1.9984	0.1254	0.3108
-2.5	0.9520	2.0233	0.1241	0.3109
-3.0	1.1859	2.1433	0.1191	0.3113
-4.0	1.5513	2.3651	0.1128	0.3116
-5.0	1.8456	2.5678	0.1090	0.3118

Table (5.19); Supports $\{-z_2', -z_1', -\sqrt{|c|}, \sqrt{|c|}, z_1', z_2'\}$ and optimal weights p_1^*, p_2^* of six point D-optimal designs on the widest choice $Z_w = (-\infty, \infty)$ for some particular values of c<0 for the double reciprocal model with $w^*(z) = w(z^2 + c)$.

c	z_1'	z_2'	p_1^*	p_2^*
-1.5	0.2929	1.7071	0.1284	0.3246
-1.6	0.4310	1.7362	0.1259	0.3247
-1.7	0.5346	1.7647	0.1236	0.3248
-1.8	0.6211	1.7928	0.1216	0.3249
-1.9	0.6970	1.8205	0.1198	0.3249
-2.0	0.7654	1.8478	0.1182	0.3250
-2.1	0.8281	1.8746	0.1167	0.3250
-2.2	0.8865	1.9011	0.1154	0.3251
-2.3	0.9417	1.9272	0.1141	0.3251
-2.4	0.9929	1.9530	0.1130	0.3252
-3.0	1.2593	2.1010	0.1079	0.3253
-4.0	1.6080	2.3269	0.1027	0.3254
-5.0	1.8936	2.5326	0.0996	0.3254

Table (5.20); Critical values of $c_1^*, c_2^*, z^*, z^\times$ and p, p_1^*, p_2^* when the D-optimal designs on the widest choice Z_w changes from four points to five points and five points to six points for the double exponential and the double reciprocal models.

Model	Four to five points			Five to six points			
	c_1^*	z^*	p	c_2^*	$z^\times$	p_1^*	p_2^*
1) DEXP	-1.017	1.632	0.191	-1.594	1.785	0.309	0.141
2) DREC	-0.988	1.562	0.176	-1.414	1.682	0.325	0.131

Table (5.21); Supports $\{0,\hat{z}_1,\hat{z}_2\}$ of three point D-optimal designs on the interval $Z=[0,\infty)$ for some particular values of c for the logistic model with $w^*(z)=w(z^2+c)$.

c	$\hat{z}_1$	$\hat{z}_2$	c	$\hat{z}_1$	$\hat{z}_2$
0.0	0.7877	1.7560	-0.1	0.8013	1.7665
0.1	0.7749	1.7461	-0.2	0.8156	1.7775
0.2	0.7629	1.7367	-0.3	0.8308	1.7890
0.3	0.7516	1.7278	-0.4	0.8468	1.8011
0.4	0.7410	1.7195	-0.5	0.8636	1.8138
0.5	0.7312	1.7116	-0.6	0.8811	1.8269
0.6	0.7220	1.7043	-0.7	0.8995	1.8405
0.7	0.7134	1.6974	-0.8	0.9187	1.8547
0.8	0.7055	1.6910	-0.9	0.9386	1.8693
0.9	0.6981	1.6850	-1.0	0.9592	1.8843
1.0	0.6913	1.6795	-2.0	1.1940	2.0547

Table (5.22); Supports $\{0, \hat{z}_1, \hat{z}_2\}$ of three point D-optimal designs on the interval $Z = [0, \infty)$ for some particular values of c for the probit model with $w^*(z) = w(z^2 + c)$.

c	$\hat{z}_1$	$\hat{z}_2$	c	$\hat{z}_1$	$\hat{z}_2$
0.0	0.6381	1.3646	-0.1	0.6554	1.3865
0.1	0.6216	1.3430	-0.2	0.6735	1.4086
0.2	0.6058	1.3217	-0.3	0.6924	1.4310
0.3	0.5906	1.3006	-0.4	0.7122	1.4536
0.4	0.5761	1.2799	-0.5	0.7329	1.4765
0.5	0.5622	1.2594	-0.6	0.7545	1.4996
0.6	0.5488	1.2393	-0.7	0.7772	1.5229
0.7	0.5359	1.2195	-0.8	0.8008	1.5464
0.8	0.5236	1.2001	-0.9	0.8255	1.5701
0.9	0.5117	1.1810	-1.0	0.8511	1.5940
1.0	0.5003	1.1622	-2.0	1.1487	1.8372

Table (5.23); Supports $\{0, \hat{z}_1, \hat{z}_2\}$ of three point D-optimal designs on the interval $Z = [0, \infty)$ for some particular values of c for the complementary log-log model with $w^*(z) = w(z^2 + c)$.

c	$\hat{z}_1$	$\hat{z}_2$	c	$\hat{z}_1$	$\hat{z}_2$
0.0	0.6052	1.1868	-0.1	0.6303	1.2185
0.1	0.5807	1.1548	-0.2	0.6559	1.2500
0.2	0.5567	1.1227	-0.3	0.6821	1.2813
0.3	0.5332	1.0905	-0.4	0.7087	1.3124
0.4	0.5104	1.0581	-0.5	0.7357	1.3432
0.5	0.4881	1.0257	-0.6	0.7633	1.3738
0.6	0.4664	0.9933	-0.7	0.7912	1.4041
0.7	0.4454	0.9609	-0.8	0.8155	1.4341
0.8	0.4249	0.9286	-0.9	0.8482	1.4638
0.9	0.4052	0.8964	-1.0	0.8772	1.4932
1.0	0.3860	0.8644	-2.0	1.1765	1.7717

Table (5.24); Supports $\{0,\hat{z}_1,\hat{z}_2\}$ of three point D-optimal designs on the interval $Z=[0,\infty)$ for some particular values of c for the complementary log-log model with $w^*(z)=w(-z^2+c)$.

c	$\hat{z}_1$	$\hat{z}_2$	c	$\hat{z}_1$	$\hat{z}_2$
0.0	0.6835	1.6678	-0.1	0.6765	1.6629
0.1	0.6914	1.6732	-0.2	0.6703	1.6586
0.2	0.7004	1.6791	-0.3	0.6648	1.6546
0.3	0.7105	1.6858	-0.4	0.6599	1.6511
0.4	0.7219	1.6931	-0.5	0.6556	1.6479
0.5	0.7348	1.7013	-0.6	0.6517	1.6450
0.6	0.7494	1.7103	-0.7	0.6482	1.6424
0.7	0.7657	1.7203	-0.8	0.6452	1.6400
0.8	0.7840	1.7313	-0.9	0.6424	1.6379
0.9	0.8044	1.7433	-1.0	0.6400	1.6360
1.0	0.8268	1.7565	-2.0	0.6258	1.6246

Table (5.25); Supports $\{0,\hat{z}_1,\hat{z}_2\}$ of three point D-optimal designs on the interval $Z=[0,\infty)$ for some particular values of c between -0.5 and 0.5 for the skewed logistic model with $w^*(z)=w(z^2+c)$ for $m=1/3$ and $m=2/3$.

c	m	$\hat{z}_1$	$\hat{z}_2$	m	$\hat{z}_1$	$\hat{z}_2$
-0.5	1/3	0.8102	1.7817	2/3	0.8361	1.7976
-0.4	"	0.7977	1.7711	"	0.8215	1.7860
-0.3	"	0.7857	1.7609	"	0.8076	1.7749
-0.2	"	0.7743	1.7512	"	0.7943	1.7643
-0.1	"	0.7634	1.7420	"	0.7818	1.7542
0.0	"	0.7530	1.7333	"	0.7699	1.7446
0.1	"	0.7432	1.7250	"	0.7586	1.7354
0.2	"	0.7340	1.7171	"	0.7480	1.7268
0.3	"	0.7252	1.7097	"	0.7381	1.7187
0.4	"	0.7170	1.7027	"	0.7287	1.7110
0.5	"	0.7093	1.6961	"	0.7200	1.7038

Table (5.26); Supports $\{0, \hat{z}_1, \hat{z}_2\}$ of three point D-optimal designs on the interval $Z = [0, \infty)$ for some particular values of c between -0.5 and 0.5 for the skewed logistic model with $w^*(z) = w(z^2 + c)$ for $m = 3/2$ and $m = 3$.

c	m	$\hat{z}_1$	$\hat{z}_2$	m	$\hat{z}_1$	$\hat{z}_2$
-0.5	**3/2**	0.9071	1.8383	**3.0**	1.0395	1.9101
-0.4	"	0.8869	1.8242	"	1.0112	1.8922
-0.3	"	0.8677	1.8106	"	0.9839	1.8748
-0.2	"	0.8495	1.7976	"	0.9575	1.8580
-0.1	"	0.8323	1.7852	"	0.9322	1.8419
0.0	"	0.8160	1.7734	"	0.9081	1.8264
0.1	"	0.8007	1.7622	"	0.8852	1.8115
0.2	"	0.7864	1.7517	"	0.8636	1.7975
0.3	"	0.7730	1.7417	"	0.8434	1.7841
0.4	"	0.7604	1.7323	"	0.8244	1.7715
0.5	"	0.7488	1.7234	"	0.8068	1.7596

Table (5.27); Supports $\{0,\hat{z}_1,\hat{z}_2\}$ of three point D-optimal designs on the interval $Z=[0,\infty)$ for some particular values of c between -0.5 and 0.5 for the skewed logistic model with $w^*(z)=w(-z^2+c)$ for $m=1/3$ and $m=2/3$.

c	m	$\hat{z}_1$	$\hat{z}_2$	m	$\hat{z}_1$	$\hat{z}_2$
-0.5	**1/3**	1.0802	2.7240	**2/3**	0.8528	2.0166
-0.4	"	1.0901	2.7259	"	0.8629	2.0216
-0.3	"	1.1008	2.7282	"	0.8736	2.0270
-0.2	"	1.1124	2.7308	"	0.8851	2.0329
-0.1	"	1.1248	2.7338	"	0.8974	2.0393
0.0	"	1.1380	2.7373	"	0.9105	2.0461
0.1	"	1.1521	2.7412	"	0.9244	2.0535
0.2	"	1.1670	2.7455	"	0.9391	2.0614
0.3	"	1.1826	2.7502	"	0.9546	2.0697
0.4	"	1.1991	2.7554	"	0.9710	2.0786
0.5	"	1.2162	2.7611	"	0.9881	2.0881

Table (5.28); Supports $\{0, \hat{z}_1, \hat{z}_2\}$ of three point D-optimal designs on the interval $Z = [0, \infty)$ for some particular values of c between -0.5 and 0.5 for the skewed logistic model with $w^*(z) = w(-z^2 + c)$ for $m = 3/2$ and $m = 3$.

c	m	$\hat{z}_1$	$\hat{z}_2$	m	$\hat{z}_1$	$\hat{z}_2$
-0.5	3/2	0.6201	1.4581	3.0	0.4546	1.0987
-0.4	"	0.6297	1.4685	"	0.4632	1.1118
-0.3	"	0.6399	1.4795	"	0.4723	1.1255
-0.2	"	0.6508	1.4911	"	0.4821	1.1400
-0.1	"	0.6625	1.5033	"	0.4925	1.1552
0.0	"	0.6748	1.5160	"	0.5036	1.1711
0.1	"	0.6879	1.5293	"	0.5153	1.1877
0.2	"	0.7018	1.5432	"	0.5278	1.2050
0.3	"	0.7164	1.5576	"	0.5409	1.2229
0.4	"	0.7318	1.5726	"	0.5548	1.2414
0.5	"	0.7480	1.5881	"	0.5694	1.2605

Table (5.29); Supports $\{0,\hat{z}_1,\hat{z}_2\}$ of three point D-optimal designs on the interval $Z=[0,\infty)$ for some particular values of c for the double exponential and the double reciprocal models with $w^*(z)=w(z^2+c)$.

The double exponential model			The double reciprocal model		
c	$\hat{z}_1$	$\hat{z}_2$	c	$\hat{z}_1$	$\hat{z}_2$
-0.25	0.5048	1.5292	-0.16	0.4028	1.5428
-0.2	0.5138	1.5357	-0.15	0.4065	1.5556
-0.1	0.5289	1.5467	-0.1	0.4245	1.6179
0.0	0.5410	1.5558	0.0	0.4576	1.7343
0.1	0.5510	1.5634	0.1	0.4879	1.8422
0.2	0.5593	1.5699	0.2	0.5159	1.9434
0.3	0.5664	1.5754	0.3	0.5423	2.0391
0.4	0.5724	1.5802	0.4	0.5672	2.1302
0.5	0.5776	1.5844	0.5	0.5910	2.2173
0.6	0.5822	1.5881	0.6	0.6138	2.3009
0.7	0.5861	1.5913	0.7	0.6356	2.3814
0.8	0.5895	1.5941	0.8	0.6567	2.4592

Table (5.30); Supports $\{0,\sqrt{|c|},\hat{z}\}$ of three point D-optimal designs on the interval $Z=[0,\infty)$ for some particular values of c for the double exponential and the double reciprocal models with $w^*(z)=w(z^2+c)$.

The double exponential model		**The double reciprocal model**	
c	$\hat{z}$	c	$\hat{z}$
-0.3	1.5463	-0.2	1.5667
-0.4	1.5822	-0.3	1.6228
-0.5	1.6155	-0.4	1.6682
-0.6	1.6472	-0.5	1.7071
-0.7	1.6776	-0.6	1.7416
-0.8	1.7069	-0.7	1.7729
-0.9	1.7355	-0.8	1.8018
-1.0	1.7633	-0.9	1.8289
-1.5	1.8950	-1.0	1.8546
-2.0	2.0175	-2.0	2.0753
-3.0	2.2436	-3.0	2.2734

Table (5.31); Supports $\{0, \tilde{z}_1, \sqrt{|c|}, \tilde{z}_2\}$ and optimal weights p_1^*, p_2^*, p_3^* of four point D-optimal designs on the interval $Z = [0, \infty)$ for some particular values of c for the double exponential model with $w^*(z) = w(z^2 + c)$.

c	$\tilde{z}_1$	$\tilde{z}_2$	p_1^*	p_2^*	p_3^*
-3.8	1.6416	2.4097	0.3331	0.0047	0.3315
-3.9	1.6671	2.4288	0.3329	0.0103	0.3294
-4.0	1.6923	2.4478	0.3326	0.0157	0.3274
-4.1	1.7173	2.4667	0.3324	0.0208	0.3256
-4.2	1.7420	2.4856	0.3322	0.0257	0.3239
-4.3	1.7665	2.5043	0.3319	0.0304	0.3223
-4.4	1.7908	2.5230	0.3317	0.0349	0.3208
-4.5	1.8147	2.5415	0.3315	0.0392	0.3194
-4.6	1.8385	2.5600	0.3312	0.0433	0.3182
-4.7	1.8620	2.5784	0.3310	0.0473	0.3170
-4.8	1.8853	2.5967	0.3307	0.0512	0.3159
-4.9	1.9083	2.6149	0.3305	0.0549	0.3148
-5.0	1.9311	2.6330	0.3302	0.0585	0.3138

Table (5.32); Supports $\{0, \tilde{z}_1, \sqrt{|c|}, \tilde{z}_2\}$ and optimal weights p_1^*, p_2^*, p_3^* of four point D-optimal designs on the interval $Z=[0,\infty)$ for some particular values of c for the double reciprocal model with $w^*(z)=w(z^2+c)$.

c	$\tilde{z}_1$	$\tilde{z}_2$	p_1^*	p_2^*	p_3^*
-9.4	2.8827	3.3500	0.3333	0.0041	0.3326
-9.5	2.8996	3.3643	0.3333	0.0058	0.3324
-9.6	2.9163	3.3785	0.3333	0.0074	0.3321
-9.7	2.9329	3.3927	0.3332	0.0090	0.3318
-9.8	2.9495	3.4069	0.3332	0.0106	0.3316
-9.9	2.9659	3.4210	0.3332	0.0122	0.3313
-10.0	2.9823	3.4350	0.3332	0.0137	0.3311
-10.1	2.9986	3.4490	0.3332	0.0152	0.3308
-10.2	3.0148	3.4630	0.3332	0.0166	0.3306
-10.3	3.0310	3.4769	0.3332	0.0181	0.3304
-10.4	3.0470	3.4908	0.3332	0.0195	0.3302
-10.5	3.0630	3.5046	0.3331	0.0209	0.3299
-11.0	3.1418	3.5730	0.3331	0.0275	0.3289

Figure (5.1)

Plot of the variance function for the global symmetric D-optimal three-point design on the widest choice Z_w for logistic model.

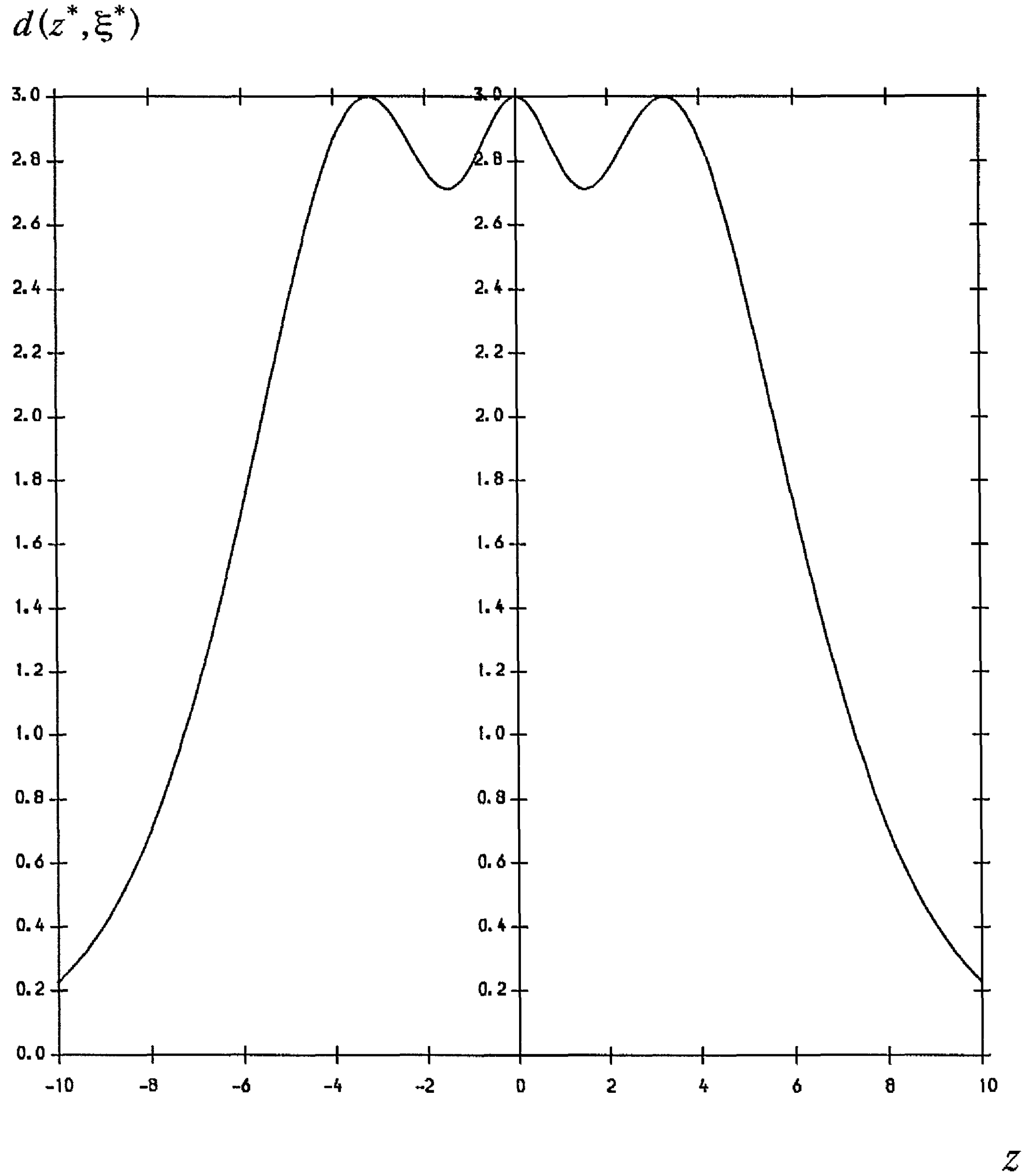


Figure (5.2)

Plot of the variance function for the global symmetric D-optimal three-point design on the widest choice Z_w for the probit model.

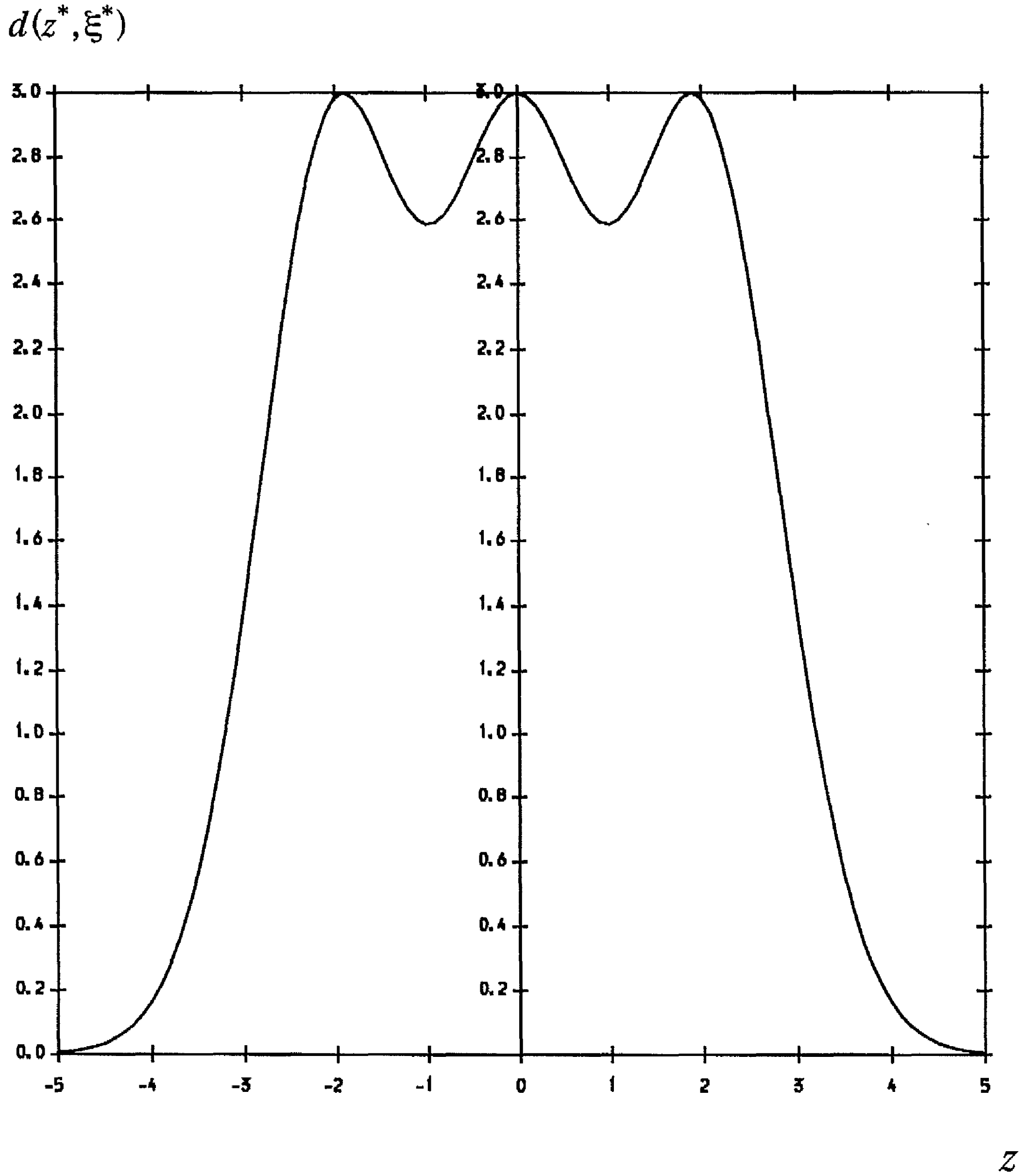


Figure (5.3)

Plot of the variance function for the global symmetric D-optimal three-point design on the widest choice Z_w for the symmetric double exponential model.

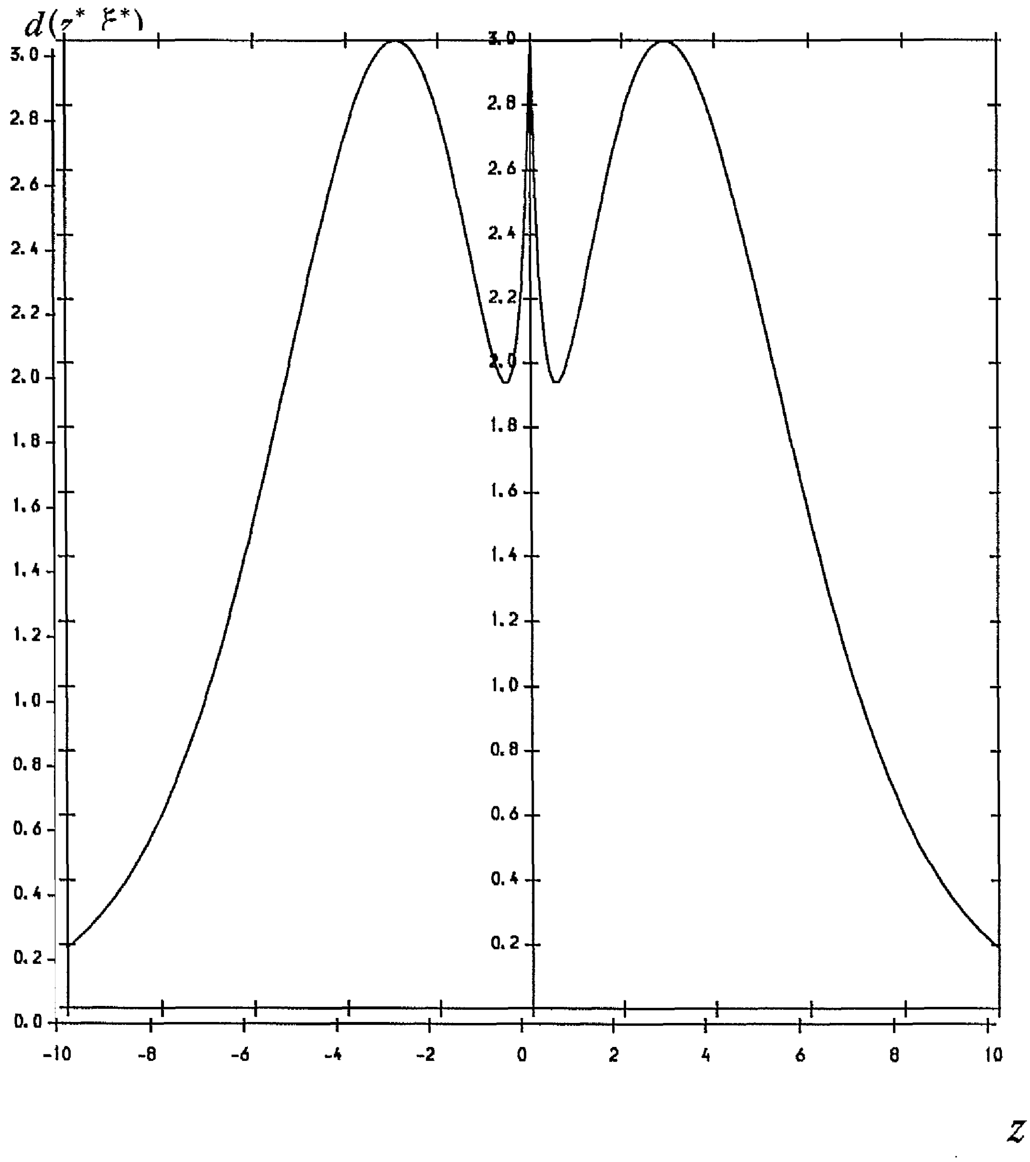


Figure (5.4)

Plot of the variance function for the global asymmetric D-optimal three-point design on the widest choice Z_w for the asymmetric complementary log-log model.

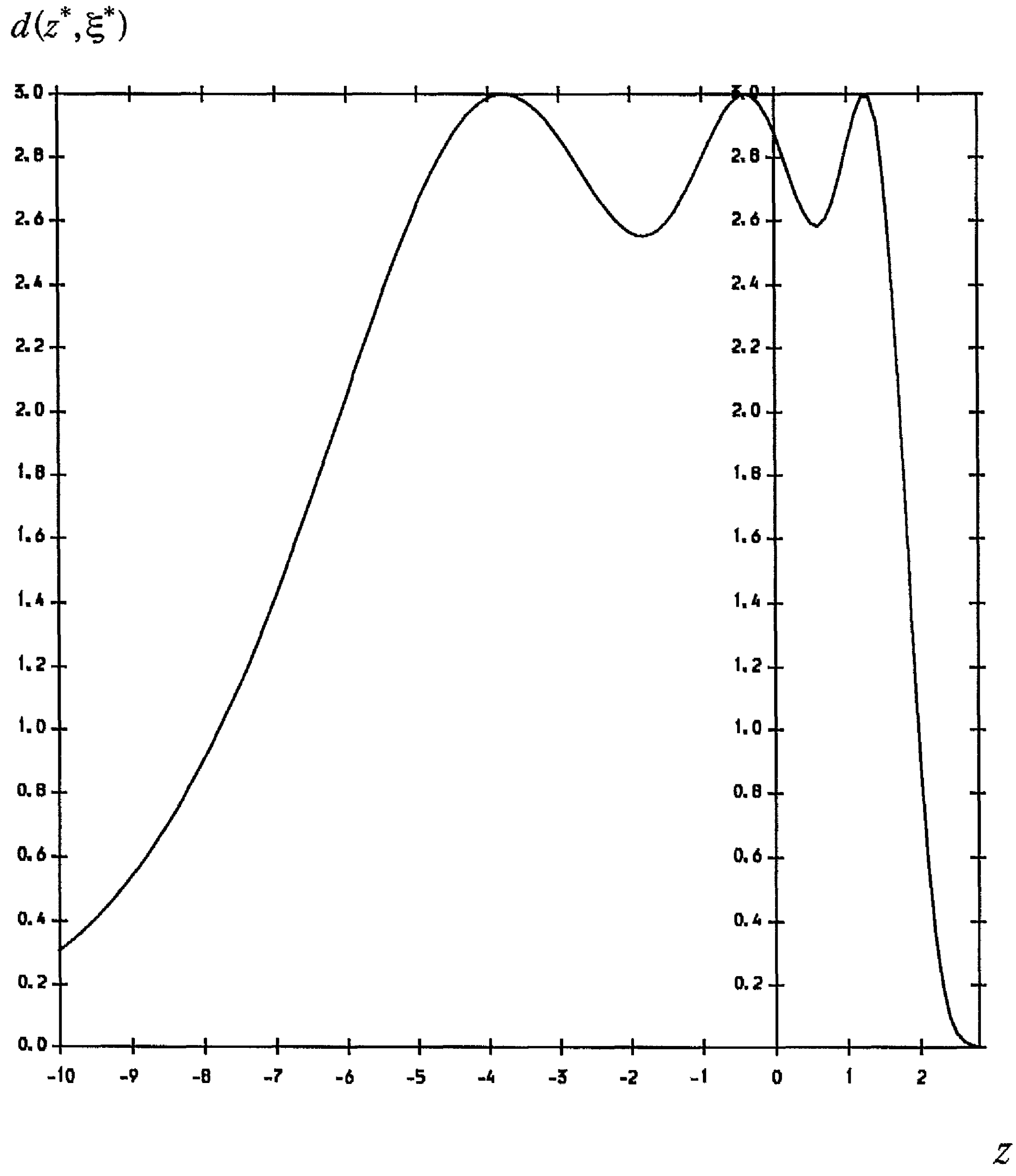


Figure (5.5)

Plot of the variance function for the global asymmetric D-optimal three-point design on the widest choice Z_w for the asymmetric skewed logistic model with $m = 3/2$.

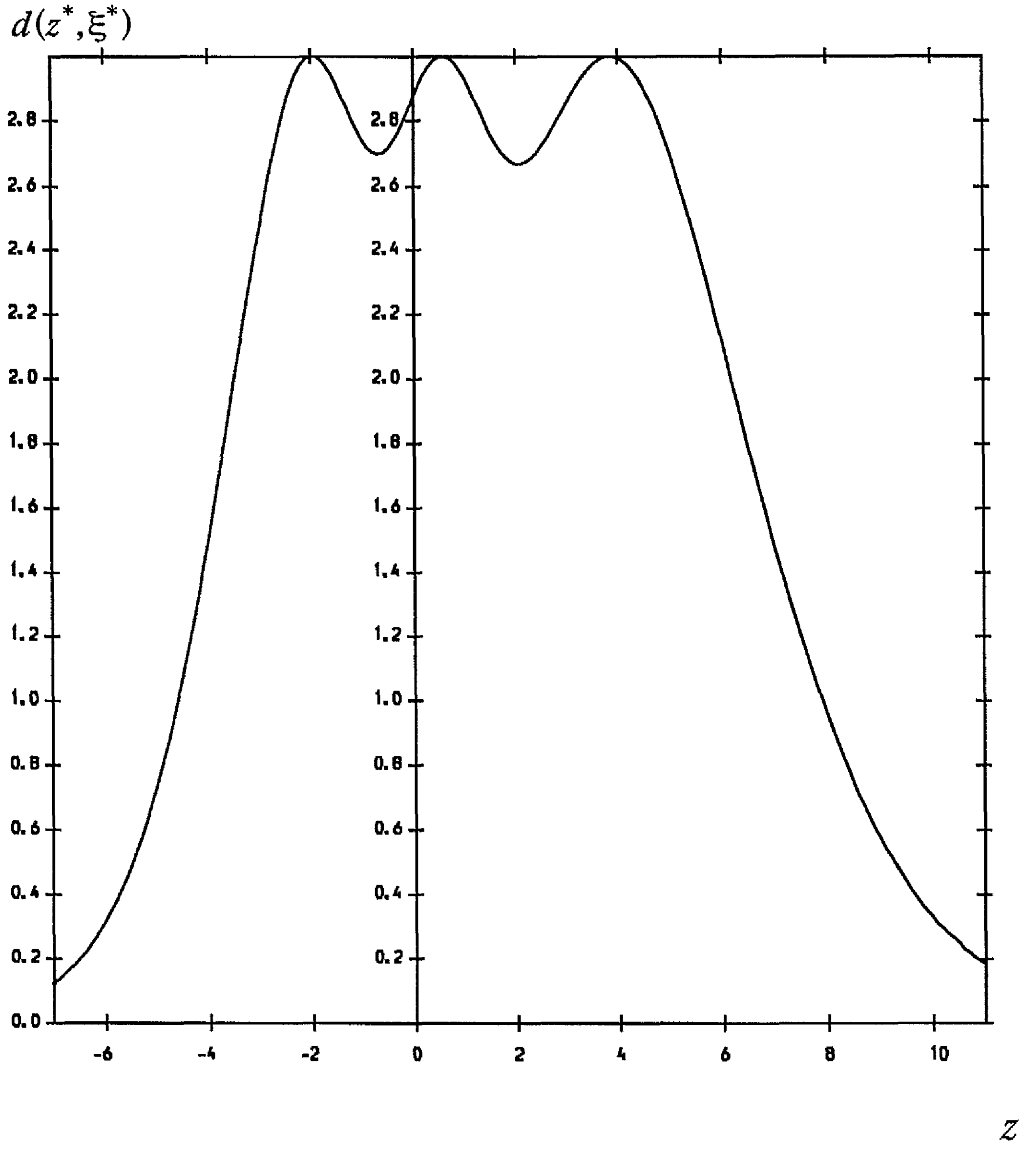


Figure (5.6)

Plot of the variance function for the global asymmetric D-optimal three-point design on the widest choice $Z_w = (-1,1)$ for the asymmetric weight function $w_1(z)$ with $(\alpha = 0.0, \beta = 1.0)$.

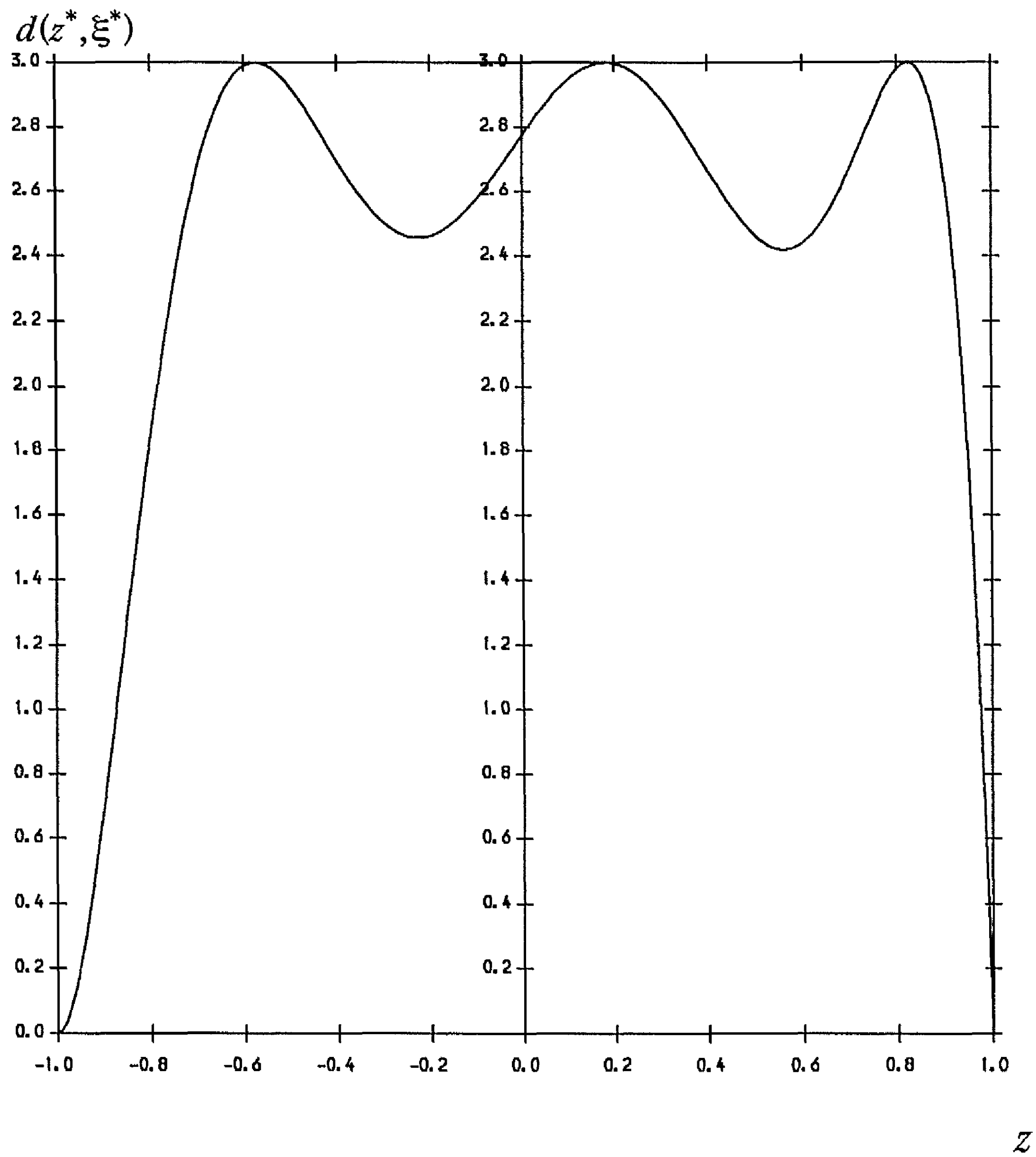


Figure (5.7)

Plot of the variance function for the global asymmetric D-optimal three-point design on the widest choice $Z_w = (0, \infty)$ for the asymmetric weight function $w_2(z)$ with $(\alpha = 1.0)$.

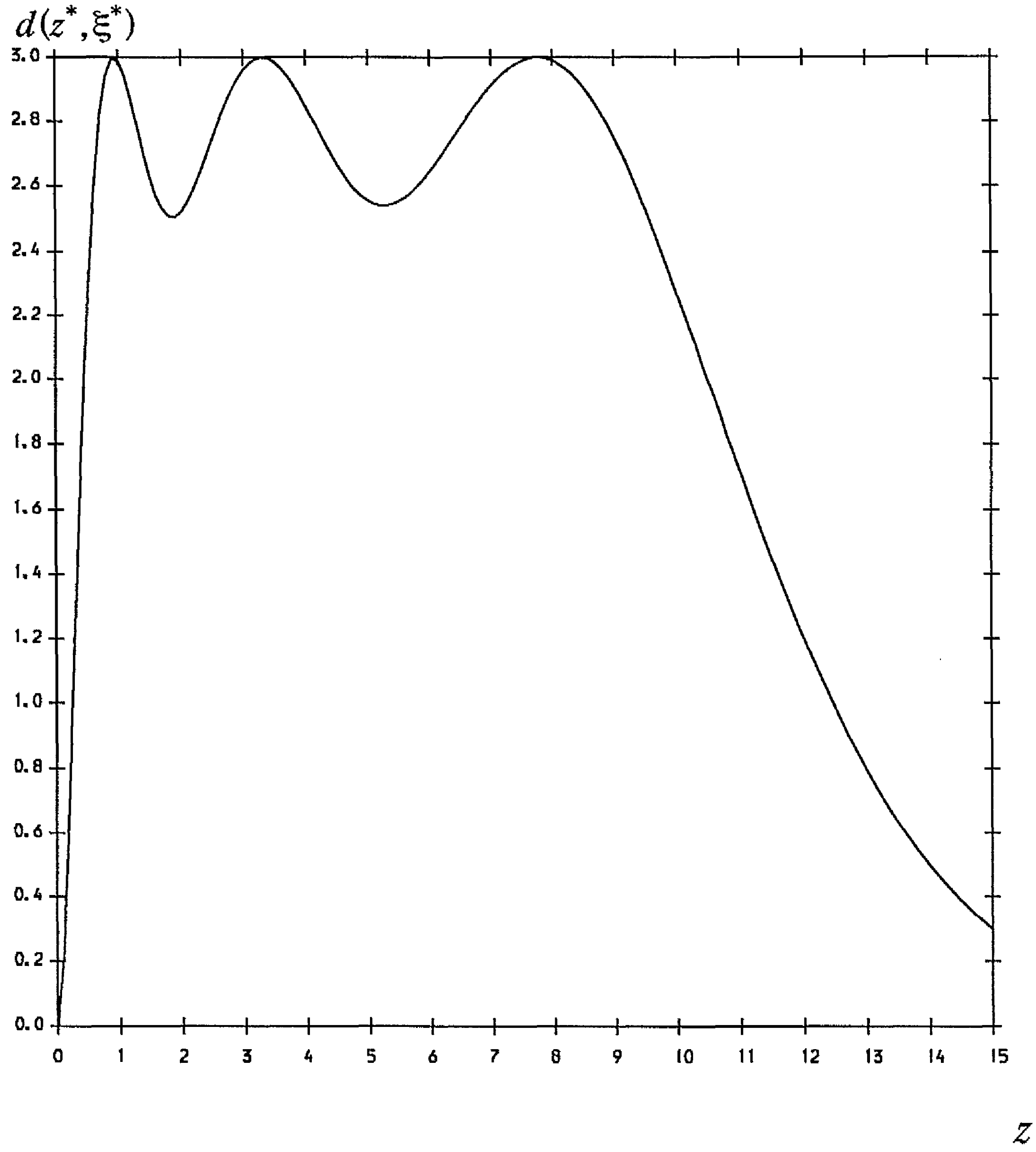


Figure (5.8)

Plot of the variance function for the global symmetric D-optimal three-point design on the widest choice $Z_w = (-\infty, \infty)$ for the symmetric weight function $w_3(z)$.

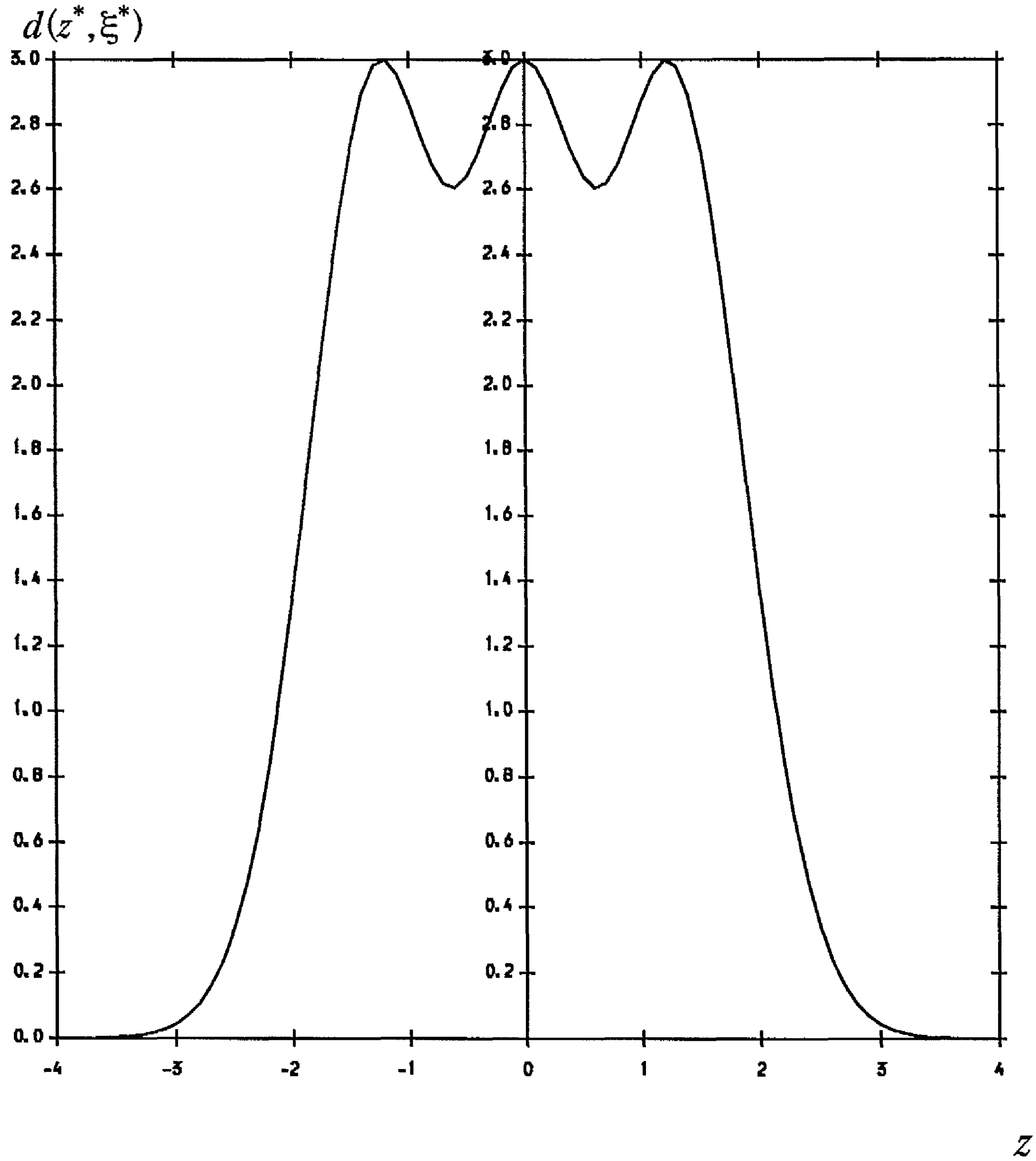


Figure (5.9)

Plot of the variance function for the global D-optimal three-point design on the interval $Z = [0, \infty)$ for the symmetric double exponential model.

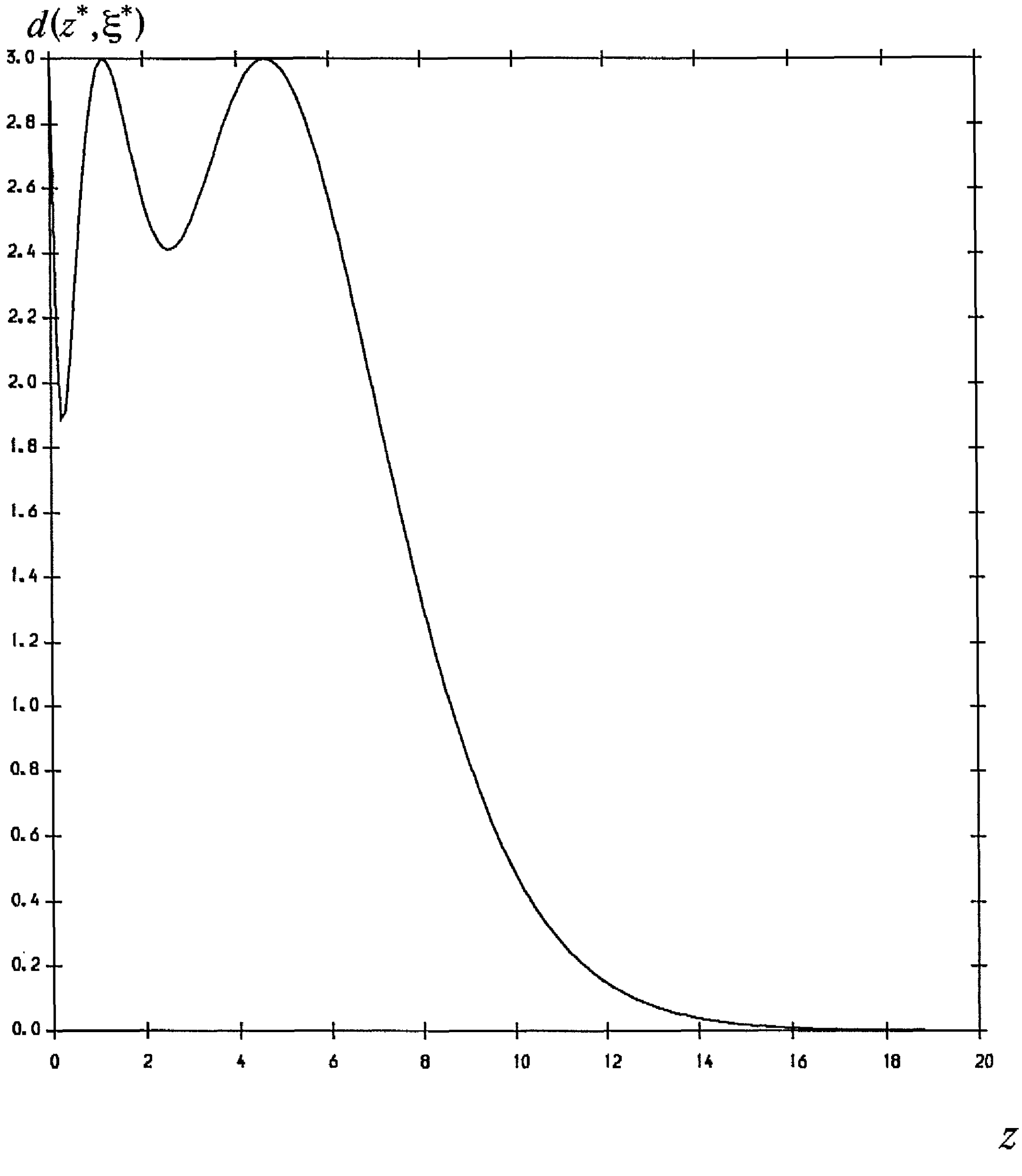


Figure (5.10)

Plot of the variance function for the global D-optimal three-point design on the interval $Z = [0, \infty)$ for the asymmetric complementary log-log model.

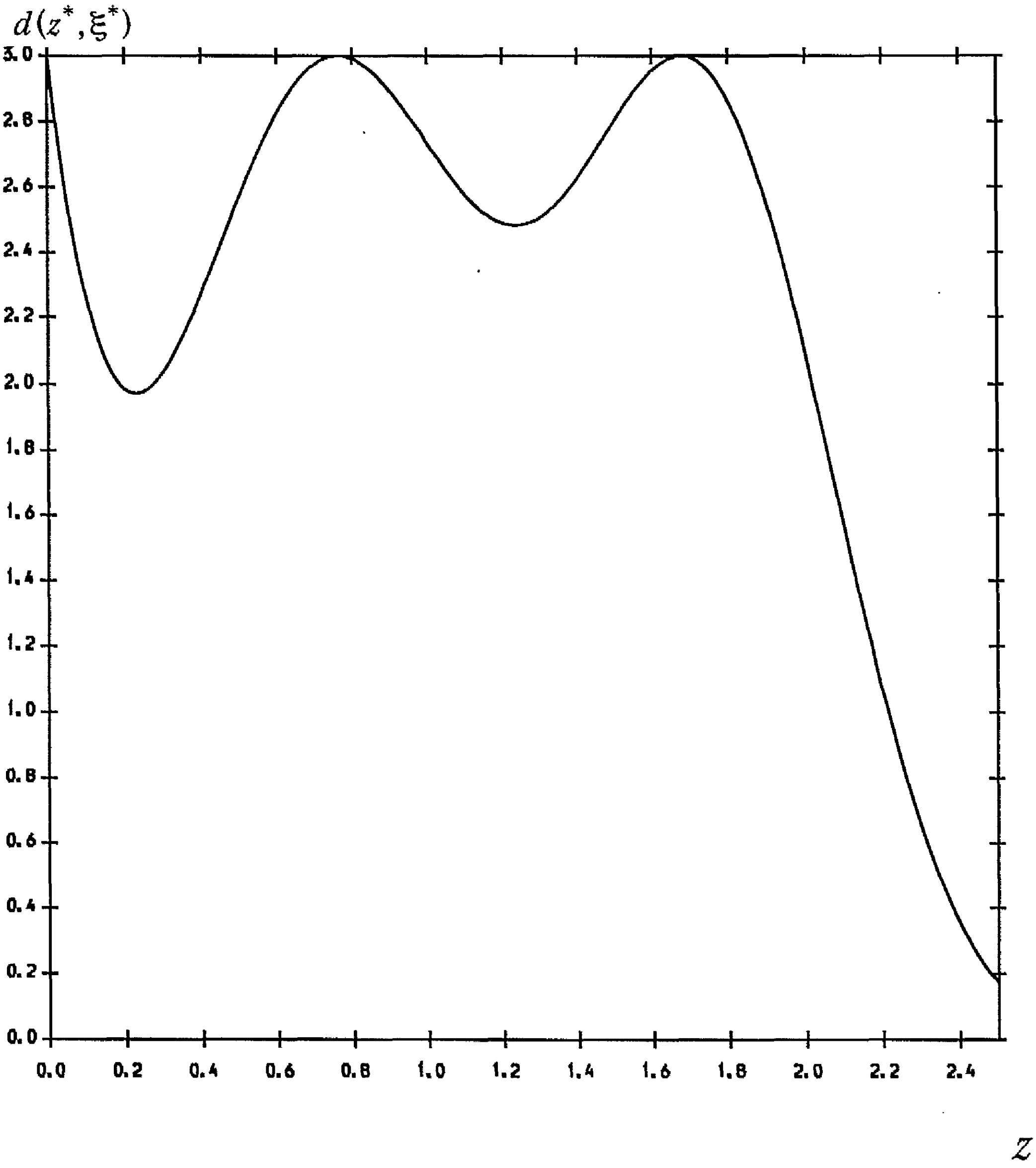


Figure (5.11)

Plot of the variance function for the global D-optimal three-point design on the widest choice Z_w for the complementary log-log model with $w^*(z^2+c)$ for $c = 0.5$.

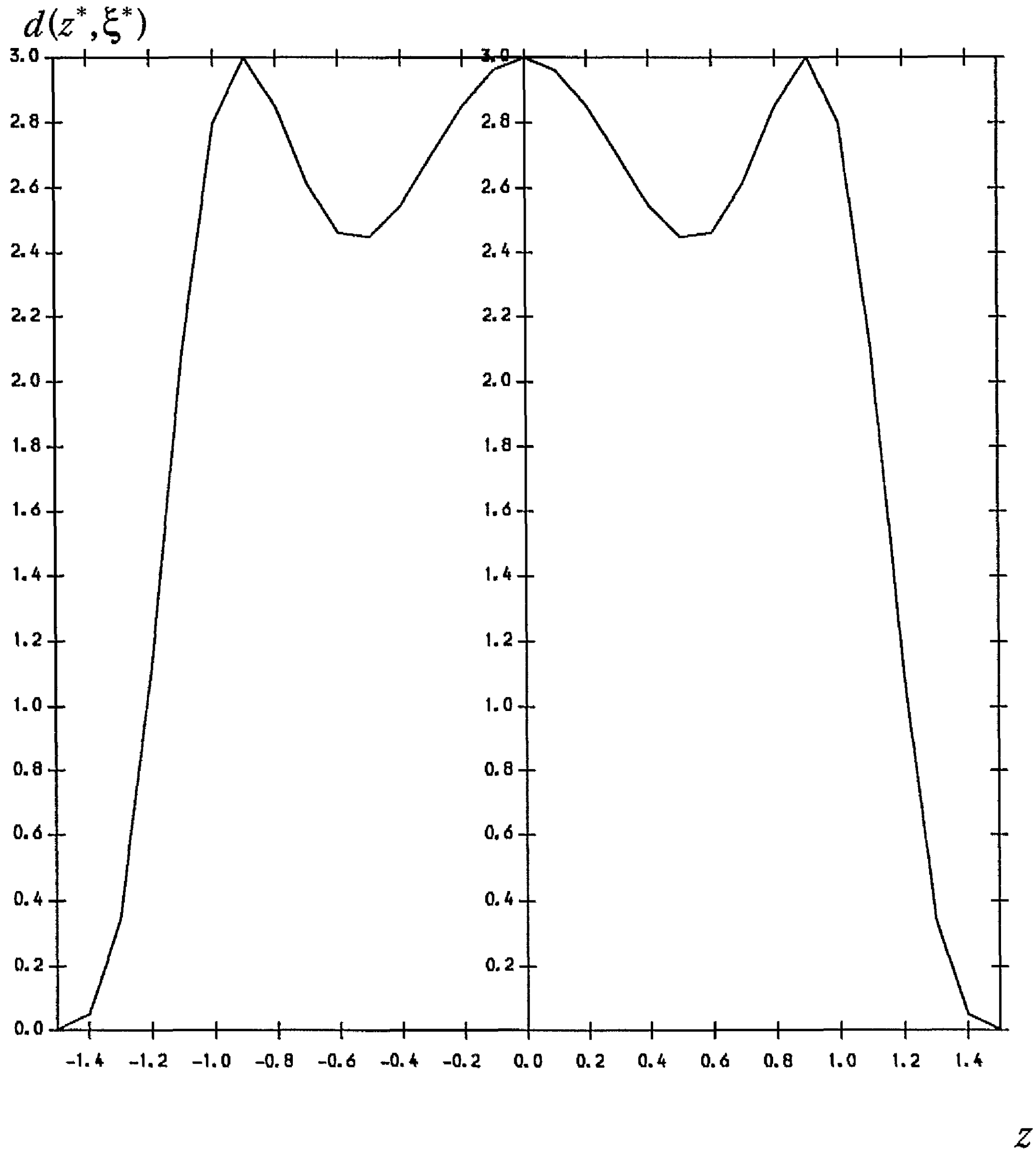


Figure (5.12)

Plot of the variance function for the global D-optimal three-point design on the widest choice Z_w for the complementary log-log model with $w^*(-z^2+c)$ for $c=-1.0$.

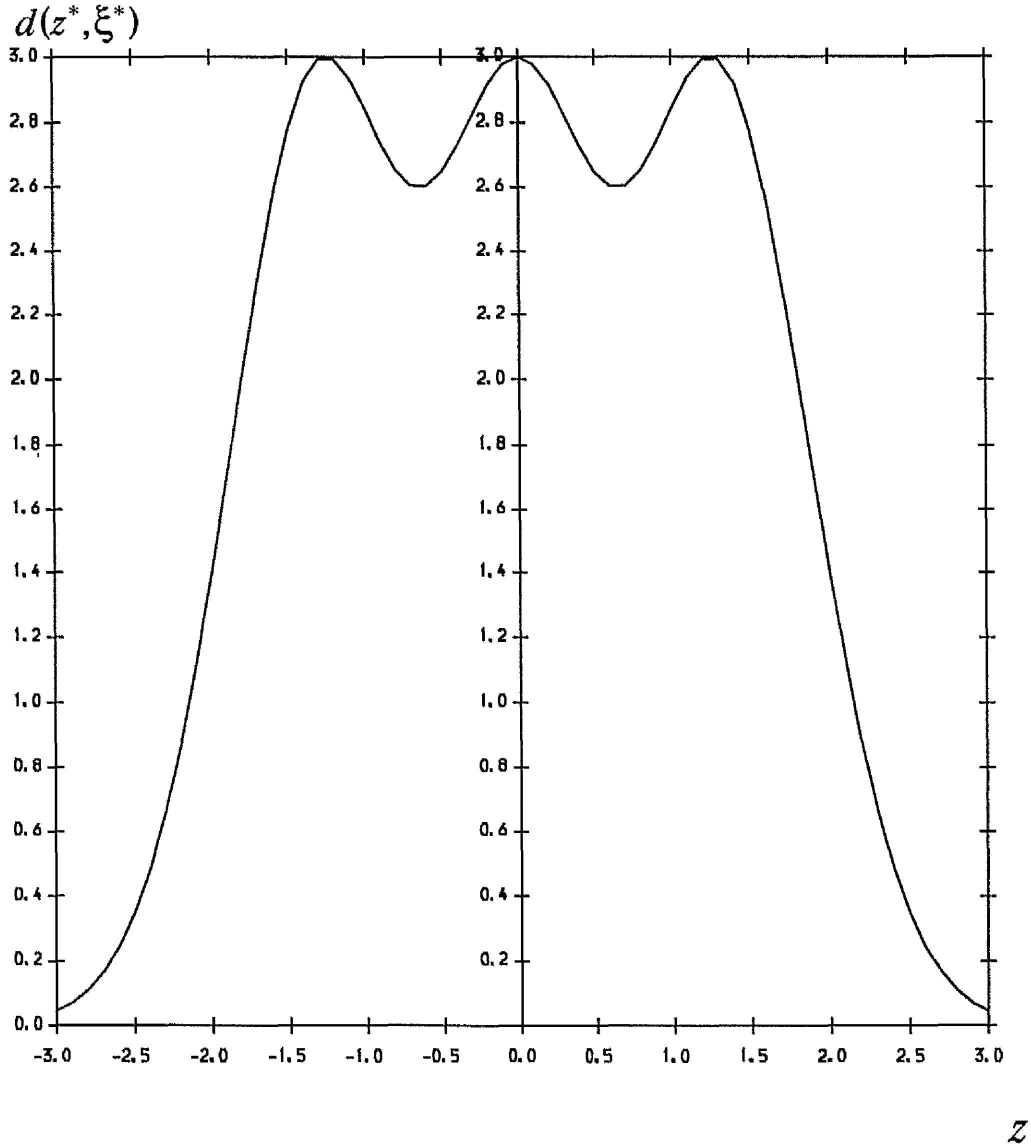


Figure (5.13)

Plot of the variance function for the global D-optimal three-point design on the widest choice Z_w for the double exponential model with $w^*(z^2+c)$ for $c=1.0$.

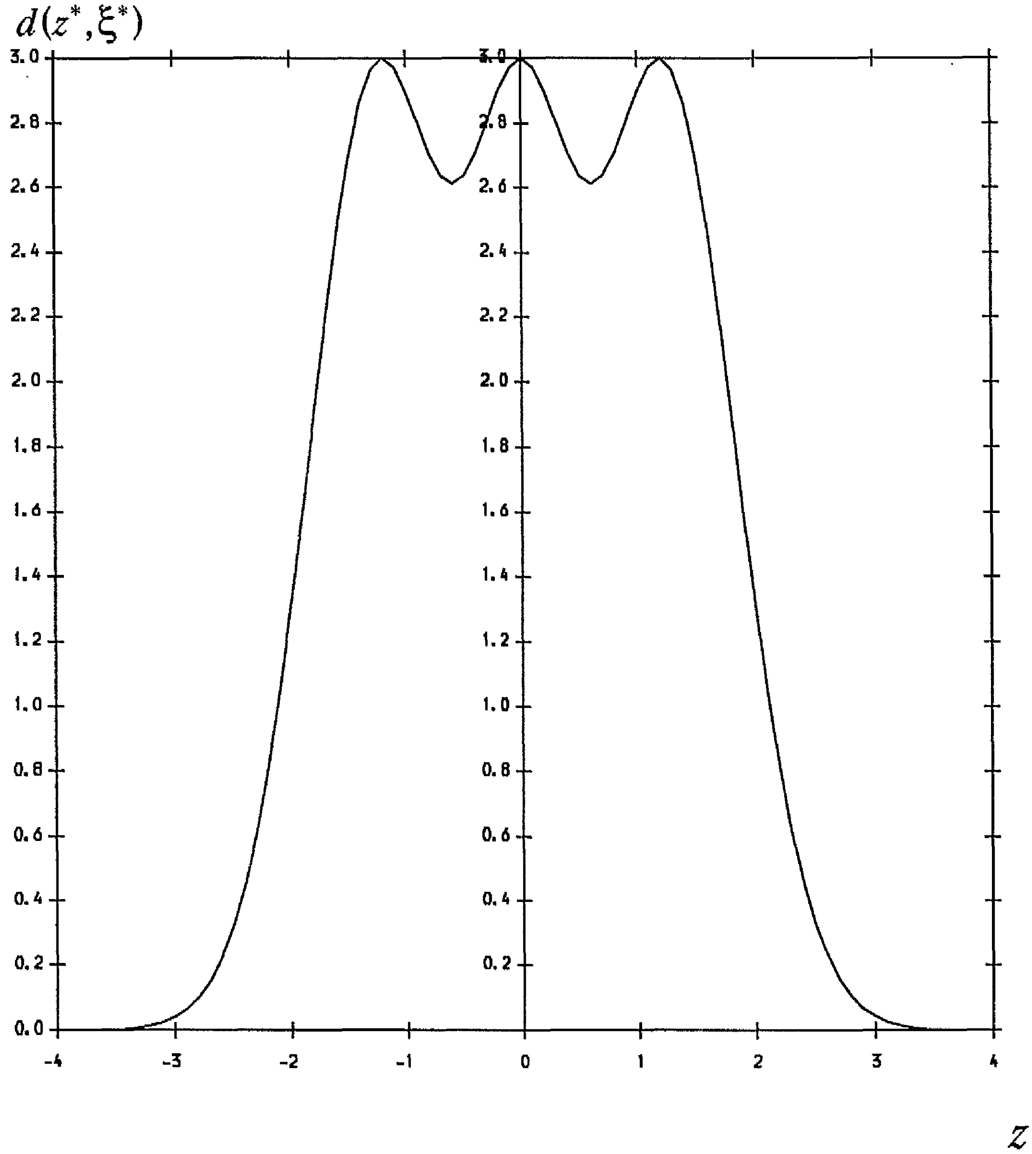


Figure (5.14)

Plot of the variance function for the global D-optimal three-point design on the widest choice Z_w for the double reciprocal model with $w^*(z^2+c)$ for $c = 0.5$.

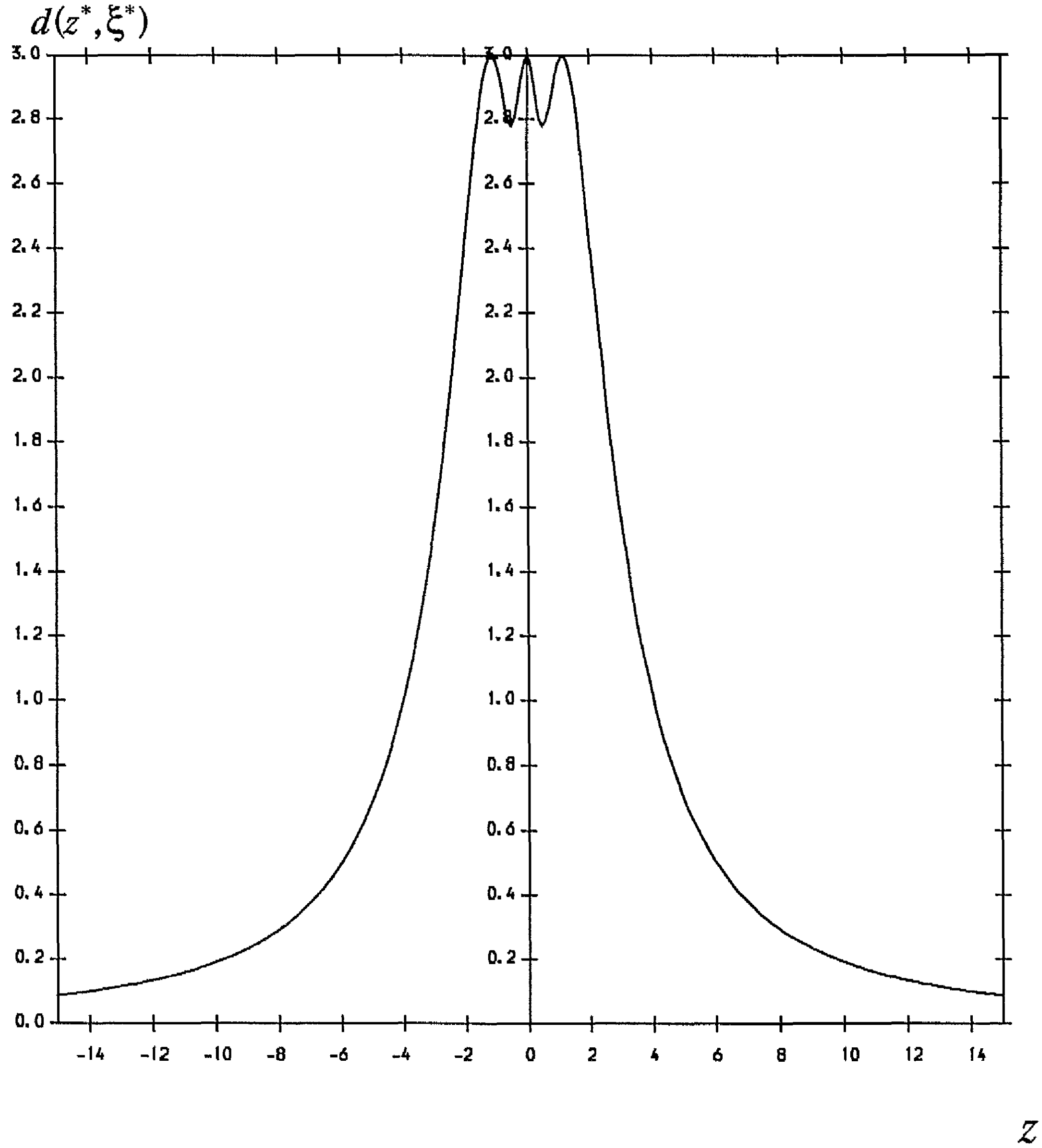


Figure (5.15)

Plot of the variance function for the global D-optimal four-point design on the widest choice Z_w for the double exponential model with $w^*(z^2+c)$ for $c=-1.0$.

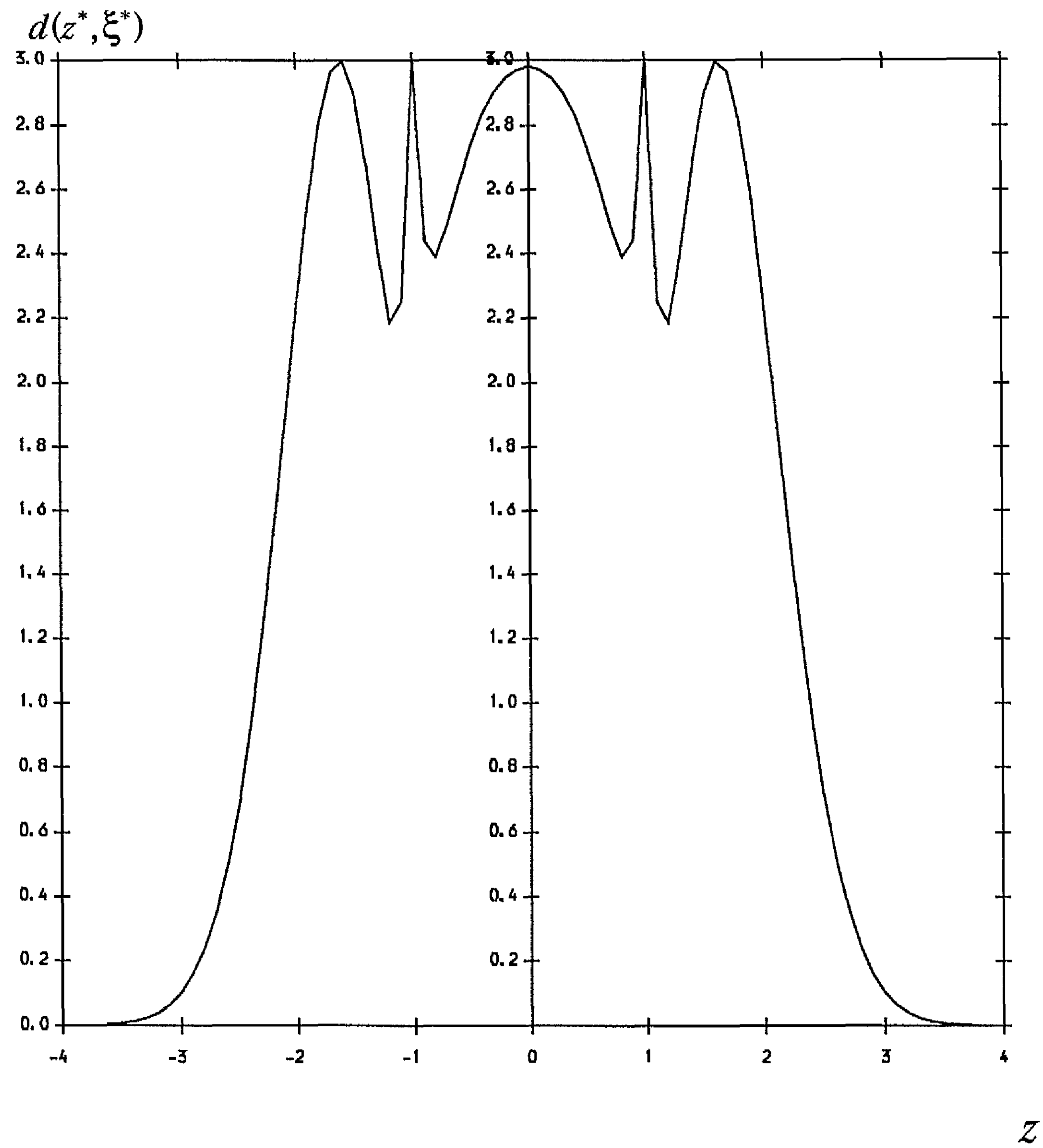


Figure (5.16)

Plot of the variance function for the global D-optimal four-point design on the widest choice Z_w for the double reciprocal model with $w^*(z^2+c)$ for $c=-0.5$.

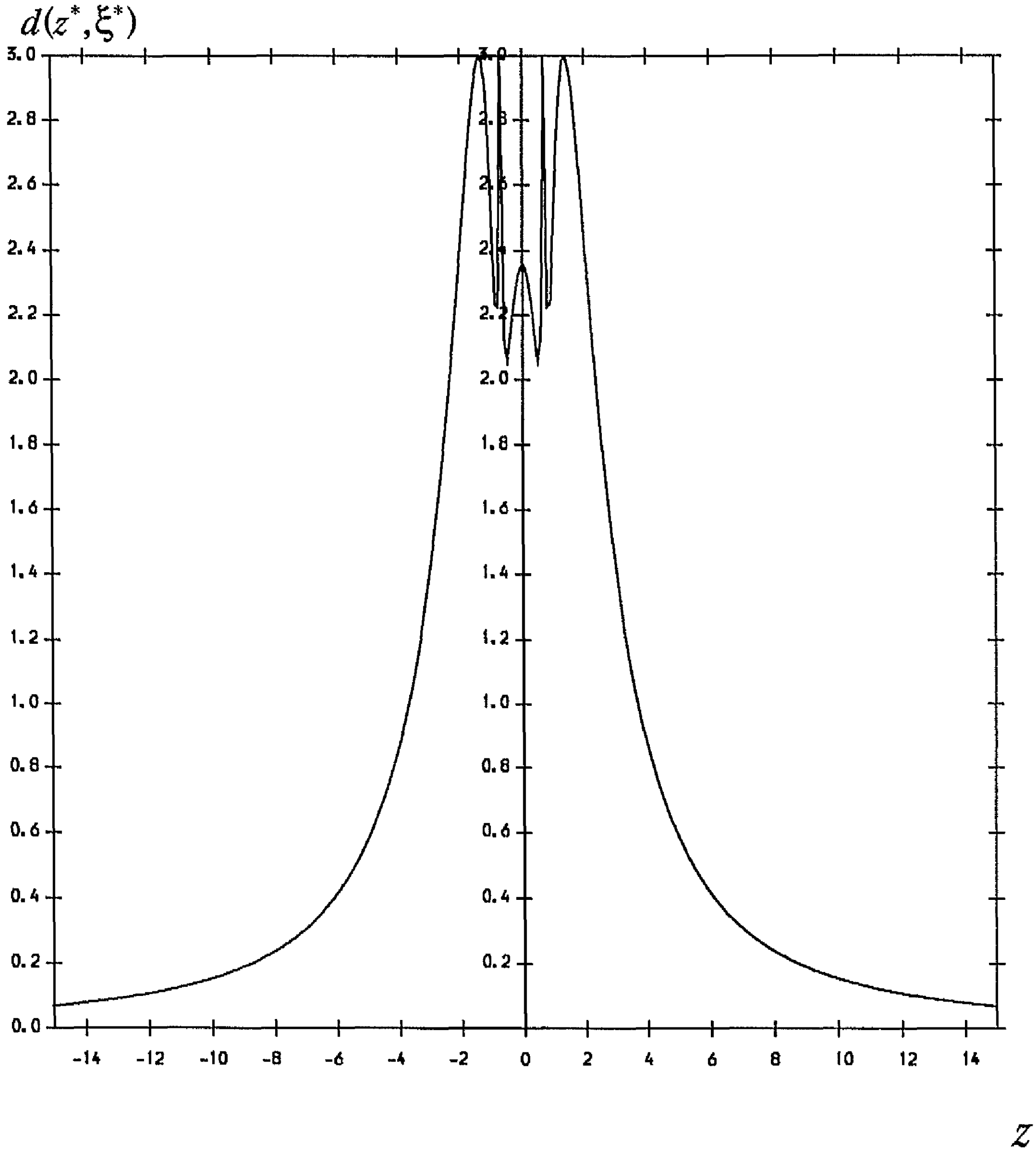


Figure (5.17)

Plot of the variance function for the global D-optimal five-point design on the widest choice Z_w for the double exponential model with $w^*(z^2+c)$ for $c=-1.5$.

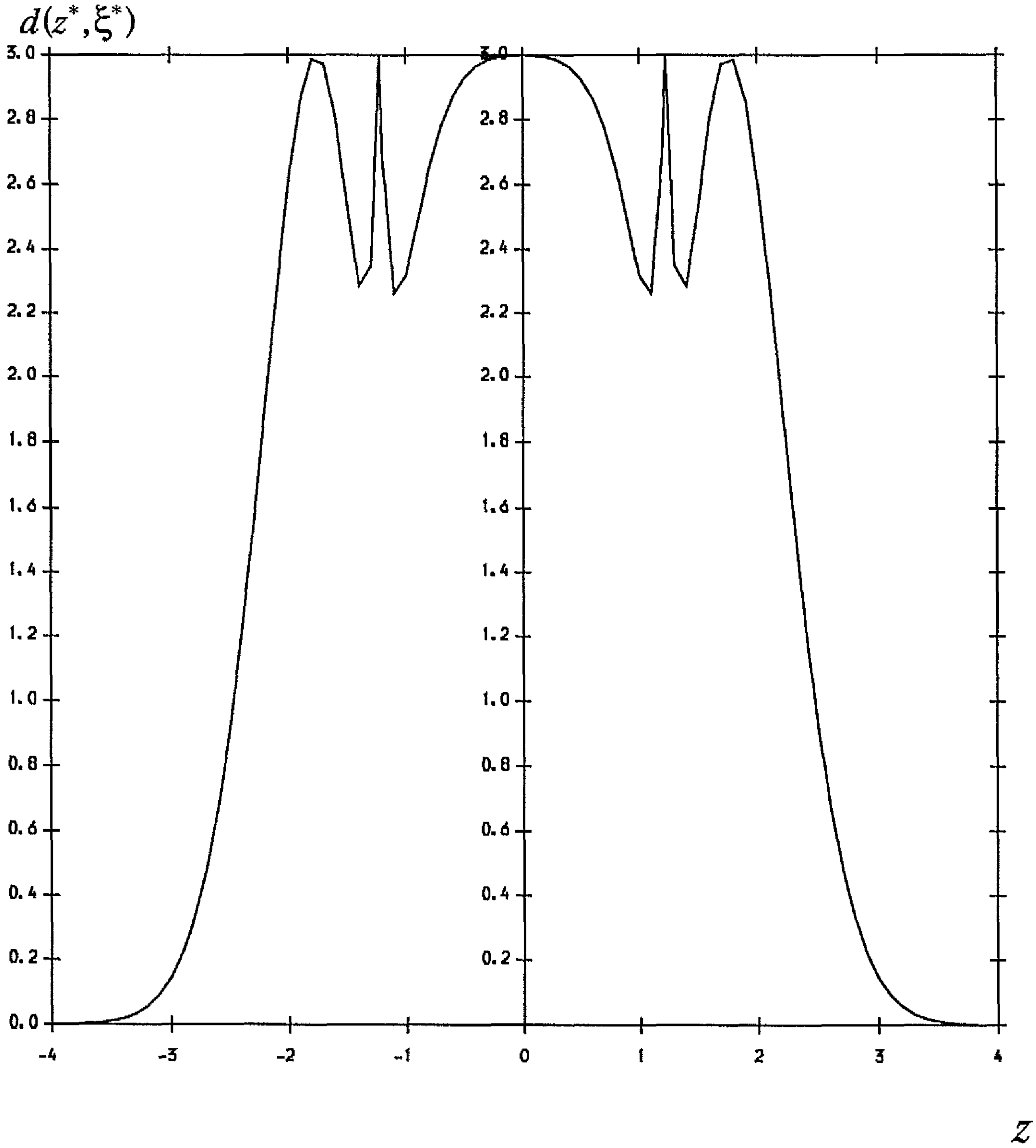


Figure (5.18)

Plot of the variance function for the global D-optimal five-point design on the widest choice Z_w for the double reciprocal model with $w^*(z^2+c)$ for $c=-1.2$.

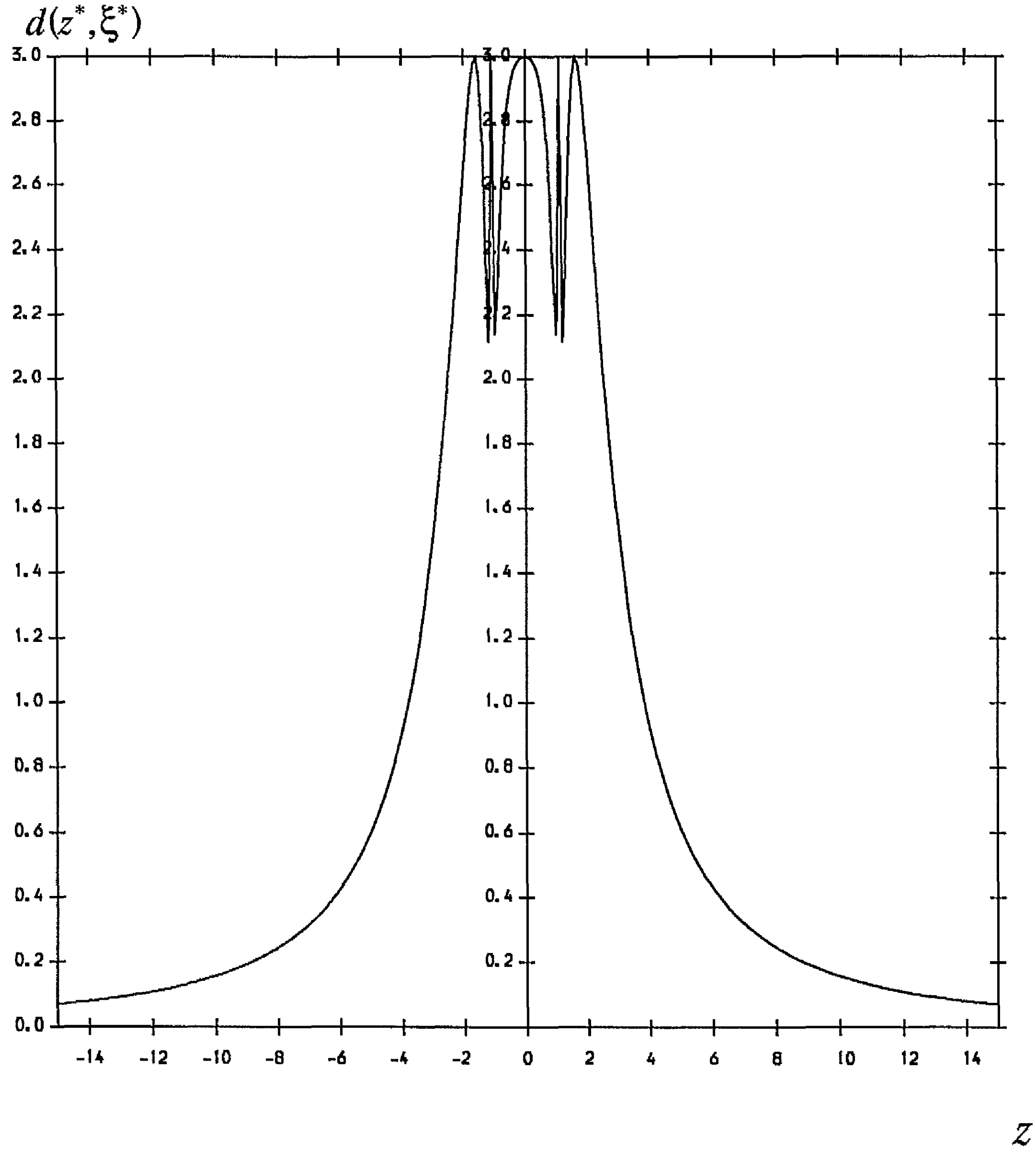


Figure (5.19)

Plot of the variance function for the global D-optimal six-point design on the widest choice Z_w for the double exponential model with $w^*(z^2+c)$ for $c=-4.0$.

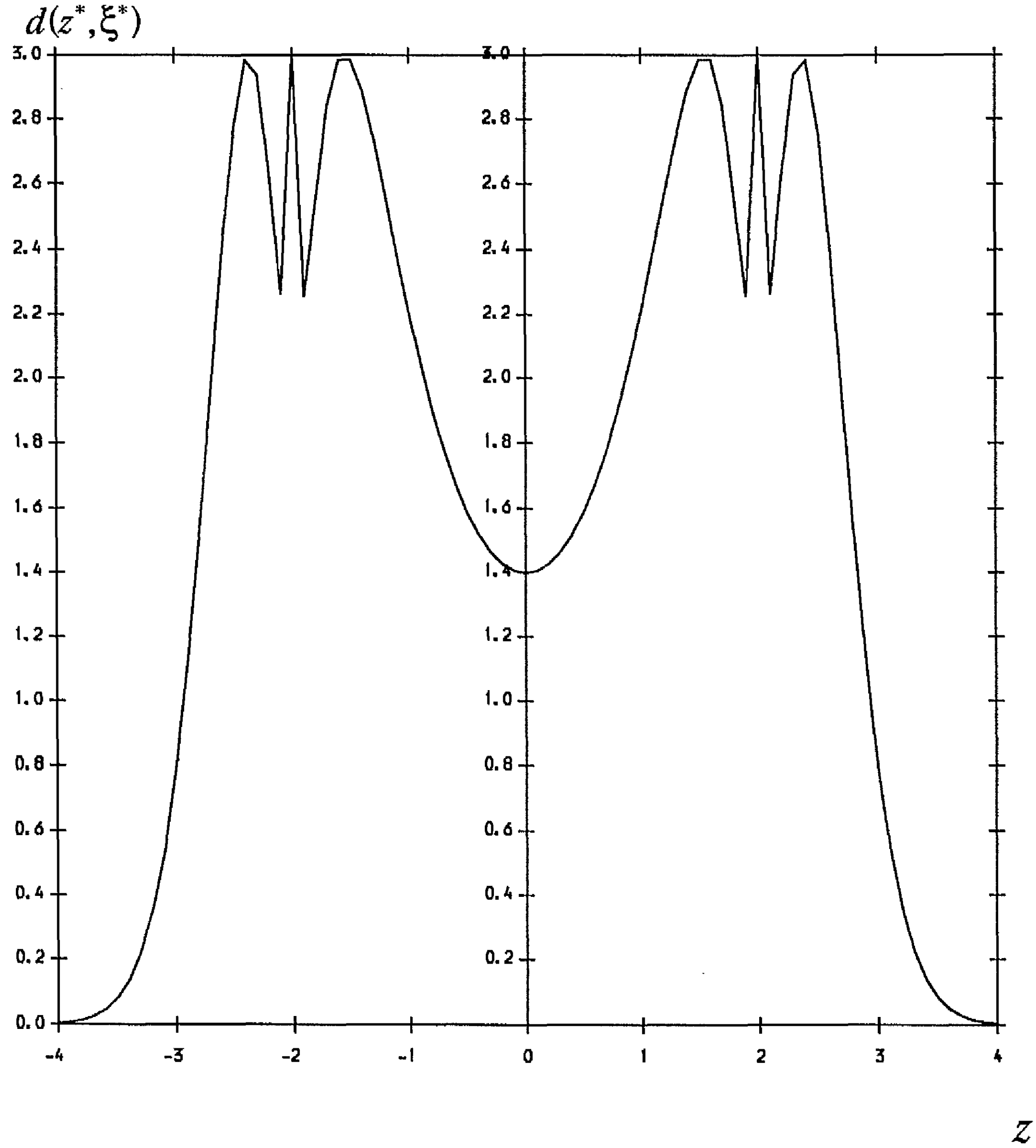


Figure (5.20)

Plot of the variance function for the global D-optimal six-point design on the widest choice Z_w for the double reciprocal model with $w^*(z^2+c)$ for $c=-4.0$.

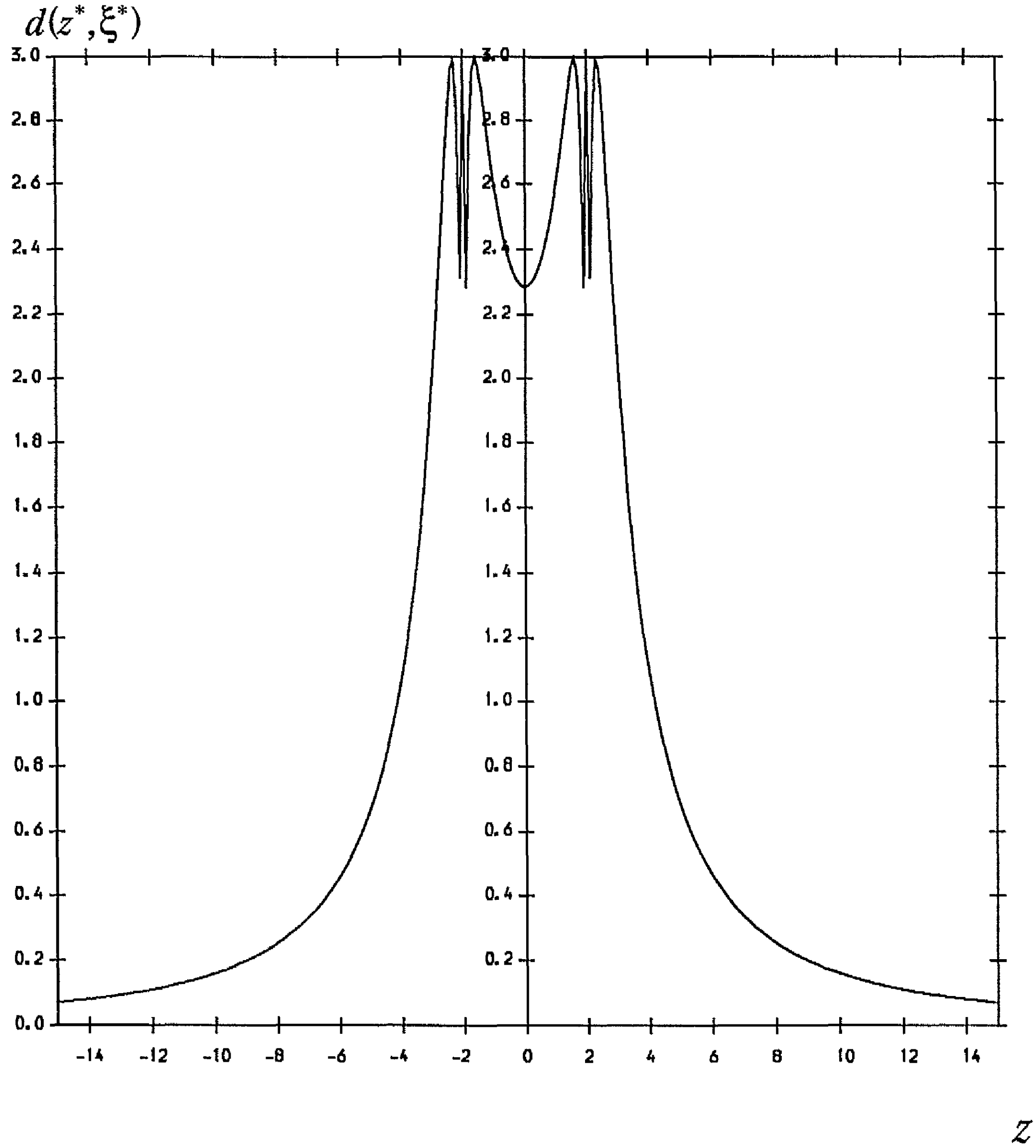


Figure (5.21)

Plot of the variance function for the global D-optimal three-point design on the interval $Z = [0, \infty)$ for the logistic model with $w^*(z^2 + c)$ for $c = 0$.

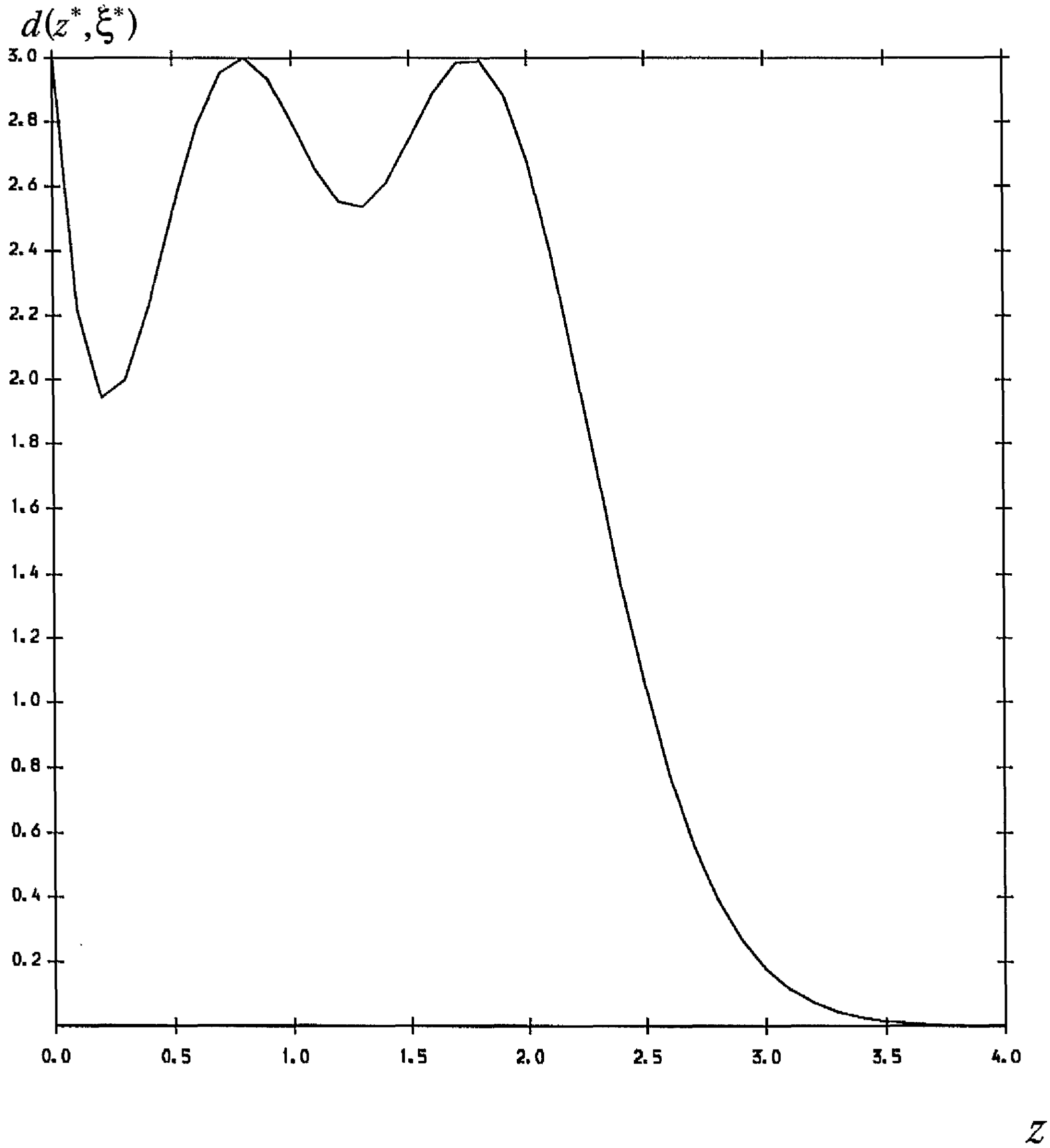


Figure (5.22)

Plot of the variance function for the global D-optimal three-point design on the interval $Z = [0,\infty)$ for the probit model with $w^*(z^2+c)$ for $c = -1.0$.

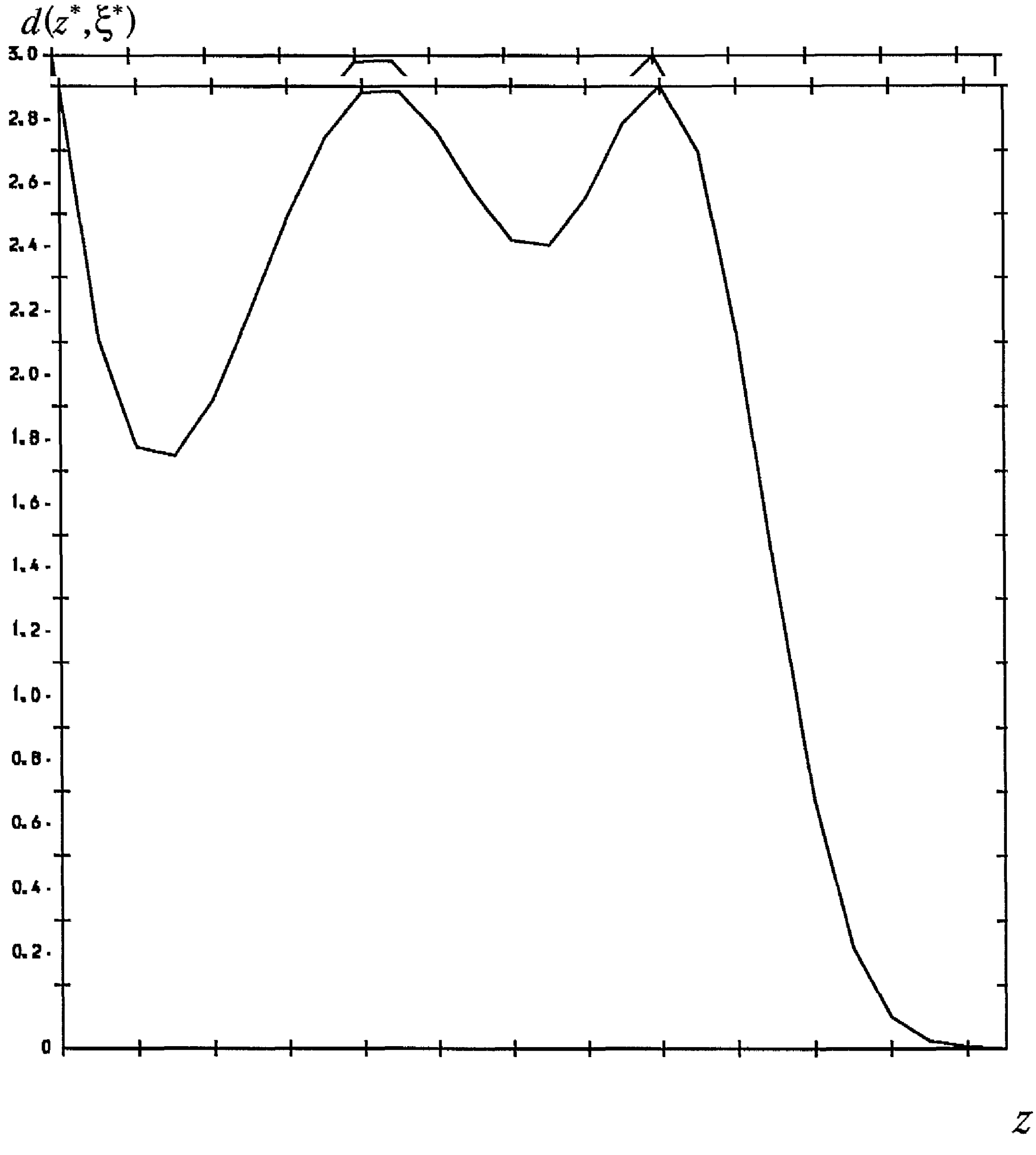


Figure (5.23)

Plot of the variance function for the global D-optimal three-point design $\{0, \hat{z}_1, \hat{z}_2\}$ on the interval $Z = [0, \infty)$ for the double exponential model with $w^*(z^2 + c)$ for $c = -0.2$.

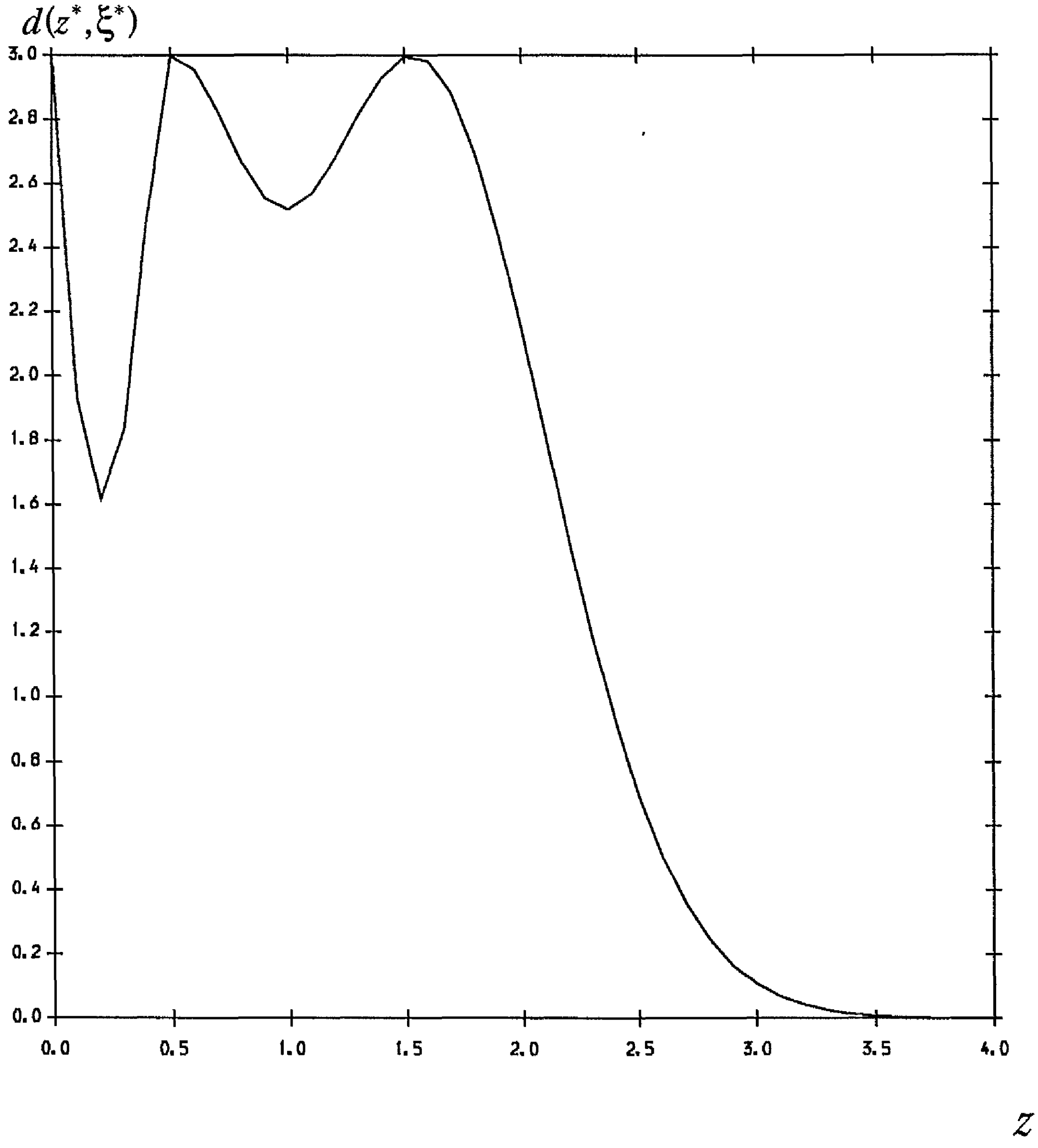


Figure (5.24)

Plot of the variance function for the global D-optimal three-point design $\{0, \hat{z}_1, \hat{z}_2\}$ on the interval $Z = [0, \infty)$ for the double reciprocal model with $w^*(z^2 + c)$ for $c = 0.5$.

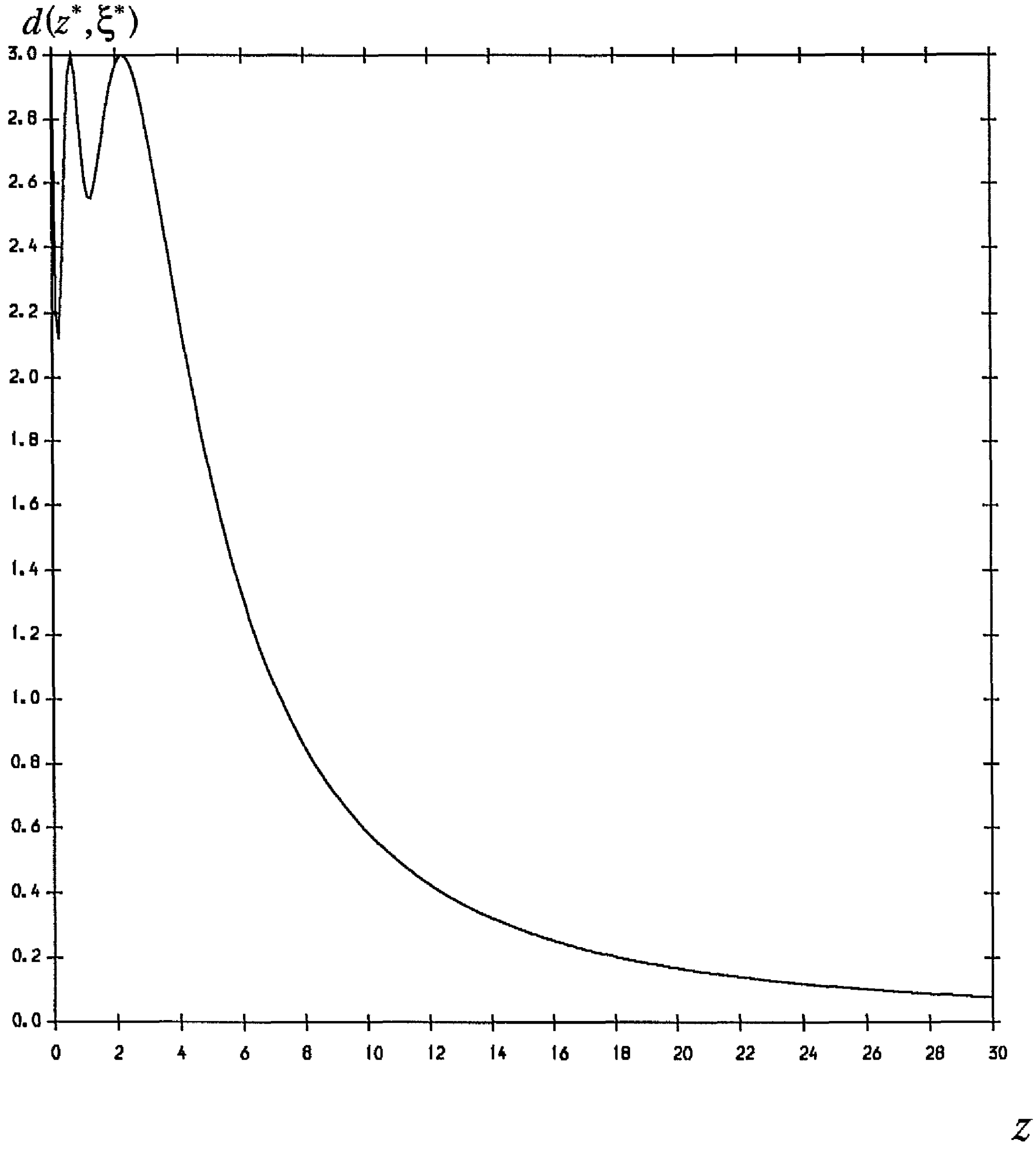


Figure (5.25)

Plot of the variance function for the global D-optimal three-point design $\{0, \sqrt{|c|}, \hat{z}\}$ on the interval $Z = [0, \infty)$ for the double exponential model with $w^*(z^2 + c)$ for $c = -1.0$.

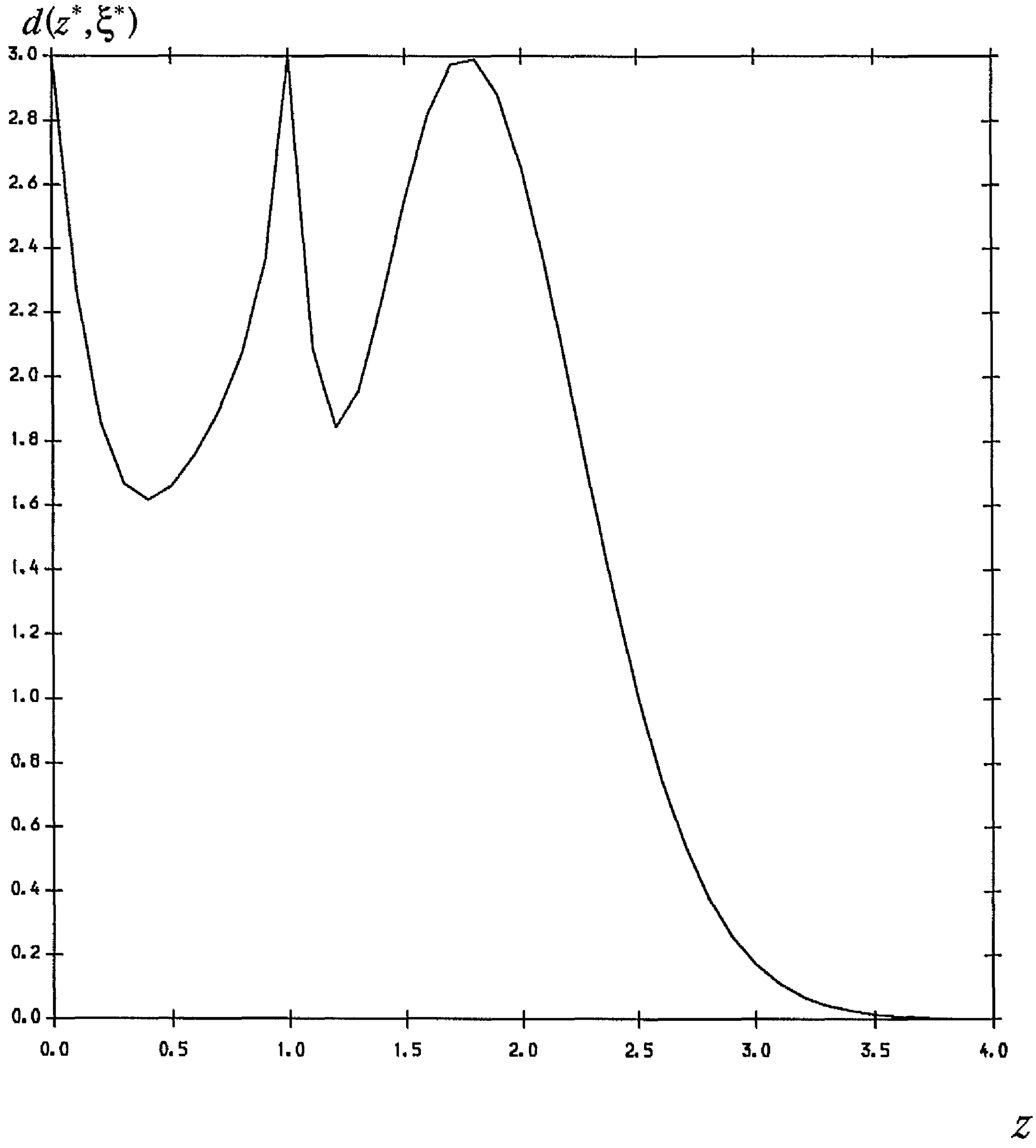


Figure (5.26)

Plot of the variance function for the global D-optimal three-point design $\{0, \sqrt{|c|}, \hat{z}\}$ on the interval $Z = [0, \infty)$ for the double reciprocal model with $w^*(z^2 + c)$ for $c = -1.0$.

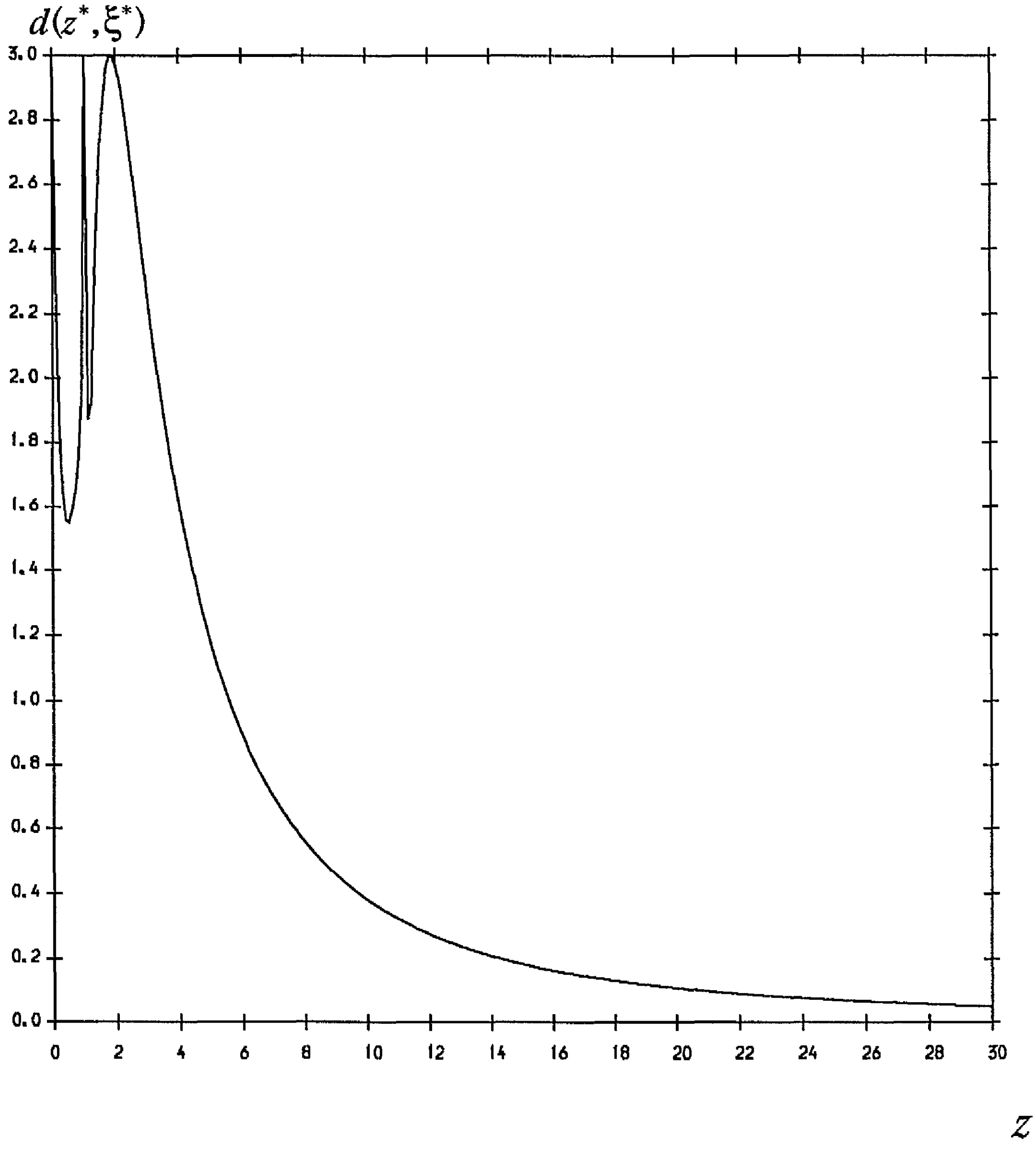


Figure (5.27)

Plot of the variance function for the global D-optimal four-point design $\{0, \tilde{z}_1, \sqrt{|c|}, \tilde{z}_2\}$ on the interval $Z = [0, \infty)$ for the double exponential model with $w^*(z^2 + c)$ for $c = -4.0$.

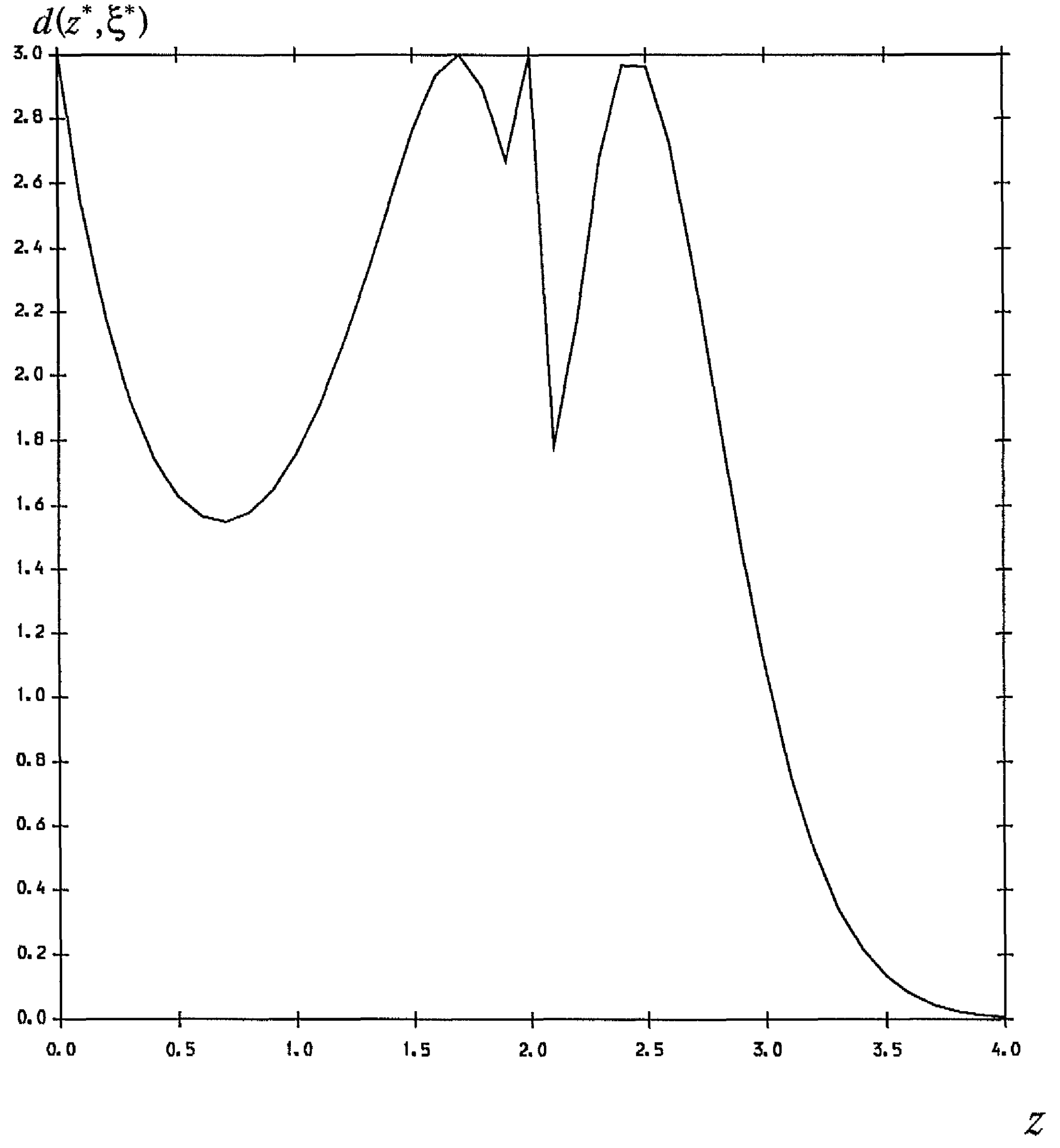
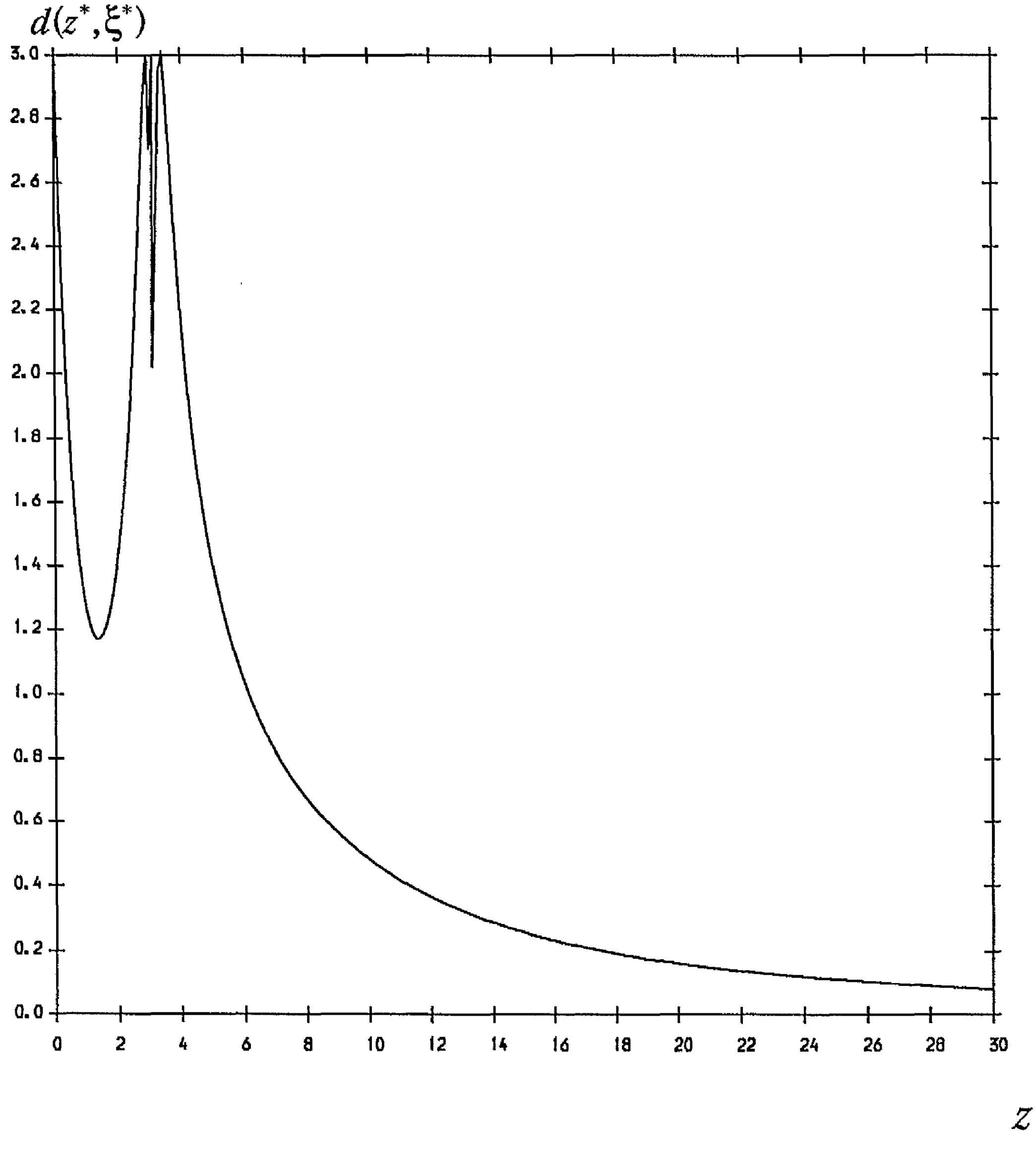


Figure (5.28)

Plot of the variance function for the global D-optimal four-point design $\{0, \tilde{z}_1, \sqrt{|c|}, \tilde{z}_2\}$ on the interval $Z = [0, \infty)$ for the double reciprocal model with $w^*(z^2 + c)$ for $c = -9.5$.



CHAPTER SIX

FURTHER WORK

The main target of this thesis was to gain knowledge, by means of theoretical and applied work, on optimal non-linear experimental design with application to binary response and to weighted regression models. The two different routes of inquiry, theoretical argument and laboratory experimentation, throughout this thesis were followed.

Ironically optimal designs for non-linear problems require knowledge of the unknown parameters. Some static designs are based on initial point estimates for the unknown parameters while others require specification of a range of plausible values or a prior distribution for the unknown parameters. More experience is needed on the application of these approaches to practical problems.

We have derived locally c-optimal and D-optimal designs for a variety of simple non-linear problems. We hope that this work will excite interest in this area and lead to further work on the construction of designs for more complex cases, particularly in the important but more difficult situations where there is more than one explanatory variable. It would be of interest to study more complex problems with more parameters. Such problems will, generally speaking, be difficult to solve although work in progress by Torsney and Sitter has proved promising. Also some interesting special cases do exist. For example as Ford, Torsney, and Wu (1992) noted in the case of uncensored exponentially distributed survival data with $\eta = \exp(\underline{\theta}' \underline{s})$, the optimal design will not depend on the unknown parameters at all (see Cox and Oakes (1984)).

APPENDIX I

AI.1 Convex sets.

Definition 1: The set S is called convex if any point $s = \alpha s_1 + (1-\alpha)s_2$, where $s_1, s_2 \in S$, and $0 \le \alpha \le 1$, belongs to this set.

Definition 2: The set of points, S^* say, with elements $s^* = \sum_{i=1}^{k} \alpha_i s_i$, where $\sum_{i=1}^{k} \alpha_i = 1$, $\alpha_i \ge 0$, $s_i \in S$ $(i = 1,2,\ldots,k, k = 1,2,\ldots)$, is a convex set.

Definition 3: The set S^* is called the convex hull of the set S.

Definition 4 : If X is a convex set, then a numerical function defined on S is called convex if for $s_1, s_2 \in S$ and all α satisfying the condition $0 \le \alpha \le 1$,

$$f[\alpha s_1 + (1-\alpha)s_2] \le \alpha f(s_1) + (1-\alpha)f(s_2),$$

and is called concave if

$$f[\alpha s_1 + (1-\alpha)s_2] \ge \alpha f(s_1) + (1-\alpha)f(s_2).$$

If these inequalities are strict for $s_1 \ne s_2$, $0 < \alpha < 1$, then the function f is called, respectively, strictly convex or strictly concave.

AI.2 Caratheodory's theorem.

Theorem: Each point s^* in the convex hull S^* of any subset S, of the n-dimensional space, can be represented in the form

$$s^* = \sum_{i=1}^{n+1} \mu_i s_i,$$

where $\mu_i \geq 0$, $\sum_{i=1}^{n+1} \mu_i = 1$, $s_i \in S$. If s^* is a boundary point of the set S^*, then μ_{n+1} can be set equal to zero. See Fedorov (1972); Silvey (1980).

AI.3 Silvapulle's theorem.

Silvapulle (1981) stated and proved the conditions under which the existence of the MLE in binary problems is guaranteed.

Let $u_1, u_2, \ldots, u_r$ be the design points corresponding to responses $y_i = 1$, $(i = 1, 2, \ldots, r)$ and $u_{r+1}, \ldots, u_n$ corresponding to responses $y_j = 1$, $(j = r+1, \ldots, n)$.

Consider the convex cones $S = \left\{ \sum_{i=1}^{r} k_i u_i,\ k_i \geq 0 \right\}$ and $T = \left\{ \sum_{j=r+1}^{n} k_j u_j,\ k_j \geq 0 \right\}$. Then the following theorem holds.

Theorem: Let the condition (L) be defined by

$$(L) \quad S \cap T \neq \varnothing \text{ or one of } S \text{ or } T \text{ is } R^m \supseteq \underline{\theta}.$$

Then for the binomial response model $\Pr = (y_i = 1) = F(u_i, \underline{\theta})$

(i) The MLE $\hat{\underline{\theta}}$ of $\underline{\theta}$ exists and the minimum set $\{\underline{\theta}\}$ is bounded only when L is satisfied.

(ii) Suppose that $\ell(\underline{\theta}) = -\sum \ln F(u_i, \underline{\theta}) - \sum \ln[1 - F(u_i, \underline{\theta})]$, is a proper closed convex function on R^m. Then the MLE $\hat{\underline{\theta}}$ exists and the minimum set $\{\hat{\underline{\theta}}\}$ is bounded if and only if (L) is satisfied.

(iii) Suppose that $-\ln F$ and $\ln(1-F)$ are convex and $u_{1i} = 1$ for every i. Then $\hat{\underline{\theta}}$ exists and the minimum set $\{\hat{\underline{\theta}}\}$ is bounded if and only if $S \cap T \neq \varnothing$. Let us further assume that F is strictly increasing at every t satisfying $0 < F(t) < 1$. Then $\underline{\theta}$ is uniquely defined if and only if $S \cap T = 0$.

APPENDIX II

AII.1 Generalised inverse.

Definition : Let $A \in M(m,n)$, with $M(m,n)$ the set of $m \times n$ matrices then A^- is the Moore-Penrose generalised inverse iff:

(i) AA^- and A^-A are symmetric.

(ii) $A^-AA^- = A^-$ and $AA^-A = A^-$.

Properties:

(1) When A^- exists it is of size $n \times m$ and it is unique.

(2) $(A^-)^- = A$.

(3) $(A^t)^- = (A^-)^t$.

(4) rank (A) = rank(A^-) = rank (AA^-) = rank (A^-A) = rank (AA^-A)= rank (A^-AA^-).

(5) If $A = A^t$ then $A^- = (A^-)^t$.

(6) If $A = A_1 + A_2 + \cdots + A_k$ and $A_i A_j^t = 0$ for all i,j=1,2,........,k $i \neq j$ then $A^- = A_1^- + A_2^- + \cdots + A_k^-$.

(7) If $\underline{a}$ is a non zero vector then $\underline{a}^- = (\underline{a}^t \underline{a})^- \underline{a}^t = \|\underline{a}\|^{-2} \underline{a}^t$.

AII.2 Newton-Raphson method.

Let f be a function $f: R^n \to R^n$ with a root ε i.e. $f(\varepsilon) = 0$. Iterative techniques are considered to evaluate such as ε. When n=1 the iteration, known as Newton-Raphson is

$$x_{i+1} = x_i - f(x_i) / f'(x_i) \ , \ \ i = 0,1,2,\ldots$$

When n>1 the above scheme is generalised to

$$\underline{x}^{(i+1)} = \underline{x}^{(i)} - \{H[\underline{x}^{(i)}]\}^{-1} \underline{f}[\underline{x}^{(i)}] \quad , \; i = 0,1,2,\ldots$$

where $\underline{f}[\underline{x}^{(i)}]$ is the gradient vector and $H[\underline{x}^{(i)}]$ is the $n \times n$ jacobian matrix with elements $\partial f_i / \partial x_j$, $i,j = 1,2,\ldots,n$. We assume that $H[\underline{x}^{(i)}]$ is non-singular.

Newton provides conditions under which the Newton-Raphson method converges, provided that the initial guess lies in the neighbourhood of the solution ε.

The method is very rapidly converging scheme. Its convergence is of quadratic order i.e.

$$\|\underline{x}^{(i+1)} - \varepsilon\| \leq k \|\underline{x}^{(i)} - \varepsilon\|^{p}, \; p \geq 2$$

where k being a constant and $\|\cdot\|$ the ℓ_2-norm.

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