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D-optimally Lack-of-Fit-Test-efficient Designs and Related Simple Designs

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Abstract: In practice it is often more popular to use a uniform than an optimal design for estimating the unknown parameters of a linear regression model. The reason is that the model can be checked by a uniform design but it cannot be checked by an optimal design in many cases. On the other hand, however, for important regression models a uniform design is not very efficient to estimate the unknown parameters. Therefore Bischoff and Miller proposed in a series of papers a compromise. It is suggested there to look for designs that are optimal with respect to a specific criterion in the class of designs that are efficient for lack-of-fit-tests. In this paper we consider the D-criterion and polynomial regression models. For polynomial regression models with degree larger than two D-optimally lack-of-fit-test-efficient designs are difficult to determine. Therefore, in this paper we determine easily to calculate and for estimating the parameters highly efficient designs that are additionally lack-of-fit-test–efficient.

Zusammenfassung: In der Praxis ist es für die Schätzung unbekannter Parameter oft populärer anstelle eines optimalen Versuchsplans, die Versuchspunkte äquidistant zu verteilen. Dies gilt insbesondere für lineare Regressionsmodelle. Der Grund ist, dass bei einem äquidistantem Versuchsplan das Modell überprüft werden kann. Mit einem optimalen Versuchsplan hingegen kann in vielen Fällen das Modell nicht auf seine Richtigkeit überprüft werden. Auf der anderen Seite ist ein äquidistanter Versuchsplan nicht sehr effizient für die Schätzung der unbekannten Parameter. Deshalb wurde in einer Serie von Aufsätzen von Bischoff und Miller folgender Kompromiss vorgeschlagen. Gesucht wird der optimale Versuchsplan bezüglich eines bestimmten Kriteriums in der Klasse von Versuchsplänen, die für das Modelltesten effizient sind. In diesem Aufsatz werden das D-Kriterium und polynomiale Regressionsmodelle betrachtet. Für polynomiale Regressionsmodelle vom Grad größer als zwei sind D-optimale Versuchspläne, die für das Modelltesten effizient sind, schwierig festzulegen. Deshalb werden in diesem Aufsatz einfach zu berechnende und für das Schätzen von Parametern hoch effiziente Versuchspläne bestimmt, die zusätzlich noch effizient für das Modelltesten sind.

Keywords: Polynomial Regression Model, Parameter Estimation, D-Criterion.

1 Introduction

Linear regression models are popular in practice since they are easy to interpret. Practitioners, however, are seldom sure whether their assumed linear model is at least approximately true for the data under consideration. Therefore, in these cases designs are of most practical interest with which the parameters cannot only be estimated but also with which the model can be checked. Known classical optimal designs for estimating a parameter of a linear model, however, are often not suitable to check the model. Therefore uniform designs which are optimal in some sense to check a linear model are more popular. On the other hand uniform designs are not very efficient to estimate the unknown parameters.

To take into consideration these concerns Bischoff and Miller suggest, see Bischoff and Miller (2006a, 2006b, 2006c, 2007) and Miller (2002), to take one part of the design points to be able to carry out a lack of fit (LOF-)test for a check of the assumed model. Then the remaining design points are determined in such a way that the whole design is as good as possible (according to a specific criterion) for inference on the unknown parameters of interest. We call such designs optimally LOF-test-efficient. In Bischoff and Miller (2006a, 2006b, 2006c) such designs are determined for the c-criterion. In Bischoff and Miller (2007) the general form of D-optimally LOF-test-efficient designs for polynomial regression models are determined. Moreover, for polynomial regression of order smaller than or equal to 2 such designs are calculated explicitly there. But note that it is difficult to determine such designs for polynomial regression of order larger than 2. The main objective of this paper is to construct easy to calculate LOF-test-efficient designs that are highly efficient to estimate the unknown parameters.

In the next section we give a short overview on D-optimally LOF-test-efficient designs for polynomial regression. Then in Section 3 we look for the structure of LOF-test-efficient designs that are easy to calculate and that are highly efficient to estimate the unknown parameters.

2 An Overview

To describe the problem and results in more detail let a regression model be given with experimental region $\mathcal{E} = [a, b] \subseteq \mathbb{R}$ and unknown, true regression function g. The observations are described by

$$Y_i(x_i) = g(x_i) + \varepsilon_i\,, \qquad i = 1, \ldots, n\,, \tag{1}$$

where $x_1, \ldots, x_n \in \mathcal{E}$, $\mathrm{E}(\varepsilon_i) = 0$, $\mathrm{cov}((\varepsilon_1, \ldots, \varepsilon_n)^\top) = \sigma^2 I_n$. The above model is a polynomial regression model of order $k-1$ if the hypothesis

$$H_0 : \;\; \exists\, \boldsymbol{\theta} = (\theta_1, \ldots, \theta_k)^\top \in \mathbb{R}^k \quad \text{with } g = f^\top \boldsymbol{\theta}$$

is true, where $f(t) := (f_1, \ldots, f_k)^\top = (1, \ldots, t^{k-1})^\top, t \in \mathcal{E} = [a, b]$. A test of the hypothesis H_0 is called "lack of fit"-test (LOF-test) for the polynomial regression model. Let $\tilde{\lambda}$ be the uniform distribution on $\mathcal{E}$, that is $\tilde{\lambda} = \frac{1}{\lambda(\mathcal{E})}\lambda$, where λ is the Lebesgue measure, and let $c > 0$. Then a meaningful set of alternatives for the polynomial regression model can be expressed by

$$\mathcal{F}_c := \left\{ f^\top \boldsymbol{\theta} + h \,\middle|\, \boldsymbol{\theta} \in \mathbb{R}^k, h \in L^2(\tilde{\lambda}) \text{ with } \int_{\mathcal{E}} h^2 \, d\tilde{\lambda} \geq c, \int_{\mathcal{E}} f_i h \, d\tilde{\lambda} = 0, \; i = 1, \ldots, k \right\}, \tag{2}$$

see Wiens (1991). Note that the following considerations and results do not depend on the constant $c > 0$. Next, we consider LOF-tests in an asymptotic way, that is when the number n of observations goes to infinity. An arbitrary design for n observations is given by $(x_1, \ldots, x_n) \in \mathcal{E}^n$ which can be identified with the probability measure $\xi_n := \frac{1}{n}\sum_{i=1}^n \delta_{x_i}$, where δ_t is the Dirac measure in $t \in \mathcal{E}$. On the other hand each probability measure ξ on $\mathcal{E}$ can be realized as an exact design for n observations by using the quantiles $F_\xi^{-1}(\frac{i-1}{n-1})$, $i = 1, \ldots, n$, of the distribution function F_ξ of ξ as design points. In this sense each probability measure can be considered as an asymptotic design. On the other hand from a practical point of view it is enough to consider asymptotic designs (probability measures) which can be decomposed into a finitely discrete part and in a part which can be expressed by a measure with a $\tilde{\lambda}$-density. The finitely discrete part corresponds to approximate designs considered in classical experimental design theory. The measure with $\tilde{\lambda}$-density corresponds to designs for LOF-tests, see below and Wiens (1991). For technical reasons we assume that the $\tilde{\lambda}$-density has bounded variation which is no restriction in practice.

By the above discussion we define the set of competing designs by

$$\Xi := \left\{ p\xi_d + (1-p)\xi_c \mid p \in [0,1], \xi_d \in \Xi_d, \xi_c \in \Xi_c \right\},$$

with

$$\Xi_d = \left\{ \sum_{i=1}^{s} q_i \delta_{t_i} \mid s \in \mathbb{N}, t_1, \ldots, t_s \in \mathcal{E}, q_1, \ldots, q_s > 0 \text{ with } \sum_{i=1}^{s} q_i = 1 \right\},$$

$$\Xi_c = \{\xi \mid \xi \text{ is a probability measure on } \mathcal{E} \text{ with } \lambda\text{-density which has bounded variation}\}.$$

Wiens (1991) and Biedermann and Dette (2001) showed for the F-test and three nonparametric LOF-tests that the uniform design $\tilde{\lambda}$ on $\mathcal{E}$ maximizes the minimal power for the alternatives given in (2). The design $\tilde{\lambda}$ is called LOF-test-optimal design.

A design is called D-optimally r-LOF-test-efficient design (for H_0) if the proportion r of design points are chosen according to the LOF-test-optimal design $\tilde{\lambda}$ and the remaining design points are chosen in such a way that the whole design is as good as possible to estimate θ by the BLUE with respect to the D-criterion. Hence, we look for a D-optimal design in

$$\Upsilon[r] := \{\xi \in \Xi \mid r\tilde{\lambda} \le \xi\},$$

i.e. we look for $\xi^* \in \Upsilon[r]$ maximizing

$$\xi \mapsto D^{(k)}(\xi) := \det\big(M(\xi)\big)^{1/k}, \quad \text{where } M(\xi) = \int_{\mathcal{E}} f(t)f(t)^\top \xi(dt). \tag{3}$$

Here $\mu_1 \le \mu_2$ for designs (probability measures) μ_1, μ_2 on $\mathcal{B}$ means $\forall B \in \mathcal{B} : \mu_1(B) \le \mu_2(B)$.

The set-up is similar to Bayesian optimum design in linear models. Namely, the fixed r-th part of observations can be considered as giving a prior under which we consider designs minimizing the determinant of the covariance matrix of the Bayesian estimator of the parameters. For more details see Pilz (1991). For the same relation with respect to c-optimality see Bischoff and Miller (2006a, p. 2020).

The D-optimal designs for polynomial regression in the classical situation are well known, see Dette and Studden (1997, p. 149), or Pukelsheim (1993, p. 214-216), see also Fedorov (1972) and Silvey (1980).

The next result shows the general form of a D-optimal design in $\Upsilon[r]$ if a polynomial regression of order $k-1$ is assumed as true model under H_0. By the same reasons as for the classical D-criterion we can choose $\mathcal{E}=[-1,1]$ without loss of generality. Then we obtain the D-optimally LOF-test-efficient design for the experimental region $\mathcal{E}=[a,b]$ by linear transforming the D-optimally LOF-test-efficient design for $\mathcal{E}=[-1,1]$ from $[-1,1]$ to $[a,b]$. The following statement is a specific result of a general equivalence theorem given in Bischoff and Miller (2006a), see also Bischoff and Miller (2007).

Theorem 1 *Let the experimental region* $\mathcal{E}=[-1,1]$, *let* $f(t)=(1,t,\ldots,t^{k-1})^T$, *let* $r\in[0,1]$ *and let*

$$d_k(t,\xi):=f(t)^\top M(\xi)^{-1}f(t)\,,\quad t\in\mathbb{R}\,,\ \xi\in\Xi\,.$$

Then the D-optimally r-LOF-test-efficient design in Ξ *for* H_0 *is symmetric with respect to 0 and has the form* $r\tilde{\lambda}+(1-r)\sum_{i=1}^{\ell}p_i\delta_{t_i}$, *where* $t_1,\ldots,t_\ell\in[-1,1]$ *are* $\ell(\le k)$ *different points with* $d(t_i,\xi)=\max_{t\in[-1,1]}d(t,\xi)$ *and* $p_1,\ldots,p_\ell\in(0,1]$ *are suitable values with* $\sum_{i=1}^{\ell}p_i=1$.

For later purposes the following fact is worth noting for the polynomial regression model $f(t)=(1,t,\ldots,t^{k-1})^\top$, $t\in\mathcal{E}=[-1,1]$, $k=2,3,\ldots$. It holds for a symmetric design $\xi\in\Xi$

$$D^{(k)}(\xi)=\det\left(\int_{\mathcal{E}}f(t)f(t)^\top\xi(dt)\right)^{1/k}=\left(\left[\int_{\mathcal{E}}t^4\xi(dt)-\left(\int_{\mathcal{E}}t^2\xi(dt)\right)^2\right]\int_{\mathcal{E}}t^2\xi(dt)\right)^{1/k}.$$

Furthermore, the fact that

$$D^{(k)}(\cdot)\ \text{ is concave}$$

is decisive for our procedure to get simple and highly efficient designs in the following.

3 Simple r-LOF-test-efficient Designs

In this section we consider straight-line, quadratic and cubic polynomial regression models, i.e., $f(t)=(1,t,\ldots,t^{k-1})$ with $k=2,3,4$. The above result can be used to calculate the optimal designs for the first two models mentioned above, see Corollary 2 and Theorem 3. By Theorem 3 we recognize that the D-optimally r-LOF-test-efficient design for the straight-line is also D-optimally r-LOF-test-efficient for the quadratic polynomial regression model if r is not too small. It is much more complicated, however, to compute the D-optimally r-LOF-test-efficient design for the cubic polynomial regression model because its design points and the corresponding weights are changing with r opposed to the straight-line and quadratic regression model. But by the experience with straight-line and quadratic polynomial regression models we get ideas on the cubic D-optimally r-LOF-test-efficient designs for r not too small. Furthermore, for smaller r we can construct simply to compute r-LOF-test-efficient designs that are highly efficient to estimate the unknown parameters. We consider the D-optimality criterion to judge the efficiency of a design for estimating the unknown parameter vector θ. The D-efficiency of an r-LOF-test-efficient design ξ is defined by

$$\text{D-eff}_r^k(\xi) := \frac{D^{(k)}(\xi)}{D^{(k)}(\xi_{r,k}^*)},$$

where $\xi_{r,k}^*$ is the D-optimally r-LOF-test-efficient design for the model $f(t) = (1, t, \ldots, t^{k-1})$.

3.1 Straight-line Regression (k = 2)

Corollary 2 *(Bischoff and Miller, 2007) Let $\mathcal{E} = [-1, 1]$, let $r \in [0, 1]$ and let $f(t) = (1\ \ t)^\top$. Then the D-optimally r-LOF-test-efficient design is given by*

$$\xi_{r,2}^* = r \cdot \tilde{\lambda} + \frac{1}{2}(1 - r)(\delta_{-1} + \delta_1).$$

The above result shows immediately that the D-optimally r-LOF-test-efficient design can be simply obtained by a linear combination of the classical D-optimal design $\xi_{0,2}^*$ and the uniform design $\xi_{1,2}^* = \tilde{\lambda}$, i.e. $\xi_{r,2}^* = r\xi_{1,2}^* + (1-r)\xi_{0,2}^*$. The D-efficiency of $\xi_{1,2}^* = \tilde{\lambda} \in \Upsilon[r]$ for each $r \in [0, 1]$ is given by

$$\text{D-eff}_r^2(\tilde{\lambda}) = \frac{1}{\sqrt{3 - 2r}}, \quad \text{D-eff}_0^2(\tilde{\lambda}) = \frac{1}{\sqrt{3}} = 0.58.$$

3.2 Quadratic Polynomial Regression (k = 3)

Theorem 3 *(Bischoff and Miller, 2007) Let $\mathcal{E} = [-1, 1]$, let $r \in [0, 1]$ and let $f(t) = (1\ \ t\ \ t^2)^\top$. Then the D-optimally r-LOF-test-efficient design is given by*

$$\xi_{r,3}^* = r\tilde{\lambda} + p^*\delta_{-1} + (1 - r - 2p^*)\delta_0 + p^*\delta_1 \in \Upsilon[r]$$

with

$$p^* = \begin{cases} \dfrac{1-r}{6} + \dfrac{\sqrt{25 - 10r}}{30}, & 0 \le r \le r_0, \\ \dfrac{1-r}{2}, & r_0 < r \le 1, \end{cases}$$

where $r_0 = (19 - \sqrt{61})/20 \approx 0.5595$.

For $r = 0$ we get the classical, approximate D-optimal design $\xi_{0,3}^* = (\delta_{-1} + \delta_0 + \delta_1)/3$ and for $r = 1$ we get the uniform design $\xi_{1,3}^* = \tilde{\lambda}$. It is worth mentioning that the D-optimally r-LOF-test-efficient design $\xi_{r,2}^* = r\tilde{\lambda} + \frac{1-r}{2}(\delta_{-1} + \delta_1) \in \Upsilon[r]$ for the straight-line regression model coincide with the D-optimally r-LOF-test-efficient design $\xi_{r,3}^*$ for the quadratic regression model if $r_0 \le r \le 1$.

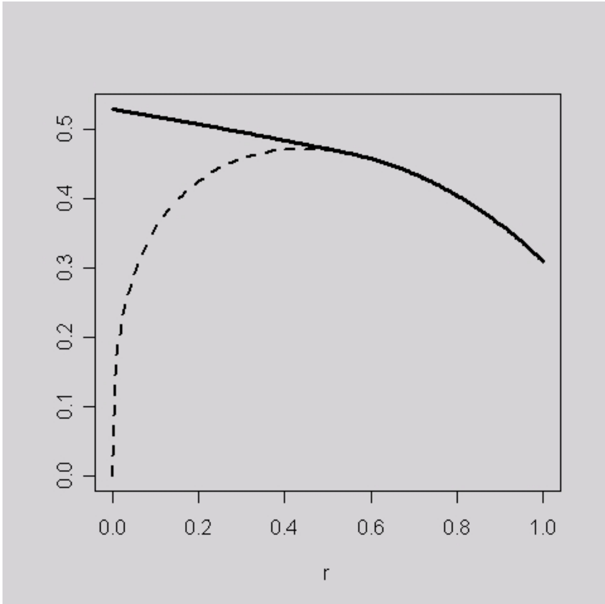

Figure 1: $D^{(3)}(\xi^*_{r,2})$ broken line and $D^{(3)}(\xi^*_{r,3})$ bold line.

For the design $\xi^*_{r,3}$ we obtain after some calculation

$$D^{(3)}(\xi^*_{r,3}) = \begin{cases} \dfrac{\sqrt[3]{10}}{15}\left(25 - 15r + 25(1 - \dfrac{2}{5}r)^{3/2}\right)^{1/3}, & 0 \le r \le r_0, \\ \dfrac{\sqrt[3]{100}}{15}\left(18r - 27r^2 + 10r^3\right)^{1/3}, & r_0 < r \le 1. \end{cases}$$

Hence, the D-efficiency of $\xi^*_{1,3} = \tilde{\lambda} \in \Upsilon[r]$ for each $r \in [0,1]$ is given by

$$\text{D-eff}^3_r(\tilde{\lambda}) = \begin{cases} \left(2.5 - 1.5r + 2.5(1 - \frac{2}{5}r)^{3/2}\right)^{-1/3}, & 0 \le r \le r_0, \\ (18r - 27r^2 + 10r^3)^{-1/3}, & r_0 < r \le 1. \end{cases}$$

Especially, we have $\text{D-eff}^3_0(\tilde{\lambda}) = 1/\sqrt[3]{5} = 0.58$. This shows the bad performance of the uniform designs $\xi^*_{1,2} = \xi^*_{1,3} = \tilde{\lambda}$ with respect to the D-efficiency. Furthermore, we obtain for $\xi^*_{r,2}$

$$D^{(3)}(\xi^*_{r,2}) = \frac{\sqrt[3]{100}}{15}\left(18r - 27r^2 + 10r^3\right)^{1/3}, \quad r \in [0,1].$$

The values $D^{(3)}(\xi^*_{r,2})$, $D^{(3)}(\xi^*_{r,3})$, $r \in [0,1]$, of the designs $\xi^*_{r,3}$, $\xi^*_{r,2} \in \Upsilon[r]$ are shown in Figure 1. Note that $\xi^*_{1,3} = \xi^*_{1,2} = \tilde{\lambda}$ and $\xi^*_{r,2} = \xi^*_{r,3}$ for $r \in [r_0, 1]$.

Although the D-optimally r-LOF-test-efficient design for r with $0 \le r < r_0$ is known we construct simple, highly efficient alternatives by the facts:

1. $\text{D-eff}^3_0(\xi^*_{r_0,2})) = 0.88$,
2. $D^{(3)}(\cdot)$ is concave.

Hence, the convex combination $\xi^c_{r,3} = (1-q)\xi^*_{0,3} + q\xi^*_{r_0,2} \in \Upsilon[r]$ with $r = qr_0$, $q \in [0,1]$, is a simple alternative for the D-optimally r-LOF-test-efficient design $\xi^*_{r,3}$ with D-eff$^3_r(\xi^c_{r,3}) \geq 0.88$, $r \in [0, r_0]$. For these designs we obtain for $r \in [0, r_0]$

$$D^{(3)}(\xi^c_{r,3}) = \frac{\sqrt[3]{2r_0}}{3r_0}\left(2r_0^2 - r_0r - \frac{6}{5}r_0^2r - r^2 + 5r_0r^2 - \frac{24}{5}r_0^2r^2 + r^3 - 4r_0r^3 + 4r_0^2r^3\right)^{1/3}.$$

Since $D^{(3)}(\cdot)$ is concave, Figure 1 implies that the designs $\xi^c_{r,3} \in \Upsilon[r]$ are highly efficient for $0 \leq r \leq r_0$. Indeed one can show numerically that D-eff$^3_r(\xi^c_{r,3}) \geq 0.9999$, $0 \leq r \leq r_0$.

3.3 Cubic Polynomial Regression (k $= 4$)

It is rather complicated to calculate the D-optimally r-LOF-efficient designs for the cubic polynomial regression model because the design points and the corresponding weights changing with r. Therefore we construct simple alternatives using the strategy developed for the quadratic regression model.

At first we investigate $d_4(t, \tilde{\lambda})$, $t \in [-1,1]$ (see Theorem 1), which is a polynomial of order 6. After some analytical calculations one can recognize that $d_4(t, \tilde{\lambda})$, $t \in [-1,1]$, has its unique maxima in $t = -1$ and $t = 1$. Let us assume that the optimal design points do not change for large r near 1. Then using Theorem 1 and the fact that $d_4(t, \cdot)$, $t \in [-1,1]$, is continuous the design $\xi^*_{r,2} = r\tilde{\lambda} + \frac{(1-r)}{2}(\delta_{-1} + \delta_1)$ coincides with the D-optimally r-LOF-efficient design $\xi^*_{r,4}$ for all $r \in [r_0, 1]$, where $r_0 \in [0,1]$ is some constant. By numerical investigations it can be recognized that $\xi^*_{r,2}$, $r \in [r_0, 1]$, is D-optimally r-LOF-efficient where $r_0 \leq 0.65 =: c$, see Figure 2.

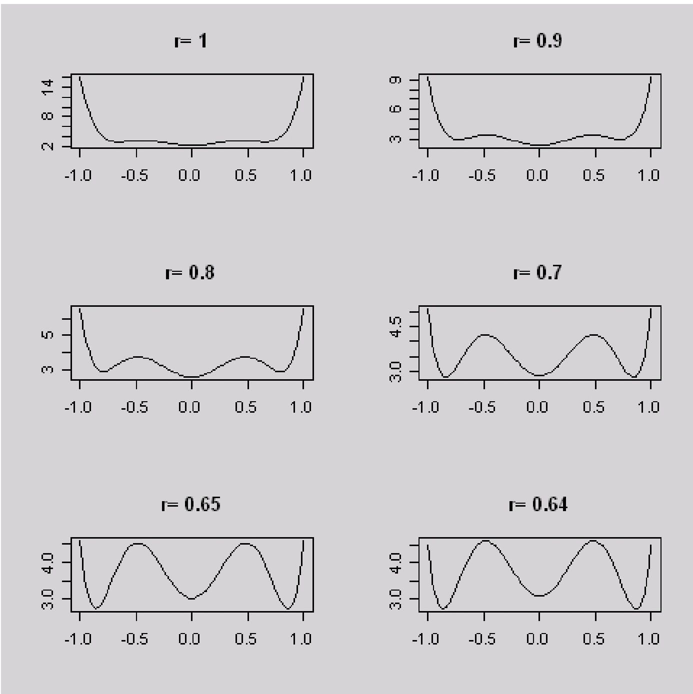

Figure 2: $d_4(t, r\tilde{\lambda} + \frac{(1-r)}{2}(\delta_{-1} + \delta_1))$, $t \in [-1,1]$, for specific r.

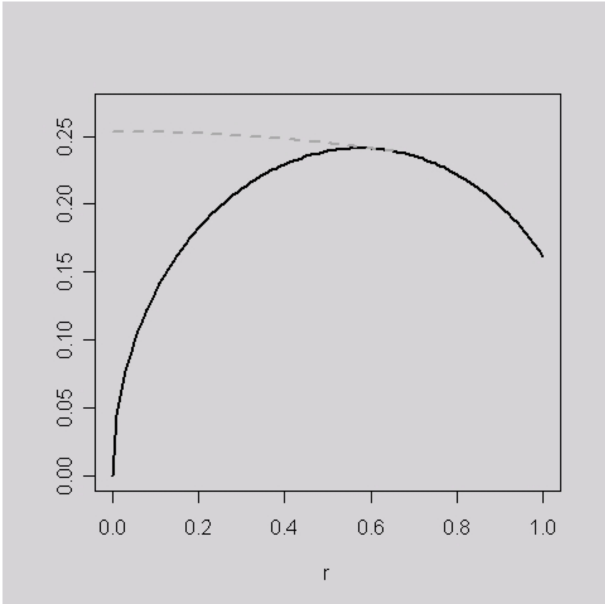

Figure 3: $D^{(4)}(\xi^*_{r,2})$ bold line, $D^{(4)}(\xi^c_{r,4})$ broken line.

The approximate D-optimal design $\xi^*_{0,4}$ is given by $\frac{1}{4}(\delta_{-1} + \delta_{-1/\sqrt{3}} + \delta_{1/\sqrt{3}} + \delta_1)$. Note that D-eff$^4_0(\tilde{\lambda}) = 0.64$ which is not very efficient, but D-eff$^4_0(\xi^*_{c,2}) \geq 0.94$ is rather large. Therefore and by the fact that $D^{(4)}(\cdot)$ is concave the convex combinations $\xi^c_{r,4} = (1-q)\xi^*_{0,4} + q\xi^*_{c,2}$ with $r = qc$, $q \in [0,1]$, is a simple alternative for the (unknown) D-optimally r-efficient-LOF-test design $\xi^*_{r,4}$. The values $D^{(4)}(\xi^*_{r,2})$, $r \in [0,1]$, $D^{(4)}(\xi^c_{r,4})$, $r \in [0,c]$, of the designs $\xi^*_{r,2}$, $\xi^c_{r,4} \in \Upsilon[r]$ are shown in Figure 3. Note that $\xi^*_{0,4} = \xi^c_{0,4}$, $\xi^*_{1,4} = \xi^*_{1,2} = \tilde{\lambda}$, and $\xi^*_{r,2} = \xi^*_{r,4}$ for $r \in [c,1]$.

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