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On locally D-optimal experimental design

1. Introduction

If one is planning an experiment it is desirable to gain maximal information by a possibly low cost. In particular, if one is going to estimate the parameters of a nonlinear growth-function it is meaningful to choose the measuring points and frequencies in an appropriate manner. For a given overall number of measurements it is useful for several reasons to have a large value of the determinant of the Fisher-information matrix (cf. [1]-[3]). This so-called D-criterion proved to yield in most cases "good" experimental designs (cf. [4]). Nevertheless, one has to be aware of the drawbacks of this approach. First of all, the unknown parameters appear in the criterion, hence one has to provide some a priori estimates. Because of this we should rather use the termini "local D-criterion" and "local D-optimal design". We drop the attribute for brevity. Further the computation time for the maximization may be so expensive, that it becomes more economic to measure twice and not to plan at all. For other criterions these difficulties occur as well (cf. [3]).

However, our goal is to overcome the problems with computing the maximum of the criterion. We succeeded to find a way for reducing the dimension of the optimization from the size of the experiment to the number of unknown parameters. For an important class of growth functions with 3 parameters the remaining optimization can be solved by elegant geometric considerations. By that way it is possible to compute relative maxima of the local D-criterion very quickly. For most growth functions it could not be proved yet whether this relative maximum is always an absolute one. For exponential regression it seems to be so, but for general situations there are counter-examples. We considered a necessary condition for an absolute maximum. This condition enabled us to construct the above counter-examples as well as an example for which the relative maximum mentioned is the absolute one. It is interesting that even if that relative

maximum is not an absolute one, the value of the local D-criterion is not worse than the absolute maximum divided by 4.5. This implies that other (expensive) numerical methods, that yield the absolute maximum, provide not more than a reduction of design size by 1.7.

It should be stressed that we considered only so-called concrete designs, i.e., we restricted ourselves to integer solutions for the frequencies. It is a simple task to modify our results for discrete designs. Analytical considerations on optimum discrete designs under several criterions are contained in [5].

2. Separation of the integer and the continuous optimization

Let us assume a growth-function

$$G: [x_1, x_u] \times \Omega \longrightarrow \mathbb{R}, \quad \Omega \subset \mathbb{R}^k,$$

$$(x, \vartheta) \longrightarrow G(x, \vartheta),$$

depending on the instant x from the time-interval $[x_1(\text{lower bound}), x_u(\text{upper bound})]$ and additionally on the parameters to be estimated. We denote the derivatives with respect to the parameters by

$$z(x) := \nabla_{\vartheta} G(x, \vartheta_0), \quad \dot{z}: [x_1, x_u] \longrightarrow \mathbb{R}^k$$

with ϑ_0 being a fixed a priori estimate for the wanted parameter vektor ϑ .

The size of the experiment to be planned is denoted by n and is assumed to be not less than k . Now we introduce a matrix-valued function

$$V: [x_1, x_u]^n \longrightarrow \mathbb{R}^{k \times n},$$

$$x = (x_1, \dots, x_n) \longrightarrow (z(x_1) \ z(x_2) \ \dots \ z(x_n)).$$

Finally, the function to be maximized is given by

$$f(x) = \det(V(x) V^T(x)),$$

$$f: [x_1, x_u]^n \longrightarrow \mathbb{R}^+.$$

The arguments x are referred to as experimental designs of the size n . If the cardinality of the set $\{x_1, \dots, x_n\}$ is 1, then x is called a 1-point-design. The set

$$\{x_1, \dots, x_n\} =: Sp(x) = \{x_{sp_1}, \dots, x_{sp_1}\}$$

together with 1 integers n_1, \dots, n_1 characterizes an experimental design up to a permutation of components. Since f is

symmetric, it is sufficient to find the support $Sp(x)$ and the frequencies n_1, \dots, n_k represented by an ordered table

$$\begin{array}{c} \underline{x_{sp_1} \quad | \quad \dots \quad | \quad x_{sp_k}} \\ n_1 \quad | \quad \dots \quad | \quad n_k \\ \\ x_1 \leq x_{sp_1} < x_{sp_2} < \dots < x_{sp_k} \leq x_u \\ n_1 + n_2 + \dots + n_k = n. \end{array}$$

Definition: If $f(x^*) = \max f(x)$, $x \in [x_1, x_u]^k$, then x^* is called a (locally D-)optimal experimental design (at $\vartheta = \vartheta_0$).

As a first step we look for optimal designs in a subset of all designs, namely in the set of all k-point designs. To this end we recollect ([6]) that

$$f(x) = |VV^T| = \sum_{i_1 < i_2 < \dots < i_k} \begin{vmatrix} v_{i_1 i_1} & v_{i_1 i_2} & \dots & v_{i_1 i_k} \\ v_{i_2 i_1} & v_{i_2 i_2} & \dots & v_{i_2 i_k} \\ \dots & \dots & \dots & \dots \\ v_{i_k i_1} & v_{i_k i_2} & \dots & v_{i_k i_k} \end{vmatrix}^2$$

Here each column of V depends on some component of x . Since there are just k different components of x all non-vanishing determinants on the right hand side must be equal; their number is the product of the frequencies $n_1 n_2 \dots n_k$. Thus we state

Lemma 1: For k-point designs the following equation is true:

$$f(x) = n_1 n_2 \dots n_k \det(z(x_{sp_1}) \dots z(x_{sp_k}))^2$$

where the n_i 's are the frequencies and the x_{sp_i} 's are the support points of x .

We conclude from this that the optimum k-point design may be found by maximizing the product $\prod_{i=1}^k n_i$ under the constraint $\sum_{i=1}^k n_i = n$ and maximizing the square of the determinant

$$\det(z(x_{sp_1}) \dots z(x_{sp_k}))$$

independently under the constraints $x_{sp_i} \in [x_l, x_u]$ for $i = 1, 2, \dots, k$.

It is not necessary to assume that $x_{sp_i} \neq x_{sp_j}$ for $i \neq j$, because $f(x)$ vanishes in such situations.

First let us treat the integer problem, of course avoiding differential calculus. We prove the following

Lemma 2: If $\prod_{i=1}^k n_i$ takes its maximum under the constraint

$$\sum_{i=1}^k n_i = n,$$

then the n_i 's are "almost equal", i.e.

$$\max_{1 \leq i < j \leq k} \{ |n_i - n_j| \} \leq 1.$$

Proof: Assume conversely that $n_{j_2} - n_{j_1} \geq 2$ for some permutation $j \in S(n)$, then

$$(n_{j_1} + 1)(n_{j_2} - 1) \prod_{i=3}^k n_{j_i} = \prod_{i=1}^k n_{j_i} + (n_{j_2} - n_{j_1} - 1) \prod_{i=3}^k n_{j_i} > \prod_{i=1}^k n_{j_i}$$

$$\text{or } \prod_{i=3}^k n_{j_i} = 0.$$

This contradicts the maximality of $\prod_{i=1}^k n_i$.

From the Lemma 2 we infer that the optimal frequencies are given by $n_i = \lfloor \frac{n}{k} \rfloor + \epsilon_i$ with $\epsilon_i \in \{0, 1\}$, $i=1, \dots, k$, and

$$\sum_{i=1}^k \epsilon_i = n - k \lfloor \frac{n}{k} \rfloor.$$

Consequently, there are $\binom{k}{n - k \lfloor \frac{n}{k} \rfloor}$ different optimal k point designs for given k and n . Only if $k|n$ the optimal design may be uniquely defined.

Remark: If we allow for discrete designs, the attribute "almost" in Lemma 2 has to be dropped. Then the frequencies for the unique optimal design are exactly equal.

Now we introduce the function

$$\varphi(x_{sp_1}, \dots, x_{sp_k}) = \det(z(x_{sp_1}) \dots z(x_{sp_k}))^2$$

and denote its maximum on $[x_1, x_u]^k$ by φ_{\max} . Further we denote the maximum of f on k -point designs by f_{kpm} and the overall maximum of f on $[x_1, x_u]^n$ by f_{\max} . Then we obtain obviously

$$f_{\max} \geq f_{kpm} \geq \left[\frac{n}{k} \right]^k \varphi_{\max}.$$

If we want f to reach a threshold f_0 , then it is sufficient to take

$$n = k \left(\left[\sqrt[k]{\frac{f_0}{\varphi_{\max}}} \right] + 1 \right).$$

Hence the support $sp(x)$ as well as the value φ_{\max} can be calculated independently of the size n by solving a low-dimensional optimization problem

$$\varphi(x_{sp_1}, \dots, x_{sp_k}) = \text{Max } f \text{ on } [x_1, x_u]^k.$$

3. Special cases

In general the above problem can be easily solved by available computer routines. Here we will focus on situations in which further reduction by analytical means is possible. To this end we make the assumption :

(A) Let $k = 3$ and the graph of the function

$$z : [x_1, x_u] \longrightarrow \mathbb{R}^3$$

is a regular curve contained in some plane ϵ with $O \notin \epsilon$. In ϵ there exists a basis $\{b_1, b_2\}$ such that the b_2 -component of z is a smooth convex function of the b_1 -component of z , i.e.,

$$z(x) = b_0 + z_1(x)b_1 + z_2(x)b_2,$$

$$z_2(x) = g(z_1(x))$$

with $g : [z_1(x_1), z_1(x_u)] \longrightarrow \mathbb{R}$ being a convex and nonlinear C^1 function.

Now we turn to

Theorem 1: Providing (A) holds and $x_{sp_1} < x_{sp_2} < x_{sp_3}$, then $\varphi(x_{sp_1}, x_{sp_2}, x_{sp_3})$ is a maximum iff $x_{sp_1} = x_1$, $x_{sp_3} = x_u$ and

$$g'(z_1(x_{sp_2})) = \frac{z_2(x_1) - z_2(x_u)}{z_1(x_1) - z_1(x_u)}.$$

Furthermore, the partial derivatives satisfy

$$\begin{aligned} \varphi_{,1}(x_1, x_m, x_u) &< 0, \\ \varphi_{,3}(x_1, x_m, x_u) &> 0, \\ \varphi_{,22}(x_1, x_m, x_u) &\leq 0 \end{aligned}$$

for each $x_m := x_{sp_2}$ fulfilling the above equality. If g is strictly convex then x_m is unique.

Proof: Let us consider the tetrahedron with the vertices $O, z(x_{sp_i}), i=1,2,3$. Its volume is given by

$$V = 1/6 \sqrt{\psi(x_{sp})}.$$

On the other hand, we have

$$V = 1/3 \text{dist}(O, \varepsilon) A(z(x_{sp_1}), z(x_{sp_2}), z(x_{sp_3}))$$

with $\text{dist}(O, \varepsilon)$ - the Eukclidean distance between the origin and the plane ε (positive due to $O \notin \varepsilon$)

and

$A(z(x_{sp_1}), z(x_{sp_2}), z(x_{sp_3}))$ - the area of the triangle with the vertices $z(x_{sp_i}), i=1,2,3$.

From the above we infer that $\varphi(x_{sp})$ is a maximum iff the area of a certain triangle is.

Hence, we obtained the equivalent but much more convenient problem of maximizing the area A of a triangle under the constraint that the vertices lie on the graph of a convex function g from an interval into the real axis.

The convexity of g yields immediately that A is an increasing function of the abscissa of the right-most vertex if the two leftmost vertices are kept constant. Moreover, the slope of that function is not less than $d \sin \alpha$ with

$$d = \text{dist}(z(x_{sp_3}), \overline{z(x_{sp_1})z(x_{sp_2})}) \text{ and } \alpha = \angle(b_2, \overline{z(x_1)z(x_2)}).$$

Analogously, A is a decreasing function of the leftmost abscissa with a negative upper bound for the slope, the remaining abscissae again assumed to be fixed.

This, together with $\varphi \sim A^2$ and the chain rule, yields the conditions

$$x_{sp_1} = x_1, \quad x_{sp_3} = x_u, \quad \varphi_{,x_1} < 0, \quad \varphi_{,x_u} > 0.$$

Now, the remaining abscissa is an inner point of the interval, hence a necessary condition for the maximality of the area may be given in terms of the derivative of the triangle's heights. This yields the expression for g' and the uniqueness in the strictly convex case.

Now, we observe that the sufficiency follows from the argument that φ is continuous on the compact set $[x_1, x_u]^3$, hence it takes on its supremum. But, on the other hand, the value of φ is the same for all points satisfying the necessary conditions. This ends the proof.

Let us consider now growth-functions G of the type

$$G(x, \alpha, \beta, \gamma) = \alpha + F(x, \beta, \gamma).$$

The definition of z yields

$$z(x) = \begin{pmatrix} 1 \\ F_{,\beta}(x, \beta, \gamma) \\ F_{,\gamma}(x, \beta, \gamma) \end{pmatrix}.$$

Hence we put $b_0 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $b_1 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ and $b_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

and $\varepsilon = b_0 + \text{span}\{b_1, b_2\}$.

The assumption A holds if the following relations are valid for each $x \in (x_1, x_u)$:

$F_{,x\beta} \neq 0$ and $\frac{F_{,xy}}{F_{,x\beta}}$ is monotonous. (The derivatives exist and satisfy the conditions.)

Especially for $F(x, \beta, \gamma) = \beta\omega(\gamma x)$ this requirements read

$$\omega'(\gamma x) \neq 0 \quad \text{and} \quad \frac{\omega''(\gamma x)}{\omega'(\gamma x)} \text{ is monotonous.}$$

Example 1: For exponential regression we have

$$\omega(\gamma x) = e^{\delta x}.$$

The above conditions turn out to be satisfied. The function g can be expressed explicitly as follows:

$$g(t) = \frac{\beta}{\delta} t \ln t.$$

As support point we obtain after some transformations:

$$x_m = \frac{x_u e^{\delta x_u} - x_1 e^{\delta x_1}}{e^{\delta x_u} - e^{\delta x_1}} - \frac{1}{\delta}.$$

Unfortunately, not always we may express x_m by a formula, as shows us

Example 2: $\omega = \tanh$

Our assumptions are satisfied whenever $0 \in (x_1, x_u)$.
The instant x_m has to be calculated from

$$x_m \tanh(\gamma x_m) = \frac{1}{2\gamma} - \frac{1}{2} \frac{x_u / (\cosh^2(\gamma x_u)) - x_1 / (\cosh^2(\gamma x_1))}{\tanh(\gamma x_u) - \tanh(\gamma x_1)}$$

Of course, this nonlinear equation can be solved quickly even by a pocket calculator - but not explicitly.

Example 3: In the case of quadratic regression

$G(x, \alpha, \beta, \gamma) = \alpha + \beta x + \gamma x^2$ we get

$$z(x) = \left(\frac{1}{x^2} \right), \quad t = x, \quad g(t) = t^2, \quad g'(t_m) = x_u + x_1$$

Hence we obtain again the well known result $x_m = \frac{x_1 + x_u}{2}$.

Regarding the case $G(x, \alpha, \beta, \gamma) = \alpha + \beta \omega(\gamma x)$ the differential equation

$$x \frac{\omega''(\gamma x)}{\omega'(\gamma x)} = \text{const}$$

is of some interest. For its solutions $\omega(x) = \begin{cases} A \ln x + C \\ A x^B + C \end{cases}$ the

above method fails. For all other monotonous functions we may choose a suitable interval $[x_1, x_u]$, so that x_m can be determined in the above way. It is evident that the failure of the method for the mentioned functions is connected with the dependence of the growth parameters. Consequently, those cases are not of interest.

It should be mentioned that the idea of maximizing $\varphi(x_{sp_1}, \dots, x_{sp_k})$ by maximizing the measure of a polyhedron with vertices lying on the graph of a convex function may be useful for other dimensions $k \neq 3$ as well. As an example with $k = 2$ we consider the so-called Michaelis-Menton-function

$$G(x, \alpha, \beta) = \frac{\alpha x}{1 + \beta x}, \quad \alpha, \beta > 0.$$

Here one obtains the problem of choosing two points on an arc of the normal parabola in such a way that the area of the triangle formed by those two points and the origin takes a maximum. The solution of that problem is geometrically obvious and implies the nice result, that the optimal support of a 2-point design consists of x_1 and the point x_m for which

$$G(x_m, \alpha, \beta) = 1/2 G(x_1, \alpha, \beta),$$

provided x_1 is sufficiently large. Otherwise we have just the ends of the observation interval in the support.

4. Designs with larger support

Up to now we considered only designs of minimal support size. Under assumption (A) we succeeded in finding the locally D-optimal one, but we don't know whether it is possible to obtain better designs by enlarging the number of support points. A general answer to this question can not be given here, but some results should be mentioned. Since our main interest is in exponential regression, in the sequel we fix $k=3$. First we will prove the following

Theorem 2: The optimal D-value for designs with an arbitrary support cannot be better than 4.5 times the optimum for 3-point designs, i.e.

$$f_{\max} < 4.5 f_{3pm}.$$

The minimal size m for which f_{\max} will be greater than f_{3pm} calculated for a given size n is greater than $n/1.7$.

Proof: The formula for determinants on page 53 Lemma 1 yields immediately

$$f_{\max} \leq \binom{m}{3} \varphi_{\max}.$$

For $n \geq 3$ and arbitrary m we have

$$\left[\frac{n+1}{3} \right]^2 (n - 2 \left[\frac{n+1}{3} \right]) > \frac{1}{27} (n-1)^3,$$

$$\binom{m}{3} < \frac{1}{6} (m-1)^3.$$

Since $f_{3pm} = \left[\frac{n+1}{3}\right](n-2\left[\frac{n+1}{3}\right])\varphi_{\max}$ we conclude $(n-1)^3 > \frac{2}{9}(n-1)^3$ and hence

$$m > \sqrt[3]{\frac{2}{9}n + (1 - \sqrt[3]{\frac{2}{9}})} > n/1.7.$$

On the other hand, for $n \geq 3$ the following inequality is true

$$\binom{n}{3} < \left[\frac{n+1}{3}\right]^2 (n - 2\left[\frac{n+1}{3}\right]) \frac{27}{6}.$$

Consequently, $f_{\max} < 4.5 f_{3pm}$. This completes the proof.

Remark: It should be pointed out that the above estimates are very pessimistic. I could not construct any example with $f_{\max} > 2f_{3pm}$. For

$$G(x, \alpha, \beta, \gamma) = \alpha + \beta e^{\gamma x}, \quad \gamma < 0,$$

and

$$G(x, \alpha, \beta, \gamma) = \alpha e^{-\exp(\beta x - \gamma)}$$

the factor is assumed to be equal to 1, i.e. $f_{\max} = f_{3pm}$ (cf. [3]).

Now we make use of the assumption (A) once more.

Lemma 3: The points x_1 and x_u belong to the support of the optimal design.

The proof runs like that of Theorem 1 applied to each of the terms in the sum - which now may differ from each other.

Let us now introduce a family of functions

$$\begin{aligned} \psi_i(u, v) = & \sum_{\substack{j < k \\ j \neq i}} \det(z(x_j) \quad z(x_k) \quad b_0 + ub_1 + vb_2)^2 \\ & + \sum_{\substack{j < k < l \\ j, k, l \neq i}} \det(z(x_j) \quad z(x_k) \quad z(x_l))^2, \quad i = 1, 2, \dots, n. \end{aligned}$$

Substituting $u = z_1(x_i)$, $v = z_2(x_i) = g(z_1(x_i))$ we obtain

$$\psi_i(u, v) = f(x).$$

Note that the functions ψ_i are quadratic semi-definite forms in (u, v) . ψ_i is positive definite iff the points $\{z(x_j) : j+i\}$ are not collinear. Otherwise x is of no interest because it cannot yield a better f than f_{3pm} . Similar functions have been used in [7] for the formulation of a sufficient criterion for $f_{\max} = f_{kpm}$.

Lemma 4: If x is an optimal design then

$$\epsilon_i := \{ (u, v) : \psi_i(u, v) \leq f(x) \}$$

is an ellipse for each i .

Theorem 3: If (A) holds and x is an optimal design then

a) $\{x_1, x_u\} \subset \text{sp}(x)$,

b) $\{(t, g(t)) : t \in [z_1(x_1), z_1(x_u)]\} \subset \bigcap_{i=1}^n \epsilon_i$.

As immediate consequences of this criterion we can state the following corollaries.

Corollary 1: Let (A) be valid and x be optimal. If $I \subset [x_1, x_u]$ is such that $z|_I$ is a straight line then $\text{sp}(x) \cap \text{int } I = \emptyset$.

Corollary 2: We cancel the smoothness of g in (A) and assume g to be continuous in $[x_1, x_u]$, nonlinear, but linear in $[x_1, x_m]$ as well as in $[x_m, x_u]$ for some $x_m \in (x_1, x_u)$. Then

a) $f_{\max} = f_{3pm}$ and

b) $f_{\max} = f(\underbrace{x_1 \dots x_1}_{\lfloor \frac{n+1}{3} \rfloor}, \underbrace{x_m \dots x_m}_{\lfloor \frac{n+1}{3} \rfloor}, \underbrace{x_u \dots x_u}_{n - 2\lfloor \frac{n+1}{3} \rfloor})$.

In order to show that the equality $f_{\max} = f_{3pm}$ in general doesn't hold let us consider the special case $n = 4$. Let z be

continuous, lie in a plane $\epsilon \neq 0$ and be linear in $[x_1, x_1]$, $[x_1, x_2]$ and $[x_2, x_u]$. If

$$\overline{z(x_1)z(x_2)} \parallel \overline{z(x_1)z(x_u)}$$

then $x = (x_1, x_1, x_2, x_u)$ is optimal. Furthermore, if $x_1 \neq x_2$ then $f_{\max} > f_{3pm}$.

Remark 1: From the above we see that the curvature of z in the neighbourhood of x_m is essential for f_{\max} to be greater or equal to f_{3pm} . Certain ellipses state indifferent cases between large curvature ($f_{\max} = f_{3pm}$) and small curvature ($f_{\max} > f_{3pm}$).

Remark 2: The examples with piecewise linear z seem to be artificial, but they occur naturally if one takes C^1 -splines of powers and logarithms as growth-functions. For an instance

$$\omega(x) = \begin{cases} x, & 0 \leq x \leq 1, \\ 2\sqrt{x} - 1, & x \geq 1, \end{cases}$$

$$G(x, \alpha, \beta, \gamma) = \alpha + \beta\omega(\gamma x), \quad \gamma > 0$$

fits the assumptions of Corollary 1.

Finally, we want to make the observation from Remark 1 above more precise. By calculating the eigenvalues of a matrix of second order derivatives we are able to give a sufficient criterion for f_{3pm} to be a relative optimum of the function f on the cube $[x_1, x_u]^n$. We remain it to the sceptical readers to do the cumbersome algebra and present here only the result. To this end the notions are introduced

$$a = \varphi_{,22}(x_1, x_m, x_u),$$

$$b_u = 2[\det(z(x_m) \ z(x_m) \ z(x_u)),_1]^2,$$

$$b_1 = 2[\det(z(x_m) \ z(x_m) \ z(x_1)),_1]^2.$$

Now we can formulate

Theorem 4: Let $\varphi : [x_1, x_u]^3 \rightarrow \mathbb{R}^+$,

$$\varphi(x_1, x_2, x_3) = \det(z(x_1) \ z(x_2) \ z(x_3))^2$$

takes a relative maximum in (x_1, x_m, x_u) , and the derivatives satisfy

$$\varphi_{,1}(x_1, x_m, x_u) < 0$$

and

$$\varphi_{,2}(x_1, x_m, x_u) > 0.$$

An experimental design x with $sp(x) = \{x_1, x_m, x_u\}$ and the

corresponding frequencies n_1, n_m, n_u is relatively optimal, if

$$\lambda := n_u n_1 a + n_m (n_1 b_1 + n_u b_u) < 0.$$

Remark: In the case of exponential regression with negative γ it is possible to show that this inequality is valid for the previously constructed relative maximum. Then the eigenvalue depends only on the ratio $\gamma/(x_u - x_1)$ and, for all n with $3|n$ or large enough, it can be proved to be negative by asymptotic expansion for arguments near zero, by limit considerations for large negative values and by numerical evaluations for the remaining case. Indeed, we have

$$a = 2\gamma e^{\gamma x_m} [e^{\gamma(\gamma - \gamma x_m - 2)} + \gamma x_m + 2] [(1 - x_m) e^{\gamma(1 + x_m)} - e^{\gamma} + x_m e^{\gamma x_m}],$$

$$b_u = 2e^{2\gamma x_m} [e^{\gamma(1 - \gamma x_m - \gamma)} - e^{\gamma x_m}]^2,$$

$$b_1 = 2e^{2\gamma x_m} [1 + \gamma x_m - e^{\gamma x_m}]^2$$

with $x_m = e^{\gamma}/(e^{\gamma} - 1) - 1/\gamma$. Using $|n_i - n_j| \leq 1$ we obtain

$$\lim_{\gamma \rightarrow -\infty} \lambda(\gamma) = -2e^{-2}(1 - 2e^{-2}) \frac{n^2}{9} \quad (+ O(n) \text{ if } 3 \nmid n)$$

and

$$\lambda(\gamma) \sim -\frac{2}{9} n^2 \gamma^2 e^{1/\gamma} - 1/2 \quad (+ O(n) \text{ if } 3 \nmid n)$$

for γ near zero.

5. Final comment

The above considerations affirm that designs of minimal size of the support yield good values of the local D-criterion and that the ends of the observation interval should belong to the support. Further it turned out that other choices of frequencies to the optimal support give us relative maxima, too. Moreover those maxima are more peak-like. On the other hand, we don't know, whether there are further maxima. But if there are such maxima, then they cannot be much better than the 3-point maximum. Problems of this kind are called frustrated. In [8], [9] we discuss algorithms for the numerical treatment of this problem. The results of that papers suggest that the above conclusions are typical for experimental design in general, not only for D-optimality.

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