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Beate Thielcke

# Zur Untergruppeneigenschaft von Klassenvereinigungen in endlichen Gruppen

Herrn Prof. Dr. L. Berg zum 60. Geburtstag gewidmet

## 1. Einleitung

In der vorliegenden Arbeit werden Vereinigungen K von Konjugiertheitsklassen einer endlichen Gruppe G betrachtet, welche die {1}-Klasse enthalten und deren Mächtigkeiten die Ordnung von G teilen. Offensichtlich bilden derartige Komplexe K, kurz CNS-Komplexe genannt, in G im allgemeinen keine Untergruppe, verhalten sich jedoch invariant gegenüber inneren Automorphismen von G. Diese Tatsache gibt Anlaß zur folgenden

Definition: Wir nennen eine endliche Gruppe G eine Converse Normal Subgroup-Gruppe (kurz CNS-Gruppe), falls jeder in G enthaltene CNS-Komplex eine Untergruppe bildet.

Natürlich sind CNS-Komplexe in CNS-Gruppen stets sogar Normalteiler. Es erweist sich, daß sowohl hinreichend komplizierte Beispiele als auch Gegenbeispiele für CNS-Gruppen existieren, deren Untersuchung teils theoretisch, teils unter Einsatz von Computern erfolgt.
Bezeichnet $Z_n$ die zylische Gruppe der Ordnung n, so ist leicht einzusehen, daß $Z_1$ und $Z_p$ für jede Primzahl p sowie die Vierergruppe $V \cong Z_2 \times Z_2$ zu den CNS-Gruppen gehören, $Z_n$ für eine zusammengesetzte Zahl n hingegen nicht.
Für das Zentrum Z(G) und für die Faktorgruppe G/G' nach der Kommutatorgruppe G' von CNS-Gruppen ergeben sich spezielle Gruppentypen, welche zur Auffindung der abelschen und der p-Gruppen unter den CNS-Gruppen führen.

## 2. Verwendete Zeichen

| | |
|---|---|
| $S_n$ | symmetrische Gruppe des Grades n |
| $A_n$ | alternierende Gruppe des Grades n |

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Petra Duchrau; Kurt Frischmuth

# A numerical search algorithm for experimental design

## 1. Introduction

In the recent years there has been paid much attention to algorithms for the construction of experimental designs which are optimal for the estimation of the parameter $\vartheta$ in models of the type

$$y_i = g(t_i,\vartheta) + \varepsilon_i, \quad i = 1 \ldots n . \tag{1}$$

Here is $\vartheta \in \Omega \subseteq \mathbb{R}^p$, $t \in I$ and $\varepsilon_i$ is some error term. Most work has been done for the case of

$$\vartheta \longrightarrow g(t_i,\vartheta)$$

being linear, say

$$g(t_i,\vartheta) = X(t_i)\vartheta$$

and the D-criterion

$$f(t) = 1/\det \Big( \sum_{i=1}^{n} X^T(t_i)X(t_i) \Big),$$

where $t = (t_1 \ldots t_n)$.

Even for this appearently simple case severe difficulties occur in the minimization. As pointed out by Mitchell [1], the main problem is to get trapped by one of the numerously existing local minima of the objective function f. In [2] Cook and Nachtsheim compared several algorithms for the linear case and the D-criterion. Most of them consist in some exchanging strategy which adds and subtracts points to the current design using properties of the determinant and the linearity of g. None of the considered algorithms was superior to all others, especially none of them did always find the best known design.

For nonlinear models an analog of the D-criterion was intro-

duced by Chernoff [3], first analytical and numerical results on optimal designs were obtained by Box and Lucas [4]. A further sophistication of the D-criterion basing on curvature measures of the solution locus as introduced by Bates and Watts [5] was given by Hamilton and Watts [6], but little attention was paid to the problem of minimizing the computed objective function.

Rasch, Rudolph and Schimke published in [7] their algorithm OPREG together with applications to a special growth model and a variety of optimality criterions derived from the asymptotic co-variance matrix. OPREG proved to be very succesful in finding the (probably) global minimizer in small sized problems ($n \leq 15$, $p = 3$), but it requires excessively high computation time even for medium problems.

Our present work is mainly aimed to provide a better understanding of the general problems with searching for optimal experimental designs, independent of the underlying statistics, and to propose a specific tool for overcoming local minima.

It turns out (see Sec. 2) that for objective functions in experimental design typical (local) minimizers exhibit only few different components. Basing on this fact we define in Sec. 3 a map U from the domain $C = I^n$ of the objective function f into its power set. This map is used lateron in order to enlarge the neighbourhoods of points, especially it selects candidates for a restart if the minimization reaches a local minimum. The idea is as follows: we start with some minimization algorithm which terminates if we find a $t \in C$ with

$$\exists\ O \text{ - open}, t \in O \quad \forall\ \tilde{t} \in O \quad f(t) \leq f(\tilde{t}). \tag{2}$$

But now, we strengthen the condition for termination demanding

$$\exists\ O \text{ - open}, t \in O \quad \forall\ \tilde{t} \in O \cup U(t) \quad f(t) \leq f(\tilde{t}). \tag{3}$$

If (2) is valid but (3) is not then we swich from our initial minimization algorithm to a supplementary algorithm for the minimization of $f_{|U(t)}$ and restart at the minimizer. Hence the risk of getting trapped in a local minimizer decreases at the cost of a more expensive search.

It turned out that for our map $U: C \longrightarrow 2^C$ the above algorithm renders the search for optimal experimental designs very economic and removes the problem of finding "wrong" minima to a

practically sufficient degree. Furthermore, for certain problems it finds even the global minimizer (see Sec. 5).

## 2. The objective function for experimental designs

For most applications the optimality criterion is based on the so called asymptotic co-variance matrix. Let $t \in C = I^n$ be an experimental design, then

$$F(t) = \sum_{i=1}^{n} [\mathrm{grad}_\vartheta\, g(t_i,\vartheta_o)]^T\, \mathrm{grad}_\vartheta\, g(t_i,\vartheta_o) \in \mathbb{R}^{P\times P} \qquad (4)$$

with a given a priori information $\vartheta_o$ is called the Fisher information matrix of $t$ and its inverse

$$V(t) = F^{-1}(t), \qquad (5)$$

if existing, is the asymptotic co-variance matrix.
Commonly used criterions are $\det(V)$, $\mathrm{tr}(V)$, and $V_{ii}$, $(i = 1 \ldots p)$, (cf. [8]).
Hamilton and Watts modify $\det(V)$ by adding a term containing second derivatives of the model function at $t$ and $\vartheta_o$ (cf. [6]).
Note that $t \longrightarrow F(t)$ is fully symmetric, hence all criterions basing on $V(t)$ are so, the criterion from [6] is fully symmetric as well. Further, smooth model functions yield smooth objective functions. Denoting $T(t) = \{t_1, \ldots, t_n\}$, we see that $F(t)$ becomes singular if $|T(t)| < p$. For such designs the objective function becomes infinite. We may assume the model function to yield finite values of the criterion otherwise.
Hence, in general, we deal with the following problem

$$f(t) = \mathrm{Min}\ ! \qquad (6)$$

with a smooth $f: C \longrightarrow \overline{\mathbb{R}^+}$ satisfying

$$f(t) = f(\pi(t)) \qquad (7)$$

for any permutation $\pi \in S(n)$ and

$$f(t) = +\infty \ \text{ iff } \ |T(t)| < p \qquad (8)$$

with some $p$, $1 < p \leq n$.

Of course, $f$ cannot be convex on $C$ since it then would take its minimum on the diagonal

$$D = \{ (\tau, \ldots, \tau) \mid \tau \in I \} \subset C$$

which is obviously not true. Further, $f$ is in general not convex even on $S \subset C$,

$$S = \{ t \in C \mid t_1 \leq t_2 \leq \ldots \leq t_n \}, \tag{9}$$

consequently the possibility of restricting $f$ to $S$ is not to much advantageous.
For the following assertion we assume $I$ to be the interval $[x_l, x_u] \subset \mathbb{R}$ and $p = 3$. Further let $D_{n_1,n_2}$, $n_1 + n_2 < n$, be the hyperdiagonal

$$\{ t \in C \mid t_1 = \ldots = t_{n_1} = x_l,\ t_{n_1+1} = \ldots = t_{n_1+n_2} = x_u,$$

$$t_{n_1+n_2+1} = \ldots = t_n \}.$$

Assertion 1: For $p = 3$, $I = [x_l, x_u] \subset \mathbb{R}$ and each pair of positive integers $n_1$, $n_2$ with $n_1 + n_2 < n$ there exists a critical point of $f$ on $D_{n_1,n_2}$.

Proof: If we introduce in the actual tangent space to $C$ at some inner point of $D_{n_1,n_2}$ the basis

$$\begin{aligned}
e_1 &= (0,0,\ldots 0,\underbrace{1,\ 1,\ \ldots,\ 1}_{n_1+n_2},\ \ldots,\ 1) \\
e_2 &= (0,0,\ldots 0,1,-1,\ 0,\ \ldots,\ 0) \\
e_3 &= (0,0,\ldots 0,0,\ 1,-1,\ 0,\ \ldots,\ 0) \\
&\vdots \\
e_{n-n_1-n_2} &= (0,0,\ldots 0,0,\ 0,\ \ldots\ 0,\ 1,-1)
\end{aligned}$$

then $df/de_i = 0$, $i = 2, \ldots, n-n_1-n_2$ due to the symmetry condition (7). Further we have

$$\lim_{\tau \to x_l(x_u)} f(x_l \ldots x_l,\ x_u \ldots x_u,\ \tau, \tau, \ldots, \tau) = \infty$$

hence due to Rolle's theorem $df/de_1$ vanishes at some point

$$t = (x_l \ldots x_l,\ x_u \ldots x_u,\ x_m \ldots x_m) \in D_{n_1,n_2}. \qquad (10)$$

We infer that the projection of grad f(t) onto the tangent space to C at t vanishes, which completes the proof. ■

Remark: Note that the mentioned tangent space is constant along $D_{n_1,n_2}$.

Assertion 2: Let $\hat{n} < n$ and $t = (t_1 \ldots t_{\hat{n}},\ 0,\ 0 \ldots 0)$ and

$$B_{\hat{n},\hat{t}} = \{\ t \mid t = t + (0,0,\ldots 0,\ \tau,\ \tau \ldots \tau),\ \tau \in I\ \}.$$
$$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad n$$

Assume a) f is convex in some neighbourhood V of $B_{\hat{n},\hat{t}}$ and

b) V contains a local minimizer of f.

Then $B_{\hat{n},\hat{t}}$ contains a local minimzer of f.

The proof is a direct consequence of (7) and Jensens's inequality, here no assumptions about I and p are needed.

There is obviously little practical use to be made from the above assertions, in Assertion 1 it remains open whether the gradient points inside or outside C, while the assumptions of Assertion 2 are practically not to be verified. But nevertheless, they give some insight why the minimization of design criterions yields usually minimizers with a minimum number (i.e., equal to the number of unknown parameters p) of different components (with exceptions!). The situation studied by Rasch, Rudolph and Schimke [7] meets the assumptions of Assertion 1, and indeed most of the results reported by them are critical points just of the form (10). Moreover, for the D-criterion and a certain class of growth functions, the existence of local minimizers of the type (10) can be proven (cf. [9]). On the other hand, there exist special cases where the assumptions of Assertion 1 are fulfilled, but not both $x_l$ and $x_u$ belong to the optimal design, e.g. for the growth function (14) below. Further "experimental" results and hypotheses on the properties of optimal experimental designs based on numerical experience are contained in Rasch a.o. [7].

The above results together with some experience suggest that for

large n and small p the terminal values of minimization algorithms are more economically represented by ordered tables

$$t \sim \left( \frac{x_1 \ \dots \ x_m}{n_1 \ \dots \ n_m} \right), \quad x_i \in I, \ n_i \in \mathbb{N}^+ \tag{11}$$

containing only the different components of t and their numbers of occurence. Now, it is quite natural to treat two such tables as neighbouring if they have a common first row and small differences in the second. This motivates the considerations of the next section.

## 3. The mapping U

Let us consider two families of sets

$$U_\varepsilon^1(t) = \{ \tilde{t} \in C \mid T(\tilde{t}) \subseteq T(t) \wedge \|n_{\tilde{t}} - n_t\| \leq \varepsilon \},$$

$$U_\varepsilon^2(t) = \{ \tilde{t} \in C \mid T(\tilde{t}) \subseteq T(t) \wedge \| n_{\tilde{t}} - n_t \| \leq \varepsilon \},$$

with $n_t(\tau) = |\{ i : t_i = \tau \}|$,

$$\|n_{\tilde{t}} - n_t\| = 1/2 \sum_{\tau \in T(t)} |n_{\tilde{t}}(\tau) - n_t(\tau)|$$

and

$$\|n_{\tilde{t}} - n_t\| = \max_{\tau \in T(t)} |n_{\tilde{t}}(\tau) - n_t(\tau)|.$$

It is easy to see :

a) For $\varepsilon < 1$ is $U_\varepsilon^1(t) = U_\varepsilon^2(t) = \{t\}$.

b) We have $|U_1^1(t)| = |T(t)| \ ( \ |T(t)| - 1 \ ) + 1,$

$$|U_1^2(t)| \leq 3^{|T(t)|}.$$

c) For each $\varepsilon$ there exists a bound $b_E$ independent of t such that

$$|U_\varepsilon^1(t)| \leq |U_\varepsilon^2(t)| < b_\varepsilon .$$

d) $U_\varepsilon^1(t) \subseteq U_\varepsilon^2(t)$.

We interpret the sets $U^i(t)$ as some "neighbourhoods" of the point t. Nevertheless, it should be pointed out that from the topological point of view the families $U^i_\epsilon(t)$, $\epsilon \geq 1$, are no bases of neighbourhoods, further the topology generated by their sum is the discrete one.

Now we define

Definition: A point $t \in C$ is called a semi-local minimizer (SLM) of f on C if

$$\exists\, \epsilon_1 > 0,\ \epsilon_2 \geq 1 \quad \forall\, \tilde{t} \in C \quad \tilde{t} \in B_{t,\epsilon_1} \cup U^i_{\epsilon_2}(t) \Longrightarrow f(\tilde{t}) \geq f(t),$$

where $B_{t,\epsilon_1}$ is the ball with radius $\epsilon_1$ and center at t and $i = 1$ or $i = 2$.

Of course, each SLM is a local minimizer, but not contrarily. In fact, the following assertion is true:

Assertion 3: A point $t \in C$ is a SLM of f on C iff

a) it is a local minimizer and
b) $f(t) = \min f_{|U^i_1(t)}$.

From now on we fix i and set $\epsilon = 1$, defining $U(t) = U^i_1(t)$. Since U(t) is for each $t \in C$ a rather small finite set the above assertion suggests a very simple algorithm for the search of SLM which will be discussed in the next section.

## 4. The search algorithm

Basing on Assertion 3 we propose the following procedure

1. $k = 0$,
2. choose a starting point $t^0$,
3. calculate an (approximative) local minimizer $t^{k+1}$, using a descent method starting at t,
4. calculate $\min f_{|U(t^{k+1})}$ $(=: f(t^{k+2}))$,
5. if $t^{k+2} = t^k$ then stop, else $k = k+2$ and go to 3.

Some details of steps 3 and 4 may be of great importance for the overall performance of the algorithm :

a) Since for $I = [x_l, x_u]$ the domain C is a cube we deal here with so called box constraints. It is either possible to transform the problem into an unconstraint minimization problem (cf. [10]) or to use some backtracking and projection method in step 3. In our implementation we used the latter approach, basing on a secant method of Broyden type (cf.[11]). In each step of the descent method the gradient of the objective function as well as the search direction are reduced, i.e. projected onto the actual tangent space of C.

b) The first application of 3. provides usually a remarkable reduction of $|T(t)|$, while the minimizer very often obeys $|T(t)| = p$. Consequently, with respect to the cardinality of U(t), we recommend to use in 4. the norm $\|\cdot\|$ until $|T(t)|$ becomes small enough and then to swich to the more expensive norm $\|\cdot\|$.

c) In the representation of designs as well as in the calculation of derivatives and updating of quasi-Hesse matrices the symmetry (7) should be used. This provides huge savings in the final stage of minimization. On the other hand, attention must be paid to the numerical method of calculating det(V), tr(V) or $V_{ii}$, respectively, for the vectors $grad_\vartheta g(t_i, \vartheta_o)$, $i = 1,\ldots,n$, are usually almost linearly dependent.

It is quite obvious that the above procedure terminates always at a SLM, provided the number of local minimizers is finite. Of course, step 3 is possible to be carried out only approximately. Step 4 may be substituted by 4a :

4a. search for $t^{k+2}$ such that $t^{k+2} = \min f_{|U(t^{k+2})}$.

Again, it is possible to swich between 4. and 4a. in dependence on the efficiency at the last taken step.

## 5. A convergence result

For the general case of the optimization problem (6)-(8) the convergence of the above algorithm to a global minimizer is not ensured. Indeed, there are examples with the norm $\|\cdot\|$ and $\varepsilon = 1$, where the global minimizer was not found for certain starting points. Nevertheless, for the special case of the criterion $f(t) = \det(V(t))$ and $p = 3$ we are

able to prove the following assertion, which applies to several models of practical interest.

Assertion 4: Let $p = 3$ and the graph of the function

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

$$z(\tau) = \mathrm{grad}_{\vartheta} g(\tau, \vartheta_o)$$

be a regular curve contained in some plane $\eta$ with $0 \notin \eta$. In $\eta$ there exists a basis $\{b_1, b_2\}$ such that the $b_2$-component of $z$ is a convex function of the $b_1$-component. Then the algorithm from the previous section solves the problem

$$f(t) = \det(V(t)) = \mathrm{Min!} \quad , \; t \in C_p$$

for each norm $\|\cdot\|$ or $|||\cdot|||$ each $\varepsilon \geq 1$ and each starting point $t_o \in C_p$ in not more then $n$ steps.
Here is $C_p = \{ t \in C : |T(t)| = p \}$.

Proof: In [9] it is proven that under the assumptions of the assertion the objective function obeys

$$f(t) = \varphi(x_t)\, \psi(n_t)$$

with $x_t$ being the first row of the representation (11) and a function $\psi$ depending only on the image of $n_t$. Further, $\varphi$ takes a unique minimum on $I^P$ and $\psi$ is a convex symmetric function of the nonvanishing values of $n$. Hence steps 3 and 4 work independently.
Consequently, the algorithm is finite, i.e., it finds a SLM. Due to the above properties of $f$, $\varphi$ and $\psi$ the conditions for a SML and for a global minimizer are the same. The bound for the number of steps follows from a simple examination of the worst case $\varepsilon = 1$. ■

The assumptions of Assertion 4 are fulfilled for the models (12) and (14) of the following section. However, we applied the algorithm succesfully in several other situations, too.

## 6. Numerical experience

We performed numerical experiments for $n = p$ (= 3 or 4), $n = 10$ and $n = 100$, using $I = [0,65]$ and objective functions calculated from the growth models

$$y = \vartheta_1 + \vartheta_2 \exp(\vartheta_3 x), \quad x \in I, \quad \vartheta = (\vartheta_1, \vartheta_2, \vartheta_3) \tag{12}$$

with $\vartheta_3 = -0.05$ and $\vartheta_3 = -0.03$,

$$y = (\vartheta_1 + \vartheta_2 \exp(\vartheta_3 x))^3, \quad x \in I, \quad \vartheta = (\vartheta_1, \vartheta_2, \vartheta_3) \tag{13}$$

with $\vartheta_1 = 5$, $\vartheta_2 = -5$, $\vartheta_3 = -0.05$,

$$y = \vartheta_1 + \vartheta_2 \exp(\exp(\vartheta_3 x)), \quad x \in I, \quad \vartheta = (\vartheta_1, \vartheta_2, \vartheta_3) \tag{14}$$

with $\vartheta_1 = 100$, $\vartheta_2 = -3$, $\vartheta_3 = 0.1$,

$$y = \vartheta_1 + \vartheta_2 \tanh(\vartheta_3 x + \vartheta_4), \quad x \in I, \quad \vartheta = (\vartheta_1, \vartheta_2, \vartheta_3, \vartheta_4) \tag{15}$$

with $\vartheta_2 = 50$, $\vartheta_3 = -3$, $\vartheta_4 = 0.1$.

For the function (12) we chose the V-criterion, for functions (13)-(15) we chose the D-criterion.
Further experiments similar to that from [2] are planned by Rasch et al. in forthcoming papers.
In order to check the danger of getting trapped in SLM's being not a global minimizer we started our algorithm from different starting points choosen to posses $m := |T(t_o)|$ different components with an uniform distribution over I. The numbers of equal components were choosen to be "almost equal" (cf.[8]). We run the algorithm with $m = 3$, $m = 4$, $m = 6$, $m = 8$ and $m = 10$. The result was for all m a design with the same value of the criterion. $|T(t)|$ was p with only two exceptions: $|T(t)|$ was p+1 for the growth model (13) with $n = 10$, $m = 6$ and for the growth model (15) with $n = 10$, $m = 8$ and $m = 10$. There was only a small difference between two components of t, but the value of the criterion was also the same like for the other m, where $|T(t)|$ was equal to p. Our experience suggests that for small values of n the starting point t with $t_i = x_l + (x_u - x_l)(i-1)/(n-1)$ is most successful, while for larger n the choice $m = p$ seems to be

sufficient. Note that usual implementations of step 3 cannot increase $|T(t)|$ with respect to the symmetry of f.

## 7. Concluding remarks

The presented concept of SLM released in an obvious manner the danger of finding local minimizers that are not global. On the other hand, the problem of constructing mappings U that ensure the SLM to be a global minimizer and result in reasonable algorithms, remains open in general. Here we mean by reasonable that U(t) should be much smaller than C (U(t) = C would of course make each SLM a global minimizer). It seems that the choice of a useful mapping U requires always some deeper understanding of the global behaviour of the objective function under consideration as provided here by Assertions 1 and 2.

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Authors

Dr. Kurt Frischmuth
W.-Pieck-Universität Rostock
Sektion Mathematik
Universitätsplatz 1
Rostock
DDR-2500

Dipl.-Math. Petra Duchrau
W.-Pieck-Universität Rostock
Sektion Informatik
Universitätsplatz 1
Rostock
DDR-2500