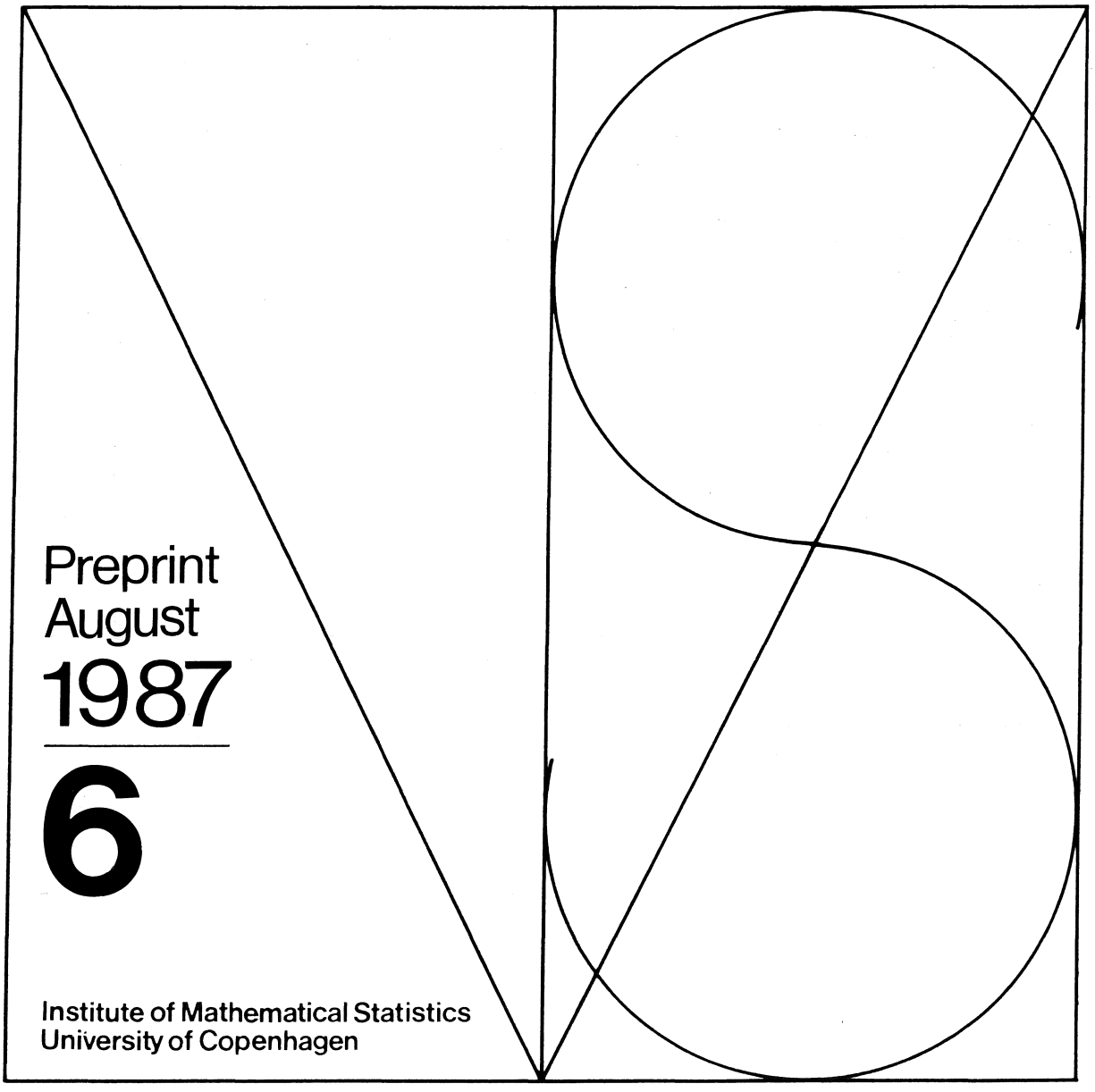
Tue Tjur

Block Designs and Electrical Networks



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BLOCK DESIGNS AND ELECTRICAL NETWORKS

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Summary.

For a given block design, an electrical network is constructed in which blocks and treatments are represented by points and observations by connections. This network has the property that the resistance between two points representing two different treatments is equal to the variance on the estimate of the corresponding treatment contrast in the usual additive "block effect plus treatment effect" model. This provides a simple tool for computation of contrast variances in many examples. Further applications are made to obtain lower bounds for contrast variances, upper bounds for efficiencies and an algorithm for the construction of optimal or nearly optimal designs.

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A-optimality, block design, efficiency, graph, network, optimal design.

1. Introduction.

Consider a *block design*, i.e. a finite set B of *blocks*, a finite set T of *treatments* and a $B \times T$ -matrix $\mathbf{N}$ of nonnegative integers n_{bt} indicating how many times treatment t occurs in block b. Draw a graph as follows: Each block and each treatment is represented by a point (vertex). Each *plot* (i.e. each occurrence of a treatment in a block) is represented by a connection (edge) between the points corresponding to the block and the treatment assigned to the plot. Thus, n_{bt} connections are drawn between the points b and t, whereas two block points or two treatment points are never directly connected (the graph is *bipartite*). Now, think of the graph as a diagram of an electrical network where the edges are connections of unit resistance (1 ohm). The properties of this network turn out to be closely related to the properties of the design. The most interesting relation is probably the following. Consider the standard "block + treatment" model, assuming that the observations (yields) on plots are independent, normally distributed with common variance σ^2 and means of the form $\alpha_t + \beta_b$. For two treatments t' and t'', let $R(t',t'')$ denote the resistance through the network between the points corresponding to t' and t''. Then,

$$\mathrm{var}(\hat{\alpha}_{t'} - \hat{\alpha}_{t''}) = \sigma^2 R(t',t'') \quad .$$

where $\hat{\alpha}_{t'} - \hat{\alpha}_{t''}$ is the (maximum likelihood or least squares) estimate of the simple contrast $\alpha_{t'} - \alpha_{t''}$.

We shall make the following applications of this basic observation:

Special designs (section 3). For many block designs (including balanced incomplete block designs, simple lattices and some other partially balanced designs) it is easy to compute the contrast variances explicitely, simply by drawing the network in a convenient manner and using the laws for parallel and serial combination of resistances.

Inequalities (sections 4 and 5). A basic observation for electrical networks is that the introduction of a new connection somewhere in the network can never increase the resistance between two points. In particular, the contraction of two or more points to a single point (by "short circuiting") can not increase any resistance through the network. This provides us with a simple tool for calculation of lower bounds for contrast variances, and thereby (via a convexity argument) upper bounds for the harmonic mean efficiency (which can be defined as the inverse proportion between the average contrast variance in the given design and the same quantity computed for a design with the same treatments repeated the same number of times in a single block).

Construction of optimal or almost optimal designs (section 6). The relation between block designs and electrical networks gives some intuitive insight in the properties of good designs (i.e. designs with small contrast variances), and suggests various algorithms for the construction of such designs. A very simple idea is to start out with a network consisting of $B + T$ isolated points, and then introduce the connections one by one, in each step adding the connection which is "most needed", in some sense. A similar idea is to start "from top" with a complete bipartite graph (corresponding to a complete block design) and then delete connections according to similar rules. As we shall see, there are simple formulas for the change of average contrast variance resulting from such changes of the network. However, designs obtained by these procedures are usually not of maximal efficiency. An additional modification can be performed by *switches*. By a switch we mean the removal of two connections (e.g. from t_1 to b_1 and t_2 to b_2) simultaneously with the addition of the two "crossing" connections (from t_1 to b_2 and from t_2 to b_1). As we shall see, it is possible (by extension of the calculations for addition and removal of connections) to give a relatively simple formula for the change of average contrast variance resulting from a switch. This makes it possible to search among all switches for the best one, that is the one that gives the maximal decrease of average contrast variance. Supplemented with a randomization

feature (to escape "local maxima" for the efficiency) this gives a cheap and efficient algorithm for construction of block designs, which is useful for situations where a "classical" solution (BIBD, PBIBD, etc.) does not exist. The algorithm is very similar to that of Jones and Eccleston (1980), but the differences seem to be important.

Section 7 contains a discussion of the relation of the present work to the work of other authors, in particular Borre and Meissl (1974, on a relation between geodetic networks and potential theory), Jones and Eccleston (1980), Paterson (1983) and Paterson and Wild (1986, on properties of a related graph derived from a block design and its relation to efficiency) and Eccleston and Hedayat (1974, on connectedness properties of designs). The probabilistic interpretation in terms of random walks on the design graph is briefly outlined. An extended design network for the case of random block effects is defined, in which the variances of estimated treatment contrasts have the same interpretation as resistances through the network.

2. *The main result.*

Notation. By I, B and T we denote the sets of plots, blocks and treatments, respectively. Elements of these sets are denoted i, i', i_1, ... $\in I$, b, b', b_1, ... $\in B$ and t, t', t_1, ... $\in T$. Whenever convenient, we assume

$$I = \{ 1, 2, \ldots, I \} ,$$
$$T = \{ 1, 2, \ldots, T \} \text{ and}$$
$$B = \{ 1, 2, \ldots, B \} .$$

Thus, I, B and T denote both the finite sets and their cardinality. This is merely for convenience, and is not likely to cause any confusion in the present context.

Formally, a design is given by two mappings $\varphi_B : I \to B$ and $\varphi_T : I \to T$, assigning factor levels to plots (cfr. Tjur 1984). The statistical properties of the design are determined by the integers $n_{bt} = \#\{ i \in I \mid \varphi_B(i)=b \text{ and } \varphi_T(i)=t \}$, constituting the $B \times T$ *incidence matrix* $\mathbf{N} = (n_{bt})$. By k_b we denote the size of block b and by r_t the number of replicates of treatment t. The incidence matrix $\mathbf{N}$ has row sums k_b, column sums r_t, and the sum of all elements is I.

The design network (not to be confused with Patersons *variety concurrence graph*, which has only the treatments as points) is formally defined as follows. The set of points of a graph is taken to be the disjoint union of B and T. On figures, we use signs $\bullet$ for treatments and $\circ$ for blocks, to distinguish. A connection from $b \in B$ to $t \in T$ is introduced for each occurence of treatment t in block b. Thus, the set of connections can (and will) be identified with I. We interprete the graph as an electrical network where these connections are unit resistances (1 ohm).

In all that follows, we shall assume that the design is *connected*, in the sense that any two treatment points t' and t'' can be joined by a

chain $t' = t_1\ b_1\ t_2\ b_2\ \dots\ b_{n-1}\ t_n = t''$ such that $n_{b_{i-1}t_i}$ $(i=2,\dots,n)$ and $n_{b_i t_i}$ $(i=1,\dots,n-1)$ are positive. This is easily seen to be equivalent to the condition that the design network is connected in the obvious graph theoretic sense (subsuming, of course, that all k_b and r_t are positive).

Theorem 2.1. *Let* $\mathbf{y} = (y_i \mid i\in I)$ *be a vector of real random variables, independent and normally distributed with common variance* σ^2 *and expectations given by*

$$\mathrm{E}\, y_i = \alpha_t + \beta_b \qquad (t = \varphi_T(i)\ ,\ b = \varphi_B(i)\ )\ .$$

Let $(\hat{\alpha}_t)$ *and* $(\hat{\beta}_b)$ *be maximum likelihood (or least squares) estimates of* (α_t) *and* (β_b) *in this statistical model. Let* $R(p',p'')$ *denote the resistance between points* p' *and* p'' *of the network. Then,*

(i) The variance of an estimated treatment contrast is given by

$$\mathrm{var}(\hat{\alpha}_{t'} - \hat{\alpha}_{t''}) = \sigma^2\, R(t',t'')\ .$$

(ii) The variance of a fitted value is given by

$$\mathrm{var}(\hat{\alpha}_t + \hat{\beta}_b) = \sigma^2\, R(t,b)\ .$$

(iii) Let $\hat{\alpha}_{t'} - \hat{\alpha}_{t''} = \Sigma_i\, a_i^{t't''} y_i$ *be the expression of the estimated* (t',t'')*-contrast as a linear combination of the observations. Then, the coefficients* $a_i^{t't''}$ *have the following interpretation as potential differences in the network: Suppose that voltages* $R(t',t'')$ *and* 0 *are kept fixed at the two points* t' *and* t''*, while all other points are left untouched. Then,* $a_i^{t't''}$ *is the current through connection* i*, signed so that current from block to treatment counts negative while current from treatment to block counts positive. Or*

(since potential difference = current through the unit resistance),

$$a_i^{t't''} = v_{\varphi_T(i)} - v_{\varphi_B(i)} ,$$

v_p *denoting the potential at the point* $p \in B \cup T$.

Remarks. We have used the term "fitted value" for the estimate $\hat{\alpha}_t + \hat{\beta}_b$. This is, perhaps, only meaningful for block-treatment combinations actually occurring in the design. For combinations which do not occur, a term like "predicted mean of hypothetical observation" would be more correct. But the result (iii) is valid in both cases.

Notice that the formula $R(t',t'') = \Sigma_i \, (v_{\varphi_T(i)} - v_{\varphi_B(i)})^2$ (which, according to (i) and (iii), merely equates two different expressions for the contrast variance) has the physical interpretation that the total energy per time unit developed by the network when a potential difference of $R(t',t'')$ between t' and t'' is kept fixed equals the sum of energies per time unit emerging from the single connections.

Notice also that (iii) suggests a way of solving the normal equations numerically by means of relatively simple physical equipment. It would be interesting to know whether such methods have been considered before the digital computer age.

Proof. Consider the $(T+B)\times(T+B)$ (or $(TUB)\times(TUB)$) matrix

$$C = (c_{pq}) = \begin{bmatrix} \mathrm{diag}(r_t) & N^* \\ N & \mathrm{diag}(k_b) \end{bmatrix}$$

with elements

$$\begin{aligned} c_{bt} &= c_{tb} = n_{bt} && \text{for } b \in B,\ t \in T , \\ c_{tt} &= r_t && \text{for } t \in T , \\ c_{bb} &= k_b && \text{for } b \in B \\ \text{and} \quad c_{pq} &= 0 && \text{for all other } (p,q) . \end{aligned}$$

This matrix plays a role, both in the analysis of the statistical model and in the analysis of the design network. In the statistical context, this role is wellknown. Let X_T denote the $I \times T$ design matrix for the factor T (cfr. Tjur 1984), i.e.

$$(X_T)_{it} = \begin{cases} 1 & \text{for } \varphi_T(i) = t \\ 0 & \text{otherwise.} \end{cases}$$

Similarly, define X_B $(I \times B)$ by

$$(X_B)_{ib} = \begin{cases} 1 & \text{for } \varphi_B(i) = b \\ 0 & \text{otherwise.} \end{cases}$$

The expectation of the random vector $\mathbf{y} = (y_i)$ under the additivity model can then be written $\mathbf{E}\,\mathbf{y} = X_T\boldsymbol{\alpha} + X_B\boldsymbol{\beta}$ ($\boldsymbol{\alpha} = (\alpha_t) \in \mathbb{R}^T$, $\boldsymbol{\beta} = (\beta_b) \in \mathbb{R}^B$). The normal equations determining the maximum likelihood estimates (up to an arbitrary constant to be added to all α_t and subtracted from all β_b) can then be written

$$\begin{bmatrix} X_T^* \\ X_B^* \end{bmatrix} \begin{bmatrix} X_T & X_B \end{bmatrix} \begin{bmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{bmatrix} = \begin{bmatrix} X_T^* \\ X_B^* \end{bmatrix} \mathbf{y}$$

or

$$\begin{bmatrix} X_T^*X_T & X_T^*X_B \\ X_B^*X_T & X_B^*X_B \end{bmatrix} \begin{bmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{bmatrix} = \begin{bmatrix} X_T^* \\ X_B^* \end{bmatrix} \mathbf{y}$$

The partitioned square matrix to the left is easily recognized as our C . Now, let C^- be a symmetric $(T+B)\times(T+B)$ matrix such that $C\,C^-C = C$ and $C^-C\,C^- = C^-$ (a *reflexive generalized inverse* for C , cfr Rao 1973). One solution to the normal equations is then given by

$$\begin{bmatrix} \hat{\alpha} \\ \hat{\beta} \end{bmatrix} = C^{-} \begin{bmatrix} X_T^* \\ X_B^* \end{bmatrix} y \quad ,$$

and the covariance matrix for this set of estimates is

$$\mathrm{cov}(\hat{\alpha} , \hat{\beta}) = \sigma^2 C^{-} \begin{bmatrix} X_T^* \\ X_B^* \end{bmatrix} \left(C^{-} \begin{bmatrix} X_T^* \\ X_B^* \end{bmatrix} \right)^* = \sigma^2 C^{-} \quad .$$

It follows that the variance on an estimated contrast $\hat{\alpha}_{t'} - \hat{\alpha}_{t''}$ is

$$\mathrm{var}(\hat{\alpha}_{t'} - \hat{\alpha}_{t''}) = (1_{t'} - 1_{t''})^* (\sigma^2 C^{-}) (1_{t'} - 1_{t''}) \quad ,$$

with an obvious notation for vectors in $\mathbb{R}^{B+T}$ which are 1 at a single coordinate and 0 elsewhere. Similarly, the variance of a fitted value $\hat{\alpha}_t + \hat{\beta}_b$ is given by

$$\mathrm{var}(\hat{\alpha}_t + \hat{\beta}_b) = (1_t + 1_b)^* (\sigma^2 C^{-}) (1_t + 1_b) \quad .$$

Now to the interpretation of C in the network context. Suppose that voltages $R(t',t'')$ and 0 are kept fixed at the two points t' and t'', while all other points are left untouched. According to Ohm's law, the current through the network from t' to t'' will then be 1 ampere. The laws of Kirchhoff, determining the potentials at all other points of the network, can be stated as follows. Let v_p $(p \in TUB)$ denote the potential at the point p. The current through a connection from t to b is then $v_t - v_b$. The currents leaving t' via connections to other (block-) points of the network must sum to 1, i.e.

$$\sum_{b \in B} (v_{t'} - v_b) n_{bt'} = 1 \qquad (2.1)$$

Similarly, the currents entering t'' must sum to 1, i.e.

$$\sum_{b \in B} (v_{t''} - v_b)\, n_{bt''} = -1 \qquad (2.2)$$

For all other points of the network, the (signed) sum of ingoing currents equals 0, i.e. for $t \neq t', t''$,

$$\sum_{b \in B} (v_t - v_b)\, n_{bt} = 0 \qquad (2.3)$$

and for $b \in B$,

$$\sum_{t \in T} (v_t - v_b)\, n_{bt} = 0 \qquad (2.4)$$

Now, (2.1), (2.2) and (2.3) can be rewritten and summarized on the form

$$r_t v_t - \sum_{b \in B} v_b\, n_{bt} = \begin{cases} 1 \text{ for } t = t' \\ -1 \text{ for } t = t'' \\ 0 \text{ otherwise} \end{cases} \qquad (2.5)$$

and (2.4) can be written similarly as

$$-k_b v_b + \sum_{t \in T} v_t\, n_{bt} = 0 \qquad (2.6)$$

These equations are conveniently put together in the matrix equation

$$\mathbf{C} \begin{bmatrix} (v_t) \\ (-v_b) \end{bmatrix} = \mathbf{1}_{t'} - \mathbf{1}_{t''} \qquad (2.7)$$

where the matrix $\mathbf{C}$ defined earlier occurs as the coefficient matrix. For $\mathbf{C}^-$ defined as above,

$$\begin{bmatrix} (v_t) \\ (-v_b) \end{bmatrix} = \mathbf{C}^- (\mathbf{1}_{t'} - \mathbf{1}_{t''}) \qquad (2.8)$$

is a solution to the network equations (not necessarily with $v_{t''} = 0$ and $v_{t'} = R(t',t'')$, but with $v_{t'} - v_{t''} = R(t',t'')$, and this is all that matters). It follows that

$$R(t',t'') = v_{t'} - v_{t''} = (1_{t'} - 1_{t''})^* \begin{bmatrix} (v_t) \\ (-v_b) \end{bmatrix}$$

$$= (1_{t'} - 1_{t''})^* C^- (1_{t'} - 1_{t''}) \quad .$$

Comparing this with our expression for the contrast variances in the statistical model, we see that (i) has been proved. The proof of (ii) is similar. Our convention that potentials of block points occur with a minus sign in the equations means that the role of $1_{t'} - 1_{t''}$ is taken over by $1_t + 1_b$, but exept for this the proof is exactly the same.

In order to prove (iii), consider the expression

$$\hat{\alpha}_{t'} - \hat{\alpha}_{t''} = (1_{t'} - 1_{t''})^* \begin{bmatrix} \hat{\alpha} \\ \hat{\beta} \end{bmatrix} = (1_{t'} - 1_{t''})^* C^- \begin{bmatrix} X_T^* \\ X_B^* \end{bmatrix} y$$

for the estimated contrast. By (2.8) above, this equals

$$\begin{bmatrix} (v_t) \\ (-v_b) \end{bmatrix}^* \begin{bmatrix} X_T^* \\ X_B^* \end{bmatrix} y$$

$$= \begin{bmatrix} (v_t) \\ (-v_b) \end{bmatrix}^* \left[\sum_i y_i (1_{\varphi_T(i)} + 1_{\varphi_B(i)}) \right] = \sum_i (v_{\varphi_T(i)} - v_{\varphi_B(i)}) y_i \ ,$$

which proves (iii).□

Remark. It should be noticed that the design-network relation relies on a somewhat artificial way of writing the network equations. From a physical point of view, the shift of sign for block point potentials is

an unnecessary complication. The canonical matrix for the network is not $\mathbf{C}$, but the matrix which can be obtained from $\mathbf{C}$ by changing the signs of all diagonal elements. Alternatively, one could obtain the relation by shifting signs of block parameters in the statistical model (as noticed by H. Brøns, see section 7). Unfortunately, this means that there is no way of extending the design-network isomorphism to additive models in designs with three or more factors. It is not even obvious how one should define the design network in that case.

3. *Explicit calculations of contrast variances, based on the design network.*

The present section illustrates, by a number of examples, the main result of the previous section. The purpose is not primarily to compute contrast variances, but rather to gain insight in the way these contrast variances are influenced by the structure of the design. The examples are important for the understanding of later sections.

Example 3.1 (*circular design with blocks of size* 2). Consider the balanced incomplete block design (BIBD) with 3 treatments arranged in 3 blocks of size 2 , i.e.

block 1 : 1 2
block 2 : 1 3
block 3 : 2 3

The design network is given by figure 1 (notice: blocks are drawn as

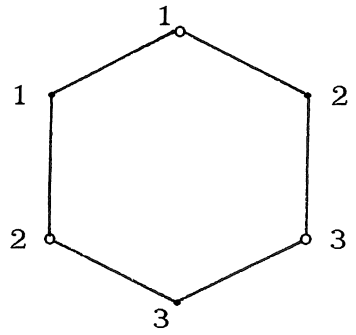

Figure 1

small circles, treatments as points). The resistance between two treatment points, e.g. 1 and 2, is easily computed. We can split this into two parallel resistances, each of which is a serial combination of unit resistances (2 and 4, respectively). By the rules for parallel and serial combination (hereby revived), we have

$$R(1,2) \quad = \quad [\ (1+1)^{-1} + (1+1+1+1)^{-1}\ ]^{-1} \quad = \quad [\ \frac{1}{2} + \frac{1}{4}\ ]^{-1} \quad = \quad 4/3\ .$$

(Notice: here and in the following, numbers like 1 and 2 in the expression $R(1,2)$ refer to treatments. When both block and treatment points are involved, we shall have to use a more careful notation, of course). Thus, $\mathrm{var}(\ \hat{\alpha}_1 - \hat{\alpha}_2\ ) \quad = \quad (4/3)\ \sigma^2$.

This is immediately generalized to designs of the form

block 1 :	1	2
block 2 :	2	3
⋮	⋮	
block T-1:	T-1	T
block T :	T	1

with T treatments arranged in $B = T$ blocks of size 2 in such a way that the design network has a circular form, similar to that of figure 1. In the same manner as above, we obtain the expression

$$R(t,t+d) \quad = \quad (\ \frac{1}{2d} + \frac{1}{2(T-d)}\ )^{-1}$$

for the resistance between two treatment points with angular distance $2\pi(d/T)$ (i.e. separated by d block points).

In order to illustrate (iii) of theorem 2.1, we return to the case $T = 3$. Figure 2 shows the potentials at different points when a

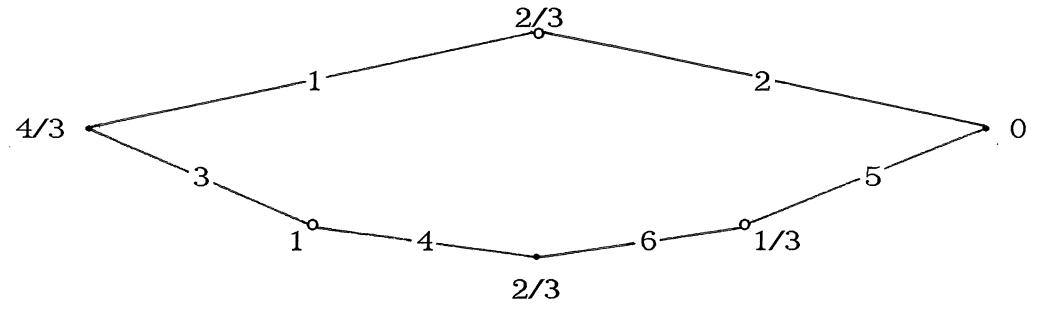

Figure 2

potential difference of $4/3$ is fixed between treatment points 1 and 2 . The numbering of connections indicates the natural ordering according to our listing of the design in the beginning of this example. By (iii) of theorem 2.1, the estimate of $\alpha_1 - \alpha_2$ is

$$\hat{\alpha}_1 - \hat{\alpha}_2 = \left(\frac{4}{3} - \frac{2}{3}\right)y_1 + \left(0 - \frac{2}{3}\right)y_2$$

$$+ \left(\frac{4}{3} - 1\right)y_3 + \left(\frac{2}{3} - 1\right)y_4 + \left(0 - \frac{1}{3}\right)y_5 + \left(\frac{2}{3} - \frac{1}{3}\right)y_6$$

$$= \frac{2}{3}[y_1 - y_2] + \frac{1}{3}[(y_3 - y_4) - (y_5 - y_6)] \ .$$

Notice how the intuitive interpretation of this expression as a weighted average of two estimates (the "direct" estimate by the two observations in block 1 and the "indirect" via the comparisons with treatment 3 in blocks 2 and 3) reflects the decomposition of the resistance into two parallel resistances. Notice also that a solution to the network equations is easy to guess in this case. Obviously, this is not always the case, but it is frequently possible when the network has some symmetry properties.

Example 3.2 *(a more complicated BIBD).* The design

1 : 1 2 4
2 : 2 3 5
3 : 3 4 6
4 : 4 5 7
5 : 5 6 1
6 : 6 7 2
7 : 7 1 3

with 7 treatments arranged in 7 blocks of size 3 is a BIBD (any two treatments meet in exactly one block). Since the design is cyclic (all blocks can be generated from the first block by addition modulo 7) we could draw the design network in a rotation-invariant form (cfr. the

previous example), but the form given by figure 3 is more convenient for

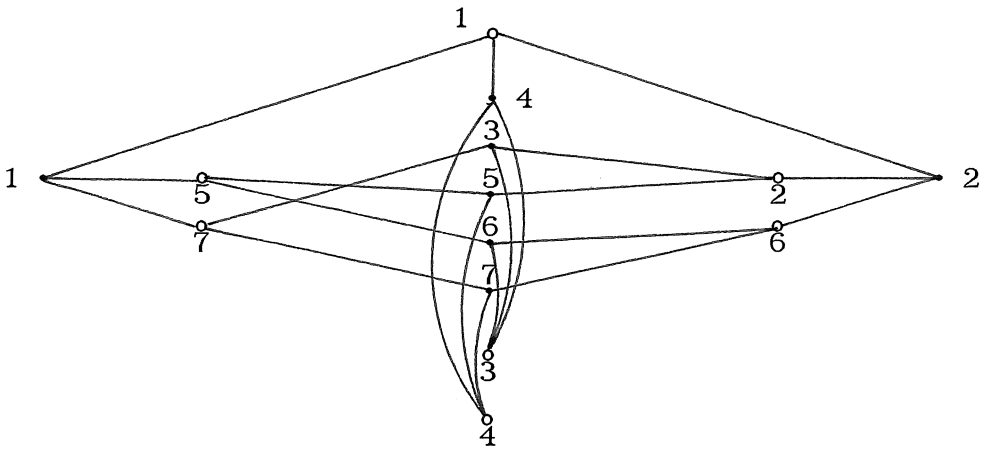

Figure 3

the purpose of determining R(1,2) . When the graph is drawn like this, it is easy to see that a constant voltage difference between treatment points 1 and 2 will induce the same potential at the points in the middle of the figure (correponding to treatments 3, 4, 5, 6 and 7 and blocks 1, 3 and 4). A more detailed argument for this can be given as follows. Suppose that block points 3 and 4 (and their six connections) are removed from the network. Then it is rather obvious that the potentials at treatment points 3,4,5,6,7 and block point 1 will be equal, namely equal to the average of the potentials kept fixed at the treatment points 1 and 2. This follows by symmetry arguments or by writing down a solution to the network equations, which is easy in this case. Now, reintroduce the connections that were removed. This will merely create some new connections between points with the same potential. Thus, none of these new connections will carry any current, and the new points will immediately take over the potential of the points they are connected to. Hence (with v_t^T denoting the potential at treatment point t, v_b^B the potential at block point b, to avoid index confusion),

$$v_1^B = v_3^B = v_4^B = v_3^T = v_4^T = v_5^T = v_6^T = v_7^T .$$

By similar arguments,

$$v_5^B = v_7^B \quad \text{and} \quad v_2^B = v_6^B$$

(indeed, this was so before the removed connections were reintroduced, and is still so because the reintroduction leaves all potentials unchanged).

Now, notice the trivial fact (already referred to once above) that resistances of connections between points with the same potential may be changed arbitrarily, without change of the potentials. In particular, points with the same potential may be "short cicuited" (i.e. connected by a 0-resistance or contracted to a single point), or the connection between them, if any, may be removed. In the present case, we may perform the following operations, without changing the solution to the network equations:

Contract block points 5 and 7 to a single point.

Contract block points 2 and 6 to a single point.

Cut the connection between block 1 and treatment 4.

Contract all points in the middle, except block 1, to a single point.

These operations create a new network (figure 4) which has the same resistance between treatment points 1 and 2 as the original network.

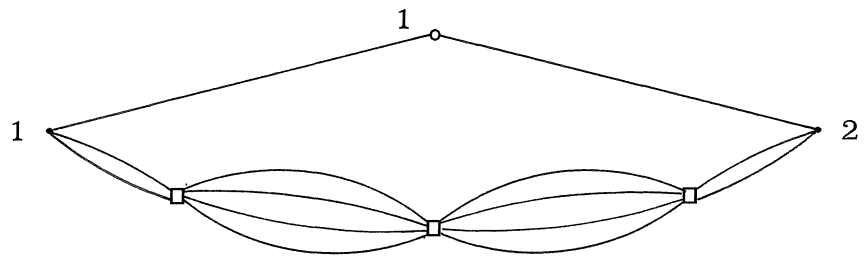

Figure 4

But in this case the resistance is easily computed:

$$R(1,2) \quad = \quad [\ (1+1)^{-1} + (\tfrac{1}{2} + \tfrac{1}{4} + \tfrac{1}{4} + \tfrac{1}{2})^{-1}\ ]^{-1} \quad = \quad 6/7\ .$$

Example 3.3 (*BIBDs in general*). Consider a design with T treatments arranged in B blocks of size k in such a way that the replicate counts r_t are all equal to the same number r (thus, $rT = kB = I$). Assume further that the design is binary (i.e. $n_{bt} \in \{0,1\}$ for all b and t) with at least one $n_{bt} = 0$, and that the numbers

$$\lambda(t',t'') \quad = \quad \#\ \{\ b\ |\ n_{bt'} = n_{bt''} = 1\ \}$$

are all equal to the same number λ (which, by a simple combinatorial argument, must then be $\lambda = r(k-1)/(T-1)$). This is the definition of a balanced incomplete block design (BIBD).

A careful examination of the arguments that were used in the reduction of the network of example 3.2 will show that similar arguments are valid for an arbitrary BIBD. We shall not give the full details, but merely outline the reasoning.

For two treatments t' and t'', imagine that the design network is drawn in a way similar to that of figure 3, with t' to the left and t'' to the right. In the middle we have all other treatment points together with all points corresponding to blocks in which neither t' nor t'' occur (bottom) and those in which both t' and t'' occur (top). Between t' and the points in the middle we place the points corresponding to blocks in which t' but not t'' occur, and similarly for t''. The crucial symmetry property which enables us to argue exactly as in example 3.2 is that any of the treatment points in the middle must have the same number of connections to the left and to the right. This is so because it meets t' and t'' in the same number of blocks. Proceeding as in example 3.2, we see that short circuiting of the following groups of points will leave $R(t',t'')$ unchanged:

I. The blocks containing t' but not t" .

II. The blocks containing t" but not t' .

III. The blocks containing both t' and t" .

IV. All treatments except t' and t" and all blocks containing neither t' nor t" .

Finally, we cut all connections between groups III and IV , and end up with the reduced network given by figure 5. On this figure, the connections are bundles of parallel unit resistances and the integers

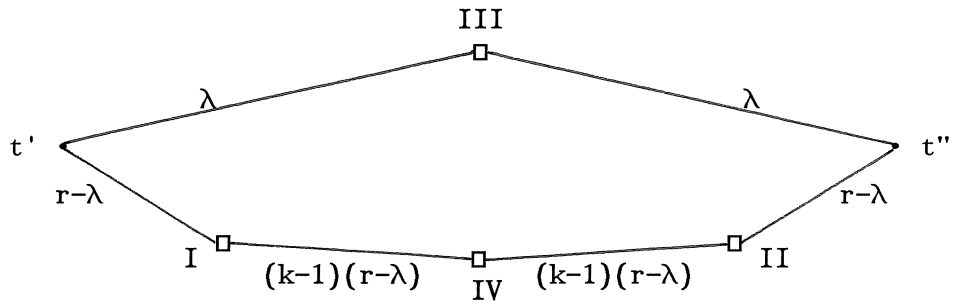

Figure 5

assigned to connections denote multiplicities or inverse resistances. The rules for parallel and serial combination gives a wellknown expression for the contrast variance in a BIBD:

$$R(t',t'') = \left[\left(\frac{2}{\lambda}\right)^{-1} + \left(\frac{2}{r-\lambda} + \frac{2}{(k-1)(r-\lambda)} \right)^{-1} \right]^{-1}$$

$$= \ldots = \frac{2}{r} \cdot \frac{1 - 1/T}{1 - 1/k} \quad .$$

Example 3.4 (*simple lattice*). Consider the design

1 :	1	2	3		
2 :	4	5	6	T = 9 ,	B = 6 ,
3 :	7	8	9	k = 3 ,	r = 2 .
4 :	1	4	7		
5 :	2	5	8		
6 :	3	6	9		

This is a special case (k=3) of the simple lattice of order k , in which $T = k^2$ treatments are arranged in B = 2k blocks of size k in such a way that the first k blocks constitute a replicate (i.e. each treatment appears exactly once) and the arrangement in the last k blocks appears as the transpose of the arrangement in the first k blocks. For reasons of symmetry, contrast variances in this design can only take one of two possible values, one for pairs of treatments which occur in the same block (like 1 and 2) and one for pairs that do not (like 1 and 5). Figures 6 and 7 show the design network drawn in two

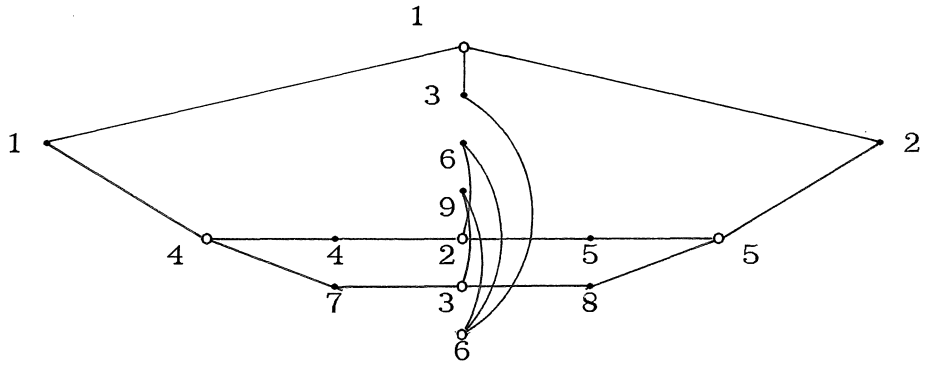

Figure 6

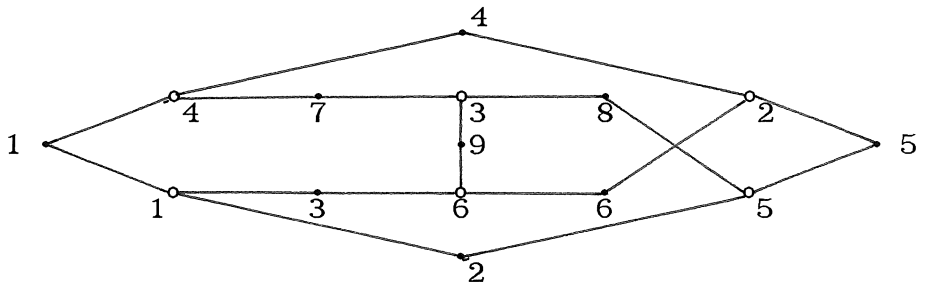

Figure 7

different ways aimed towards the determination of R(1,2) and R(1,5), respectively. Reasoning similar to that of example 3.2 leads to the reduced networks of figures 8 and 9, giving the result

$$R(1,2) = \left[(1+1)^{-1} + (1+ \tfrac{1}{2} + \tfrac{1}{2} + \tfrac{1}{2} + \tfrac{1}{2} +1)^{-1} \right]^{-1} = 4/3 ,$$

$$R(1,5) = \tfrac{1}{2} + \left[(\tfrac{1}{2} + \tfrac{1}{2})^{-1} + (\tfrac{1}{2} + \tfrac{1}{2} + \tfrac{1}{2} + \tfrac{1}{2})^{-1} \right]^{-1} + \tfrac{1}{2} = 5/3 .$$

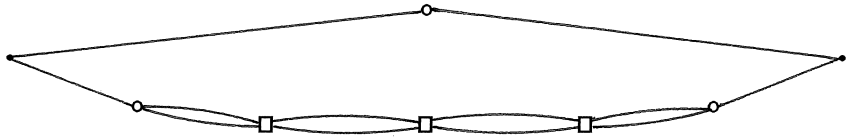

Figure 8

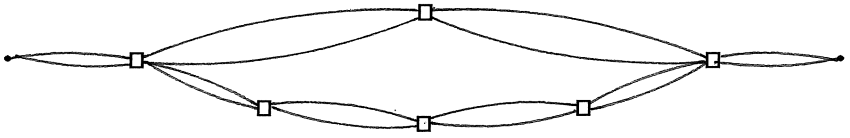

Figure 9

This is easily generalized to the case of a simple lattice of order k, where the result is

$$\operatorname{var}(\hat{\alpha}_{t'} - \hat{\alpha}_{t''}) = \begin{cases} \frac{k+1}{k}\sigma^2 & \text{for } t' \text{ and } t'' \text{ occurring in the same block} \\ \frac{k+2}{k}\sigma^2 & \text{otherwise.} \end{cases}$$

Example 3.5 (*complete block design with a missing observation*). Consider a complete block design with $B = r = 4$ and $T = k = 3$. Figure 10 shows the design network stretched out between treatment points 1 and 2. Obviously, the contrast variance is given by

$$\sigma^2 R(1,2) = \sigma^2 \left(\frac{1}{4} + \frac{1}{4} \right) = \sigma^2/2 .$$

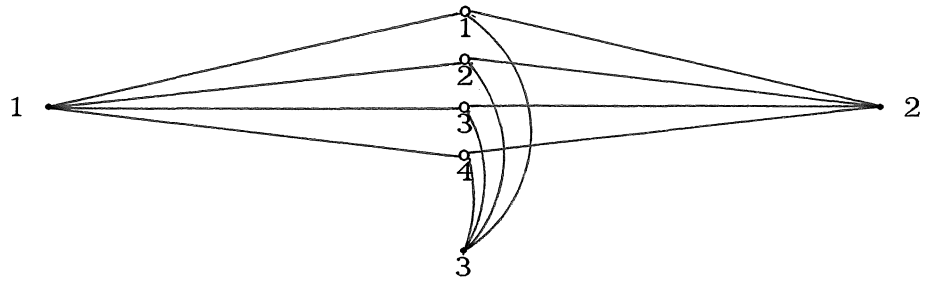

Figure 10

Now, consider what happens if a single connection is removed from the network. The removal of one of the connections to treatment point 3 will leave $R(1,2)$ unchanged. The statistical interpretation of this is that a missing observation in a complete block design does not affect contrast variances in which the treatment of the experimental unit removed is not directly involved. But the removal of, say, the connection from treatment 2 to block 4 will give a picture like figure 11. The resistance

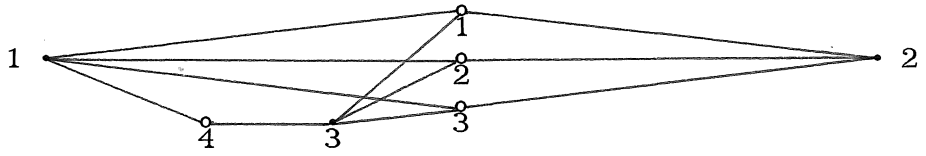

Figure 11

between treatment points 1 and 2 now becomes

$$R(1,2) = \frac{1}{3} + \left[3 + \left(\frac{1}{3} + 1 + 1 \right)^{-1} \right]^{-1} = 5/8 .$$

Figure 12 shows the short circuited network for the general case of an arbitrary complete block design (k = T , r = B , all $n_{bt} = 1$) with a

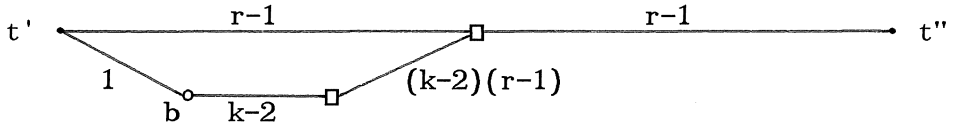

Figure 12

missing observation (t" in block b). The result is

$$R(t',t'') = \frac{1}{r-1} + \left[(r-1) + \left(1 + \frac{1}{k-2} + \frac{1}{(k-2)(r-1)} \right)^{-1} \right]^{-1}$$

$$= \ldots = \frac{(k-1)(2r-1) + 1}{r(r-1)(k-1)} .$$

This is for treatments involved, i.e. for either t' or t" the treatment of the experimental unit that was lost. All other contrast variances are unchanged (= $2\sigma^2/r$). The formula is wellknown (see e.g. Cochran and Cox 1957), but the proof would usually involve a lot of matrix algebra.

4. *Lower bounds for contrast variances.*

In this section we shall derive lower bounds for contrast variances by short circuiting of the design network. The idea can be illustrated by the following argument, which gives a very rough bound. Suppose, for an arbitrary block design, that all blocks are contracted (short circuited) to a single point. This gives a network of the form indicated by figure 13. Obviously, the resistance from t' to t" in this

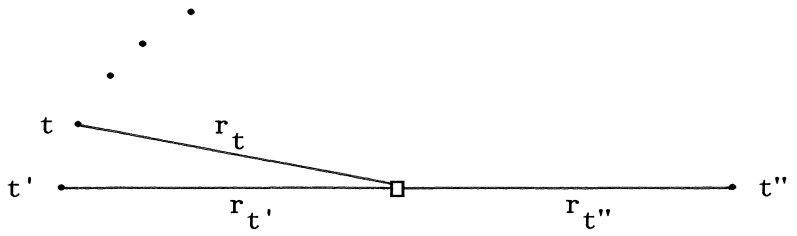

Figure 13

network is $1/r_{t'} + 1/r_{t"}$. Since this network was obtained from the original network by the introduction of some new (0-resistance) connections, this resistance can never be smaller than the original resistance. Hence, we have proved the inequality

$$\mathrm{var}(\hat{\alpha}_{t'} - \hat{\alpha}_{t"}) \quad \geq \quad \left(\frac{1}{r_{t'}} + \frac{1}{r_{t"}} \right) \sigma^2$$

stating that a contrast variance can never be smaller than the contrast variance for the same two treatments in a (hypothetical) design with the same treatments repeated the same number of times in a single block (and with the same σ^2).

In fact, we can say a little more than this. The situations where the above inequality is an equality must obviously be those where a difference in potential between t' and t" induces the same potential at all block points. With a little bit of intuition, it is not difficult to see that this happens if and only if the occurrence counts for t'

and t'' in blocks are proportional, i.e. $n_{bt'} = cn_{bt''}$ for some constant c independent of b. Thus, equality for *all* pairs of treatments occurs if and only if the design is *orthogonal* in the sense that all columns of $\mathbf{N}$ are proportional, cfr. Tjur (1984).

The above result is classical. More refined inequalities come out by less drastic short circuiting of the design network. We shall prove two such inequalities, one that gives a bound similar to the expression for the contrast variance in a BIBD, and a more complicated inequality based on a short circuiting procedure similar to that followed in example 3.4.

Proposition 4.1. *Suppose that the design is binary, that all block sizes are equal* ($k_b = k$) *and that all replicate counts are equal* ($r_t = r$). *Then*

$$R(t',t'') \geq \frac{2}{r}\left[1 - \frac{r-\lambda(t',t'')}{kr}\right]^{-1}$$

where $\lambda(t',t'')$ *denotes the number of blocks in which both* t' *and* t'' *occur.*

Proof. Short circuiting exactly as in example 3.3, we obtain a reduced network like that of figure 5, the only difference being that $\lambda = \lambda(t',t'')$ now depends on t' and t'' (but the removal of all connections between groups III and IV is still possible, for reasons of symmetry). The first expression for the resistance through the short circuited network of example 3.3 is still valid when λ is replaced by $\lambda(t',t'')$, but in this case it should be regarded as a lower bound for $R(t',t'')$. The algebraic manipulations required to transform this expression to that stated by the proposition are straightforward. The last expression for $R(t',t'')$, given in example 3.3, is not valid here, because it depends on the formula for λ in a BIBD.□

Proposition 4.2. *In addition to the assumptions of proposition 4.1, assume that the numbers* $\lambda(t',t'')$ *are all* ≤ 1 . *Define*

$$\Lambda(t',t'') \quad = \quad \#\{\, t \neq t',t'' \mid \lambda(t,t') = \lambda(t,t'') = 1 \,\}$$

(= the number of other treatments that meet both t' *and* t'' *). Then*

$$R(t',t'') \quad \geq \quad \left[\frac{\lambda}{2} + \left[\frac{2r}{r(k-1)(r-\lambda-1) + \Lambda + \lambda} + \frac{2}{r-\lambda} \right]^{-1} \right]^{-1}$$

where Λ *and* λ *are short for* $\Lambda(t',t'')$ *and* $\lambda(t',t'')$.

Proof. The following sets of points are contracted to single points by short circuiting:

I The blocks containing t' and t'' .

II_1 The blocks containing t' but not t'' .

II_2 The blocks containing t'' but not t' .

III The blocks containing neither t' nor t'' .

IV_1 The treatments occurring in a block together with t' , but not with t'' .

IV_2 The treatments occurring in a block together with t'' , but not with t' .

V The treatments occurring in blocks with both t' and t'' .

VI The treatments that never occur in a block with t' or t'' .

Figure 14 shows the reduced network (still with the brief notation λ =

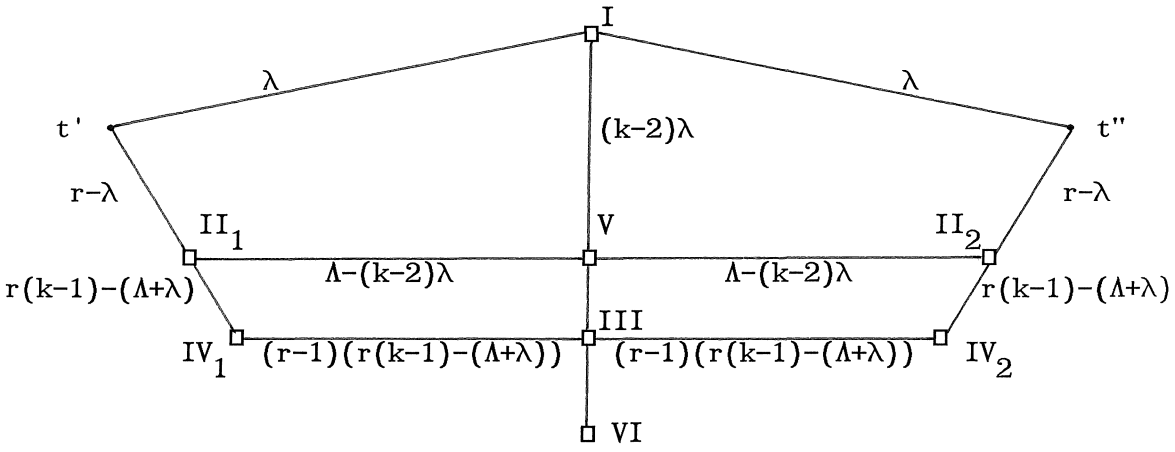

Figure 14

$\lambda(t',t'')$ and $\Lambda = \Lambda(t',t'')$). For reasons of symmetry, the vertical connections can be removed, and it follows that we have the lower bound

$$\left[\frac{\lambda}{2} + \left[\frac{2}{r-\lambda} + \left[\left(\left(2+\frac{2}{r-1}\right) \frac{1}{r(k-1)-(\Lambda+\lambda)} \right)^{-1} + \left(\frac{2}{\Lambda-(k-2)\lambda}\right)^{-1} \right]^{-1} \right]^{-1} \right]^{-1}$$

for $R(t',t'')$. The proposition follows, after some straightforward algebraic manipulations.□

5. *Upper bounds for efficiencies.*

The *efficiency* (or *harmonic mean efficiency*) E of a block design with equal block sizes and equal replicate counts can be defined as the harmonic mean of the $T-1$ nonzero eigenvalues of the matrix $\frac{1}{r} C_T$, where

$$C_T = r\, I_{T\times T} - \frac{1}{k} N^* N$$

is the information matrix for the set of treatment parameters (see e.g. Paterson 1983). However, we shall refer to the following (equivalent) definition, which can be regarded as an intuitive justification of the efficiency as a measure of design quality. Define

$$\overline{R} = \frac{2}{T(T-1)} \sum_{t'< t''} R(t',t'')$$

(= the average resistance between pairs of treatment points in the design network). Then,

$$E = \frac{2/r}{\overline{R}} .$$

Notice that $\overline{R}\,\sigma^2$ is the average contrast variance for the given design, while $(2/r)\,\sigma^2$ is the same quantity for a complete block design with each treatment repeated r times. Thus, it follows from the discussion in the beginning of section 4 that $E \leq 1$ (and, in fact, that $E = 1$ if and only if the design is orthogonal). According to example 3.3, the efficiency of a BIBD is

$$E = \frac{1 - 1/k}{1 - 1/T} = \frac{T(k-1)}{(T-1)k} .$$

Our definition of the efficiency E implies that any lower bound for the contrast variance $\sigma^2 \overline{R}$ gives an upper bound for the average contrast variance, and vice versa. In section 4, lower bounds for contrast variances were given as resistances through short circuited networks in which the inverse resistances (= multiplicities) of connections are linear expressions in combinatorial quantities like $\lambda(t',t'')$ and $\Lambda(t',t'')$. It is easy to derive expressions for sums or averages of such combinatorial quantities over all pairs of distinct treatments. Thus, in order to "average" the lower bounds for contrast variances to obtain lower bounds for average contrast variances (or upper bounds for efficiencies), we need the convexity property stated by the following lemma.

Lemma 5.1. *Consider a connected graph with* P *as its set of points and* I *as its set of connections. We think of the graph as an electrical network with variable resistances. By* z_i *we denote the inverse resistance of connection* i *. For two selected, distinct points* p' *and* p'' *, let* $R(z) = R((z_i))$ *denote the resistance through the network from* p' *to* p'' *. Then, the function* R *on* $[0,+\infty)^I$ *is convex.*

Remark. Notice that one or more zeroes among the z_i may give the value $+\infty$ of $R(z)$, due to disconnectedness. However, it will follow from the proof that R is also convex in the (obvious) extended sense. We shall use the term *conductance* for inverse resistance.

Proof. We give a heuristic proof, based on the kind of physical reasoning applied in section 4. In the two applications, which we shall make of the lemma, more direct proofs of the convexity can easily be given.

We begin by noticing that it suffices to show that $1/R(z)$ is a concave function of z . Indeed, if for all $\lambda \in (0,1)$ and for any z', $z'' \in [0,+\infty)^I$ we can show that

$$R(\lambda z' + (1-\lambda)z'')^{-1} \geq \lambda R(z)^{-1} + (1-\lambda) R(z'')^{-1}$$

then it follows easily (by monotonicity and convexity of the function $R \to 1/R$) that R is convex. Now, consider two copies of the network, equipped with conductances $z' = (z'_i)$ and $z'' = (z''_i)$, respectively. Multiply all conductances of the first network by λ and multiply all conductances of the second by $(1-\lambda)$. After this, we obviously have conductances $\lambda R(z')^{-1}$ and $(1-\lambda)R(z'')^{-1}$, respectively, between the points p' and p'' in the two networks. Now, consider the following two ways of short circuiting the two networks to a single network:

(1) (cfr. figure 15) The points called p' in the two networks are short circuited; similarly for p''.

(2) (cfr. figure 16) *All* pairs of corresponding points of the two networks are short circuited.

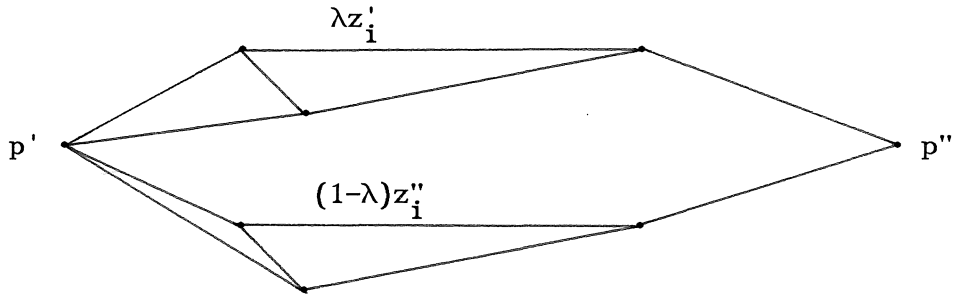

Figure 15

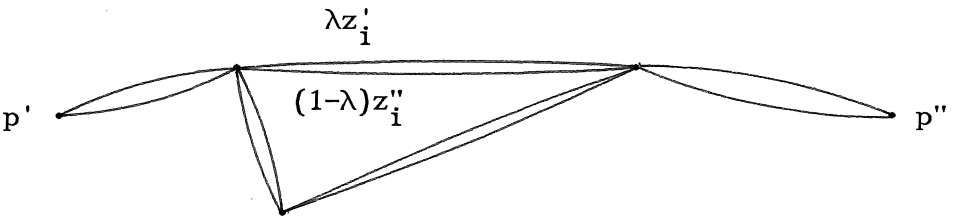

Figure 16

By the rule for parallel combination of resistances, the conductance from

p' to p" in the network given by (1) is

$$\lambda\, R(z')^{-1} + (1-\lambda)\, R(z")^{-1} \quad .$$

By the same rule, applied to each double connection of the network given by (2), the conductance from p' to p" in that network is

$$R(\, \lambda z' + (1-\lambda)z"\,)^{-1} \quad .$$

However, since (2) is obtained from (1) by further short circuiting, the conductance through (2) must be greater than or equal to the conductance through (1). The lemma follows immediately.□

Example. Consider the inequality

$$R(t',t") \;\geq\; \frac{1}{r_{t'}} + \frac{1}{r_{t"}}$$

derived in the beginning of section 4 from the network of figure 13. In this simple case, we conclude from lemma 5.1 that $1/r_{t'} + 1/r_{t"}$ is a convex function of $\mathbf{r} = (r_t)$. By Jensen's inequality,

$$\bar{R} = \frac{2}{T(T-1)} \sum_{t'< t"} R(t',t") \;\geq\; \frac{2}{T(T-1)} \sum_{t'< t"} \left(\frac{1}{r_{t'}} + \frac{1}{r_{t"}} \right) \;\geq\; 2/\bar{r}$$

where $\bar{r}$ is the average (in principle over all pairs of distinct treatments, but equivalently over all treatments) of the replicate counts r_t. Since this is

$$\bar{r} = \frac{1}{T} \Sigma_t\, r_t = I/T \quad ,$$

we have proved that $\bar{R} \geq 2T/I$, i.e. the average contrast variance is at least $(2T/I)\sigma^2$. This is not particularly exciting, but the example illustrates very well what is going on in the following under more

complicated circumstances.

Proposition 5.2. *Under the assumptions of proposition 4.1,*

$$E \leq \frac{1 - 1/k}{1 - 1/T} .$$

Remark. Under the usual definition of E given at the beginning of this section, this is merely the inequality stating that the harmonic mean of the $T-1$ eigenvalues of $\frac{1}{r} C_T$ is less than or equal to the arithmetic mean of these. Hence, the result is wellknown, but we include it because our proof does not refer to the spectral decomposition of C_T .

Proof. The inequality of proposition 4.1 was derived from a short circuited design network (figure 5) in which the conductances are affine functions of $\lambda = \lambda(t',t'')$. It follows, by lemma 5.1, that the inequality still holds when $R(t',t'')$ on the left hand side is replaced by $\bar{R}$ and $\lambda(t',t'')$ on the right hand side is replaced by $\bar{\lambda}$ = the average of $\lambda(t',t'')$ over all pairs of distinct treatments. Now, since the design is assumed to be binary, we have $n_{bt}^2 = n_{bt}$. Hence,

$$\bar{\lambda} = \frac{2}{T(T-1)} \sum_{t'<t''} \lambda(t',t'') = \frac{2}{T(T-1)} \sum_{t'<t''} \Sigma_b \, n_{bt'} n_{bt''}$$

$$= \frac{2}{T(T-1)} \frac{1}{2} \left[\sum_{t',t'',b} n_{bt'} n_{bt''} - \sum_{t,b} n_{bt}^2 \right]$$

$$= \frac{1}{T(T-1)} \left[\Sigma_b \left(\Sigma_t \, n_{bt} \right)^2 - \sum_{b,t} n_{bt} \right]$$

$$= \frac{1}{T(T-1)} \left(B k^2 - I \right) = \frac{Bk(k-1)}{T(T-1)} .$$

The substitution of this expression in the "averaged" inequality

$$\bar{R} \geq \frac{2}{r} \left(1 - \frac{r - \bar{\lambda}}{kr} \right)^{-1}$$

followed by a little algebra, gives the desired result.□

Proposition 5.3. *Under the assumptions of proposition 4.2,*

$$E \leq \frac{k-1}{T-1} + \left[\frac{r}{(k-1)(r-1)} + \frac{T-1}{T-k} \right]^{-1} .$$

Proof. By arguments similar to those applied in the proof of proposition 5.2, a lower bound for $\overline{R}$ can be obtained from proposition 4.2 by replacement of $\lambda(t',t'')$ and $\Lambda(t',t'')$ by the averages of these quantities over pairs of distinct treatments. An expression for $\overline{\lambda}$ was obtained in the proof of the previous proposition. In order to compute $\overline{\Lambda}$, notice that our assumptions imply that $\lambda(t',t'')^2 = \lambda(t',t'')$. Thus,

$$\sum_{t'<t''} \Lambda(t',t'') = \sum_{t'<t''} \sum_{t:t\neq t',t''} \lambda(t,t')\,\lambda(t,t'')$$

$$= \frac{1}{2} \sum_{t'\neq t''} \sum_{t:t\neq t',t''} \lambda(t,t')\,\lambda(t,t'')$$

$$= \frac{1}{2} \Sigma_t \sum_{t':t'\neq t} \lambda(t,t') \sum_{t'':t''\neq t,t'} \lambda(t,t'')$$

$$= \frac{1}{2} \Sigma_t \sum_{t':t'\neq t} \lambda(t,t') \left[(k-1)r - \lambda(t,t')\right]$$

$$= \frac{1}{2} \Sigma_t \left[(k-1)r \sum_{t':t'\neq t} \lambda(t,t') - \sum_{t':t'\neq t} \lambda(t,t')^2 \right]$$

$$= \frac{1}{2} \Sigma_t \left[((k-1)r)^2 - (k-1)r \right] = \frac{1}{2} T \left[(k-1)r - 1\right](k-1)r .$$

Thus, $\overline{\Lambda}$ equals this expression divided by $T(T-1)/2$, which is

$$\overline{\Lambda} = \frac{r(k-1)(r(k-1)-1)}{T-1} = (r(k-1)-1)\,\overline{\lambda} .$$

The inequality following from proposition 4.2 by "averaging" is

$$\overline{R} \geq \left[\frac{\overline{\lambda}}{2} + \left[\frac{2r}{r(k-1)(r-\overline{\lambda}-1) + \overline{\Lambda} + \overline{\lambda}} + \frac{2}{r - \overline{\lambda}} \right]^{-1} \right]^{-1}$$

or

$$E \leq \frac{2}{r} \left[\frac{\overline{\lambda}}{2} + \left[\frac{2r}{r(k-1)(r-\overline{\lambda}-1) + \overline{\Lambda} + \overline{\lambda}} + \frac{2}{r - \overline{\lambda}} \right]^{-1} \right]$$

Noting that the relation $\overline{\Lambda} = (r(k-1)-1)\overline{\lambda}$ gives a considerable simplification of the complicated denominator involved here, this inequality is easily rewritten to that stated by the proposition.□

Example 5.1. Paterson and Wild (1986) study an α-lattice with 40 treatments arranged in 32 blocks of size 5. The efficiency of this design is 0.79048. They derive upper bounds for the efficiency under various conditions. The sharpest among those proved under the general assumptions of proposition 5.3 is $E \leq 0.79740$. Proposition 5.3 gives $E \leq 0.79335$, which is less than half as far from the true efficiency as the bound reported by Paterson and Wild.

Example 5.2. Jarrett (1977) gives an upper bound for the efficiency which, in the case $B = 15$, $T = 20$, $k = 4$ and $r = 3$, is $E \leq 0.7549$ (without additional assumptions, like resolvability etc.). Our bound in this case is $E \leq 0.7505$. Jarrett gives an example (an α-lattice) with $E = 0.7447$.

It is tempting to conjecture, on the background of these examples, that our result is better than those obtained by Jarrett (1977) and Paterson and Wild (1986) by methods based on the spectral decomposition of C_T. However, the bounds given in these papers are very complicated expressions, and we have not been able to make a direct comparison. It should be noticed that our bound applies only to the case where all

$\lambda(t',t'')$ are either 0 or 1. There seems to be no immediate generalization to regular graph designs in general (i.e. designs in which any value of $\lambda(t',t'')$ is either λ_0 or λ_0+1, for some λ_0).

6. *Optimization of designs.*

The design-network isomorphism suggests various algorithms for construction of optimal or nearly optimal designs. We shall describe one such algorithm which, on the basis of several test runs, is found to be relatively successful. A more detailed description of some of these test runs is found later in this section. A listing of the program (written in UNIVAC OS1100 Pascal) is available from the author. The possibility of a Turbo Pascal version for personal computers is considered, but some problems with RAM capacity can be expected.

For given design constants I, B, T, r and k (with $I = Bk = Tr$) our problem is to find a design of these dimensions with efficiency as close as possible to 1; or, equivalently, to construct a network with $\overline{R}$ as small as possible. We proceed as follows.

Phase 1. Our starting point is a totally disconnected graph consisting of $B + T$ points. We introduce the I connections one by one, according to the following principles. As long as the network is disconnected, each new connection should join two connected components of the graph, thus decreasing the number of such components by one. Connections between points with few connections to other points are preferred. For example, as long as isolated points of both block and treatment type exist, any new connection should connect such two. Each new connection should, of course, be allowed in the sense that the two points have "vacant entries". Among the connections satisfying these conditions, the one to be added may be chosen at random.

Connectedness is obtained in step no. $B + T - 1$, where the number of connected components is decreased from 2 to 1. From then on, it makes sense to talk about $\overline{R}$ (since all $R(t',t'')$ are welldefined now), and we can choose the "best" connection to be added as the one among those allowed that decreases $\overline{R}$ as much as possible. A simple and computationally cheap formula for the decrease of $\overline{R}$ when a given

connection is added is given in proposition 6.3.

Phase 2. The design coming out of phase 1 is usually a good one, but it is rarely optimal. In order to improve the design, we proceed as follows. By a *switch* we mean an operation of the form

$$\begin{aligned} n_{b_1t_1} &:= n_{b_1t_1} - 1 \\ n_{b_2t_2} &:= n_{b_2t_2} - 1 \\ n_{b_1t_2} &:= n_{b_1t_2} + 1 \\ n_{b_2t_1} &:= n_{b_2t_1} + 1 \end{aligned}$$

which removes two connections and adds two other connections in such a way that the design constants (block sizes and replicate counts) are unchanged. Among all possible switches we select, in each step, one according to the following criteria. Switches that would make the design disconnected are not taken into account. Also, switches that would make the design "less orthogonal" than it was before are ignored; by this we mean that only switches satisfying

$$n_{b_1t_1}/k_{b_1} > n_{b_2t_1}/k_{b_2} \quad \text{and} \quad n_{b_2t_2}/k_{b_2} > n_{b_1t_2}/k_{b_1}$$

are taken into account (remark: under the assumption that all block sizes are equal to k, this condition can be written on a simpler form; however, our algorithm is applicable to the more general situation where block sizes and/or replicate counts are different, therefore this general form). Among the switches allowed, we choose the one that gives the maximal decrease of $\overline{R}$. The algorithm is stopped when no switch decreases $\overline{R}$.

It is easy to show that any design can be transformed by a sequence of switches to any other design with the same design constants. We may regard the mininum number of switches required for the transformation of one design into another as a kind of distance between the two designs.

Under this distance measure, the design found by phase 2 is "locally optimal", in the sense that any of its "neighbours" (i.e. any design that can be reached in a single switch) has a lower efficiency. This does not guarantee that the design is (globally) optimal. The choice of a reasonable starting point (the result of phase 1) may be crucial for this. For small design constants, the algorithm consisting of phase 1 and phase 2 turns out to work well. For large designs, phase 2 is more frequently "trapped" by locally optimal designs. This problem can, to some extend, be solved by the addition of a third phase:

Phase 3. A procedure for randomized search, which may be regarded as a primitive version of simulated annealing (see e.g. Geman and Geman 1984) is as follows. Proceed as in phase 2, with the result of phase 2 as the starting point, but add during the search for the optimal switch a small random pertubation to each change of $\bar{R}$ computed. Thus, as the next switch to be performed, we select the one (among those allowed) with the smallest value of, say,

$$\bar{R}(b_1,t_1,b_2,t_2)\ (\ 1 + A\ z_{b_1t_1b_2t_2}\ )\ ,$$

where $\bar{R}(b_1,t_1,b_2,t_2)$ is the value of $\bar{R}$ after the switch determined by (b_1,t_1,b_2,t_2), $z_{b_1t_1b_2t_2}$ is a pseudo-random number on [0,1], and A is a suitable scaling factor. For small values of A, this gives a procedure which tends to decrease $\bar{R}$ "on average", while still (if A is not *too* small) able to escape local minima for $\bar{R}$. Phase 3 is terminated when no significant improvement has been observed for some time. Then, A is set to zero again, and phase 2 is repeated. Of course, A may also be changed during the algorithm. In our test runs, we have used an interactive program which allows the user to choose A (and the number of steps to follow with switches chosen by that A) on the basis of the list of previous efficiencies. A successful strategy seems to be to "shake" the system occasionally by relatively long sequences of switches chosen with a large value (say, 0.01 or 0.001) of

A , alternating with (shorter) local optimization sequences with $A = 0$. Another strategy, more in the spirit of simulated annealing, would be to decrease A slowly.

The purpose of the algorithm described here is to provide a unified method for construction of good (optimal or almost optimal) designs for experimental situations where no classical solution (BIBD, PBIBD etc.) is available. The algorithm has been presented here only for the case where block sizes and replicate counts are equal, but it can easily be adapted (our present version is in fact adapted) to the case of different block sizes and/or different replicate counts. It is also easy to modify the algorithm to search for minimum values of other linear combinations of the contrast variances than $\overline{R}$, e.g. the average of contrast variances between test treatments and a single baseline treatment. However, since little can be said about optimality in complicated situations, the only way of testing the algorithm is to apply it to situations where the optimal design is known, by proof or by qualified conjecture. The following reports on test runs show some strong and weak points.

Example 6.1 *(a sample of BIBDs).* For given T and $k < T$, let B be the smallest integer such that both $r = kB/T$ and $\lambda = k(k-1)B/(T(T-1))$ are integer. The algorithm was applied to the 51 sets of design constants (B,T,k,r) of this form satisfying $3 \leq T \leq 12$ and $B \leq 56$. In all cases, a BIBD is known to exist, and it is known (Kiefer 1958) that BIBDs are optimal when they exist (in fact, this follows also from proposition 5.2). A BIBD was found as the result of phase 2 in 40 out of the 51 cases. The number of switches required by step 2 was less than 12 in these cases. In 10 of the 11 remaining cases, a BIBD was found in phase 3 in less than 40 switches. Only in one case, $(B,T,k,r) = (33,12,8,22)$ the search was given up after 60 randomized switches; surprisingly, perhaps, the complementary BIBD to this was found in phase 2 after 8 switches.

This test run was later extended to cover the 57 cases with $13 \leq T \leq 22$ (still assuming $B \leq 56$). Randomized search was not tried in these

cases, and the finding of a BIBD by phase 2 was a rare event, which occurred only in the 10 cases with $T = B = k+1 = r+1$. It is remarkable, however, that the efficiencies of the locally optimal designs found by phase 2 came very close to those of the corresponding BIBDs. Only in three cases did that difference exceed 0.01, and it never exceeded 0.02. The maximal number of switches required by phase 2 to obtain local optimality was 28.

Example 6.2 (*a sample mainly consisting of regular graph designs*). John and Mitchell (1977) list 145 triples (T,k,r) for which the optimal design has been found by systematic search among all possible designs. In all but 9 cases, a design with the same efficiency as the optimal design (reported with 3 significant digits by John and Mitchell) was found by phase 2. In the remaining 9 cases, designs with at least that efficieny minus 0.001 was found. The number of switches performed was less than 8 in all cases.

Example 6.3 (*simple lattices for* k = 3, 4, 5 and 6). The algorithm was applied to design constants of the form $B = 2k$, $T = k^2$, $r = 2$, for k = 3, 4, 5 and 6. A simple lattice (cfr. example 3.4) was found by phase 2 after 1, 3, 2 and 5 switches, respectively.

Example 6.4 (*two α-lattices*). The algorithm was applied to the two situations of example 5.1 and 5.2, where very efficient (optimal?) α-lattices are known to exist. For example 5.1 (B=32, T=40, k=5, r=4) a design of efficiency 0.79020 -i.e. only 0.00028 less than the efficiency of the α-lattice- was found in phase 2 after 16 switches. For example 5.2 (B=15, T=20, k=4, r=3), a locally optimal design with efficiency 0.7441 was found after 5 switches. This is 0.0006 less than the efficiency of the α-lattice.

The conclusion of these and several other less systematic test runs is that the algorithm consisting of phase 1 and 2 is excellent for finding designs which are almost as efficient as those believed to be optimal. Quite frequently, the (conjectured or proved) optimal design is actually

found. The addition of phase 3 improves considerably the ability to find these designs, but for large design constants the increasing number of switches required (and the increasing size of the search taking place in each step) makes the algorithm expensive.

Our experiences confirm the conjecture put forward by John and Mitchell (and several other authors) that the optimal design is a regular graph design whenever such a design exists. Indeed, the switches chosen in phase 2 tend to shrink the distribution of the values of $\lambda(t',t'')$ whenever possible. Only 10 of the 145 designs found in the test run described by example 6.2 were not regular graph designs (and some of these were of dimensions for which a regular graph design does not exist). Also conjectures about the optimality of α-lattices were confirmed. We tried to take the two α-lattices referred to in example 6.4 as starting points for phase 2 and 3. Both were found to be locally optimal, and even careful "shaking" by phase 3 tended to create designs, which were transformed back to the initial α-lattice when phase 2 was repeated.

Computations. The performance of our algorithm relies heavily on the following propositions which result in simple and computationally cheap expressions (proposition 6.3) for the change of $\bar{R}$ resulting from the addition of a connection or a switch.

Proposition 6.1. *For a given design (or design network), consider the operation which adds a connection of unit resistance between block point* b_0 *and treatment point* t_0 *. The change of the resistance between* t' *and* t'' *resulting from this operation is given by*

$$R_{new}(t',t'') = R(t',t'') - \frac{[\,(1_{t'} - 1_{t''})\, C^{-}\, (1_{b_0} + 1_{t_0})\,]^2}{1 + R(b_0,t_0)} \quad .$$

(with notation as in section 2).

Proof. Consider what happens to the fundamental matrix C when a connection from b_0 to t_0 is added. Obviously,

$$C_{new} = C + (1_{b_0} + 1_{t_0})(1_{b_0} + 1_{t_0})^* .$$

Hence, the network equations determining the potentials of the new network when current 1 from t' to t" is induced can be written (cfr. the proof of theorem 2.1)

$$(C + (1_{b_0} + 1_{t_0})(1_{b_0} + 1_{t_0})^*) \begin{bmatrix} v_t \\ -v_b \end{bmatrix} = 1_{t'} - 1_{t''}$$

or

$$C \begin{bmatrix} v_t \\ -v_b \end{bmatrix} = -(v_{t_0} - v_{b_0})(1_{b_0} + 1_{t_0}) + (1_{t'} - 1_{t''}) .$$

Assuming that $C^-C \begin{bmatrix} v_t \\ -v_b \end{bmatrix} = \begin{bmatrix} v_t \\ -v_b \end{bmatrix}$ (which is merely to assume that the solution to the new network equations satisfies the same uniqueness constraint as assumed for the old one by our choice of C^-, e.g. $\Sigma v_t + \Sigma v_b = 0$ or $v_{t''} = 0$), multiplication by C^- from the left of this equation gives

$$\begin{bmatrix} v_t \\ -v_b \end{bmatrix} = -(v_{t_0} - v_{b_0}) C^- (1_{b_0} + 1_{t_0}) + C^- (1_{t'} - 1_{t''}) \quad (6.1)$$

Further multiplication by $(1_{b_0} + 1_{t_0})^*$ from the left yields the equation

$$v_{t_0} - v_{b_0} = -(v_{t_0} - v_{b_0}) R(b_0, t_0) + (1_{b_0} + 1_{t_0})^* C^- (1_{t'} - 1_{t''})$$

which can be solved for $v_{t_0} - v_{b_0}$, giving

$$v_{t_0} - v_{b_0} = \frac{(1_{b_0} + 1_{t_0})^* C^- (1_{t'} - 1_{t''})}{1 + R(b_0, t_0)} .$$

Substitution of this in (6.1), followed by multiplication from the left with $(1_{t'} - 1_{t''})$, gives

$$v_{t'} - v_{t''} =$$

$$-(v_{t_0} - v_{b_0}) [(1_{t'} - 1_{t''})^* C^- (1_{b_0} + 1_{t_0})] + (1_{t'} - 1_{t''})^* C^- (1_{t'} - 1_{t''})$$

$$= - \frac{[(1_{t'} - 1_{t''})^* C^- (1_{b_0} + 1_{t_0})]^2}{1 + R(b_0, t_0)} + R(t', t'') .$$

which concludes the proof.□

Remark. A similar formula for *removal* of an existing connection between b_0 and t_0 is

$$R_{new}(t', t'') = R(t', t'') + \frac{[(1_{t'} - 1_{t''})^* C^- (1_{b_0} + 1_{t_0})]^2}{1 - R(b_0, t_0)} .$$

Notice that the denominator here must be positive if the operation is allowed. Of course, $R(b_0, t_0)$ is always ≤ 1 when a connection between b_0 and t_0 is present. If $R(b_0, t_0)$ is equal to 1, this connection represents the only path from b_0 to t_0 in the network, and only in that case does the removal create a disconnected design.

Proposition 6.2. *Consider the switch operation on the design network which removes the two connections* $b_1 t_1$ *and* $b_2 t_2$ *and adds the two "crossing" connections* $b_1 t_2$ *and* $b_2 t_1$. *The effect of this on the resistance between two arbitrary treatment points* t' *and* t'' *is given by*

$$R_{new}(t',t'') = R(t',t'') +$$

$$\frac{(\delta_t^* C^- \delta_t)(\Lambda^* C^- \delta_b)^2 + (\delta_b^* C^- \delta_b)(\Lambda^* C^- \delta_t)^2 + 2(1-\delta_b^* C^- \delta_t)(\Lambda^* C^- \delta_t)(\Lambda^* C^- \delta_b)}{(1 - \delta_b^* C^- \delta_t)^2 - (\delta_t^* C^- \delta_t)(\delta_b^* C^- \delta_b)}$$

where

$$\begin{aligned} \delta_t &= 1_{t_1} - 1_{t_2} \quad , \\ \delta_b &= 1_{b_1} - 1_{b_2} \quad \text{and} \\ \Lambda &= 1_{t'} - 1_{t''} \quad . \end{aligned}$$

Proof. The proof is similar to that of the previous proposition, except that the updating of C required by a switch amounts to the addition of a matrix of rank 2; therefore, the equation for $v_{t_0} - v_{b_0}$, which was solved in the proof of proposition 6.1, is replaced by two equations in the two variables $v_{t_1} - v_{t_2}$ and $v_{b_1} - v_{b_2}$. We start by noticing that the change of C due to the switch operation can be written

$$C_{new} = C - (1_{b_1} - 1_{b_2})(1_{t_1} - 1_{t_2})^* - (1_{t_1} - 1_{t_2})(1_{b_1} - 1_{b_2})^*$$

$$= C - \delta_b \delta_t^* - \delta_t \delta_b^* \quad .$$

Thus, the network equations for current 1 from t' to t" (after the switch) can be written

$$(C - \delta_b \delta_t^* - \delta_t \delta_b^*) \begin{bmatrix} (v_t) \\ (-v_b) \end{bmatrix} = 1_{t'} - 1_{t''}$$

or

$$C \begin{bmatrix} (v_t) \\ (-v_b) \end{bmatrix} = (v_{t_1} - v_{t_2})\, \delta_b - (v_{b_1} - v_{b_2})\, \delta_t + \Lambda \quad .$$

Imposing the same uniqueness constraint on the potentials v_t and v_b as before the switch (i.e. assuming that $\begin{bmatrix} (v_t) \\ (-v_b) \end{bmatrix}$ is a linear

combination of the columns of C^-) multiplication from the left yields

$$\begin{bmatrix} (v_t) \\ (-v_b) \end{bmatrix} = (v_{t_1} - v_{t_2})\, C^- \delta_b - (v_{b_1} - v_{b_2})\, C^- \delta_t + C^- \Lambda \qquad (6.2)$$

Further multiplication from the left by δ_t^* and δ_b^* gives the two equations

$$(v_{t_1} - v_{t_2}) = (\delta_t^* C^- \delta_b)(v_{t_1} - v_{t_2}) - (\delta_t^* C^- \delta_t)(v_{b_1} - v_{b_2}) + \delta_t^* C^- \Lambda$$

$$-(v_{b_1} - v_{b_2}) = (\delta_b^* C^- \delta_b)(v_{t_1} - v_{t_2}) - (\delta_b^* C^- \delta_t)(v_{b_1} - v_{b_2}) + \delta_b^* C^- \Lambda$$

which can be regarded as two linear equations in the two variables $(v_{t_1} - v_{t_2})$ and $-(v_{b_1} - v_{b_2})$. The determinant

$$(1 - \delta_t^* C^- \delta_b)^2 - (\delta_t^* C^- \delta_t)(\delta_b^* C^- \delta_b)$$

is positive in the situations where the switch will not create a disconnected design. This follows from a seperate argument, given at the end of the proof. It remains to solve the equations for $(v_{t_1} - v_{t_2})$ and $(v_{b_1} - v_{b_2})$, insert the result in (6.2) and multiply by Λ^* from the left to obtain an explicit formula for $R_{new}(t',t'') = v_{t'} - v_{t''}$. These lengthy but straightforward calculations are omitted.

In order to see that the determinant must be positive, suppose that a current in the network (as it was before the switch) of 1 ampere from t_1 to b_1 is induced by a potential difference of $R(t_1,b_1)$ between the points t_1 and b_1 . Schematically, this situation will be as illustrated by figure 17. The resistance $R(t_1,b_1)$ can be decomposed

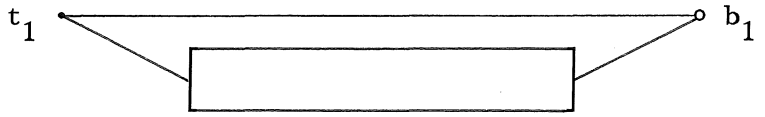

Figure 17

as a parallel combination of two, the unit resistance to be removed by the switch and the rest of the network represented by the box. The current through the single connection is $R(t_1,b_1)$, and the current through the remaining part of the network must then be $1 - R(t_1,b_1)$. It follows that the current through any single connection in the remaining part of the network must be less than or equal to $1 - R(t_1,b_1)$. In particular, the current from b_2 to t_2 through the other connection to be removed by the switch is less than or equal to $1 - R(b_1,t_1)$. This current is equal to the difference between the potentials at b_2 and t_2 , which (cfr. the proof of theorem 2.1) is

$$v_{b_2} - v_{t_2} = -(1_{t_2} + 1_{b_2})^* \begin{bmatrix} (v_t) \\ (-v_b) \end{bmatrix} = -(1_{t_2} + 1_{b_2})^* C^- (1_{t_1} + 1_{b_1}) .$$

Thus,

$$- (1_{t_2} + 1_{b_2})^* C^- (1_{t_1} + 1_{b_1}) \leq 1 - R(t_1,b_1) ,$$

or, introducing the expression for $R(t_1,b_1)$ in terms of C^-,

$$- (1_{t_2} + 1_{b_2})^* C^- (1_{t_1} + 1_{b_1}) \leq 1 - (1_{t_1} + 1_{b_1})^* C^- (1_{t_1} + 1_{b_1}) ,$$

which can also be written

$$(\delta_t + \delta_b)^* C^- (1_{t_1} + 1_{b_1}) \leq 1 \qquad (6.3)$$

The same argument with (t_1,b_1) and (t_2,b_2) interchanged gives

$$- (\delta_t + \delta_b)^* C^- (1_{t_2} + 1_{b_2}) \leq 1 \qquad (6.4)$$

(the change of sign is due to the change of sign for δ_t and δ_b). Adding (6.3) and (6.4), we obtain

$$(\delta_t + \delta_b)^* C^- (\delta_t + \delta_b) \leq 2$$

which can also be written

$$\delta_t^* C^- \delta_t + \delta_b^* C^- \delta_b \leq 2 (1 - \delta_t^* C^- \delta_b) .$$

Dividing by 2 and squaring both sides, and finally applying to the left hand side the inequality $(\frac{a+b}{2})^2 \geq ab$ (valid for all a , b , with equality if and only if $a = b$) we obtain

$$(\delta_t^* C^- \delta_t) (\delta_b^* C^- \delta_b) \leq (1 - \delta_t^* C^- \delta_b)^2 \qquad (6.5)$$

which is exactly the condition for the determinant occurring earlier in the proof to be nonnegative.

Now, consider the situation where (6.3) is an equality. This means that all current not passing through the connection from t_1 to b_1 passes through the other connection to be removed. This corresponds to the situation outlined by figure 18. The removal of the two connections

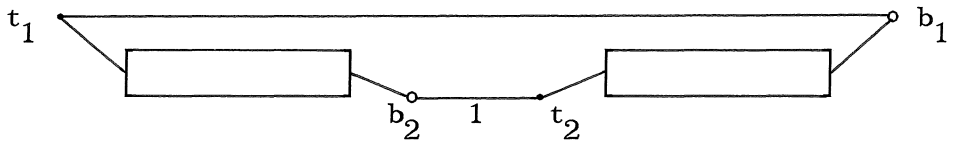

Figure 18

in this case would obviously create a disconnected network, and this disconnectedness would not disappear when the two new connections from t_1 to b_2 and from t_2 to b_1 were introduced. Conversely, if the

switch creates a disconnected design, the situation must be like this. It follows that if a switch is allowed, then (6.3), and thereby (6.5), will be sharp. On the other hand, if the switch creates a disconnected design, both (6.3) and (6.4) are equalities, and - since $\delta_t^* C^- \delta_t = R(t_1,t_2) = R(b_1,b_2) = \delta_b^* C^- \delta_b$ in this case - so is (6.5).□

Remark. The fact that a switch creates a disconnected design if and only if (6.5) is satisfied can be applied in the algorithm to avoid a tedious combinatorial check for connectedness. It suffices to check, for each switch considered, that (6.5) (which involves quantities that have to be computed anyway) is sharp.

In principle, formulas for the change of average contrast variance due to a new connection or a switch can be obtained by averaging over all pairs of distinct treatments in the formulas of proposition 6.1 and 6.2. However, it is computationally cheaper to build this averaging into an initial computation of a matrix to be formed *before* the search among all possible extensions by a single connection or all possible switches. The computational formulas for this are given by the following proposition.

Proposition 6.3. *Define*

$$\mathbf{M} = C^- \begin{bmatrix} \frac{2}{T-1} I_{T\times T} - \frac{2}{(T-1)T} J_{T\times T} & 0_{T\times B} \\ 0_{B\times T} & 0_{B\times B} \end{bmatrix} C^-$$

where $I_{T\times T}$ *is the* $T \times T$ *identity matrix and* $J_{T\times T}$ *is the* $T \times T$ *matrix with all entries equal to* 1 . *Then, the change of average contrast variance created by the addition of a (unit resistance) connection from* t_0 *to* b_0 *is given by*

$$\bar{R}_{new} = \bar{R} - \frac{(1_{b_0} + 1_{t_0})^* \mathbf{M} (1_{b_0} + 1_{t_0})}{1 + R(b_0,t_0)} .$$

The change of average contrast variance created by a switch (involving b_1 , t_1 , b_2 *and* t_2 *as in proposition 6.2) is given by*

$$\bar{R}_{new} = \bar{R} + \frac{(\delta_t^* C^- \delta_t)(\delta_b^* M \delta_b) + (\delta_b C^- \delta_b)(\delta_t M \delta_t) + 2(1 - \delta_b^* C^- \delta_t)(\delta_t^* M \delta_b)}{(1 - \delta_b^* C^- \delta_t)^2 - (\delta_t^* C^- \delta_t)(\delta_b^* C^- \delta_b)} .$$

Remark. Once $\mathbf{M}$ has been computed, the change of average contrast variance due to a switch (or the addition of a connection) is essentially expressed in "matrix operation free" terms. Obviously, expressions like $\delta_b^* C^- \delta_t$ or $\delta_t^* \mathbf{M} \delta_b$ are not matrix products from a computational point of view because they involve only the addition or subtraction of four elements of a square matrix.

Proof. We shall only prove the formula for addition of a connection. The switch formula is proved in essentially the same manner.

The formula for change of a single resistance $R(t_1, t_2)$ when a connection from b_0 to t_0 is added is given by proposition 6.1. The important term, involving t_1 and t_2 , is the nominator

$$[\ (1_{t'} - 1_{t''})^* C^- (1_{b_0} + 1_{t_0})\ ]^2$$

$$= (1_{b_0} + 1_{t_0})^* [\ C^- (1_{t'} - 1_{t''})\ (1_{t'} - 1_{t''})^* C^-\ ]\ (1_{b_0} + 1_{t_0}) .$$

The averaging of this over all pairs (t', t'') of distinct treatments amounts to the averaging of the matrix in brackets, which is easily seen to result in our matrix $\mathbf{M}$. The desired result follows immediately.□

7. *Notes and remarks.*

This section outlines relations to results and ideas put forward by other authors, and indicates some directions for further research.

Borre and Meissl (1974). This paper seems to be the first presentation of a relation between potential theory and covariance structures. As noticed by H. Brøns (lecture around 1974, unpublished), the theory presented by Borre and Meissl contains the main result of the present paper (theorem 2.1) as a special case. However, their exposition is based on the probabilistic interpretation of potential theory (the "electrical network" interpretation is found in an appendix), and the statistical problem investigated is the following. Suppose that measurements of height differences between certain points in a landscape are given. Denote the meaurements y_i , $i \in I$, and let p_i' and p_i'' be the two correponding points, so that y_i is a measurement of $\alpha_{p_i'} - \alpha_{p_i''}$, where α_p denotes the true level (over the sea surface, say) of point p . The classical statistical model for "smoothing" of such data states that the y_i are normally distributed, independent with $E\, y_i = \alpha_{p_i'} - \alpha_{p_i''}$ and (for simplicity) known variances $\mathrm{var}(y_i) = \sigma_i^2$. The maximum likelihood or weighted least squares estimates $\hat{\alpha}_p$ of the true levels (given up to a common additive constant) are obtained by minimization of

$$\Sigma_i \, (y_i - (\alpha_{p_i'} - \alpha_{p_i''}))^2/\sigma_i^2 \quad .$$

Now, the "electrical version" of the connection to potential theory can be explained as follows. Draw, for each measurement y_i , a line on the map between the points p_i' and p_i'' . Think of the resulting graph (which is assumed to be connected) as an electrical network in which the connection corresponding to the i'th measurement has a resistance of σ_i^2 ohm. Then, $\mathrm{var}(\hat{\alpha}_{p'} - \hat{\alpha}_{p''})$ equals the resistance through the network from p' to p'' . The probabilistic interpretation in terms of random

walks on the graph will be given later in this section.

The observation made by Brøns was the following. Suppose that the graph is bipartite and that all σ_i^2 are equal. Denoting the two sets of points by B and T, and denoting the levels of the two different kinds of points by α_t $(t \in T)$ and β_b $(b \in B)$, we have the model

$$y_i \sim N(\alpha_{t_i} - \beta_{b_i}, \sigma^2)$$

which is merely the two-way additive model with a slightly unusual ("subtractive") parametrization. The above mentioned electrical network is recognized as our design network (with resistances σ^2 instead of 1), and (i) and (ii) of theorem 2.1 come out as special cases of the above mentioned result. In fact, (iii) can also be deduced from results in Borre and Meissl (1974).

Dynkin (1980). In this paper, a relation between Markov processes and Gauss fields is presented. Roughly, the idea is that the Greens function (or potential operator) of a time homogeneous symmetric Markov process is a positive definite matrix which can be taken as the covariance matrix for a set of normal random variables. Interesting relations between properties of the Markov process and properties of the Gauss field are derived. The most striking result is probably the fact that conditional independence of two sets of variables in the Gauss field, given a third, occurs if and only if passage between the two sets of states in the Markov proces can only take place via the third. Relations to Markov random fields and statistical mechanics are discussed. More recently,

Ylvisaker (1986) followed up some of these ideas and noticed their relation to design and prediction problems of a more general nature.

The following probabilistic considerations indicate the connections between Dynkin's approach, the random walk approach followed by Borre and Meissl and the electrical network approach followed in the present paper.

Consider a graph with P (= B U T , if desired) as its set of points and let $n_{p'p''}$ denote the number of connections (or an arbitrary weight assigned to the connection) between points p' and p'' . Consider a continuous time Markov process on P , jumping between points of the graph with intensities equal to the multiplicities $n_{p'p''}$. Thus, the intensity matrix $\mathbf{A}$ (= the generator of the transition semigroup) for this process has off-diagonal elements $n_{p'p''}$, and the diagonal elements are determined by the convention that row sums (and thereby column sums, in the symmetric case) should be zero. The semigroup of transition matrices is

$$\mathbf{P}^t = \exp(t\mathbf{A}) = \sum_{n=0}^{\infty} \frac{t^n}{n!} \mathbf{A}^n .$$

If the graph is connected, this Markov process is ergodic, and the unique stationary distribution is easily seen to be the uniform distribution on P . The *potential operator* $\mathbf{G}$ is formally defined by

$$\mathbf{G} = \int_0^{\infty} \mathbf{P}^t \, dt .$$

This integral is divergent, but $\mathbf{G}$ is welldefined as a linear operator on the subspace

$$U = \{ \mathbf{u} \in \mathbb{R}^P \mid \Sigma u_p = 0 \} .$$

Indeed, the spectral decomposition of the symmetric matrix $\mathbf{P}^t$ can be shown to be of the form

$$\mathbf{P}^t = \mathbf{P}_1 + \sum_{j=2}^{|P|} \lambda_j^t \mathbf{P}_j$$

with $\mathbf{P}_1$ = the matrix with all entries $1/|P|$ (the orthogonal projection onto $U^{\perp}$) and $0 \leq \lambda_j < 1$. It follows that the integral

$$\mathbf{G}u \;=\; \int_0^\infty \mathbf{P}^t\, u\, dt \;=\; \int_0^\infty \Big(\sum_{j=2}^{|P|} \lambda_j^t\, \mathbf{P}_j u \Big)\, dt$$

is welldefined for $u \in U$. The potential operator $\mathbf{G}$ is a (restriction of a) generalized inverse of $-\mathbf{A}$ in the sense that

$$\mathbf{A}\,\mathbf{G}\,u \;=\; \mathbf{G}\,\mathbf{A}\,u \;=\; -u \quad \text{for} \quad u \in U\ .$$

This follows by integration from 0 to ∞ of the identity

$$\mathbf{A}\,\mathbf{P}^t\,u \;=\; \mathbf{P}^t\,\mathbf{A}\,u \;=\; \frac{d}{dt}\,\mathbf{P}^t\,u\ .$$

Since the matrices $\mathbf{P}^t$ are positive definite ($\mathbf{P}^t = \mathbf{P}^{t/2}\,\mathbf{P}^{t/2} = \mathbf{P}^{t/2}\,(\mathbf{P}^{t/2})^*$), so is any positive linear combination or integral of these matrices. In particular, $\mathbf{G}$ is positive definite in the sense that it can be taken as the "covariance" for a Gaussian distribution on $\mathbb{R}^P$; the fact that $\mathbf{G}$ is only defined on U means that this distribution is only given up to an additive (random or deterministic) constant to be added to all coordinates. Or, equivalently, only variances on (and covariances between) random variables of the form $\Sigma\, a_p z_p$, $\Sigma\, a_p = 0$, are determined by $\mathbf{G}$. This is Dynkins construction of a Gauss field on P for the special case of a finite set P and a non-defective semigroup $(\mathbf{P}^t)$.

In order to relate this construction to the electrical network, consider a stochastic system where particles are generated according to a Poisson process of intensity 1 at the point p' and absorbed (killed) at the point p'' . The particles are assumed to behave independently according to the transition semigroup $(\mathbf{P}^t)$ (except for the absorbtion at p''). After a long time, the system will be in equilibrium, and we can define

$$\mathbf{v} \;=\; (v_p) \;=\; (\,\mathbf{E}\, n_p(t)\,)$$

= the vector of expected numbers of particles in the different states at

time t . Straightforward arguments, concerning the expected numbers of transitions in a small time interval, show that these expected counts satisfy the matrix equation

$$-A\,\mathbf{v} \;=\; 1_{p'} - 1_{p''}$$

which is recognized as the matrix equation summarizing the laws of Kirchhoff (cfr. section 2) for current 1 from p' to p'' , under the usual interpretation of the graph as an electrical network. This confirms an obvious (and wellknown) interpretation of electricity as a large number of charged particles moving around in a random fashion. At the same time, it follows from what was said about the potential operator above that a solution to the network equations is given by

$$\mathbf{v} \;=\; G\,(\,1_{p'} - 1_{p''}\,) \;=\; \int_0^\infty P^t\,(\,1_{p'} - 1_{p''}\,)\,dt \quad ,$$

and the resistance of the network from p' to p'' is

$$\begin{aligned} R(p',p'') \;&=\; v_{p'} - v_{p''} \;=\; (1_{p'} - 1_{p''})^{*}\mathbf{v} \\ &=\; (1_{p'} - 1_{p''})^{*}\,G\,(1_{p'} - 1_{p''}) \quad . \end{aligned}$$

In the special case of a bipartite graph ($P = B \cup T$, $n_{p'p''} = 0$ for p' and p'' both in B or both in T) this means that the covariance of the set of estimates in the additive model (section 2) coincides with the covariance of Dynkin's Gauss field (apart from our change of signs for block parameters). A similar interpretation can be given to the covariance of the set of estimates in the more general levelling type problem considered by Borre and Meissl, when the integer multiplicities $n_{p'p''}$ are replaced by arbitrary intensities (or precisions) $1/\sigma_i^2$.

The resistance $R(p',p'')$ can be given a more concrete interpretation in the Markov process framework. Assuming that particles are absorbed at p'' , we have $v_{p''} = 0$, and thus $R(p',p'') = v_{p'}$. Now, $v_{p'}$ is the expected number of particles at state p' when the system is in

equilibrium. Since particles are created at p' at a rate of 1 per time unit, and since a particle present at p' leaves p' after an exponentially distributed waiting time of expected duration $1/(-a_{p'p'})$ (where a_{pp} is the p'th diagonal element of $\mathbf{A}$, or minus the number of connections to p), we have

$$R(p',p'') = v_{p'}$$
$$= \text{expected number of particles present at } p'$$
$$= \frac{\text{expected number of visits at } p' \text{ of a single particle}}{-a_{p'p'}} .$$

The last expression gives the interpretation emphasized by Borre and Meissl. The chain of states visited by a particle starting at p' can be described as a random walk on the graph which, in each step, jumps to a random state among those connected to the present state, until the absorbing state p'' is reached for the first time. Thus, $R(p',p'')$ equals the expected number of visits (including the initial "visit") at p' of a random walk starting in p' before it hits p'', divided by the number of connections to p'. Notice that this gives a very simple probabilistic interpretation of contrast variances in terms of random walks on the design network. We shall make an application of this in the discussion of the variety-concurrence graph below. For a more careful exposition of the relation between Markov chains and electrical networks, see Kemeny, Snell and Knapp (1976).

Paterson (1983) and Paterson and Wild (1986). For a binary design with blocks of equal size k, define the *variety concurrence graph* as follows. As the set of points in this graph we take the set T of treatments, and a connection between t' and t'' is introduced for each block in which both t' and t'' occur. Thus, there are $\lambda(t',t'')$ connections between t' and t'', in the notation of proposition 4.1. Now, a very brief outline of the main result on which Patersons 1983-paper is based can be given as follows. Consider the information matrix

$$\mathbf{C}_T = r\,\mathbf{I} - \frac{1}{k}\mathbf{N}^*\mathbf{N} = r(\mathbf{I} - \frac{1}{kr}\mathbf{N}^*\mathbf{N})$$

for treatment effects, cfr. the beginning of section 5. Formally, an inverse to this is given by the Taylor expansion

$$\frac{1}{r}\left[\sum_{n=0}^{\infty}\left(\frac{1}{kr}\mathbf{N}^*\mathbf{N}\right)^n\right] .$$

Unfortunately, $\mathbf{C}_T$ is not regular and the series is not convergent, but it can be seen that the infinite sum is welldefined as an operator on the subspace U of vectors with coordinate sum 0 in the same sence as the potential operator $\mathbf{G}$ defined earlier in this section, and that this operator is (a restriction of) a generalized inverse to $\mathbf{C}_T$ in the same sense as $\mathbf{G}$ was an inverse to $\mathbf{A}$. It follows that contrast variances can be computed as convergent sums

$$\mathrm{var}(\hat{\alpha}_{t'}-\hat{\alpha}_{t''}) = \sigma^2\frac{1}{r}\sum_0^{\infty}(\mathbf{1}_{t'}-\mathbf{1}_{t''})^*\left(\frac{1}{kr}\mathbf{N}^*\mathbf{N}\right)^n(\mathbf{1}_{t'}-\mathbf{1}_{t''}) ,$$

and the average contrast variance can, accordingly, be computed as a convergent sum in which the important (design-dependent) quantities will be traces of powers of $\mathbf{N}^*\mathbf{N}$. Now, the trace of $(\mathbf{N}^*\mathbf{N})^n$ can be expressed as a linear combination of the numbers of cycles of lengths 2, 3, ..., n in the variety concurrence graph, and so the average contrast variance (and thereby the harmonic mean efficiency) can be expressed in terms of these combinatorial quantities. Paterson did this and concluded that high efficiency of a design can be expected when the variety-concurrence graph has few cycles of low order. The paper conjectures that optimal designs are characterized by the property that the number of two-cycles is minimal, the number of three-cycles given the number of two-cycles is minimal etc. Paterson and Wild (1986) followed this up by giving exact upper bounds for the efficiency in terms of the number of triangles under various conditions.

The variety-concurrence graph does not, as opposed to our design network, contain the full information about the structure of the design. For example, a BIBD with $\lambda = 1$ and a design consisting of a single complete block will have the same variety-concurrence graph. However, it follows

from Patersons results that this graph does (together with the block size) give information about contrast variances etc. It is tempting to ask, in the present context, whether it makes sense to think of the variety-concurrence graph as an electrical network. This turns out to be the case, and there are two very simple ways of seeing it.

The first argument is probabilistic. Consider a random walk on the design network, as discussed earlier in this section. The bipartiteness of this graph implies that the state of such a random walk will alternate between treatment and block type. Thus, if we start at (discrete) time 0 in a treatment point and consider the states at even times only, we have a Markov chain with state space T . It is easy to see that this chain behaves like a random walk on the variety concurrence graph, except that it remains in its present state with a certain positive probability in each step. The probability of "no shift" is obviously $1/k$, because return to the same treatment once more from the intermediate block state is always $1/k$. Notice that equal block sizes and the fact that the design is binary are essential here. Now, for a proper random walk on the variety-concurrence graph (i.e. one that makes a proper shift each time), we know (by arguments similar to those applied earlier in this section to the design network) that the expected number of visits in t' for a random walk starting at t' and being killed at its first visit to t'' is

$$(k-1)\, r_t\, R_{vc}(t',t'')$$

where $R_{vc}(t',t'')$ denotes the resistance through the variety-concurrence graph from t' to t'' , when the graph is regarded as an electrical network with connections of unit resistance (the number of connections to t' in this graph is $(k-1)r_t$). We know, on the other hand, that the expected number of visits to t' of our "delayed" random walk on the variety-concurrence graph is equal to $r_t\, R(t',t'')$, because this is the expected number of visits to t' for the random walk on the design network from which the chain was constructed. But the "delayed" chain can be modelled as a proper random walk with a geometrically distributed waiting time following each shift. Thus, the expected time spent in t'

by the "delayed" chain equals the expected time spent there by a proper random walk, multiplied by the factor

$$(1 + \frac{1}{k} + (\frac{1}{k})^2 + \ldots) \quad = \quad \frac{k}{k-1} \quad ,$$

which is the expected duration of each visit to t' . It follows that

$$r_t \, R(t',t'') \quad = \quad \frac{k}{k-1} \, (k-1) \, r_t \, R_{vc}(t',t'') \quad ,$$

or

$$R(t',t'') \quad = \quad k \, R_{vc}(t',t'') \quad .$$

An alternative proof of this simple relation can be based on the socalled *star-delta transform* for electrical networks, see e.g. Bollobás (1979). According to this rule, a point in an electrical network and its connections to other points (a "star") can be replaced by a set of connections between the points connected to it (a "delta"), without affecting the resistances between other points of the network. The formula for the resistances of the new connections implies that a "star" with k "rays" of unit resistance should be replaced by a "delta" consisting of $\binom{k}{2}$ edges of resistance k . If we apply this transformation to all block points of the design network, we obviously end up with the variety-concurrence graph, except that all resistances will be k instead of 1 . The above relation between R and R_{vc} follows immediately.

Thus, for binary designs with equal block sizes, we have an interpretation of resistances through the variety-concurrence graph which is similar to our interpretation of resistances through the design network. The only difference is that the resistances should be multiplied by $k \, \sigma^2$ instead of σ^2 to give the contrast variances. Unfortunately, this seems not to simplify the situation in concrete applications like those made in section 3. The variety concurrence graph has fewer points than the design network, but the number of connections is much larger. There seems not to be any relation between our upper

bounds for efficiences based on short circuiting and those given by Paterson and Wild in terms of the number of triangles.

Eccleston and Hedayat (1974) discuss concepts of connectedness which are clearly equivalent to, or at least closely related to, graph theoretical connectedness properties of the design network. Up to small modifications, their concepts can be characterized as follows. Connectedness in the usual sense is called *local connectedness*, and the following two stronger conditions are considered:

Pseudo-global connectedness : After the removal of any treatment point and its connections to block points, the graph is still connected.

Global connectedness : After the removal of any two treatment points and their connections to block points, the graph is still connected.

This description seeems not to be quite correct, because Eccleston and Hedayat work with a version of the basic "path definition" of connectedness according to which a chain $t_1b_1t_2b_2\ldots$ must not contain a treatment which has itself as its neighbours neighbour, i.e. ...tbt... is not allowed. This makes no difference as to the definition of local connectedness, but for the two more complicated concepts it means that our description is not quite precise. However, apart from such divergencies the above characterization is roughly correct, and probably a sufficient description as far as the main results of their paper are concerned. These results state that designs which are optimal in a certain sense must, under suitable conditions on the dimensions, posess one or both of the two last connectedness properties. The concept of optimality referred to is roughly equivalent to S-optimality (Shah 1960), which amounts to the minimization of the square sum of the eigenvalues of the information matrix for treatment effects. The proofs are based on the idea that if such connectedness properties are not present, then it is possible to find a switch which improves the design. There is no immediate way of generalizing these results to the concept of optimality

based on the harmonic mean efficiency (A-optimality), but since the criterion on which S-optimality is based can be regarded as (a transformation of) a second order approximation to the efficiency, their results strongly suggest that such connectedness properties are important. A study of these ideas in connection with graph theoretical concepts of connectedness might very well turn out to be fruitful.

Jones (1976) and Jones and Eccleston (1980). Our algorithm for optimization of designs (section 6) can be regarded as a further improvement of an algorithm originally due to Jones (1976) and improved by Jones and Eccleston (1980). The main differences lie in the strategy for choice of switches and the computational tools on which these choices are based. The algorithm of Jones used an approximation to the inverse of the information matrix C_T after a switch. The improved algorithm of Jones and Eccleston can be descibed as follows. In a first stage, an initial (almost arbitrary) design of the desired dimensions is modified by a sequence of *exchange procedures*. An exchange procedure is, in our terminology, the removal of a single connection followed by the addition of a new connection from the same block point to an other treatment point. Notice that block sizes are unchanged, while replicate counts are changed. In each step, the choice of the next exchange procedure to be performed is based on computational formulas similar to our formula for change of $\overline{R}$ when a new connection is added (proposition 6.3) or deleted. The strategy is roughly based on the principle that $\overline{R}$ should be decreased as much as possible by each exchange, but since the computational tools give only the result of a single (delete or add) operation, a more complicated strategy must be used. When this strategy fails to give further improvement of the design, a second phase consisting of a sequence of *interchange procedures* (i.e. switches) is initiated. In this phase, switches are performed according to a rather complicated strategy. The need for a complicated strategy is obvious, since the computational tools are still the same, so the final result of a switch is not visible before the switch has almost been performed. A direct comparison with our algorithm is difficult on the basis of the paper by Jones and Eccleston, but we have worked with similar ideas, and

it is our experience that the final result of a switch is very difficult to predict from such "single step forecasts".

At the end of their paper, Jones and Eccleston have an interesting remark concerning designs with $k = 2$ and $B = T$. It appears that the circular designs (cfr. our example 3.1) are not always optimal here when the replicate counts are allowed to vary freely. For $B = T = 10$, 11 and 12 designs of higher efficiency than the circular design (and with unequal replicates, of course) were found. Incidentally, this is a situation where the network approach gives a complete solution to the optimization problem, and since this is a very illustrative example the arguments will be briefly outlined here.

For $B = T$ and $k = 2$ the design network must necessarily be of the form illustrated by figure 19 for the case $B = T = 10$, i.e. a circular subgraph equipped

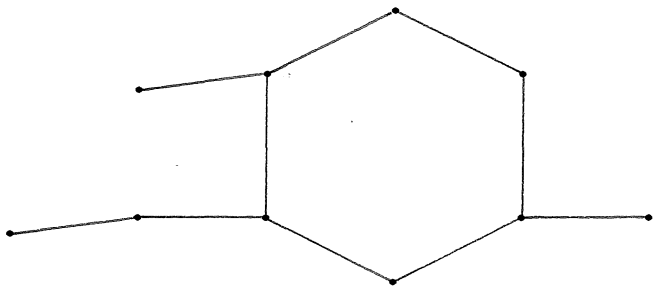

Figure 19

with a number of "rays" (figure 19 is actually the varity concurrence graph, but the design network comes out of it if we imagine a block point at the midpoint of each connection). This is so for combinatorial reasons. A connected graph with $B + T$ points and $B + T - 1$ connections is a *tree*, i.e. a graph without cycles, and if a single connection is added to this, a graph with exactly one cycle comes out of it. Now, it is easy to see that the operation which collects all the rays in the same treatment point (without changing their lengths) will

improve the design. For example, the design of figure 20 is better than

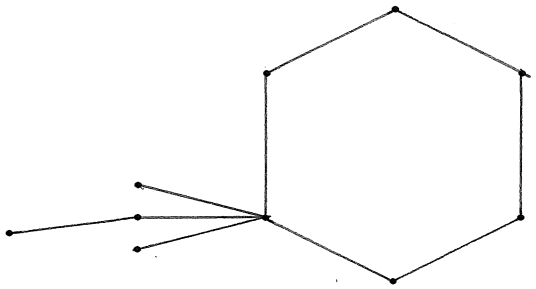

Figure 20

that of figure 19 because resistances between treatment points on the rays are either decreased or unchanged by this operation, while the average of the remaining contrast variances is obviously unchanged. Similarly, it is easy to see that the operation which breaks a long ray into pieces and fixes these pieces as shorter rays at the same point of the cycle, will improve the design. Thus, the design of figure 21 is better than

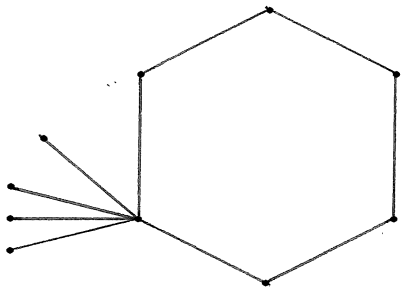

Figure 21

that of figure 20. These arguments show that an optimal design in this case is always of the form indicated by figure 21, i.e. a circular design involving some of the treatments, extended by a number of blocks in which the remaining treatments occur together with a selected treatment from the circular design. By the rules for parallel and serial combination and some straightforward summations, it is not difficult to compute the

average contrast variance of a design like this. It turns out to be

$$\overline{R} = \frac{(c-1)(c+1)(\frac{1}{3}B - \frac{1}{6}c) + 2(B-c)(B-1)}{B(B-1)/2}$$

where c is the number of treatments in the circular design. A straightforward analysis of the behaviour of this third order polynomial in c for fixed B gives the following surprisingly complicated solution to our optimization problem:

For $B \leq 8$ the circular design ($c = B$) is optimal.

For $9 \leq B \leq 12$ the design with $c = 4$ is optimal. The replicate counts of this design are $B-2, 2, 2, 2, 1, 1, \ldots, 1$.

For $12 \leq B$ the design with $c = 3$ is optimal. The replicates are $B-1, 2, 2, 1, 1, \ldots, 1$, and the design can be regarded as a design with $B-1$ blocks in which a selected "baseline treatment" is compared with the remaining $B-1$ treatments, extended by a single block with two arbitrary (non-baseline) treatments.

The overlap for $B = 12$ means that the two designs with $c = 3$ and 4 have the same efficiency. The complexity of the solution confirms the impression that optimization of designs is a difficult matter.

Recovery of interblock information. One final result deserves to be mentioned here because it indicates that the design-network relation goes deeper than we have been able to decover. It turns out that the recovery of interblock information by a model with random block effects has a natural counterpart in the network context. More specifically, we are thinking of a design with equal blocksizes and an additive model of the usual form, in which the block parameters β_t are assumed to be independent normally distributed random variables with the same mean and the same variance ω^2. Consider the design network as defined in section 2, but (for simplicity) with connections of resistance σ^2

instead of 1, so that contrast variances in the model with fixed block effects are simply equal to the corresponding resistances. Extend this network by the addition of a single point with a connection of resistance ω^2 to each block point. The resistances between treatment points in this extended network turn out to be equal to the corresponding variances on (generalized least squares or maximum likelihood) estimates of treatment contrasts in this variance component model. The proof of this is straightforward, but too lengthy to be given here. Notice how the two extreme situations ω^2/σ^2 large (almost no gain over the fixed effects model) and ω^2/σ^2 small (almost equivalence with the model without block effects, corresponding to a network created from the present one by contraction of all block points to a single point) are nicely reflected by the properties of this network.

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