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FURTHER RESULTS ON A PROBLEM OF DOEHLERT AND KLEE

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ABSTRACT. In this paper we investigate a class of (r,λ)-designs which arises naturally in the consideration of a certain experimental design. These designs satisfy the condition

$$r^2 = \lambda b ,$$

where b is the number of blocks. We are interested in determining the maximum number of elements in such designs. We obtain some general results in this area and settle some specific values.

1. *Introduction.*

In [3] it is shown that the vertex set of the d-dimensional cuboctahedron is useful as an experimental design for estimating a response over a spherical region.

Doehlert and Klee [2] considered the problem of rotating such a design so as to minimize the number of levels at which the experimental variables are required to appear. They show that this problem is intimately related to the problem of finding m proper subsets $X_1, X_2, \ldots, X_m$ of $\{1,2,\ldots,v\}$ such that

$$\frac{|X_s||X_t|}{|X_s \cap X_t|} = v \tag{1.1}$$

for all $s \neq t$.

If one lets F_m be any family of equicardinal subsets with property (1.1), then it is desired to evaluate $T^*(v)$, the maximum value of F_m.

If the cardinality of each element of F_m is denoted by k, then condition (1.1) shows that $|X_s \cap X_t|$ is a constant d and that

$$k^2 = vd. \tag{1.2}$$

We prefer to consider the dual of the above problem and hence require the following definitions.

UTILITAS MATHEMATICA Vol. 12 (1977), pp. 263-271.

An (r,λ)-design D is a collection of b subsets (called blocks, some of which may be empty), chosen from a finite set of v elements (called varieties), such that

(i) every variety occurs in r blocks;

(ii) every unordered pair of distinct varieties is contained in precisely λ blocks.

If every block of D has the same cardinality k, then D is called a balanced incomplete block design (BIBD). The parameters of a BIBD are listed as (v,b,r,k,λ).

Suppose we have a family F_m of equicardinal subsets of size r, taken from a set of b elements. If we interchange the roles of elements and subsets in the incidence relation of F_m, we obtain an (r,λ)-design D having b blocks and m varieties in which

$$r^2 = \lambda b \quad (1.3)$$

We shall refer to any (r,λ)-design satisfying (1.3) as a Doehlert-Klee design (or DK-design). The problem then is to find, for a given b, the maximum v such that a DK-design exists; we shall call this maximum $K(b)$. Note that the original requirement that F_m contain proper subsets $(k < v)$ means that $r < b$ in our formulation.

In the paper by Doehlert and Klee [2], $K(b)$ was evaluated for a number of values of b. In [5], several other values of $K(b)$ for $b \le 100$ were obtained. In this paper, we generalize some of the results of [5], and consider the unknown values of $K(b)$ for $b \le 100$.

2. *Preliminaries.*

If, in a BIBD, $b = v$, then the design is called a symmetrical BIBD or an SBIBD. In this case, $r = k$, and the parameters are listed as (v,k,λ). It is well known [6] that in any (r,λ)-design $b \ge v$, with equality if and only if the design is an SBIBD. The following results can be found in [5].

THEOREM 2.1. *For all positive integers* $b \ge 2$

$$K(b) \ne b .$$

THEOREM 2.2. $K(b) = b-1$ *if and only if there eixists a* $(b-1,b/2,b/4)$ - *SBIBD*.

THEOREM 2.3. *The complement of a DK-design is a DK-design.*

Theorem 2.4 is proved in [4].

THEOREM 2.4. *Let* D *be a* $DK(r,\lambda)$-*design having* b *blocks and* v *varieties. If* k_i *is the cardinality of the* i^{th} *block in* D

$$k_i \le \frac{(r-\lambda)(b-1)-\lambda v}{b-2r}, \quad i = 1,2,\ldots,b .$$

Noting that $K(b) = 1$ if b is the product of distinct primes, and that $K(4a) = 4a - 1$ for $a \le 25$ (this is the Hadamard matrix problem), it is possible to evaluate $K(b)$ for all values of $b \le 100$ except for 9,18,25,27,45,49,50,54,63,75,81,90,98, and 99. In [5], $K(b)$ is evaluated for $b = 9,18,25,27$, and 81. This paper determines $K(49)$, gives a general construction, and improves the upper bounds for the remaining values of $b \le 100$.

3. *Conditions for the Existence of DK-Designs.*

From Theorems 2.1 and 2.2, we immediately deduce that $K(b) \le b-2$ if $b \neq 2r$.

THEOREM 3.1. *Let* t *be a positive integer which is square free. Then* $K(9t) = 9t-2$ *if and only if there exists a* $(9t-2,3t,t)$-*SBIBD*.

Proof. Since t is square free, the only values of r and λ satisfying $\lambda 9t = r^2$ are $r = 3t$, $\lambda = t$, and the complementary set of parameters. Suppose k is the cardinality of a block B in D. By Theorem 2.4

$$k \le \frac{2t(9t-1)-tv}{9t-6t} .$$

If $v = 9t - 2 + \varepsilon$, where $0 \le \varepsilon \le 2$, then

$$k \le \frac{2(9t-1)-9t+2-\varepsilon}{3} = 3t - \frac{\varepsilon}{3} .$$

This implies that $k \le 3t$. Consider any variety x in D. x is contained in $3t$ blocks $B_1, B_2, \ldots, B_{3t}$ of D and is contained in

$\sum_{i=1}^{3t} (|B_i|-1)$ pairs in these blocks. But the number of pairs that contain x in D is $\lambda(v-1) = t(9t - 2 + \varepsilon - 1)$. Thus

$$(3.1) \qquad t(9t - 2 + \varepsilon - 1) = \sum_{i=1}^{3t} (|B_i|-1) \le 3t(3t-1) ,$$

which implies $\varepsilon \le 0$. For $\varepsilon > 0$, there are no DK-designs. If $\varepsilon = 0$, then (3.1) implies that every non-empty block in D has size $3t$. Thus D is a $(9t-2,3t,t)$-SBIBD. This completes the proof.

Suppose we consider $K(45)$. By Theorem 3.1, $K(45) = 43$ if and only if there exists a $(43,15,5)$-SBIBD. Since this design is ruled out by the Bruck-Ryser-Chowla theorem, $K(45) \le 42$.

COROLLARY 3.1.

(a) $K(63) = 61$ *if and only if there exists a* $(61,21,7)$*-SBIBD.*
(b) $K(99) = 97$ *if and only if there exists a* $(97,33,11)$*-SBIBD.*

Theorem 2.2 states that $K(b) = b-1$ if and only if there exists a Hadamard matrix of order b. We now give a necessary condition for $K(b)$ to equal $b-2$.

THEOREM 3.2. *Let* k *be the cardinality of any block in a* DK(r,λ)*-design* D *having* b *blocks and* $b-2$ *varieties. Let* $n=r-\lambda$ *and* $a = \{r+\lambda(b-3)\}$. *A necessary condition for the existence of* D *is*

(1) if b *is odd, then* $(nb-a)-k(b-2r)$ *is a perfect square;*
(2) if b *is even,* $n\{(nb-a)-k(b-2r)\}$ *is a perfect square.*

Proof. Let A be the incidence matrix of D. That is, $A = (a_{ij})$ is a $(b-2)\times b$ matrix of zeros and ones such that

$$a_{ij} = \begin{cases} 1, & \text{if variety } i \text{ is in block } j, \\ 0, & \text{otherwise.} \end{cases}$$

Form a new matrix

$$A^* = \begin{bmatrix} & & A & & \\ 1 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 1 & \cdots & 1 \end{bmatrix} .$$

A^* is a $b\times b$ matrix. Let k be the number of ones in the first column of A and assume that they occur in the first k positions.

Thus,

$$A^*(A^*)^T = \begin{bmatrix} r & \lambda & \cdots & \lambda & 1 & r \\ \lambda & r & \cdots & \lambda & 1 & r \\ \cdot & & & \cdot & \cdot & \cdot \\ \cdot & & & \cdot & \cdot & \cdot \\ \cdot & & & \lambda & 1 & r \\ \lambda & & \cdots & & 0 & r \\ \cdot & & & \cdot & \cdot & \cdot \\ \cdot & & & \cdot & \cdot & \cdot \\ \cdot & & & \cdot & \cdot & \cdot \\ \lambda & \lambda \ldots \lambda & \ldots & r & 0 & r \\ 1 & 1 \ldots 1 & 0.0 & & 1 & 1 \\ r & r \ldots r & r.r & & 1 & b \end{bmatrix} .$$

Applying Lemma 3.1 of [1]

$$\det A^*(A^*)^T = n^{b-3}[(nb-a)-k(b-2r)] .$$

But

$$\det A^*(A^*)^T = (\det A^*)^2 .$$

Thus, if b is odd, $b-3$ is even and the result follows.

THEOREM 3.3. *Let* D *be a* $DK(r,\lambda)$*-design having* b *blocks and* $b-2$ *varieties. Then* $r \le 3\lambda$ *with equality if and only if* D *is a* $(9\lambda-2, 3\lambda, \lambda)$*-SBIBD.*

Proof. Let $B_1, B_2, \ldots, B_b$ be the blocks of D and let $k_i = |B_i|$, $1 \le i \le b$. From Theorem 3.2, $(nb-a)-k_i(b-2r)$ or $n[(nb-a)-k_i(b-2r)]$ (where $n = r - \lambda$, $a = \{r+\lambda(b-3)\}$) must be a perfect square for each k_i. Let

$$t_i = (nb-a) - k_i(b-2r)$$
$$= -(r-3\lambda) - (b-2r)(k_i-r), \quad 1 \le i \le b.$$

Suppose $r \ge 3\lambda$. This implies $b - 2r > 0$ and, since $t_i \ge 0$, $k_i \le r$. Let x be any variety in D. The total number of pairs in D containing x is $\lambda(b-3)$. But, in any block containing x, x occurs in at most $r-1$ pairs. Thus

(3.2) $$\lambda(b-3) \le r(r-1) .$$

Since D is a DK-design, $\lambda b = r^2$; thus (3.2) implies that $r \leq 3\lambda$, which is a contradiction unless $r = 3\lambda$. This gives equality in (3.2) and thus every nonempty block of D must have cardinality r. Therefore, D is a $(9\lambda-2,3\lambda,\lambda)$-SBIBD. The result now follows.

If t is a divisor of $b-2r$, then the following result follows immediately from Theorem 3.2.

THEOREM 3.4. *A necessary condition for the existence of a* $DK(r,\lambda)$-*design having* b *blocks and* $b-2$ *varieties is that in the ring of integers modulo* t,

(1) if b *is odd,* $3\lambda-r$ *be a perfect square;*
(2) if b *is even,* $n(3\lambda-r)$ *be a perfect square.*

As an application of this theorem, consider K(50). We know that $K(50) \leq 48$. Does there exist a $DK(r,\lambda)$-design having 50 blocks and 48 varieties such that $\lambda 50 = r$? The possible values of r and λ are

$b = 50$	r	λ
	10	2
	20	8
	30	18
	40	32

Since the parameters come in complementary pairs, we need only consider (10,2)-designs and (20,8)-designs. By Theorem 3.3, there is no (10,2)-design having 50 blocks and 48 varieties since $r > 3\lambda$. Applying Theorem 3.4 to the (20,8)-design with $n = 12$, $t = 5$ we see that 12.3.8 must be a perfect square in the integers modulo 5. But $12.3.8 \equiv 3$ mod 5 and 3 is not a square. Hence, there is no DK(20,8)-design and therefore $K(50) \leq 47$.

4. *A Construction for DK-Designs.*

In this section, we give a construction for DK-designs having $b-3$ varieties and show that in certain cases and possibly infinitely often these designs are extremal.

For this section let $a = (2t+1)^2$, where t is any positive integer and $v = a - 3$.

THEOREM 4.1. *If there exists a Hadamard matrix of order* $\frac{v}{2}+1$ *and if there exists a* $\left(2t(t+1)+1, t^2, t(t-1)/2\right)$*- SBIBD, then there exists a* $DK(2t^2+t, t^2)$*-design having* $(2t+1)^2$ *blocks and* $(2t+1)^2-3$ *varieties.*

Proof. If there exists a Hadamard matrix of order $\frac{v}{2}+1$ (this is possible and conjectured to be true since $\frac{v}{2}+1 \equiv 0 \pmod 4$), then there exists a $\left(\frac{v}{2}, \frac{v-2}{4}, \frac{v-6}{8}\right)$-SBIBD. Let the blocks of this design be $B_1, B_2, \ldots, B_{v/2}$. We form a new design D^* by adjoining a new element ∞ to the variety set of the SBIBD and the blocks of D^* are $B_1\cup\{\infty\}, B_2\cup\{\infty\}, \ldots, B_{v/2}\cup\{\infty\}, \bar{B}_1, \bar{B}_2, \ldots, \bar{B}_{v/2}$, where $\bar{B}_i$ is the complement of B_i. D^* is a $\left(\frac{v}{2}+1, v, \frac{v}{2}, \frac{v+2}{4}, \frac{v-2}{4}\right)$-BIBD and it has the property that

$$|(B_i\cup\{\infty\}) \cap \bar{B}_i| = 0,$$
$$|(B_i\cup\{\infty\}) \cap B_j| = \frac{v+2}{8}, \quad i \neq j, \quad \text{and}$$
$$|(B_i\cup\{\infty\}) \cap \bar{B}_j| = \frac{v+2}{8}, \quad i \neq j.$$

(D^* is called an affine resolvable design.)

Now consider the $\left(2t(t+1)+1, t^2, \frac{t(t-1)}{2}\right)$-SBIBD, D'. This design has $\frac{v}{2}+2$ blocks. Let $C_1, C_2, \ldots, C_{v/2}$ be any distinct set of $v/2$ of the $\frac{v}{2}+2$ blocks. Let V_1 be the variety set of D^* and V_2 be the variety set of D'. Choose V_1 and V_2 such that $V_1 \cap V_2 = \emptyset$. Form a new configuration C^* on the variety set $V_1 \cup V_2$ such that C^* contains all blocks of the form

$$\left.\begin{aligned} C^*_{1i} &= B_i\cup\{\infty\} \cup C_i, \\ C^*_{2i} &= \bar{B}_i \cup C_i, \end{aligned}\right\} \quad 1 \le i \le \frac{v}{2}.$$

The blocks of C^* have the property that

(a) $|C^*_{ji}| = 2t^2+t, \quad 1 \le j \le 2, \quad 1 \le i \le \frac{v}{2}$;

(b) $|C^*_{1i} \cap C^*_{2i}| = t^2, \quad 1 \le i \le \frac{v}{2}$;

(c) $|C^*_{ji} \cap C^*_{\ell k}| = t^2, \quad 1 \le j, \ell \le 2, 1 \le i, k \le \frac{v}{2}$.

Thus any two blocks of C^* have precisely t^2 varieties in common. If we dualize C^*, that is, interchange the roles of variety and block in the incidence relation, we obtain a $(2t^2 + t, t^2)$-design having a blocks and v varieties. It is easily seen that this design is a DK-design and the proof is complete.

COROLLARY 4.1. *and* $K(25) \geq 22$ *and* $K(49) \geq 46$.

Proof. Since there exists a Hadamard matrix of order 12 and a (13,4,1)-SBIBD, Theorem 4.1 implies the existence of a DK(10,4)-design having 22 varieties and 25 blocks. Thus, $K(25) \geq 22$.

Since there exists a Hadamard matrix of order 24 and a (25,9,3)-SBIBD, there exists a DK(21,9)-design having 46 varieties and 49 blocks. Therefore, $K(49) \geq 46$.

K(25) has been shown [5] to be 22. We now prove a result which allows us to determine K(49).

THEOREM 4.2. *Let* p *be a prime number congruent to* 5 *or* 7 *modulo* 12. *Then* $K(p^2) \leq p^2-3$.

Proof. Since p^2 is not divisible by 4, $K(p^2) \leq p^2-2$. Let D be a $DK(r,\lambda)$-design having p^2 blocks and p^2-2 varieties. Then $r=p\ell$, $\lambda = \ell^2$ for some ℓ, $1 \leq \ell \leq \frac{p-1}{2}$. By Theorem 3.4, 3λ must be a perfect square in the integers modulo p. But λ is a perfect square and hence 3 must be a perfect square in the integers modulo p. Applying the law of quadratic reciprocity

$$(3/p) = (-1)^{\left(\frac{3-1}{2}\right)\left(\frac{p-1}{2}\right)}(p/3) ,$$

where $(3/p)$ is the Legendre symbol. Since $p \equiv 5$ or $7 \pmod{12}$, we have that $(3/p) = -1$ and hence 3 is not a perfect square. Therefore, no DK-designs exist having p^2-2 varieties and the result follows.

COROLLARY 4.2. $K(25) = 22$ *and* $K(49) = 46$.

This follows immediately from Corollary 4.1 and Theorem 4.2.

Summary.

We now summarize the results of the previous sections as they apply to K(b), b = 9, 18, 25, 27, 45, 49, 50, 54, 63, 75, 81, 90, 98, and 99.

Theorem 3.1 and the existence of certain SBIBD's gives $K(9) = 7$, $K(18) = 16$, $K(27) = 25$, $K(45) \leq 42$, $K(54) \leq 51$, $K(81) = 79$, and $K(90) \leq 87$. Corollary 3.1 provides a partial answer for K(63) and K(99). Corollary 4.2 yields $K(25) = 22$ and $K(49) = 46$. We have seen that Theorem 3.4 can be used to show $K(50) \leq 47$. Theorem 3.2 and Theorem 2.4 can be applied to show that $K(75) \leq 72$ and $K(98) \leq 95$.

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Received June 22, 1977.