REPEATED MEASUREMENTS DESIGNS, II1

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Repeated measurements designs are concerned with scientific experiments in which each experimental unit is assigned more than once to a treatment, either different or identical. It is shown that a family of balanced repeated measurements designs which are very popular among experimenters are universally optimal in a relatively large class of competing designs.

1. Introduction and the need for repeated measurements. Experimenters in many fields of research perform experiments designed in such a way that each experimental unit (subject) is assigned more than once to a treatment (test), either different or identical. These designs are given several names in the literature of statistical designs: repeated measurements designs (briefly RM designs), crossover or changeover designs, (multiple) time series designs, and before-after designs. An extreme form of an RM design is the one in which the entire experiment is planned on a single experimental unit. Details on latter designs can be found in Williams (1952), Finney and Outhwaite (1956), and Kiefer (1960). A brief history of the subject with a bibliography containing 136 directly related references is given in Hedayat and Afsarinejad (1975).

The use of RM designs rather than the classical designs, for which the number of experimental units is the same as the number of observations, can be justified in many settings such as when:

- (i) One of the objectives of the experiment is to determine the effect of different sequences of treatment applications as in drug, nutrition or learning experiments.
- (ii) The experimenters might be interested in discovering whether or not a trend can be traced among the responses obtained by successive applications of several treatments on a single experimental unit. For example, if one wants to measure the degree of adaptation to darkness over time, the most efficient use of subjects requires that each subject be tested at all times of interest.
- (iii) Experimental units are scarce and have to be used repeatedly. This is often the case in small clinics or in the development of large military systems, such as aerospace vehicles, airplanes, radar, computers, etc.
- (iv) The nature of the experiment is such that it calls for special training over a long period of time. Therefore, to minimize cost and time, the experimenter

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Received August 1975; revised March 1977.

Research supported in part by NSF Grants MPS75-07570, MCS-07217 and AFOSR76-3050.

AMS 1970 subject classifications. Primary 62K05, 62K10, 62K15; Secondary 05B05, 05B10.

Key words and phrases. Repeated measurements designs, crossover designs, changeover designs, universal optimal repeated measurements designs.

should take advantage of the trained experimental units for repeated measurements.

To this point, RM designs have been used on the grounds of balance and simplicity of computations. While such criteria may still be attractive in some cases, they cannot be justified on statistical grounds. This paper shows that some families of RM designs which are very popular among experimenters are "universally optimal" in a relatively large class of competing designs (Section 3.1). Existence and nonexistence of such designs are discussed in Section 3.2.

2. Preliminaries and universal optimality. The search for an optimum design involves the determination, in a specified class of competing designs, of the design which is best according to some well defined criteria under a given model for observations. In this paper we are concerned exclusively with the following setup: t treatments are to be tested and studied via n experimental units. Each experimental unit is used in p periods resulting in $r_i \ge 1$ observations for the ith treatment, $r_1 + r_2 + \cdots + r_t = np$. Clearly there are numerous ways of performing the experiment. Let D denote the set of all such arrangements, to which we shall refer as designs. If d is a design in D, then let d(i, j) denote the treatment assigned by d in the ith period to the jth experimental unit. Throughout this paper the following model is assumed for the response obtained under d(i, j):

$$(2.1) Y_{ij} = \mu + \alpha_i + \beta_j + \tau_{d(i,j)} + \rho_{d(i-1,j)} + e_{ij}$$

$$i = 1, 2, \dots, p; \quad j = 1, 2, \dots, n; \quad \rho_{d(0,j)} \equiv 0 \quad \text{for all} \quad j,$$

where the unknown constants μ , α_i , β_j , $\tau_{d(i,j)}$ and $\rho_{d(i-1,j)}$ are respectively called the overall mean, the effect of the *i*th period, the effect of the *j*th experimental unit, the *direct effect* of treatment d(i,j) and the *first order residual effect* (or *carryover effect*) of treatment d(i-1,j). We assume that e_{ij} 's are homoscedastic with means zero.

We are interested in specifying a design d in D which is connected with respect to all contrasts in direct and residual effects and is "universally optimal" in a specified class of competing designs.

2.1. Universal optimality. In vector notation the np responses under Model (2.1) can be written as

$$Y_d = X_{1d}\theta_1 + X_{2d}\theta_2$$

where θ_1 consists of parameters of interest for study. In our case, θ_1 consists of direct treatment effects or residual effects or both. Let

$$C_d(\theta_1) = X'_{1d}X_{1d} - X'_{1d}X_{2d}(X'_{2d}X_{2d})^-X'_{2d}X_{1d}$$

and

$$Q_d(\theta_1) = X'_{1d}Y_d - X'_{1d}X_{2d}(X'_{2d}X_{2d})^-X'_{2d}Y_d$$

then $C_d(\theta_1)$ is the information matrix associated with θ_1 since it is well known that a linear parametric function $\xi = l'\theta_1$ is estimable under d if l' is in the row

space of C_d , and the best linear unbiased estimator of ξ is given by

$$\hat{\xi} = l'(C_d)^- Q_d$$
 with $\operatorname{Var}(\hat{\xi}) = l'(C_d)^- l \sigma^2$.

In this case we say d is connected for ξ . Now suppose d is connected for a set of t-1 independent orthonormal contrasts $A'\theta_1$. Then by the above argument the covariance of the best linear unbiased estimator of $A'\theta_1$ is given by

$$V_d \sigma^2 = A' C_d^- A \sigma^2 = (A' C_d A)^{-1} \sigma^2$$
.

This leads to consideration of an optimality functional ψ on $(t-1) \times (t-1)$ matrices and to determination of a design d which minimizes $\psi(V_d)$. Some commonly used optimality criteria are:

 $\begin{array}{ll} \textit{D-} \text{optimality:} & \phi(V_d) = \det V_d \ ; \\ \textit{A-} \text{optimality:} & \phi(V_d) = \operatorname{tr} V_d \ ; \\ \textit{E-} \text{optimality:} & \phi(V_d) = \operatorname{maximum \ eigenvalue \ of} & V_d \ . \end{array}$

The relationship between these optimality criteria is well known and may be found in Kiefer (1958, 1959, 1975). In some settings it is possible to introduce an optimality criterion which includes D-, A- and E-optimality as special cases. One such setting together with a sufficient condition under which a design is optimal is given by Kiefer (1975) and will be utilized throughout this paper.

A major difficulty is the computation of $(A'C_dA)^{-1}$ for each competing design d. Since in our case, as will be seen later, each row (hence each column) of C_d adds up to zero, we can utilize the recent result of Kiefer (1975) on universal optimality and avoid the computation of $(A'C_dA)^{-1}$ for each d. We shall now briefly review the concept of universal optimality. Suppose that R_t consists of $t \times t$ nonnegative definite matrices. Let \bar{R}_t consist of those elements of R_t , all of whose row and column sums are zero. Let Ω be the set of all functions ω from \bar{R}_t to $(-\infty, +\infty]$ with properties:

- (i) $\omega(\cdot)$ is convex;
- (2.2) (ii) $\omega(bR)$ is nonincreasing in the scalar $b \ge 0$, $R \in \bar{R}_t$;
 - (iii) $\omega(\cdot)$ is invariant under each simultaneous permutation of rows and columns of $R \in \bar{R}_t$.

In our setting $C_d \in \bar{R}_t$.

A very useful concept of optimality in this setting is:

DEFINITION 2.1. A design d^* is universally optimal in the class of competing designs under consideration if $\omega(C_d^*) \leq \omega(C_d)$ for each $\omega \in \Omega$.

If d^* is universally optimal, then it is D-, A-, and E-optimal. In some situations it is possible to identify the universally optimal design without actually computing $\omega(C_d)$ for each d. One such situation has been identified by Kiefer (1975), and is formally stated here. First we need the following definition.

DEFINITION 2.2. A design d is said to be completely symmetric with respect to

 θ_1 if its corresponding C_d is of the form $aI_t + bJ_t$, where a and b are scalars, I_t is the identity matrix of order t and J_t is the matrix of order t whose entries are all ones.

THEOREM 2.1. If the class of competing designs contains a design d* such that

- (i) d* is completely symmetric;
- (ii) tr $C_d^* \ge \text{tr } C_d$, for all $d \in \bar{R}_t$,

then d* is universally optimal.

In the following sections we have characterized universally optimal designs in some classes of competing designs which we know are connected for the parameters under consideration.

3. Universally optimal repeated measurements designs. In this section we shall search for a universally optimal design (if it exists) in a class of uniform RM designs. The existence and nonexistence of such optimal designs are studied in the final part of this section. First we need some notation and definitions. An arbitrary RM design based on np observations resulting from the application of t treatments to n experimental units during p periods is denoted by RM (t, n, p). The set of all such arbitrary RM designs is designated by $\mathcal{RM}(t, n, p)$. Our study here is limited to the case where p = t and $n = \lambda t$, λ a positive integer.

DEFINITION 3.1. A design d in $\mathcal{RM}(t, n, p)$ is said to be uniform on the experimental units if $d(i, j) \neq d(i', j)$, $i \neq i'$ for all j.

DEFINITION 3.2. A design d in $\mathcal{RM}(t, n, p)$ is said to be uniform on the periods if, in each period, d assigns the same number of experimental units to each treatment.

DEFINITION 3.3. A design d in $\mathcal{RM}(t, n, p)$ is said to be *uniform* if it is uniform on both the experimental units and periods.

The subset of all uniform designs in $\mathcal{RM}(t, n = \lambda t, t)$ is denoted by $\mathcal{URM}(t, \lambda t, t)$.

3.1. Search for a universal optimal design in $\mathscr{URM}(t, \lambda t, t)$. Our interest here mainly lies in unbiased estimation of linear parametric functions of direct treatment effects and residual effects under Model 2.1. So, under the notation of Section 2.1, the parametric vector θ_1 consists of either all direct effects or all first order residual effects. The information matrix associated with the entire set of parameters of Model 2.1, rewritten as

$$Y_{ij} = au_{d(i,j)} +
ho_{d(i-1,j)} + lpha_i + eta_j + \mu + e_{ij}$$

for an arbitrary d in $\mathcal{URM}(t, n = \lambda_1 t, t)$ is given by

$$(3.1) \qquad (X_d'X_d)\sigma^{-2} = \begin{bmatrix} nI & M_d & \lambda J_1 & J_2 & n1_t \\ M_d' & \lambda(t-1)I & E_d & N_d & \lambda(t-1)1_t \\ \lambda J_1' & E_d' & nI & J_2 & n1_t \\ J_2' & N_d' & J_2' & tI & t1_n \\ n1_t' & \lambda(t-1)1_t' & n1_t' & t1_n' & nt \end{bmatrix} \sigma^{-2}$$

where

I is the identity matrix of order t;

 M_d is the incidence matrix of direct effects and first order residual effects under d;

 J_1 is a square matrix of order t with all entries ones;

 J_2 is a $t \times n$ matrix with all entries ones;

 1_r is an $r \times 1$ vector of ones;

 E_d is the incidence matrix of first order residual effects and period effects under d:

 N_d is the incidence matrix of first order residual effects and experimental unit effects under d.

LEMMA 3.1. The information matrix of the joint direct treatment effects and first order residual effects is given by

(3.2)
$$C_d(\tau, \rho)\sigma^{-2} = \begin{bmatrix} nI - \lambda J_1 & M_d - \frac{\lambda(t-1)}{t}J_1 \\ M_d - \frac{\lambda(t-1)}{t}J_1 & \lambda\left(\frac{t^2 - t - 1}{t}\right) \left[I - \frac{1}{t}J_1\right] \end{bmatrix} \sigma^{-2}.$$

PROOF. If we write $X_d'X_d$ as partitioned in (3.1) in the following way

$$X_d'X_d = \begin{bmatrix} Z'_{1d} \, Z_{1d} & Z'_{1d} \, Z_{2d} \\ Z'_{2d} \, Z_{1d} & Z'_{2d} \, Z_{2d} \end{bmatrix},$$

then

(3.3)
$$C_d(\tau, \rho) = Z'_{1d} Z_{1d} - Z'_{1d} Z_{2d} (Z'_{2d} Z_{2d})^- Z'_{2d} Z_{1d},$$

where

$$(Z_{2d}'Z_{2d})^{-} = \begin{bmatrix} nI & J_{2} & n1_{t} \\ J_{2}' & tI & t1_{n} \\ n1_{t}' & t1_{n}' & nt \end{bmatrix}^{-} = \begin{bmatrix} \frac{1}{n}I + \frac{1}{nt}J_{1} & \frac{-1}{nt}J_{2} & 0 \\ \frac{-1}{nt}J_{2}' & \frac{1}{t}I & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

After some algebra (3.3) reduces to (3.2).

THEOREM 3.1. A design d^* in $\mathcal{URM}(t, \lambda t, t)$ is universally optimal for the estimation of direct treatment effects if $M_{d^*} = \lambda(J_1 - I)$.

PROOF. Utilizing the joint information matrix of the vector of direct treatment effects and residual effects as given in (3.2), one can derive the information matrix of the vector of direct effects as

(3.4)
$$C_d(\tau) = nI - \frac{t}{\lambda(t^2 - t - 1)} M_d M_{d'} + \frac{\lambda(2 - t)}{t^2 - t - 1} J_1.$$

It can be argued that for any d in $\mathcal{URM}(t, \lambda t, t)$

$$M_d J_1 \equiv J_1 M_{d'} \equiv \lambda (t-1) J_1$$

and therefore

$$C_d(\tau)1_t=0,$$

meaning that the sum of the entries in each row and column of $C_d(\tau)$ is zero. Therefore, by Theorem 2.1, a design d^* in $\mathscr{URM}(t,\lambda t,t)$ is universally optimal if $C_{d^*}(\tau)$ is completely symmetric and $\operatorname{tr} C_{d^*}(\tau) \geq \operatorname{tr} C_d(\tau)$ for any other d in the class. Clearly $C_{d^*}(\tau)$ is completely symmetric if d^* is such that $M_d^* = \lambda(J_1 - I)$. From the expression for $C_d(\tau)$ it is obvious that $\operatorname{tr} C_d(\tau)$ is maximum if and only if $\operatorname{tr} M_d M_d'$ is minimum. But since the sum of each row of M_d is $\lambda(t-1)$, $\operatorname{tr} M_d M_d'$ is minimum if and only if $M_d = \lambda(J_1 - I)$.

THEOREM 3.2. A design d^* in $\mathcal{UPM}(t, \lambda t, t)$ is universally optimal for the estimation of first order residual effects if $M_d^* = \lambda (J_1 - I)$.

Since the information matrix of the first order residual effects, $C_d(\rho)$, from (3.2), is

(3.5)
$$C_d(\rho) = \lambda \left(\frac{t^2 - t - 1}{t} \right) I - \frac{1}{n} M_d M_d' + \frac{\lambda (2 - t)}{t^2} J_1,$$

the proof is analogous to the proof of Theorem 3.1.

The problem of the existence and nonexistence of a universally optimal design in $\mathcal{URM}(t, \lambda t, t)$ will now be studied.

3.2. Existence and nonexistence of a universally optimal design in $\mathscr{URM}(t, \lambda t, t)$. First we shall give a combinatorial interpretation of the structure of a design in $\mathscr{URM}(t, \lambda t, t)$ whose incidence matrix of direct treatment effects and first order residual effects, M_d , is of the form $\lambda(J_1 - I)$. Then we shall investigate the existence and nonexistence of such designs. First we need the following definition.

DEFINITION 3.4. A design d in $\mathcal{UPM}(t, \lambda t, t)$ is said to be balanced with respect to the set of direct treatment effects and first order residual effects if in the order of application each treatment is preceded λ times by each other treatment, i.e., the collection of ordered pairs $(d(i, j), d(i+1, j)), 1 \le i \le t-1;$ $1 \le j \le \lambda t$ contains each ordered pair of distinct treatments precisely λ times. If d satisfies the above requirement we shall simply say that d is balanced.

Example 3.1. Let t = 3 and $\lambda = 4$. Then the following design is balanced.

Experimental Units

		1	2	3	4	5	6	7	8	9	10 2 3 1	11	12
	1	1	2	3	2	3	1	1	2	3	2	3	1
Periods	2	3	1	2	3	1	2	3	1	2	3	1 ·	2
	3	2	3	1	1	2	3	2	3	1	1	2	3

LEMMA 3.2. M_d is of the form $\lambda(J_1 - I)$ if and only if d is balanced, i.e., d is universally optimal if it is balanced.

The proof follows directly from the definition of first order residuals effect in Model 2.1 and the fact that under the stated condition the diagonal entries of M_d are zeros and off diagonal entries are λ .

If d_i is a balanced RM $(t, \lambda_i t, t)$ design, i = 1, 2, then by patching d_1 and d_2 side by side we shall obtain a balanced RM $(t, \lambda t, t)$ design with $\lambda = \lambda_1 + \lambda_2$. Therefore to construct a balanced RM $(t, \lambda t, t)$ design it is sufficient to study the existence of a balanced RM (t, t, t) design. But it should be clear that if a balanced RM (t, t, t) design does not exist then we *cannot* conclude the non-existence of balanced RM $(t, \lambda t, t)$ designs with $\lambda > 1$, as we shall see shortly.

Several authors have studied the existence and nonexistence of balanced RM (t, t, t) designs either directly in the context of experimental design or in algebraic systems equivalent to such designs. For an extensive bibliography on the subject the reader is referred to Hedayat and Afsarinejad (1975). Here we shall update the information on balanced designs given in Hedayat and Afsarinejad (1975).

Family one. t = 2m, $\lambda = 1$. It is known that balanced RM (t, t, t) designs exist for all values of m. For example, if we number the experimental units and periods by $1, 2, \dots, t$, then d is balanced if d assigns treatment d(i, j) in the ith period to the jth experimental unit in the following way:

$$d(i,j) = \left(\frac{2t-i}{2}\right) + j \mod 2m \quad \text{if} \quad i \text{ is even}$$
$$= \left(\frac{i-1}{2}\right) + j \mod 2m \quad \text{if} \quad i \text{ is odd.}$$

Family two. t = 2m + 1, $\lambda = 1$. It is known that no balanced RM (t, t, t) design exists if t = 3, 5, or 7. According to E. Sonnemann² the following design for t = 9 was found via an electronic computer by K. B. Mertz.

Experimental Units

		1	2	3	4	5	6	7	8	9
	1	1	2	3	4	5	6	7	8	9
	2	9	7	8	6	4	5	1	2	3
	3	7	8	9	2	3	1	4	5	6
	4	6	4	5	3	1	2	9	7	8
Periods	5	4	5	6	9	7	8	2	3	1
	6	8	9	7	1	2	3	6	4	5
	7	5	6	4	8	9	7	3	1	2
	8	3	1	2	7	8	9	5	6	4
	9	2	3	1	5	6	4	8	9	7

E. Sonnemann has found the following design for t = 15 by mimicking the pattern of the design discovered by Mertz.

² Personal communication to A. Hedayat.

Experimental Units

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	1	6	11	2	3	4	5	7	8	9	10	12	13	14	15
2	3	12	6	4	5	1	2	13	14	15	11	7	8	9	10
3	7	14	1	8	9	10	6	15	11	12	13	2	3	4	5
4	15	1	7	11	12	13	14	2	3	4	5	8	9	10	6
5	8	11	3	9	10	6	7	12	13	14	15	4	5	1	2
6	9	2	12	10	6	7	8	3	4	5	1	13	14	15	11
7	11	5	8	12	13	14	15	1	2	3	4	9	10	6	7
8	12	8	5	13	14	15	11	9	10	6	7	1	2	3	4
9	5	10	13	1	2	3	4	6	7	8	9	14	15	11	12
10	4	15	10	5	1	2	3	11	12	13	14	6	7	8	9
11	6	13	4	7	8	9	10	14	15	11	12	5	1	2	3
12	10	3	15	6	7	8	9	4	5	1	2	11	12	13	14
13	14	4	9	15	11	12	13	5	1	2	3	10	6	7	8
14	13	9	2	14	15	11	12	10	6	7	8	3	4	5	1
15	2	7	14	3	4	5	1	8	9	10	6	15	11	12	13

Experimental Units

	1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27
	1	A	Y	K	Н	0	α	Z	Е	J	X	В	$\overline{\mathbf{C}}$	F	L	N	D	U	S	w	I	V	P	T	M	R	o	I
	2	M																										
	3																									Н		
	4																									Q		
	5	X	\mathbf{o}	D	V	Α	Q	P	S	\mathbf{C}	N	Y	\mathbf{Z}	T	\mathbf{E}	G	α	K	R	M	\mathbf{w}	L	Ι	J	F	В	Н	U
	6	N	Н	α	L	\mathbf{X}	A	I	R	\mathbf{Z}	G	\mathbf{o}	P	J	S	U	Q	\mathbf{D}	В	F	M	\mathbf{E}	\mathbf{w}	\mathbf{C}	T	\mathbf{Y}	V	K
	7	R	I	Y	P	\mathbf{v}	В	Α	M	\mathbf{X}	Н	J	K	N	\boldsymbol{z}	S	L	Ε	\mathbf{C}	G	Q	F	U	D	α	W	T	O
	8	F	\mathbf{X}	M	D	J	\boldsymbol{z}	Y	Α	L	w	G	Н	В	N	P	Ι	T	α	\mathbf{v}	E	U	R	S	o	K	Q	\mathbf{C}
	9	S	P	В	Z	Н	R	Q	W	Α	\mathbf{o}	T	U	\mathbf{X}	\mathbf{C}	E	\mathbf{v}	L	J	N	α	M	G	K	\mathbf{D}	I	F	Y
	10	Q	В	U	o	α	\mathbf{D}	\mathbf{C}	L	T	Α	R	J	M	\mathbf{v}	\mathbf{X}	K	G	\mathbf{E}	I	P	Н	Z	F	\mathbf{W}	S	Y	N
	11	I	α	P	G	\mathbf{M}	T	S	\mathbf{D}	\mathbf{o}	Z	Α	В	E	Q	J	\mathbf{C}	\mathbf{w}	U	Y	Н	\mathbf{X}	L	V	R	N	K	F
	12	Н	T	L	F	R	\mathbf{v}	U	\mathbf{C}	K	S	I	A	D	M	o	В	Y	\mathbf{w}	α	G	Z	Q	X	N	J	P	\mathbf{E}
ç s	13	E	\mathbf{Z}	R	\mathbf{C}	o	S	α	I	Q	Y	F	G	Α	J	L	Н	V	T	X	D	W	N	U	K	P	M	В
Periods	14	W	Q	I	U	F	J	R	α	Н	P	X	Y	S	Α	C	Z	M	K	O	V	N	\mathbf{E}	L	В	G	D	T
Pe	15	α	R	G	Y	D	K	J	V	F	Q	S	T	W	H	Α	U	N	L	P	Z	О	C	M	Ι	\mathbf{E}	В	X
	16	G	V	Q	E	N	X	W	В	P	U	Н	Ι,	· C	R	K	Α	α	Y	T	F	S	M	Z	J	O	L	D
	17	K	Ε	X	R	U	G	F	O	W	D	L	M	P	Y	α	N	Α	H	C	J	В	T	I	Z	V	S	Q
	18	-	_	_	•																					α		
	19																									Z		
	20																									M		
	21											_																M
	22		-																	-						C		
	23																									T		
	24																											V
	25																											W
	26																									D		
	27	D	S	N	В	K	U	T	Н	M	α	Е	F	I	О	Q	G	X	V	Z	C	Y	J	W	P	L	R	Α

An example of balanced RM (21, 21, 21) is given in Hedayat and Afsarinejad (1975). An example of balanced RM (27, 27, 27) is given above. The group theoretic equivalent structure of the last design was first discovered by Keedwell (1974).

In an abstract, Wang (1973) has claimed the existence of a certain pattern in nonabelian groups of orders 39, 55 and 57 which when translated to our setup implies the existence of balanced RM (t, t, t) designs with t = 39, 55 and 57. But we have not seen the announced results. No other published or announced results are known to us.

The story of balanced RM (t, t, t) design with t odd is somewhat discouraging but, as we shall see shortly, such designs exist for all t if $\lambda = 2$.

Family three. t=2m+1, $\lambda=2$. In this case $n=\lambda t=2(2m+1)$ experimental units. Partition the experimental units into two groups each of size 2m+1. Number the periods and experimental units in each group by $1, 2, \dots, t$. Then d is balanced if d assigns treatment d(i, j) in the ith period to the jth experimental unit in the following way:

In the first group:

$$d(i,j) = \left(\frac{2t-i}{2}\right) + j \mod 2m + 1$$
 if i is even,
 $= \left(\frac{i-1}{2}\right) + j \mod 2m + 1$ if i is odd.

In the second group:

$$d(i,j) = \left(\frac{t-1+i}{2}\right) + j \mod 2m + 1 \quad \text{if} \quad i \text{ is even,}$$
$$= \left(\frac{t-i}{2}\right) + j \mod 2m + 1 \quad \text{if} \quad i \text{ is odd.}$$

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