Gower, J. C. and Preece, D. A. 1972. Generating successive incomplete blocks with each pair of elements in at least one block. *Journal Of Combinatorial Theory Series A.* 12 (1), pp. 81-97.

JOURNAL OF COMBINATORIAL THEORY (A) 12, 81–97 (1972)

Generating Successive Incomplete Blocks with Each Pair of Elements in at Least One Block

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Communicated by J. M. Hammersley

Received September 9, 1969

This paper examines solutions to the following combinatorial problem: Produce an ordered set of blocks of M elements chosen from N such that (i) any pair of the N elements occurs together in at least one block, and (ii) the total number of element changes in forming each new block from the previous one is minimised. For certain values of N and M, the only known solutions have no known generalisation. However, several general algorithms are described that produce sets of blocks satisfying (i) and either satisfying or nearly satisfying (ii). Other, related, combinatorial problems are outlined; all are relevant to organizing a certain type of data in a computer.

BACKGROUND

This work arose from a problem of data organization within a computer. The results are, however, of general combinatorial interest.

Many statistical calculations begin by computing a symmetric matrix of coefficients from data arranged in a rectangular matrix X; for example $X'X$ or XX' may be required. More elaborate coefficients than sums of products exist, but the basic requirement is still that every cell of the symmetric matrix is computed from a *pair* of columns (or rows) of X. If only M columns (rows) out of a total of N are available at any one time, the order of the computations is important. Various criteria may be used to define an optimum order. Different criteria give rise to different combinatorial problems, some of which are discussed in this paper.

On a computer, the matrix X will probably be held on backing store such as magnetic tape or disc, with the elements stored successively by columns (i.e., the last value in the first column of X will be followed by the first value in the second column, etc.). As transfer of data from backing store to a working store is slower than arithmetic operations, an algorithm might be required that makes as few transfers of columns as possible.

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But the computation of coefficients from sets of columns will usually be done by a subroutine, use of which can be time-consuming too. Thus we may wish to minimise not the number T of transfers of columns, but the number B of different sets of M columns that have to be set up, or a function of T and B. These problems are discussed below.

An important practical constraint on the order of transferring columns of X applies when the backing store is magnetic tape. Here, efficiency demands that the machinery should not have to wind unnecessarily through tape containing columns not required at the time. With machinery that can read tape either forwards or backwards, unproductive winding can be avoided if—as with Nelder's algorithm described below—the next column to be transferred is always the next or previous one on the tape. With machines that can read only forwards, general conditions for efficient winding are difficult to state. These matters are not, however, considered further in this paper.

We have found few relevant publications. Jowett [3] and Hammersley [2] are concerned with using the fewest operations to compute a particular coefficient ("Sums of Squares and Products") on hand-operated calculating machines. Their problem differs from ours because they can deal straightforwardly only with $M = 2$; also they are concerned with certain checks (particularly sum checks) that are important with hand calculation, but unlikely to be useful on stored-program computers.

The many balanced incomplete block designs (see, for example, the tables given by Fisher and Yates [1]) provide poor solutions to the transfer problem. Except with the cyclic and near-cyclic designs, there is no simple algorithm for generating the elements of successive blocks. With the cyclic designs there must be M new transfers for every block, so that, when λ (the number of times every pair of columns occurs) $= 1$, we have

$$T = \left\{\binom{N}{2}\Big/\binom{M}{2}\right\} \times M = N(N-1)/(M-1);$$

this is about twice as many transfers as in the designs discussed below, but the number of blocks $B = T/M$ is the smallest possible. T can be made smaller by reordering the cyclically generated blocks so that there are M transfers for the first block and $M - 1$ thereafter, whence

$$T = 1 + \left\{\binom{N}{2}\Big/\binom{M}{2}\right\} \times (M-1) = 1 + N(N-1)/M;$$

this is still far from optimum.

1. Introduction

Nelder [4] posed his combinatorial problem as follows: Produce an ordered set of blocks of M elements chosen from N such that

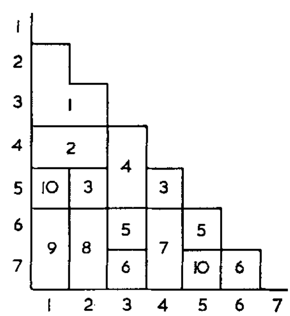
(i) any pair of the N elements occurs together in at least one block, and

(ii) the total number of element changes (i.e., transfers of single elements) in forming each new block from the previous one is minimised.

A solution for $N = 7$, $M = 3$ is

$$\begin{array}{cccccccccc} \textcircled{1} & 1 & \textcircled{5} & 5 & 5 & \textcircled{7} & 7 & 7 & 7 & 7 \\ \textcircled{2} & 2 & 2 & \textcircled{3} & 3 & 3 & \textcircled{4} & \textcircled{2} & \textcircled{1} & 1 \\ \textcircled{3} & \textcircled{4} & 4 & 4 & \textcircled{6} & 6 & 6 & 6 & 6 & \textcircled{5} \end{array} \qquad (1)$$

where the ten blocks run vertically from left to right, and changes are ringed. This solution can also be represented by the following triangular diagram:



(2)

The numbers down the left side of the diagram and along the bottom denote the elements; the numbers in the body of the diagram denote the blocks in which the corresponding pairs of elements appear together for the first time. The triangular diagram (2) shows that condition (i) is satisfied by (1); condition (ii) is satisfied because only one element is transferred for each new block, and after transfer the new element appears for the first time with each of the other elements in the block.

In what follows, triangular diagrams, with one block number for each pair of elements, are used for solutions of Nelder's and other problems. But such a diagram does not necessarily correspond to only one solution, and a block number in the body of a diagram need not indicate the *first* appearance of a pair of elements. (This will be illustrated below by Figure 5.)

2. Nelder's Algorithm and the Minimum Number of Transfers of Single Elements

As is proved in Nelder's paper, a lower bound to the minimum number of transfers of single elements is

$$\max\left\{\left[M+\frac{\binom{N}{2}-\binom{M}{2}}{M-1}\right],\ 2N-M\right\},$$

where $[x]$ denotes the least integer $\geqslant x$. This bound cannot, however, always be attained.

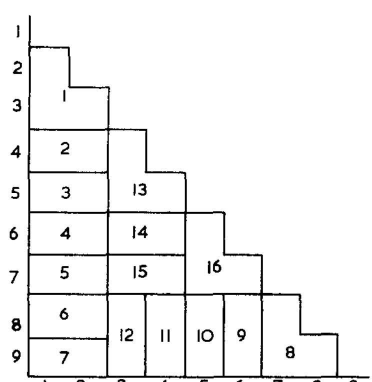
Nelder gave a very simple algorithm which is near-optimum in the sense that the total number, T, of transfers of single elements is never more than 20 per cent larger than the above lower bound. The algorithm gives $T =$ lower bound when $M = 2$, and when $N < 2M$, $M > 2$.

For $N = 9$, $M = 3$ Nelder's algorithm gives

1							7	6	5	4	3				5	
2							8					4			6	(3)
3	4	5	6	7	8	9						5	6	7		

(only the elements that change are shown)

which has the triangular diagram:



Here $T = 21$, whereas the lower bound, which is attainable (see below), is 20. In general, for Nelder's algorithm,

$$T = N(1+p) - \tfrac{1}{2}Mp(1+p) + \tfrac{1}{2}p(p-1),$$

where p is the integral part of $(N-2)/(M-1)$. Values of T for $M \leqslant N \leqslant 12$, and the corresponding lower bounds, are in Table 1.

TABLE 1

Values of T, $N \leqslant 12$

Lower bound

M \ N	2	3	4	5	6	7	8	9	10	11	12
2	2	4	7	11	16	22	29	37	46	56	67
3		3	5	7	9	12	16	20	24	29	35
4			4	6	8	10	12	14	17	21	24
5				5	7	9	11	13	15	17	19
6					6	8	10	12	14	16	18
7						7	9	11	13	15	17
8							8	10	12	14	16
9								9	11	13	15
10									10	12	14
11										11	13
12											12

Nelder's algorithm

M \ N	2	3	4	5	6	7	8	9	10	11	12
2	2	4	7	11	16	22	29	37	46	56	67
3		3	5	7	10	13	17	21	26	31	37
4			4	6	8	10	13	16	19	23	27
5				5	7	9	11	13	16	19	22
6					6	8	10	12	14	16	19
7						7	9	11	13	15	17
8							8	10	12	14	16
9								9	11	13	15
10									10	12	14
11										11	13
12											12

The outlined areas of the tables indicate the values of M and N for which Nelder's algorithm gives more transfers than the lower bound.

3. Non-Isomorphism of Solutions

A representation such as (1) will be called a "design." Two designs for a given set of values (N, M) will be said to be "non-isomorphic" (or "distinct," or "structurally different") if one cannot be changed into the other by any combination of (a) renaming the elements, (b) rearranging the rows, and (c) reading the design from right to left instead of from left to right.

It is easily seen that interchanging the 7th and 8th blocks of (1) produces a design that is still optimum, but not isomorphic to (1). A further, deeper type of non-isomorphism can be demonstrated by comparing (1) with the following, which is also optimum and for $N = 7$, $M = 3$:

$$\begin{array}{cccccccccc} 1 & & 5 & & & & & 6 & & \\ 2 & & & 3 & 6 & 7 & & & & \\ 3 & 4 & & & & & 1 & & 3 & 2 \end{array} \qquad (4)$$

Designs (1) and (4) can most readily be seen to be non-isomorphic by comparing the corresponding distributions of the number of times elements are transferred: writing a_i for the number of elements transferred i times, we have

Solution	a_1	a_2	a_3
(1)	2	5	0
(4)	3	3	1

and $a_i = 0$ for $i > 3$. In general, the a_i must, for an optimum design, satisfy

$$\sum a_i = N, \qquad \sum i a_i = T, \qquad a_1 \leqslant M,$$

and (5)

$$A \leqslant (N-1)/(M-1),$$

where A is the greatest number of transfers of any element. The inequality for a_1 holds because elements transferred only once must occur together in some block. The inequality for A holds because at each transfer of an element it occurs with $M - 1$ out of the other $N - 1$ elements.

The existence of a set $\{a_i\}$ satisfying (5) does not necessarily imply the existence of a corresponding design. For $N = 7$, $M = 3$, the only possible sets $\{a_i\}$ are the two given above, but for $N = 10$, $M = 3$ there are 14 sets, as follows:

a_1	a_2	a_3	a_4	Whether solution found
0	6	4	0	Yes
1	4	5	0	Yes
2	2	6	0	Yes
3	0	7	0	No
0	7	2	1	No
1	5	3	1	Yes
2	3	4	1	Yes
3	1	5	1	Yes
0	8	0	2	No
1	6	1	2	No
2	4	2	2	Yes
3	2	3	2	Yes
2	5	0	3	Proved impossible
3	3	1	3	Proved impossible

We define the complement, C, of a design D as the design such that (a) each block of C contains the elements absent from the corresponding block of D, and (b) if, in D, element i overwrites element j when block $x + 1$ is formed from block x, then, in C, j overwrites i at the corresponding place.

The complement of an optimum design with $N = 2M$ is also optimum, but not necessarily isomorphic to the original design. (Indeed no selfcomplementary optimum design has been found.) For example, the complementary designs

1		5	6					4	3			2		
2				3		1	and	5		1				3
3	4				5			6			5		4	

are non-isomorphic.

The complement of an optimum design with $N > 2M$ will often be a poor design. For example, the complement of (4) has $N = 7$, $M = 4$, $T = 13$, whereas an optimum design with $N = 7$, $M = 4$ has $T = 10$.

4. On the Number of Blocks in a Solution

Different algorithms can use the *same* number of transfers of single elements, but *different* numbers of blocks. One of the most important ways in which this can happen is illustrated by comparing Nelder's algorithm with a less simple variant, to be referred to as algorithm $N1$. This can conveniently be done using the specimen values $N = 15$, $M = 4$.

The two triangular diagrams are Figures 1a and 1b. With both procedures, the diagrams are divided into nested L-shaped bands, the L's being "frayed" at their tips but otherwise of width $M - 1$. The bands are filled with block numbers successively, starting with the outermost. Once the second band is begun, it is filled by the same procedure as for the first, and so on. Any small region remaining after the innermost L has been filled is filled last. When deriving a design from Figure 1b, care should be taken that element 4 in block 21 is not overwritten in blocks 22 or 23, and likewise that element 7 in block 32 is not overwritten in blocks 33 or 34. If this precaution is taken, the number of single element transfers required for the Nelder design is the same as for the variant design, although the former has 31 blocks and the latter 35.

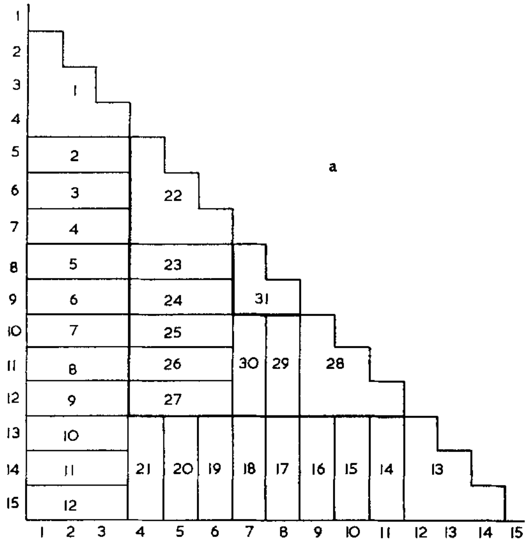
In general the number of blocks produced by the Nelder algorithm is

$$B = T - N + p + 1$$

and a lower bound for B is

$$\max\left\{\left[\frac{N(N-1)}{M(M-1)}\right], \left[\frac{N}{M}\right] + \left[\frac{N-M}{M-1}\right]\right\}.$$

An obvious variant of Nelder's original problem seeks to minimize B instead of T (see algorithm $N5$ below).



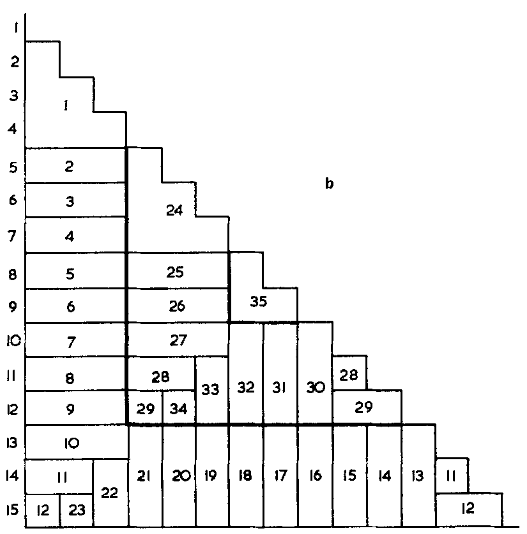


FIG. 1. Triangular diagrams—N = 15, M = 4: (a) Nelder's algorithm. (b) algorithm $N1$.

5. Other Algorithms

(a) *Algorithm N2*

This is illustrated for $N = 15$, $M = 4$ in Figure 2a, and for $N = 10$, $M = 5$ in Figure 2b. Once again the triangular diagrams are divided into nested L-shaped regions, but now each of these regions is filled with block numbers in the opposite direction from the previous one. Block numbers run consecutively round the outside of each L except in its last $M - 2$ positions. The distinctive feature of this algorithm is the method

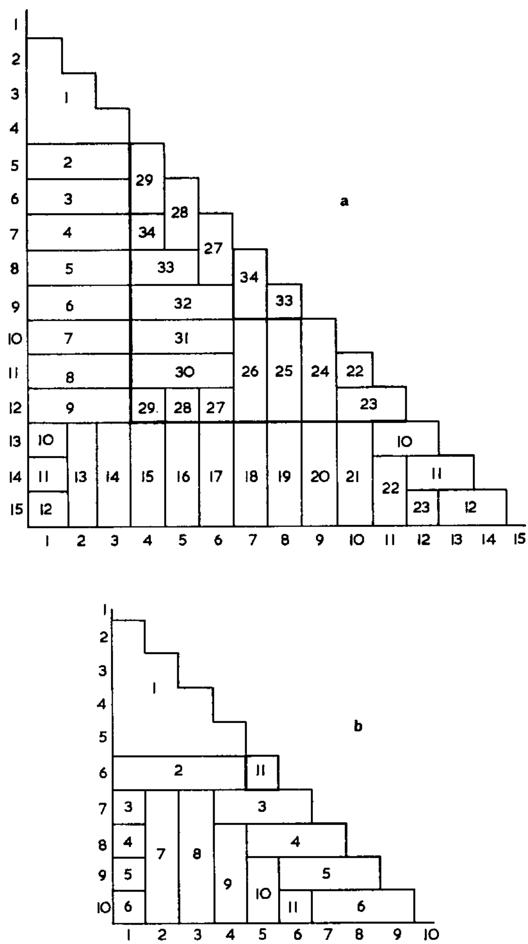


Fig. 2. Triangular diagrams—algorithm $N2$: (a) $N = 15$, $M = 4$. (b) $N = 10$, $M = 5$.

TABLE 2

Values of $T, M \geqslant 3, 2M \leqslant N \leqslant 12$

Lower bound

M \ N	6	7	8	9	10	11	12
3	9	12	16	20	24	29	35
4			12	14[a]	17	21	24
5					15	17	19
6							18

Nelder's algorithm

M \ N	6	7	8	9	10	11	12
3	10	13	17	21	26	31	37
4			13	16	19	23	27
5					16	19	22
6							19

Algorithm N2

M \ N	6	7	8	9	10	11	12
3	9	12	16	20	24	29	35
4			13	15	18	22	26
5					16	19	21
6							19

Algorithms N3 + N4

M \ N	6	7	8	9	10	11	12
3	9	12	16	20	24	29	35
4			12	15	18	22	26
5					15	18	21
6							18

Designs with the smallest known values of T

M \ N	6	7	8	9	10	11	12
3	9	12	16	20	24	29	35
4			12	15	18[b]	21	25[b]
5					15	18	21
6							18

[a] This lower bound has been proved to be unattainable.
[b] See Section 6.

TABLE 3

Values of B, $M \geqslant 3$, $2M \leqslant N \leqslant 12$

Lower bound

M \ N	6	7	8	9	10	11	12
3	5	7	10	12	15	19	22
4			5	6	8	10	11
5					5	6	7
6							5

Nelder's algorithm

M \ N	6	7	8	9	10	11	12
3	7	9	13	16	21	25	31
4			8	10	12	16	19
5					9	11	13
							10

Algorithm N2

M \ N	6	7	8	9	10	11	12
3	7	10	14	18	22	27	33
4			9	11	14	18	22[a]
5					11	13	15
							13

Algorithm N3

M \ N	6	7	8	9	10	11	12
3	7	10	14	18	22	27	33
4			9	12	14	18	22[a]
5					11	14	16
6							13

Algorithm N4

M \ N	6	7	8	9	10	11	12
3	7	10	14	18	22	27	33
4			9	11	14	18	22[a]
5					11	13	15
6							13

[a] These values can all be reduced to 21 by making the last two transfers simultaneously.

for forming blocks $N - 2M + 3$, $N - 2M + 4, \ldots, N - M + 1$ in the first L, and the corresponding blocks in the other L's.

If $N \geqslant 3M - 4$, then $M - 2$ elements must be transferred to form the $(N - 2M + 3)$th block; however if $N = 3M - 5$ only $M - 3$ need be transferred, if $N = 3M - 6$ only $M - 4$, and so on.

Tables 2 and 3 show how the values of T and B for this algorithm compare with the lower bounds, and with the values for Nelder's algorithm, when $N \leqslant 12$ and when Nelder's algorithm gives $T >$ lower bound. It will be seen that Nelder's algorithm produces values of B less than or equal to those for $N2$, but values of T greater than or equal to those for $N2$.

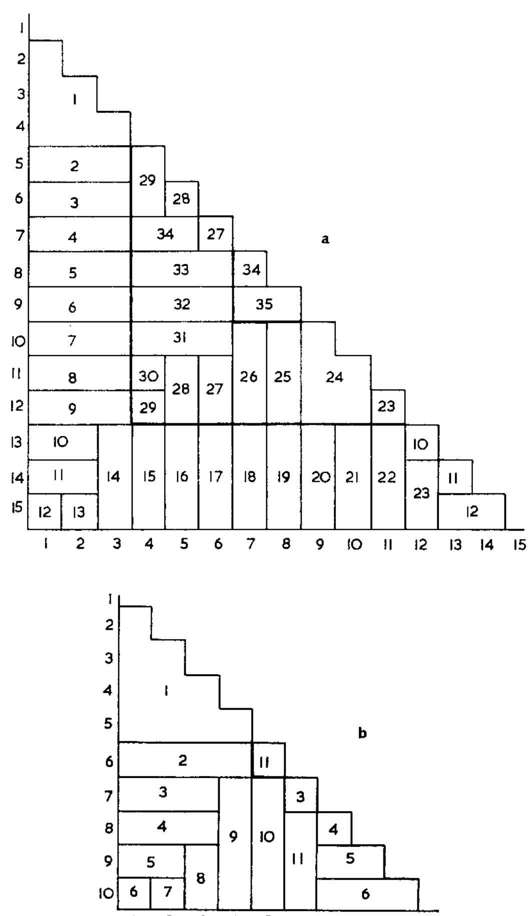
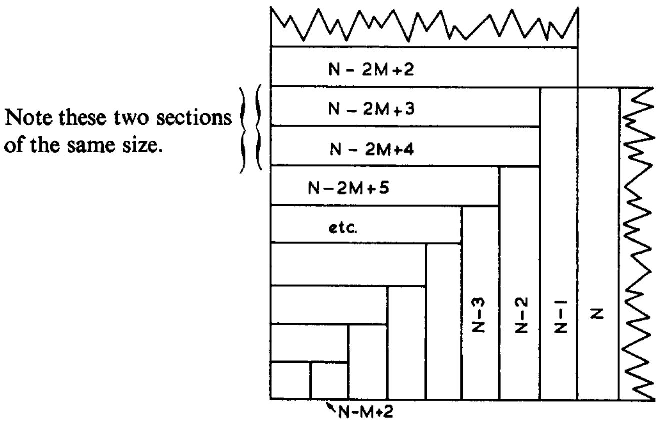


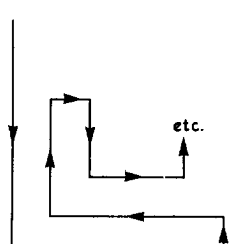
FIG. 3. Triangular diagrams—algorithm $N3$: (a) $N = 15$, $M = 4$. (b) $N = 10$, $M = 5$.

(b) *Algorithm N*3

This is illustrated in Figure 3. Comparison of Figures 2 and 3 shows that algorithms $N2$ and $N3$ are very similar; indeed they are identical for $M = 3$. The first difference for $M > 3$ is brought about by the way in which the corner of each L-shaped region is treated; for $N3$ the pattern in the first region is:



(When constructing designs from the triangular diagrams, care must be taken in the first L that blocks $N - M + 2$, $N - M + 3, \ldots, N - 2$ are so formed as to permit the formation of block $N - 1$. Similar care is required for each subsequent L.) The other difference is in the formation of the second block for each L after the first; these blocks are got by transferring more than one variate. Going round all but the last $M - 3$ positions on the outside of each L, block numbers fall consecutively as follows:



Tables 2 and 3 show that, when $N \leqslant 12$ and Nelder's algorithm gives $T >$ lower bound, there is little to choose between $N2$ and $N3$. Values of T are the same for the two algorithms, except that, for four sets of M

and N, T is one less for $N3$ than for $N2$. For only three sets of M and N are values of B different, and then the value for $N3$ is one more than the value for $N2$.

(c) *Algorithm* $N4$

This is so similar to previous algorithms that it is not described in detail. Figure 4 and Table 2 provide the relevant information. Algorithms $N2$, $N3$, and $N4$ are equivalent for $M = 3$.

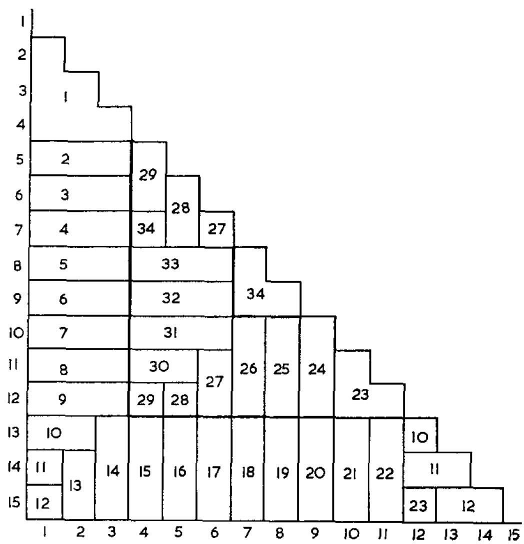


FIG. 4. Triangular diagrams—$N = 15$, $M = 4$: algorithm $N4$.

(d) *Algorithm* $N5$

This generalisation of Nelder's algorithm is illustrated by Figure 5, for which $N = 13$ and $M = 6$, and by the corresponding design

1					8	7	5	
2					9	6		
3					10			7
4					11			8
5	7	9	11	13				9
6	8	10	12					0

The algorithm differs from Nelder's in that v variates, and not just one variate, are overwritten in the "straightforward" parts of the process. (In the example, $v = 2$.) This usually makes possible a reduction in the

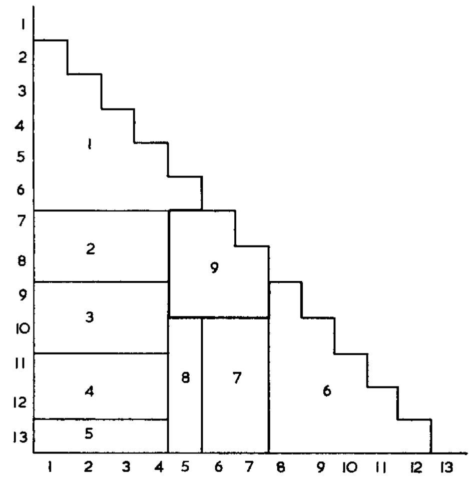


FIG. 5. Triangular diagram—$N = 13$, $M = 6$: algorithm $N5$ with $\nu = 2$.

number of blocks at the expense of an increease in the number of transfers. (In the example $T = 23$ and $B = 9$, whereas with $v = 1$ the corresponding values are 22 and 12.) In general,

$$T = N(1 + p) - \tfrac{1}{2}Mp(1 + p) + \tfrac{1}{2}vp(p - 1),$$

where p is the integral pair of $(N - v - 1)/(M - v)$. The number B is more difficult to compute when $v > 1$, because of incomplete rectangular "blocks" like numbers 5 and 8 in Figure 5; the approximation

$$B_v = ((T - N)/v) + p + 1$$

is an underestimate obtained by assuming that all "blocks" are complete.

Tables 4 and 5 list values of T and B_v for $M = 10$ and $M = 20$ and various values of N and v. The final column of Table 4 gives exact values of B when $N = 20$; the values agree well with those of B_v especially for the smaller values of v. In Tables 4 and 5, B_v is minimum when $v = \tfrac{1}{2}M$; this result cannot be universally true as it must require modification when M is odd, but it is fairly clear that the minimum is very close to

$$v = [\tfrac{1}{2}M].$$

TABLE 4

Values of B_v and T for $M = 10$, $N = 100, 50, 20$ and $v = 1(1)9$

	$N = 100$		$N = 50$		$N = 20$		
v	T	B_v	T	B_v	T	B_v	B (exact)
1	595	506	160	116	31	14	14
2	652	289	170	66	32	9	9
3	724	222	185	52	33	8	8
4	820	196	204	47	34	7	7
5	955	190	230	45	35	6	6
6	1158	217	270	48	38	7	8
7	1615	248	337	56	42	9	10
8	2170	305	470	74	52	10	12
9	4195	546	8870	133	75	18	22

TABLE 5

Values of B_v and T for $M = 20$, $N = 100, 50$ and $v = 1(1)19$

$M = 20$	$N = 100$		$N = 50$	
v	T	B_v	T	B_v
1	310	216	91	44
2	320	116	92	24
3	330	83	93	18
4	340	66	94	14
5	355	58	95	12
6	370	52	98	12
7	387	49	101	12
8	408	47	104	11
9	432	46	107	11
10	460	45	110	10
11	496	46	116	11
12	540	48	122	11
13	598	52	130	13
14	674	56	140	13
15	780	63	155	14
16	940	71	178	17
17	1207	99	215	21
18	1740	138	290	31
19	3340	257	515	56

6. Two Other Solutions Optimum for T

No known algorithm always gives the smallest possible value of T. This is shown by the following two schemes, each of which has T less than could be obtained, for the same N and M, by any algorithm given above:

(i)

1	5		7	8						11							
2		6					5	7	10								
3					1						4	3	2				5
4						9								6	8	7	

$N = 11, \quad M = 4, \quad T = 21 = \text{lower bound} \quad$ (see Table 2).

(ii)

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

$$N = 12, \quad M = 4, \quad T = 25 = 1 + \text{lower bound}.$$

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