CHARACTERIZATION OF THE MAXIMUM PROBABILITY FIXED MARGINALS r imes c CONTINGENCY TABLES *

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Abstract:

• In this paper operators i[j] and [j]k are defined, whose effects on an $r \times c$ contingency table X are to subtract 1 from x_{ij} and to add 1 to x_{kj} , respectively, so that the composition i[j]k of the two operators changes the j-th column of the contingency table without altering its total. Also a loop is defined as a composition of such operators that leaves unchanged both row and column totals. This is used to characterize the $r \times c$ contingency tables of maximum probability over the fixed marginals reference set (under the hypothesis of row and column independence). Another characterization of such maximum probability tables is given using the concept of associated U tables, a $U = \{u_{ij}\}$ table being defined as a table such that $u_{ij} > 0$, $1 \le i \le r$ and $1 \le j \le c$, and for a given set of values r_h $1 \le h < r$, $u_{h+1,j} = r_h u_{hj}$ for all j. Finally, a necessary and sufficient condition for the uniqueness of a maximum probability table in the fixed marginals reference set is provided.

Key-Words:

• $r \times c$ contingency table; maximum probability $r \times c$ contingency table; network algorithm; Fisher's exact test.

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1. INTRODUCTION

Let $X = \{x_{ij}\}$ denote an $r \times c$ contingency table, with $x_{ij} \in \mathbb{N}$ the entry in row i and column j, and let R_1, \ldots, R_r be the sums of rows, C_1, \ldots, C_c the sums of columns and $N = \sum_i R_i = \sum_j C_j$. Given the marginal sums R_i and C_j , $i = 1, \ldots, r, j = 1, \ldots, c$, let

$$\mathcal{F} = \left\{ X \mid \sum_{j=1}^{c} x_{ij} = R_i, \quad \sum_{i=1}^{r} x_{ij} = C_j \right\}$$

be the reference set of all possible $r \times c$ tables with the aforementioned marginal sums. Then, under the hypothesis of row and column independence, it is well known that for $X \in \mathcal{F}$,

(1.1)
$$P(X) = \frac{\prod_{i} R_{i}! \prod_{j} C_{j}!}{N! \prod_{ij} x_{ij}!}.$$

A problem that is of interest is that of obtaining a table $X \in \mathcal{F}$ which maximizes (1.1), i.e. a maximum probability fixed marginals $r \times c$ table (MPT). This problem arises, for example, as part of the best known and most efficient algorithm for calculating the p-value of Fisher's exact test in unordered $r \times c$ contingency tables: the network algorithm of Mehta and Patel [2]. The application of this algorithm to an observed $r \times c$ table requires, for many of the nodes in the network, the calculation of the longest subpath from each node to the terminal node, and this involves (many) repeated applications of the calculation of maximum probability $r \times c'$ tables ($c' \le c$) for given fixed marginal sums.

Methods for obtaining these MPTs have been proposed by Mehta and Patel [2] and by Joe [1]. The most general is that of Joe, which is based on a necessary condition for the MPTs, and generally involves the (recursive) construction of a subset of \mathcal{F} in which the MPTs are contained, and obtaining these by inspecting the probabilities of the tables of this subset. However, the computation time for the Joe method grows exponentially when r or c increase, and it is practically unviable for relatively large values of r and c.

In the particular case of $2 \times c$ tables, Requena and Martín [3] present a necessary and sufficient condition for the MPTs. Based on this characterization, Requena and Martín [4] propose a general and very efficient method for obtaining the MPTs, and Requena and Martín [5] present some modifications in the network algorithm of Mehta and Patel for $2 \times c$ tables, which produce a drastic reduction in computation time.

In order to obtain general and more efficient methods for obtaining the MPTs, in the general case of $r \times c$ tables, it is important that these methods are based on necessary and sufficient conditions for the MPTs. In this sense,

in this paper, two necessary and sufficient conditions are presented in order to characterize the MPTs. However, this characterization is not a generalization of the one previously shown in Requena and Martín [3]; it is completely different, although logically in the particular case of $2 \times c$ tables, the characterization presented in this paper is equivalent to that of Requena and Martín [3].

In Section 2 of this paper, we define and study the concepts of sequence and loop which we will use in the characterization of the MPTs, which is presented in Sections 3 and 5. In Section 3 we present the characterization as a more theoretical result, while in Section 5, with a more applied purpose, the characterization is presented in terms of a particular type of tables (U tables), which we define and study in Section 4. Finally, in Section 6 we provide a necessary and sufficient condition of the uniqueness of the MPT.

2. SEQUENCES AND LOOPS

The characterization of the MPTs which we set out in the following sections is based on the concepts of *sequence* and *loop*. In order to define these concepts, we will start by defining some operators, which are applied to an $r \times c$ table $X = \{x_{ij}\}.$

We define the operator i[j] whose effect on X is to subtract 1 from x_{ij} leaving all the other entries unchanged, and the operator [j]k whose effect on X is to add 1 to x_{kj} leaving all the other entries unchanged. Based on these operators, we define the operator i[j]k as the composition of i[j] with [j]k ($i[j] \circ [j]k = i[j]k = [j]k \circ i[j]$). It is clear that i[j]k changes the j-th column of the table without altering its sum. Also, as i[j]i is the identity operator, i[j] and [j]i are inverse of each other.

Definition 2.1. Given an $r \times c$ table $X = \{x_{ij}\}$, and given the rows $i_0, i_1, ..., i_k$ (with $i_{h-1} \neq i_h$) and columns $j_1, ..., j_k$ (not all equal), a sequence is the composition of $i_0[j_1]i_1$ with $i_1[j_2]i_2, ...$ with $i_{k-1}[j_k]i_k$, which for simplicity we denote by $i_0[j_1]i_1[j_2]i_2....i_{k-1}[j_k]i_k$ ($1 \leq i_h \leq r$ and $1 \leq j_h \leq c$).

Definition 2.2. Given an $r \times c$ table $X = \{x_{ij}\}$, a loop is a sequence in which $i_k = i_0$, i.e. $i_0[j_1]i_1[j_2]i_2....i_{k-1}[j_k]i_0$.

From this point onward in the text, when we write a sequence as

$$i_0[\cdot]i_1....i_{k-1}[\cdot]i_k$$

it will be understood that it is a sequence for an unspecified set of columns $j_1, ..., j_k$.

In terms of the effect of applying a sequence or a loop to a table X, we can understand a sequence or a loop as a succession of operators $i_{h-1}[j_h]$ and $[j_h]i_h$ (or as a succession of operators $i_{h-1}[j_h]i_h$), h=1,2,...,k, applied in a successive manner: each operator is applied to the table obtained by applying the previous one (the first one is applied to X). For example, applying the sequence 1[2]2[3]4 to a 4×4 table has the effect of adding 1 in x_{43} , subtracting 1 in x_{23} , adding 1 in x_{22} and subtracting 1 in x_{12} . A sequence applied to X does not alter the column sums, but it alters the i_0 -th and the i_k -th row sum. However a loop does not alter neither the column sums nor the row sums.

Logically, if one removes pairs of inverse operators from a sequence (or loop) in an appropriate way, one would obtain a new and more reduced sequence (or loop), but one which would have the same effect on X as the previous one. In this sense, we give the following definition:

Definition 2.3. Given an $r \times c$ table $X = \{x_{ij}\}$, two sequences (or two loops) are *equivalent* when they have the same effect on X.

Thus, we have classes of equivalent sequences (or loops). Within a same class, the difference between two sequences (or two loops) is a set of pairs of inverse operators.

In the same way, we will define the equivalence between a sequence (or loop) and a group of several sequences (or loops), based on the understanding that the sequences (or loops) which compose the group are applied in a successive manner: each sequence (or loop) is applied to the table obtained by applying the previous one.

Because the effect of an operator [j]i on X is to add 1 to x_{ij} , and the effect of an operator i[j] is to subtract 1 from x_{ij} , and denoting the number of operators [j]i and i[j] in the loop by n_{ij} and n'_{ij} , respectively, any loop can be represented by means of a table $D = \{d_{ij}\}$, defined as $d_{ij} = n_{ij} - n'_{ij}$, i = 1, ..., r and j = 1, ..., c. It is easy to see that a table D defined thus has all its marginal sums equal to 0. Reciprocally, any table $D = \{d_{ij}\}$, with d_{ij} being integer numbers and marginal sums equal to 0, will represent a loop or a group of loops. Moreover, applying a loop to a table X is equivalent to adding the corresponding table D to it, thereby obtaining a new table X' with entries $x'_{ij} = x_{ij} + d_{ij}$, and with the same marginal sums as X. But X' is not necessarily an $r \times c$ table, because some of the entries x'_{ij} could be negative. If this happens (although we can consider such a loop) we would not consider that table X'. This is taken into account in Section 3.

Example 2.1. Let us consider the loop 2[1]3[4]1[1]3[2]4[3]2. Applying this loop to a 4×4 table X, we will obtain a new 4×4 table X'. Let us see it for some i's and j's. For i=2 and j=1, because there is only one operator $2[1](n'_{21}=1)$ and no operator $[1]2(n_{21}=0)$, $d_{21}=0-1=-1$ and we have to subtract 1 from $x_{21}(x'_{21}=x_{21}-1)$. Likewise, for i=3 and j=1 there are two operators $[1]3(n_{31}=2)$ and no operator $3[1](n'_{31}=0)$, therefore $d_{31}=2-0=2$

and we have to add 2 to x_{31} ($x'_{31} = x_{31} + 2$). In a similar way for the other *i*'s and *j*'s. The complete table *D* that represent this loop is

-1	0	0	1
-1	0	1	0
2	-1	0	-1
1	1	-1	0

and adding this table D to the table X we obtain the table X'.

If in a sequence (or loop) B we invert the order of the i_h 's and also of the j_h 's (each operator would be substituted by its inverse one), we will obtain a new sequence (or loop): we will call it *inverse* of B. For example, the sequence inverse of 1[2]2[3]4 is 4[3]2[2]1. Furthermore, if $D = \{d_{ij}\}$ represents a loop B, then $-D = \{-d_{ij}\}$ will represent the inverse of B.

Let us now define a particular type of loop which we will use in the characterization of the MPTs.

Definition 2.4. For $1 < k \le \min(r, c)$, an order k simple loop, is a loop $i_0[j_1]i_1[j_2]....i_{k-1}[j_k]i_0$ in which all the k rows $i_0, i_1,, i_{k-1}$ are different and all the k columns $j_1,, j_k$ are different. We will call these the k rows and the k columns of the loop.

Observe that such simple loop leaves r-k rows and c-k columns of X unchanged.

In order to distinguish them from the general case, we will write the tables D which represent order k simple loops as $E = \{e_{ij}\}$. In an order k simple loop, since all of its rows i_h (and all of its columns j_h) are different, both n_{ij} and n'_{ij} can only be equal to 1 or 0, and $n_{ij} + n'_{ij} \leq 1$. Therefore, the corresponding table E will have all of its entries e_{ij} equal to 0, except for a 1 and a -1 in each of the k rows and in each of the k columns of the loop. Moreover, any table E of this type will represent an order k simple loop. For example, the table

0	-1	0	1	0
-1		0	0	0
1		0	-1	0
0	0	0	0	0

represents the order 3 simple loop 2[1]3[4]1[2]2.

It is obvious that if one subtracts from a table D (different to any table E) a table E whose $e_{ij} \neq 0$ have the same sign as the corresponding d_{ij} in D, this will result in another type D table (or type E). Therefore, it is easy to deduce that

any table D is the sum of several type E tables, i.e. any loop (represented by D) can be broken down into a group of simple loops, which together are equivalent to D. For example:

The loop represented by the table D on the left-hand side is broken down into the (equivalent) group of three simple loops on the right-hand side (the first and the second are order 2 and the third order 3).

Finally, for any $r \times c$ table $X = \{x_{ij}\}$ and for any loop, from this point onward we will use expressions of the type

(2.1)
$$Q = \prod_{j \in J} \frac{x_{bj} + 1}{x_{aj}},$$

where J represents the set of columns j's (which are not necessarily all different) corresponding to the [j]'s of the operators a[j]b in the loop, and a and b are the rows of these operators. In this type of expression, a one-to-one relation between the terms of the product and the set of operators a[j]b of the loop is established. For example, for the loop 2[1]4[5]1[3]2

$$Q = \frac{x_{41} + 1}{x_{21}} \cdot \frac{x_{15} + 1}{x_{45}} \cdot \frac{x_{23} + 1}{x_{13}}.$$

3. CHARACTERIZATION OF THE MAXIMUM PROBABILITY r imes c TABLES

The simple loops defined in the previous section are used in the following result to characterize the MPTs.

Theorem 3.1. The necessary and sufficient condition for $X = \{x_{ij}\} \in \mathcal{F}$ to be an MPT is that

$$(3.1) \qquad \prod_{j \in J} \frac{x_{bj} + 1}{x_{aj}} \ge 1$$

for every order k simple loop $E = \{e_{ij}\}$ and every k, $1 < k \le \min(r, c)$, where J is the set of the k columns of the loop, and for each $j \in J$, k and k are the rows such that k are the rows such that k and k are the rows such that k and k are the rows such that k are the

Proof: Let X be an MPT, and let us consider X' = X + E, for any order k simple loop E, $1 < k \le \min(r, c)$. All of the elements of X and X' will be identical, except $x'_{bj} = x_{bj} + 1$ and $x'_{aj} = x_{aj} - 1$ for $j \in J$, and a, b and J previously defined. Firstly, if E is an order k simple loop such that x'_{aj} is a negative integer (for some a and j), that is, X' is not an $r \times c$ table, then $x_{aj} = 0$ and, hence, the condition (3.1) is fulfilled for that E. Secondly, if (on the contrary) E is such that X' is an $r \times c$ table ($X' \in \mathcal{F}$), then from expression (1.1), and because $P(X) \ge P(X')$, we obtain

$$\frac{P(X)}{P(X')} = \prod_{j \in J} \frac{(x_{bj} + 1)! (x_{aj} - 1)!}{x_{bj}! x_{aj}!} = \prod_{j \in J} \frac{x_{bj} + 1}{x_{aj}} \ge 1.$$

Therefore, for an MPT, (3.1) is fulfilled for all E of order k.

In order to prove the sufficient condition one must note, in the first place, that if an $r \times c$ table fulfils (3.1) for every simple loop, it will fulfil said expression for an order k simple loop E, and also for the inverse loop -E (which is also an order k simple loop). For this reason

$$(3.2) \qquad \prod_{j \in J} \frac{x_{aj} + 1}{x_{bj}} \ge 1$$

will also be fulfilled with a, b and J defined for E as in the formulation of the theorem. Thus, for each E, (3.1) and (3.2) will be fulfilled. The proof of the sufficient condition in the case that there is only one $r \times c$ table of \mathcal{F} fulfilling (3.1) is trivial. Therefore, we will assume that there is more than one. Let $X \in \mathcal{F}$ be an MPT which will obviously fulfil (3.1). It will be necessary to prove that for any $X' \in \mathcal{F}$ satisfying (3.1) for all order k simple loops, P(X') = P(X) must be fulfilled.

It is clear that X' can always be written as X' = X + D, when D is a table representing a loop (or group of loops), which can be broken down into a group of tables E's (simple loops). According to this type of decomposition (as we have seen in the previous section), for any of these E's, considering $j \in J$, a and b defined as before, the signs of e_{aj} and e_{bj} should be the same as those of their corresponding d_{aj} and d_{bj} in table D. Moreover, because X' fulfils (3.1) and (3.2) for any of these E's, we can write

(3.3)
$$\prod_{j \in J} \frac{x'_{bj}}{x'_{aj} + 1} = \prod_{j \in J} \frac{x_{bj} + d_{bj}}{x_{aj} + d_{aj} + 1} \le 1$$

for each E, and because X also fulfils (3.1), we have that

$$(3.4) \qquad \prod_{j \in J} \frac{x_{bj} + 1}{x_{aj}} \ge 1$$

for each E. From this expression, and because the d_{bj} 's are positive and the d_{aj} 's are negative,

(3.5)
$$Q' = \prod_{j \in I} \frac{x_{bj} + d_{bj}}{x_{aj} + d_{aj} + 1} \ge 1$$

will be fulfilled. Moreover, if any $d_{bj} > 1$ or any $|d_{aj}| > 1$ we will obtain Q' > 1, which would contradict (3.3). Hence $d_{bj} = 1$ and $d_{aj} = -1$, and from (3.3) and (3.5) we obtain

(3.6)
$$\prod_{j \in J} \frac{x_{bj} + 1}{x_{aj}} = 1.$$

Since the above is valid for any of the E's in which D is broken down, on the one hand we will obtain $|d_{hl}| \leq 1$ for all h and l, hence for every $d_{hl} \neq 0$ there will be one and only one of the loops E's such that $e_{hl} = d_{hl}$. On the other hand, considering the expression (3.6) for all the E's in which D has been broken down, we will obtain

(3.7)
$$\frac{\prod_{hl \in D+} (x_{hl} + 1)}{\prod_{hl \in D-} x_{hl}} = 1$$

where D+ and D- are the sets of subindices hl such that $d_{hl}=1$ and $d_{hl}=-1$, respectively. Finally, from (1.1)

$$\frac{P(X)}{P(X')} = \frac{\prod_{hl \in D+} (x_{hl} + 1)! \prod_{hl \in D-} (x_{hl} - 1)!}{\prod_{hl \in D+} x_{hl}! \prod_{hl \in D-} x_{hl}!} = \frac{\prod_{hl \in D+} (x_{hl} + 1)}{\prod_{hl \in D-} x_{hl}}$$

is obtained, and from (3.7) we will obtain P(X') = P(X).

From this theorem, and from what has been said in the proof, the two following results are easily deduced:

Theorem 3.2. If X is an MPT and E an order k simple loop for which

(3.8)
$$\prod_{j \in J} \frac{x_{bj} + 1}{x_{aj}} = 1$$

holds, where J, a and b are defined as in Theorem 3.1, then X' = X + E is also an MPT.

Theorem 3.3. If two tables, X and X', belonging to \mathcal{F} are MPTs, then the difference between both tables is one or several simple loops, such that (3.8) holds for X and for each of these simple loops. Moreover the following always holds

$$|x'_{hl} - x_{hl}| \le 1$$
 $\forall h, l$

Finally, the following result extends expression (3.1) to any loop.

Theorem 3.4. Given the expression Q defined in (2.1), if X is an MPT, for any loop the following always holds

(3.9)
$$Q = \prod_{j \in J} \frac{x_{bj} + 1}{x_{aj}} \ge 1$$

where J is the set of columns j's corresponding to the [j]'s of the loop, and a[j]b are the operators that compose the loop.

Proof: From Theorem 3.1, for simple loops it is obvious that (3.9) is fulfilled. In the case of non-simple loops, if the loop is represented by a table D, it can be decomposed into a set of n simple loops. Representing the expression (2.1) for the simple loop h ($1 \le h \le n$) by Q_h , we will obtain that

$$Q = \prod_{h=1}^{n} Q_h$$

and because $Q_h \geq 1$ for all h (from Theorem 3.1), we obtain $Q \geq 1$. Finally, if the loop is not represented explicitly by any type D table, there will always be an equivalent loop represented by a table D, and the difference between both loops will only be a set of pairs of inverse operators. Without loss of generality, let us suppose that the difference is the pair a[b], [b]a. Then, according to what was said when defining expression (2.1), and decomposing (as before) the loop D into n simple loops, we will obtain

$$Q = \frac{x_{ab} + 1}{x_{ab}} \prod_{h=1}^{n} Q_h > 1.$$

Therefore, to sum up, (3.9) is fulfilled for every loop.

4. A PARTICULAR TYPE OF TABLES: THE *U* TABLES

We will now proceed to define and study a type of tables (U tables) that is particularly important in a new characterization of the MPTs.

Definition 4.1. A U table is a table $\{u_{ij}\}$ with r rows and c columns $(1 \le i \le r \text{ and } 1 \le j \le c)$, in which u_{ij} are strictly positive real values $(u_{ij} > 0)$ and such that, for a given set of values r_h , $1 \le h < r$, $u_{h+1,j} = r_h u_{hj}$ for all j.

Given this definition, from this point onward $r_h = u_{h+1,j}/u_{hj}$ will represent the ratio between the consecutive rows h and h+1 of the U table. On the other hand, it is obvious that for any two rows h and i, the ratio $r_{hi} = u_{ij}/u_{hj}$ is constant for all j, and $r_{ih} = 1/r_{hi}$. In particular, $r_{h,h+1} = r_h$. Moreover, for h < i, r_{hi} coincides with the product of the ratios between consecutive rows from

row h to row i, i.e., $r_{hi} = r_h r_{h+1} \dots r_{i-1}$. So we will also denote this product by r_{hi} . For example, $r_{14} = r_1 r_2 r_3$. Furthermore, it will always be understood that $r_{hh} = 1$.

Let us consider some properties of this type of table, the proofs for which are very straightforward.

Property 4.1. If any row or column of a U table is multiplied by a constant, or the rows (or columns) of a U table are interchanged, another U table is obtained.

Property 4.2. For any two rows h and i of a U table, $r_{hi} = 1/r_{ih}$ is always fulfilled. Moreover, given the rows h, s and i ($h \le s \le i$) of a U table, $r_{hi} = r_{hs}r_{si}$ will always hold.

Property 4.3. In a U table $\{u_{ij}\}$ the following always holds:

$$\prod_{j \in J} \frac{u_{bj}}{u_{aj}} = 1$$

for every order k simple loop $E = \{e_{ij}\}$, and every k, $1 < k \le \min(r, c)$, where J is the set of the k columns of the loop, and for each $j \in J$, k and k are the rows such that k are the rows such that k and k are the rows such that k and k are the rows such that k are th

The following are two examples of U tables.

Example 4.1. A table $\{u_{ij}\}$ in which all the elements in each row are equal (that is, $u_{ij} = A_i > 0$ for all j) is a U table.

Example 4.2. Given an $r \times c$ table, with marginal sums $\{R_i\}$ and $\{C_j\}$, the table of expected frequencies $\{E_{ij}\}$, defined as $E_{ij} = R_i C_j / N$, is a U table. In this case, the ratios between the rows are $r_{hi} = R_i / R_h$. It would also be a U table if R_i and C_j were strictly positive real values.

The following definition establishes a link between the U tables and the $r \times c$ tables.

Definition 4.2. We say that a U table $\{u_{ij}\}$ is associated with an $r \times c$ table $X = \{x_{ij}\}$ if the following holds

$$(4.1) 0 \le u_{ij} - x_{ij} \le 1 \forall i, j, \quad 1 \le i \le r, \quad 1 \le j \le c$$

From this definition and from the definition of U tables, it is easy to deduce that the U table associated with an $r \times c$ table, if it exists, is not necessarily unique (and generally it is not so).

Given an $r \times c$ table $X = \{x_{ij}\}$, is there always a U table $\{u_{ij}\}$ associated with it? In order for such a U table to exist, $u_{ij} = x_{ij} + \varepsilon_{ij}$ would have to be

fulfilled for all i and j, with $0 \le \varepsilon_{ij} \le 1$. Now, because the ratios between the rows in the U table would be

$$r_{hi} = u_{ij}/u_{hj} = (x_{ij} + \varepsilon_{ij})/(x_{hj} + \varepsilon_{hj})$$
 $\forall j,$

and so, for a given j, the minimum and the maximum value for r_{hi} would be $x_{ij}/(x_{hj}+1)$ and $(x_{ij}+1)/x_{hj}$, respectively, then, r_{hi} should fulfil

$$m_{hi}^{o} \leq r_{hi} \leq M_{hi}^{o}$$
,

where

$$m_{hi}^{\text{o}} = \max_{j} \{x_{ij}/(x_{hj}+1)\}$$
 and $M_{hi}^{\text{o}} = \min_{j} \{(x_{ij}+1)/x_{hj}\}.$

In the particular case of consecutive rows (i.e., i = h + 1), the limits for the ratios r_h would be

$$(4.2) m_{h,h+1}^{o} \le r_h \le M_{h,h+1}^{o} 1 \le h < r.$$

Moreover, because $r_{hi} = r_h r_{h+1} \dots r_{i-1}$, the limits for the products of ratios r_{hi} should likewise be

(4.3)
$$m_{hi}^{o} \le r_{hi} \le M_{hi}^{o} \qquad 1 \le h < i - 1 < r.$$

Therefore, in principle, in order for the said U table to exist, there must be a set of ratios r_h that fulfil (4.2) and whose products r_{hi} fulfil (4.3).

Remark 4.1. If $X = \{x_{ij}\}$ is an MPT, applying expression (3.1) to all order 2 simple loops, we obtain $x_{ij'}/(x_{hj'}+1) \leq (x_{ij}+1)/x_{hj}$ for all h, i, j and j'. Hence the following will always be fulfilled

$$m_{hi}^{\mathrm{o}} \leq M_{hi}^{\mathrm{o}} \qquad \forall h,\, i, \quad \ 1 \leq h < i \leq r.$$

Remark 4.2. For any two rows h and i, and from the definition of the limits m_{hi}^{o} and M_{hi}^{o} , we easily obtain that

$$M_{hi}^{\rm o} = 1/m_{ih}^{\rm o}$$
.

We can use this expression to obtain m_{pq}^{o} and M_{pq}^{o} for p > q.

We will call these limits $m_{h,h+1}^{\text{o}}$, $M_{h,h+1}^{\text{o}}$, m_{hi}^{o} and M_{hi}^{o} (for each ratio r_h and each product r_{hi}) initial limits and, in general, we will refer to them (without specifying the subindices) as limits m^{o} 's and limits M^{o} 's.

Example 4.3. In order for there to be a U table associated with the 3×3 table

there must be a set of ratios, r_1 and r_2 , that fulfils (4.2) and whose product $r_{13} = r_1 r_2$ fulfils (4.3). In this case, the initial limits are: $0.714 \le r_1 \le 0.750$, $0.417 \le r_2 \le 0.429$ and $0.294 \le r_{13} \le 0.300$. In principle, we can take appropriate values of r_1 and r_2 in order to construct an associated U table.

If there are appropriate values of r_h such that (4.2) and (4.3) are fulfilled, and considering the initial limits m° 's and M° 's as the current limits for r_h and r_{hi} , they can be redefined (in the sense that we will show below) given the limits of the other products and ratios, thus obtaining new and more accurate limits for r_h and r_{hi} . In general we will denote these new limits as m_{hi} and M_{hi} .

For example, in $3 \times c$ tables, for the product r_{13} , because $r_{13} = r_1 r_2$, the restriction $m_{12}^{\rm o} m_{23}^{\rm o} \leq r_{13} \leq M_{12}^{\rm o} M_{23}^{\rm o}$ must also be fulfilled, which means r_{13} should fulfil $m_{13} \leq r_{13} \leq M_{13}$, and the new limits will be

$$m_{13} = \max\{m_{13}^{\text{o}}, m_{12}^{\text{o}}m_{23}^{\text{o}}\} \text{ and } M_{13} = \min\{M_{13}^{\text{o}}, M_{12}^{\text{o}}M_{23}^{\text{o}}\}.$$

Likewise, for the ratio r_1 , because $r_1 = r_{13}/r_2$, the restriction $m_{13}^o m_{32}^o \le r_1 \le M_{13}^o M_{32}^o$ must also be fulfilled, and the new limits for r_1 will be

$$m_{12} = \max\{m_{12}^{\text{o}}, m_{13}^{\text{o}}m_{32}^{\text{o}}\} \text{ and } M_{12} = \min\{M_{12}^{\text{o}}, M_{13}^{\text{o}}M_{32}^{\text{o}}\}.$$

In a similar way, the new limits for r_2 are

$$m_{23} = \max\{m_{23}^{\circ}, m_{21}^{\circ}m_{13}^{\circ}\} \text{ and } M_{23} = \min\{M_{23}^{\circ}, M_{21}^{\circ}M_{13}^{\circ}\}.$$

Example 4.3 revisited. Starting from the previously calculated initial limits in Example 4.3, we calculate the new limits at the second stage as indicated in the previous paragraph, and we obtain

$$0.298 \le r_{13} \le 0.300$$
, $0.714 \le r_1 \le 0.720$ and $0.417 \le r_2 \le 0.420$.

In $4 \times c$ tables, for the product r_{13} , because from Property 4.2 $r_{13} = r_1 r_2$ and $r_{13} = r_{14}/r_3$, the restrictions $m_{12}^o m_{23}^o \le r_{13} \le M_{12}^o M_{23}^o$ and $m_{14}^o m_{43}^o \le r_{13} \le M_{13}^o M_{43}^o$ must also be fulfilled, which means r_{13} has to fulfil $m_{13} \le r_{13} \le M_{13}$, and the new limits will be:

$$m_{13} = \max\{m_{13}^{\text{o}}, m_{12}^{\text{o}}m_{23}^{\text{o}}, m_{14}^{\text{o}}m_{43}^{\text{o}}\}$$

and

$$M_{13} = \min \{ M_{13}^{\text{o}}, M_{12}^{\text{o}} M_{23}^{\text{o}}, M_{14}^{\text{o}} M_{43}^{\text{o}} \}.$$

Likewise, for the ratio r_2 , because $r_2 = r_{13}/r_1$, $r_2 = r_{24}/r_3$ and $r_2 = r_{14}/(r_1r_3)$, the following restrictions must be fulfilled:

$$m_{21}^{\mathrm{o}} m_{13}^{\mathrm{o}} \le r_2 \le M_{21}^{\mathrm{o}} M_{13}^{\mathrm{o}},$$

$$m_{24}^{\mathrm{o}} m_{43}^{\mathrm{o}} \le r_2 \le M_{24}^{\mathrm{o}} M_{43}^{\mathrm{o}},$$

$$m_{21}^{\mathrm{o}} m_{14}^{\mathrm{o}} m_{43}^{\mathrm{o}} \le r_2 \le M_{21}^{\mathrm{o}} M_{14}^{\mathrm{o}} M_{43}^{\mathrm{o}}.$$

Thus r_2 must fulfil that $m_{23} \le r_2 \le M_{23}$, and the new limits will be:

$$m_{23} = \max\{m_{23}^{\text{o}}, m_{21}^{\text{o}}m_{13}^{\text{o}}, m_{24}^{\text{o}}m_{43}^{\text{o}}, m_{21}^{\text{o}}m_{14}^{\text{o}}m_{43}^{\text{o}}\},$$

$$M_{23} = \min\{M_{23}^{\text{o}}, M_{21}^{\text{o}} M_{13}^{\text{o}}, M_{24}^{\text{o}} M_{43}^{\text{o}}, M_{21}^{\text{o}} M_{14}^{\text{o}} M_{43}^{\text{o}}\}.$$

In a similar way for r_1 , r_3 , r_{14} and r_{24} .

Remark 4.3. It is evident that the new limits will fulfil $m_{hi}^{o} \leq m_{hi}$ and $M_{hi} \leq M_{hi}^{o}$, and if $m_{hi} \leq M_{hi}$, the new intervals (m_{hi}, M_{hi}) will be contained in the corresponding initial (current) intervals (m_{hi}^{o}, M_{hi}^{o}) , both for the ratios r_h and for the products r_{hi} .

Remark 4.4. For any two rows h and i, from Remark 4.2 and from the definition of the new limits, we easily obtain that $M_{hi} = 1/m_{ih}$.

Now, taking the limits m_{hi} and M_{hi} as the current limits for the ratios and products, we can recalculate the limits in the same sense as before, obtaining new limits (for the ratios and products) which we will also denote as m_{hi} and M_{hi} . Thus we will have a recursive process, where, at each stage, the newly calculated limits will have the same property as the current limits. At each stage, we always obtain the new limits m_{hi} and M_{hi} for h < i, and we can use Remark 4.4 for h > i. In general, and at any stage of the process, we will refer to these limits (without specifying the subindices) as limits m's and limits M's.

In this process, because from Property 4.2, $r_{hi} = r_{hs}r_{si}$, $1 \le h < s < i \le r$, and $r_{hi} = r_{h'i'}/(r_{h'h}r_{ii'})$, $1 \le h' \le h < i \le i' \le r$, it is easy to see that the general expressions of the new limits, m_{hi} and M_{hi} , for r_{hi} $(1 \le h < i \le r)$ in terms of the current limits can be written as:

(4.4)
$$\max_{i',h',s} \{ m_{hs} m_{si}, h < s < i ; m_{hh'} m_{h'i'} m_{i'i}, 1 \le h' \le h < i \le i' \le r \}$$

$$(4.5) \quad \min_{i'.h'.s} \left\{ M_{hs} M_{si} , \ h < s < i ; \ M_{hh'} M_{h'i'} M_{i'i} , \ 1 \le h' \le h < i \le i' \le r \right\},$$

where the terms on the right-hand side of the expressions correspond to the current limits of the ratios and products (these will coincide with the initial limits m^{o} 's and M^{o} 's in the first stage of the process), and where we understand that $m_{qq} = M_{qq} = 1$.

In particular, taking i = h + 1 in (4.4) and (4.5) we will obtain the limits for the ratios r_h :

(4.6)
$$m_{h,h+1} = \max_{i',h'} \left\{ m_{hh'} m_{h'i'} m_{i',h+1}, \quad 1 \le h' \le h < i' \le r \right\},$$

$$(4.7) M_{h,h+1} = \min_{i',h'} \{ M_{hh'} M_{h'i'} M_{i',h+1}, 1 \le h' \le h < i' \le r \}.$$

If all the intervals (m_{hi}, M_{hi}) are not empty $(m_{hi} \leq M_{hi})$ (this we will see in Section 5), and because the new intervals (m_{hi}, M_{hi}) are contained in the corresponding current intervals, the process will converge and we will be able to obtain *final limits* for the ratios and products, and we will continue to represent these by m_{hi} and M_{hi} .

Example 4.3 revisited. For the 3×3 table of Example 4.3, given the second stage limits, the new limits obtained at the third stage are the same limits as at the second stage. Therefore, the final limits are

$$0.298 \le r_{13} \le 0.300$$
, $0.714 \le r_1 \le 0.720$ and $0.417 \le r_2 \le 0.420$.

Once the final limits have been obtained, we can answer the question posed previously more precisely. Given an $r \times c$ table X, in order for there to be a U table associated with it, there must be a set of ratios r_h that fulfils (4.2) and whose products r_{hi} fulfil (4.3), but taking (in these expressions) the final limits m_{hi} and M_{hi} instead of the initial ones. In greater detail, and taking r_h successively, there must be: first, a value r_1 such that $m_{12} \leq r_1 \leq M_{12}$; second, a value r_2 such that $m_{23} \leq r_2 \leq M_{23}$ and with the product $r_1r_2 = r_{13}$ such that $m_{13} \leq r_1r_2 \leq M_{13}$, i.e. a value r_2 such that

$$\max\{m_{23}, m_{13}/r_1\} < r_2 < \min\{M_{23}, M_{13}/r_1\},\$$

and so on. Moreover, the associated U table $\{u_{ij}\}$ would be of the form: $u_{1j} = x_{1j} + \varepsilon_{1j} \ (0 \le \varepsilon_{1j} \le 1)$ and $u_{ij} = u_{1j}r_{1i}, \ 1 < i \le r, \ 1 \le j \le c$.

We can express all this in general form by saying that, given an $r \times c$ table X, in order for there to be a U table associated with X, it must be possible to take successively a set of ratios r_h , h = 1, 2, ..., r - 1, such that

(4.8)
$$\max_{1 \le s \le h} \{ m_{s,h+1}/r_{sh} \} \le r_h \le \min_{1 \le s \le h} \{ M_{s,h+1}/r_{sh} \}$$

(in which $r_{sh} = r_s r_{s+1} \cdots r_{h-1}$ and we understand that $r_{hh} = 1$) and a set of ε_{1j} ($1 \le j \le c$) (for the first row of the U table) such that (4.1) is fulfilled.

Further on in this paper, we will see that an associated U table exists for the MPTs, and only for these.

Example 4.3 revisited. Given de final limits we have calculated in this example, in order to obtain a U table associated with the 3×3 table, we can take $r_1 = 0.716$ (for example). In this case, from (4.8) we have to take a value r_2 such that $0.417 \le r_2 \le 0.419$: it may be $r_2 = 0.418$. With these ratios, and taking appropriate values for ε_{1j} , for example, $\varepsilon_{11} = 0.74$, $\varepsilon_{12} = 0.02$ and $\varepsilon_{13} = 0.99$ (we will see how to take these values in Section 5) we obtain the associated U table

16 + 0.74	10 + 0.02	6 + 0.99	
$16.74\cdot0.716$	$10.02\cdot0.716$	$6.99 \cdot 0.716$	=
$16.74 \cdot 0.716 \cdot 0.418$	$10.02 \cdot 0.716 \cdot 0.418$	$6.99 \cdot 0.716 \cdot 0.418$	

16.74	10.02	6.99
11.98	1.174	5.005
5.010	2.999	2.092

5. CHARACTERIZATION OF THE MPTs IN TERMS OF THE U TABLES

In order to characterize the MPTs in terms of the U tables we will use products of limits M's, m's, M's and m's (which we will denote by ΠM , Πm , $\Pi M^{\rm o}$ and $\Pi m^{\rm o}$, respectively), the subindices of which are chained in the sense that we are going to define.

Definition 5.1. We will say that ΠM is a product whose subindices are chained if it can be written as $M_{i_0i_1}M_{i_1i_2}...M_{i_{h-1}i_h}$. When $i_h=i_0$ we will say that the subindices of the product are circularly chained. We will say the same for products Πm , ΠM° , and Πm° .

From this definition we see that the chained subindices of a product

$$M_{i_0i_1}M_{i_1i_2}...M_{i_{h-1}i_h}$$

form a sequence $i_0[\cdot]i_1[\cdot]i_2.....i_{h-1}[\cdot]i_h$ (without specifying the columns), and if $i_h = i_0$ they would form a loop. Let us give some examples. The subindices of the product $M_{23}M_{35}M_{54}$ are chained, and they form the sequence $2[\cdot]3[\cdot]5[\cdot]4$. The subindices of the product $m_{13}m_{34}m_{42}m_{21}$ are circularly chained, and they form the loop $1[\cdot]3[\cdot]4[\cdot]2[\cdot]1$. Logically there will be some products whose subindices are not chained, e.g. $M_{12}M_{34}$.

We will now provide a result about products of terms M's, which we will use in the characterization of the MPTs in terms of the U tables.

Theorem 5.1. Given an MPT $X = \{x_{ij}\}$, for a product of terms M's (ΠM) whose subindices are circularly chained, the following will always hold

$$(5.1) \Pi M \ge 1.$$

Proof: As we have seen previously, the terms M's and m's are obtained by a recursive process from the M's and m's of the previous step. Specifically, from (4.5), M_{hi} is either a product $M_{hs}M_{si}$ or a product $M_{hh'}M_{h'i'}M_{i'i}$ of terms of

the previous step, whose subindices (in both cases) are chained, and they form a sequence beginning in row h and ending in row i. Now, by going back one step in the recursive process, the same can be applied to each of these M_{hs} , M_{si} , $M_{hh'}$, In this way, by going back to the initial step in the process, we will obtain that M_{hi} can always be written as a product of terms M° 's whose subindices are chained, and they form a sequence beginning in row h and ending in row h.

Thus, and in accordance with what has just been said, the product on the left-hand side of (5.1), whose subindices are circularly chained, can always be expressed as a product $\Pi M^{\rm o}$ whose subindices are circularly chained. Therefore, in order to demonstrate the theorem we will have to prove that $\Pi M^{\rm o} \geq 1$ whenever the subindices of the product are circularly chained, and they form a loop. Let the product be

$$\Pi M^{\rm o} = M^{\rm o}_{i_0 i_1} M^{\rm o}_{i_1 i_2} M^{\rm o}_{i_{s-1} i_0}$$

which, according to the definition of the terms M° 's, can be written as

$$\Pi M^{o} = \prod_{h=1}^{s} \frac{x_{i_h j_h} + 1}{x_{i_{h-1} j_h}}$$

where $j_1, j_2,, j_s$ are columns that correspond to the terms M° 's of the product, and where $i_s = i_0$. Then, if $j_1 = j_2 = = j_s$ it is evident that $\Pi M^{\circ} > 1$. Otherwise, we can consider the loop $i_0[j_1]i_1[j_2]i_2.....i_{s-1}[j_s]i_0$, which is determined by the subindices of the product, and from the expression (3.9) of the Theorem 3.4 one will obtain $\Pi M^{\circ} \geq 1$.

The following result characterizes the MPTs in terms of the U tables.

Theorem 5.2. An $r \times c$ table $X = \{x_{ij}\}$ is an MPT if, and only if, a U table $\{u_{ij}\}$ exists associated with it.

Proof: Let $\{u_{ij}\}$ be a U table associated with X. From the Property 4.3,

$$\prod_{j \in J} \frac{u_{bj}}{u_{aj}} = 1$$

for every order k simple loop, $1 < k \le \min(r, c)$, and J, a and b defined as in the said property. In addition, from (4.1) we will obtain

$$x_{aj} \le u_{aj}$$
, $x_{bj} \le u_{bj}$ and $x_{bj} + 1 \ge u_{bj}$.

Hence, for every order k simple loop, $1 < k < \min(r, c)$,

$$1 = \prod_{j \in J} \frac{u_{bj}}{u_{aj}} \le \prod_{j \in J} \frac{x_{bj} + 1}{x_{aj}}$$

and, therefore, X fulfils the condition of Theorem 3.1 and will be an MPT.

It remains to be demonstrated that if X is an MPT, there will always be a U table associated with it. For this purpose, and in accordance with what was said previously in Section 4, on the one hand we must demonstrate that there will always be a set of ratios r_h , $1 \le h < r$, which fulfil (4.8).

Firstly, in order to demonstrate that we can always take at least one value for each of the ratios r_h , $1 \le h < r$, within the respective intervals $(m_{h,h+1}, M_{h,h+1})$, which would be true if $m_{hi} \le M_{hi}$ for h < i, it will be sufficient to prove that any of the expressions which appear on the right-hand side of (4.4) is less than or equal to any of those on the right-hand side of (4.5), i.e.

$$M_{hs'}M_{s'i}/(m_{hs}m_{si}) = M_{hs'}M_{s'i}M_{is}M_{sh} \ge 1,$$

$$M_{hh'}M_{h'i'}M_{i'i}/(m_{hs}m_{si}) = M_{hh'}M_{h'i'}M_{i'i}M_{is}M_{sh} \ge 1,$$

$$M_{hs}M_{si}/(m_{hh'}m_{h'i'}m_{i'i}) = M_{hs}M_{si}M_{ii'}M_{i'h'}M_{h'h} \ge 1,$$

$$M_{hh'}M_{h'i'}M_{i'i}/(m_{hh''}m_{h''i''}m_{i''i}) = M_{hh'}M_{h'i'}M_{i'i}M_{ii''}M_{i''h''}M_{h''h} \ge 1,$$

for all s, h' and i' within the established limits in (4.4) and (4.5), and all s', h'' and i'' with the same limits of s, h' and i', respectively. But all these inequalities are true from Theorem 5.1, because the subindices of each one of the products are circularly chained.

Secondly, we will demonstrate by induction that, given the final limits, there will always be at least one set of these ratios (taken successively, r_1 , r_2 ,, r_{r-1}) that fulfil (4.8). We can always take one value for the first ratio r_1 from inside (m_{12}, M_{12}) , and it is obvious that this r_1 fulfils (4.8).

Now we have to prove that if we take a subset of ratios $r_1, r_2,, r_{h-1}$ (1 < h < r) such that they fulfil (4.8), we can always take an r_h which also fulfils (4.8). It is easy to see that if $r_1, r_2,, r_{h-1}$ fulfil (4.8), we will have

(5.2)
$$m_{ss'} \le r_{ss'} \le M_{ss'}$$
 $1 \le s < s' \le h$.

Now, for an r_h that fulfils (4.8) to exist it will be enough to prove that

(5.3)
$$m_{s,h+1}/r_{sh} \le M_{s',h+1}/r_{s'h}$$
 $\forall s, s', 1 \le s \le h 1 \le s' \le h.$

For s = s' it is obvious that this inequality is fulfilled, because we have already proved that $m_{hi} \leq M_{hi}$. For s < s', and taking into account Remark 4.4, expression (5.3) is reduced to

$$m_{s,h+1}m_{h+1,s'} \le r_{ss'}$$
 $1 \le s < s' \le h$

which is true, because from (4.4) and (5.2) we have

$$m_{s,h+1}m_{h+1,s'} \le m_{ss'} \le r_{ss'}$$
 $1 \le s < s' \le h$.

This is proved in a similar way for s > s'.

Finally, given a set of ratios $r_1, r_2, ..., r_{r-1}$ that fulfil (4.8), we must demonstrate that there will always be a U table $\{u_{ij}\}$, with $u_{1j} = x_{1j} + \varepsilon_{1j}$ ($0 \le \varepsilon_{1j} \le 1$) and $u_{ij} = u_{1j}r_{1i}$, $1 < i \le r$, $1 \le j \le c$, which is associated with X. In other words, we have to prove that there will always be values ε_{1j} , $1 \le j \le c$, such that (4.1) is fulfilled, i.e., such that

$$0 \le (x_{1j} + \varepsilon_{1j}) r_{1i} - x_{ij} \le 1 \qquad 1 \le i \le r,$$

from which it follows that the ε_{1j} , $1 \leq j \leq c$, should satisfy

(5.4)
$$\max_{1 \le i \le r} \left\{ \frac{x_{ij}}{r_{1i}} - x_{1j} \right\} \le \varepsilon_{1j} \le \min_{1 \le i \le r} \left\{ \frac{x_{ij} + 1}{r_{1i}} - x_{1j} \right\}.$$

Let us see that for every j there is a value ε_{1j} which satisfies (5.4). For this purpose, it is enough to prove that for any j and any i and i' the following holds

$$x_{ij}/r_{1i} \leq (x_{i'j}+1)/r_{1i'}$$
.

For i = i' it is trivial that this is true. For i < i' it is also true, because $r_{1i'}/r_{1i} = r_{ii'}$, and because from (4.8) (taking s = i and h + 1 = i') and from the definition of the limits M's and the limits M0's we can obtain

$$r_{ii'} \leq M_{ii'} \leq M_{ii'}^{\text{o}} \leq (x_{i'j} + 1)/x_{ij} \qquad \forall j.$$

This is proved in a similar way for i > i'.

The last part of the proof of the Theorem 5.2 shows us how we can easily obtain a U table associated with an MPT. This is summarized in the next result.

Corollary 5.1. Given an MPT $X = \{x_{ij}\}$ and a set of ratios r_h , $1 \le h < r$, fulfilling (4.8), a table $\{u_{ij}\}$ with

$$u_{ij} = \begin{cases} x_{1j} + \varepsilon_{1j} & i = 1, & 1 \le j \le c \\ u_{1j} r_{1i} & 1 < i \le r, & 1 \le j \le c \end{cases}$$

where $r_{1i} = r_1 r_2 \dots r_{i-1}$ and ε_{1j} satisfies (5.4) for all j, is a U table associated with X.

6. ON THE UNIQUENESS OF A MAXIMUM PROBABILITY $r \times c$ TABLE

The following result, based on the previous results, is a necessary and sufficient condition which characterizes the uniqueness of an MPT.

Theorem 6.1. An MPT $X = \{x_{ij}\}$ is unique if and only if

(6.1)
$$\prod_{j \in J} \frac{x_{bj} + 1}{x_{aj}} > 1$$

for every order k simple loop $E = \{e_{ij}\}$ and every k, $1 < k \le \min(r, c)$, where J is the set of the k columns of the loop, and for each $j \in J$, k and k are the rows such that k are the rows such that k and k are the rows such that k and k are the rows such that k are the

Proof: Let X be the unique MPT, which obviously will fulfil (3.1). If (3.8) is fulfilled for a simple order k loop E, then, from Theorem 3.2, X' = X + E would be an MPT, which would contradict the initial hypothesis and, thus, (6.1) is fulfilled. Reciprocally, let X be an MPT fulfilling (6.1), and let us suppose that X' is also an MPT. Then, from Theorem 3.3, the difference between both will be one or several simple loops, such that (3.8) will be fulfilled for X and for each of these simple loops, which would contradict (6.1). Hence, X is the only MPT.

7. CONCLUSIONS

The most efficient algorithm (network algorithm) to calculate the p-value of the Fisher's exact test in an $r \times c$ table requires us to calculate many times maximum probability $r \times c'$ ($c' \le c$) contingency tables, and to perform a great amount of comparisons in which the probabilities of these tables are involved. At present, the general method to obtain maximum probability fixed marginals contingency tables is based on a necessary condition for these tables, which makes that method insufficiently efficient, especially for a relatively large r or c. In this paper, we present two necessary and sufficient conditions for these maximum probability tables. This characterization, especially that which is expressed based on U tables, will allow us to construct a general algorithm for obtaining the aforementioned maximum probability contingency tables.

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