A CLASS OF STATISTICAL MODELS TO WEAKEN INDEPENDENCE IN TWO-WAY CONTINGENCY TABLES

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In this paper we study a new class of statistical models for contingency tables. We define this class of models through a subset of the binomial equations of the classical independence model. We use some notions from Algebraic Statistics to compute their sufficient statistic, and to prove that they are log-linear. Moreover, we show how to compute maximum likelihood estimates and to perform exact inference through the Diaconis-Sturmfels algorithm. Examples show that these models can be useful in a wide range of applications.

1. Introduction. One of the most popular statistical models for two-way contingency tables is the independence model. It has became a reference tool in applied research where categorical variables are concerned. In many applications the independence model is sufficient to describe and model the data, but this is not always the case. There are situations where the independence model does not fit the data and one has to detect more complex relations between the random variables. Thus, different models have been introduced in order to identify some structures in the contingency tables. Most of these models belong to the class of log-linear models. Among these, we recall the quasi-independence model, the quasi-symmetry model, the logistic regression model. As a general reference for these models see again [3]. Such models have a wide spectrum of applications in, e.g., biology, psychology and medicine. The books by Fienberg [15], Fingleton [17], Le [26] and Agresti [3] present a great deal of examples with real data sets coming from the most disparate disciplines.

A recent development in the area of statistical models for contingency tables involves the use of some tools from Algebraic Geometry to describe the structure and the properties of the models. This field is currently known under the name of Algebraic Statistics. While the first work on this direction relates to a method for exact inference, see [13], following papers have focused their attention on the geometry of the statistical models through polynomial algebra. The algebraic and geometric point of view in the analy-
ysis of probability models allows us to generalize statistical models in presence of cells with zero probability (toric models), to study its exponential structure, and to make inference feasible also in models with complex structure. This approach has been particularly useful in the fields of log-linear and graphical models. Some relevant works on these recent topics are [20], [18], [19], and [31]. An exposition of such theory, with a view toward applications to computational biology, can be found in [27].

The theoretical advances mentioned above also have a computational counterpart. In fact, many symbolic softwares traditionally conceived for polynomial algebra now include special functions or packages specifically designed for Algebraic Statistics, see e.g. CoCoA [9], 4ti2 [1], and LattE [12].

In this paper we consider statistical models for two-way contingency tables with strictly positive cell probabilities. We introduce a class of models in order to weaken independence, starting from the binomial representation of the independence model. The independence statement means that the table of probabilities has rank 1, and therefore that all $2 \times 2$ minors vanish. In the strictly positive case, this is equivalent to the vanishing of all $2 \times 2$ adjacent minors. Our models, which we call weakened independence models, are defined through a subset of the independence binomial equations. As a consequence, the independence statements hold locally and the resulting models allow us to identify local patterns of independence in contingency tables. We study the main properties of such models. In particular, we prove that they belong to the class of log-linear models, and we determine their sufficient statistic. Moreover, we compute the corresponding Markov bases, in order to apply the Diaconis-Sturmfels algorithm without symbolic computations. The relevance of our theory is emphasized by some examples on real data sets. We also show that our models have connections with a problem recently stated by Bernd Sturmfels in the field of probability models for Computational Biology, the so-called “100 Swiss Francs Problem”, see [32].

While most of the papers in Algebraic Statistics uses algebraic and geometric methods to describe and analyze existing statistical models, or to make exact inference, the main focus of this paper is the definition of a new class of models, by exploiting the Algebraic Statistics way of thinking.

Notice that we restrict the analysis to adjacent minors. Therefore, the applications are mainly concerned with binary or ordinal random variables. At the end of the paper we will give some pointers to follow-ups and extensions of this work.

In Section 2 we define the weakened independence models and we give some examples, while in Section 3 we provide the computation of a suffi-
cient statistic. In Section 4 we prove that these models belong to the class of toric models (and therefore they are log-linear for strictly positive probabilities), and we explicitly write down some consequences, such as a canonical parametrization of the models. In Section 5 we compute the Markov bases for weakened independence models and we present some examples with real data. In particular, Example 5.3 is devoted to the discussion of some interesting relationships between our models and the “100 Swiss Francs Problem”. Section 6 highlights the main contributions of our theory and provides some pointers to future developments.

2. Definitions. A two-way contingency table collects data from a sample where two categorical variables, say $X$ and $Y$, are measured. Suppose that $X$ has $I$ levels and $Y$ has $J$ levels. The sample space for a sample of size one is $\mathcal{X} = \{1, \ldots, I\} \times \{1, \ldots, J\}$ and a joint probability distribution for an $I \times J$ contingency table is a table of raw probabilities $(p_{i,j})_{i=1,\ldots,I, j=1,\ldots,J}$ in the simplex

$$\Delta = \left\{ (p_{i,j})_{i=1,\ldots,I, j=1,\ldots,J} \in \mathbb{R}_{+}^{I \times J} : \sum_{i,j} p_{i,j} = 1 \right\}.$$ 

A statistical model for an $I \times J$ contingency table is then a subset of $\Delta$ defined through equations on the raw probabilities $p_{1,1}, \ldots, p_{I,J}$. In this paper, we do not allow any $p_{i,j}$ to be zero, and we assume strict positivity of all probabilities.

The independence model can be defined in parametric form through the power product representation, i.e. by the set of equations

$$p_{i,j} = \zeta_0 \zeta_i^X \zeta_j^Y$$

for $i = 1, \ldots, I$ and $j = 1, \ldots, J$, where $\zeta_i^X$ and $\zeta_j^Y$ are unrestricted positive parameters and $\zeta_0$ is the normalizing constant, see [28]. In term of log-probabilities, Eq. (2.1) assumes the most familiar form

$$\log p_{i,j} = \lambda + \lambda_i^X + \lambda_j^Y$$

where $\lambda = \log \zeta_0$, $\lambda_i^X = \log \zeta_i^X$ for $i = 1, \ldots, I$ and $\lambda_j^Y = \log \zeta_j^Y$ for $j = 1, \ldots, J$. As an equivalent representation, one can derive implicit formulae on the raw probabilities $p_{i,j}$. Eliminating the $\zeta$ variables from Eq. (2.1), one obtains the set of equations below:

$$p_{i,j}p_{k,m} - p_{i,m}p_{k,j} = 0$$
for all \(1 \leq i < k \leq I\) and \(1 \leq j < m \leq J\). In other words, in the independence model all \(2 \times 2\) minors of the table vanish. It is well known, see e.g. [3], that in the positive case, the equalities in Eq. (2.3) are redundant and it is enough to set to zero the adjacent minors:

\[
(2.4) \quad p_{i,j}p_{i+1,j+1} - p_{i+1,j}p_{i,j+1}
\]

for all \(1 \leq i < I\) and \(1 \leq j < J\).

**Remark 2.1.** In the framework of toric models as defined in [28], where structural zeros are allowed, the implicit representations (2.3) and (2.4) are not equivalent, as they differ on the boundary. For a description of such phenomenon, see [31].

In algebraic terms, let

\[
\mathcal{C} = \{p_{i,j}p_{i+1,j+1} - p_{i+1,j}p_{i,j+1} : 1 \leq i < I, \ 1 \leq j < J\}.
\]

The set \(\mathcal{C}\) is the set of all \(2 \times 2\) adjacent minors of the table of probabilities. Moreover, let \(\mathbb{R}[p]\) be the polynomial ring in \(I \times J\) indeterminates with real coefficients.

From the geometric point of view, the independence model is the variety

\[
V_{\mathcal{C}} = \{p_{i,j} : \mathcal{C} = 0\} \cap \Delta,
\]

i.e., the set of the points of the simplex where all binomials in \(\mathcal{C}\) vanish.

The choice of a subset of \(\mathcal{C}\) leads us to the definition of a new class of models.

**Definition 2.2.** Let \(\mathcal{B}\) be a subset of \(\mathcal{C}\). The \(\mathcal{B}\)-weakened independence model is the variety

\[
V_{\mathcal{B}} = \{p_{i,j} : \mathcal{B} = 0\} \cap \Delta.
\]

Of course, \(V_{\mathcal{C}} \subseteq V_{\mathcal{B}}\) for all subsets \(\mathcal{B}\) of \(\mathcal{C}\). The meaning of the class of models in Definition 2.2 is quite simple. In fact, the choice of a given set of minors means that we allow the binomial independence statements to hold locally, i.e., we determine patterns of independence.

**Example 2.3.** As a first applications, we consider a \(2 \times J\) contingency table. A table of this kind could derive, e.g., from the observation of a binary random variable \(X\) at different times.

The model defined through the set of binomials

\[
\mathcal{B} = \{p_{1,1}p_{2,2} - p_{1,2}p_{2,1}, p_{1,2}p_{2,2} - p_{1,3}p_{2,2}, \ldots, p_{1,j'}-1p_{2,j'} - p_{1,j'}p_{2,j'-1}\},
\]

for all \(1 \leq i < I\) and \(1 \leq j < J\).
where $j' < J$, is presented in Figure 1. This choice of $\mathcal{B}$ means that there is independence between $X$ and the time up to the instant $j'$ and not after. In literature, the point $j'$ in this model refers to the detection of the change-point in a logistic regression model. A recent paper about this topic is [21].

**Example 2.4.** Let us consider a $I \times I$ contingency table. A table of this kind could derive from a rater agreement analysis. Suppose that 2 raters independently classify $n$ objects using a nominal or ordinal scale with $I$ categories. If we set

$$\mathcal{B} = \{p_{1,1}p_{2,2} - p_{1,2}p_{2,1}\}$$

the corresponding model yields that categories 1 and 2 are indistinguishable. A reference for the notion of category indistinguishability is, e.g., [11]. This model can be generalized using the set of binomials

$$\mathcal{B} = \{p_{i,j}p_{i+1,j+1} - p_{i,j+1}p_{i+1,j} : 1 \leq i \leq i', 1 \leq j \leq i'\}$$

meaning that the categories $1, \ldots, i'$ are indistinguishable. The first paper in the direction of modelling patterns of agreement is [2]. An example with 5 categories and 3 indistinguishable categories is presented in Figure 2. More examples on the models for rater agreement problems will be presented later in the paper.

**Remark 2.5.** In the next sections, our approach will proceed somehow backwards with respect to the classical log-linear models theory. In fact, we will define the model through the binomials and then we will use them to determine a sufficient statistic and a parametrization.

**3. Sufficient statistic.** As noticed in the Introduction, the independence model is defined through the log-linear form in Eq. (2.2). One can easily check that for the independence model a sufficient statistic $T$ for the sample of size 1 is given by the indicator functions of the $I$ rows and the
indicator functions of the $J$ columns. More precisely, we denote the indicator function of the $i$-th row by $\mathbb{I}_{(i,+)}$ and the indicator function of the $j$-th column by $\mathbb{I}_{(+,j)}$. Writing the sample space as $\mathcal{X} = \{1, \ldots, I\} \times \{1, \ldots, J\}$, a sufficient statistic for the independence model is

$$ T = \left( \mathbb{I}_{(1,+)}, \ldots, \mathbb{I}_{(I,+)}, \mathbb{I}_{(+,1)}, \ldots, \mathbb{I}_{(+,J)} \right) . $$

A single observation is an element of the sample space $\mathcal{X}$ and its table has a single count of 1 in one cell and 0 otherwise. This observation yields a value of 1 in the corresponding row and column indicator functions in $T$.

Therefore, the sufficient statistic $T$ for a sample of size 1 is a linear map from $\mathcal{X}$ to $\mathbb{N}^{I+J}$. The function $T$ can be extended to a linear homomorphism $T : \mathbb{R}^{IJ} \to \mathbb{R}^{I+J}$.

In Section 4 we will prove that weakened independence models, as the independence model, are log-linear. Thus, the sufficient statistic for a sample of size $n$ is the sum of the sufficient statistics of all components of the sample and it will be formed by the sum of appropriate cell counts, as familiar in the field of categorical data analysis, see e.g. [3]. However, in this section it is more convenient to work with a sample of size one and with the indicator functions. This approach has been fruitfully used in [22] and, more recently, in [28].

Hereinafter, we write the table as a column vector, i.e. the table of probabilities is written as

$$ p = (p_{1,1}, \ldots, p_{1,J}, \ldots, p_{I,1}, \ldots, p_{I,J})^t , $$

where $t$ denotes the transposition. Moreover, we use a vector notation, i.e. we write a binomial in the form $p^a - p^b$, meaning $p_{1,1}^{a_{1,1}} \cdots p_{1,J}^{a_{1,J}} - p_{1,1}^{b_{1,1}} \cdots p_{1,J}^{b_{1,J}}$. 

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig2.png}
\caption{Binomials for Example 2.4.}
\end{figure}
We briefly review the relationship between the sufficient statistic and the binomials in Eq. (2.4). Writing the table as a column vector of length $IJ$, the matrix representation of $T$ is a matrix $A_C$. This matrix has size $IJ \times (I + J)$ and its rank is $I + J - 1$.

Moreover, consider the log-vector of a $2 \times 2$ minor to be defined in the following way:

$$
\Lambda : \mathbb{R}^p \longrightarrow \mathbb{R}^{IJ}
$$

$$
p^a - p^b \mapsto a - b
$$

We denote by $Z_C$ the sub-vector space of $\mathbb{R}^{IJ}$ generated by the vectors $\Lambda(m)$, for all $2 \times 2$ adjacent minors $m$. It is well known, see for example [6], that $Z_C$ has dimension $(I - 1)(J - 1)$ and the sequence of log-vectors $\Lambda(m)$ with $m \in \mathcal{C}$ is a sequence of $(I - 1)(J - 1)$ linearly independent vectors orthogonal to $A_C$. Hence the column space $A_C$ is the orthogonal of $Z_C$. Thus, from a vector-space perspective, the exponents of the binomials are the orthogonal complement of the matrix $A_C$. In the sequel, we will use the same symbol to denote a matrix $A$ and the sub-vector space of $\mathbb{R}^{IJ}$ generated by the columns of $A$, although this should be considered as a slight abuse of notation.

The procedure described above is quite general and it provides a method to actually compute the relevant binomials of a statistical model with a given sufficient statistic. For more details, see [28].

In order to analyze the weakened independence models in Definition 2.2, we use the theory sketched above for the independence model. We start with a set of binomials, we compute a sufficient statistic and the parametric representation of the model.

**Remark 3.1.** We will prove in Section 4 that weakened independence models are log-linear. Therefore, the orthogonal to the log-vectors of the chosen binomials is the matrix representation of a sufficient statistic. In order to keep notation as simple as possible, we call this orthogonal a sufficient statistic even before showing that the models are log-linear.

**Lemma 3.2.** The log-vectors of $d$ distinct adjacent minors are linearly independent.

**Proof.** Let $\mathcal{B}_d$ be a set of $d$ distinct adjacent minors and let $L_d$ be the set of their log-vectors. We proceed by induction on $d$. For $d = 1$ the statement is clearly true. We assume that the elements of $L_i$ are linearly independent for all $i < d$ and we will show that the same holds for $L_d$. Let $m \in \mathcal{B}_d$ be the
minor involving the indeterminate having the lex-smallest index, say $p_{i,j}$, and notice that no other element in $B_d$ involves $p_{i,j}$. Let $l = \Lambda(m) \in L_d$ and notice that $l$ is not a linear combination of the element of $L_d \setminus \{l\}$ which are linearly independent by hypothesis. Hence the element of $L_d$ are linearly independent.

**Remark 3.3.** Lemma 3.2 is false when we consider log-vectors of non-adjacent minors. As a counterexample, take a $2 \times 3$ table and all three minors.

Now, consider a $B$-weakened independence model with set of adjacent minors $B$ of cardinality $m$. Let $Z_B$ be the matrix of the log-vectors of the adjacent minors in $B$. In view of Lemma 3.2, the orthogonal of $Z_B$ has dimension $(IJ - m)$. Thus, the explicit computation of $A_B$, the orthogonal of $Z_B$, requires to find at least $(IJ - m)$ vectors orthogonal to $Z_B$. Although this can be done simply with a linear algebra algorithm, it is very useful to investigate the structure of the the matrix $A_B$.

Given a $B$-weakened independence model for $I \times J$ contingency tables, we define a graph in the following way.

**Definition 3.4.** Given a set $B$ of adjacent minors, we define a graph $G_B$ as follows: the set of vertices is the set of cells and each binomial defines 4 edges. The binomial $p_{i,j}p_{i+1,j+1} - p_{i,j+1}p_{i+1,j}$ defines the edges $(i,j) \leftrightarrow (i+1,j)$, $(i+1,j) \leftrightarrow (i+1,j+1)$, $(i,j+1) \leftrightarrow (i+1,j+1)$ and $(i,j) \leftrightarrow (i,j+1)$.

The edges associated to a binomial are the 4 sides of the square with vertices on the 4 cells involved in the binomial.

**Definition 3.5.** A cell $(i,j)$ is a free cell if no edge of $G_B$ involves $(i,j)$.

Equivalently, a cell $(i,j)$ is a free cell if and only if the indeterminate $p_{i,j}$ does not appear in any of the binomials in $B$.

**Definition 3.6.** The sequence of cells $(i,j),(i,j+1),\ldots,(i,j+h)$ is a connected component of the $i$-th row if each pair of consecutive cells is connected by an edge of $G_B$. The sequence forms a maximal connected row component (MCR) if the sequence is no more connected when one adds $(i,j-1)$ or $(i,j+h+1)$.

One can define similarly the maximal connected column component (MCC). We illustrate the definitions above with an example.
Example 3.7. In the model for a $4 \times 4$ contingency table defined through the binomials in Figure 3, we have 4 MCRs, 5 MCCs and 2 free cells.

Proposition 3.8. Consider a $\mathcal{B}$-weakened independence model with set of binomials $\mathcal{B}$ and let $Z_{\mathcal{B}}$ be the matrix of the log-vectors of the minors in $\mathcal{B}$. The indicator vectors of the free cells, the indicator vectors of the MCRs and the indicator vectors of the MCCs are orthogonal to the column space $Z_{\mathcal{B}}$.

Proof. If $(i,j)$ is a free cell, then no monomial in $\mathcal{B}$ involves the corresponding variable. Hence the indicator vector of $(i,j)$ is orthogonal to the column space of $Z_{\mathcal{B}}$. Given a MCR, its indicator function is clearly orthogonal to the columns of $Z_{\mathcal{B}}$ corresponding to minors not involving the cells of the MCR. If a minor involves a cell of the MCR, then it involves two cells with alternating signs. A similar argument works for MCCs. Hence the orthogonality follows.

Now, two questions arise: one about the linear independence of the vectors defined in Proposition 3.8 and the other about the dimension of the sub-vector space generated by such vectors. In other words, we have to investigate whether these vectors generate the space orthogonal to $Z_{\mathcal{B}}$ or not. Let us start with two simple examples.

Example 3.9. Consider a weakened independence model for $4 \times 4$ tables defined through the adjacent minors in Figure 4. In this situation, $Z_{\mathcal{B}}$ has rank 3 and there are 4 MCRs, 4 MCCs and 6 free cells. Here, the 14 vectors corresponding to the MCRs, to the MCCs and to the free cells generate a sub-vector space of dimension 13. Thus, they are enough to define the matrix $A_{\mathcal{B}}$. 
Consider now a weakened independence model for $4 \times 4$ tables defined through the adjacent minors in Figure 5. The model above only leaves out one minor, namely the central one. In this case, $Z_B$ has rank 8 and there are 4 MCRs and 4 MCCs. The 8 vectors corresponding to the MCRs and to the MCCs generate a sub-vector space of dimension 7 and therefore they are not enough to generate the orthogonal space $A_B$.

The dimension of the vector space generated by the indicator function of the MCRs, the MCCs and the free cells can be computed and we have the following results.

**Proposition 3.11.** For any connected component of $B$ with $r$ MCRs and $c$ MCCs, the vector space generated by the MCRs and by the MCCs has dimension $(r + c - 1)$.

**Proof.** Clearly the log-vectors of the MCRs and of the MCCs are not linearly independent as their sums are equal. To show that this is the only relation we proceed by induction on the number of minors in the connected
component. Let this number be $d$. If $d = 1$ the result is trivial. Now, assume that the result holds for $d$. If the connected component involves $d+1$ minors, let $r_1, \ldots, r_t$ be the indicator functions of the $MCR$s and $c_1, \ldots, c_s$ be the indicator functions of the $MCC$s. Also assume that $c_1$ and $r_1$ involve the lex-smallest cell. Notice that $c_1$ and $r_1$ are the only vectors involving this cell. Given a linear combination

$$\sum \lambda_i c_i = \sum \mu_i r_i$$

we must have $\lambda_1 = \mu_1$. Then the linear combination (3.1) can be read in $B' = B \setminus \{m\}$, where $m$ is the minor involving the lex-smallest cell and the $c_i$’s and the $r_i$’s represent the log-vectors of the $MCR$s and the $MCC$s of $B'$. By the inductive hypothesis we get $\lambda_i = \mu_i = 1$ for all $i$.

As distinct connected components and free cells act on spaces which are orthogonal to each other, Proposition 3.11 leads to the following corollary.

**Theorem 3.12.** Consider a $B$-weakened independence model defined by a set of binomials $B$ whose graph has $k$ connected components and with $r$ $MCR$s, $c$ $MCC$s and $f$ free cells. The dimension of the vector space generated by $MCR$s, $MCC$s and the indicator functions of the free cells is $(r + c + f - k)$.

**Proof.** The indicators of the free cells are clearly independent with the indicators of the $MCC$s and of the $MRC$s. Moreover, indicators of $MCC$s and $MRC$s of different connected components are linearly independent as they do not share any cell. By Proposition 3.11 each connected component gives exactly one relation among the indicators of the $MCR$s and the $MCC$s. Hence the result follows.

In the results above, we have addressed dimensional issues. Now, we use them to find a procedure to determine a sufficient statistic. Moreover, the examples of this section show that in some cases the vectors of $MCC$s, $MCR$s and free cells are sufficient to generate the space orthogonal to $Z_B$. Clearly, these vectors are not sufficient when the graph $G_B$ of the binomials in $B$ present a hole, i.e., when we remove some minors with 4 double edges from the complete set of binomials $C$. Removing such a minor adds a new vector to the orthogonal. On the other hand, it does not add anything in terms of $MCR$s, $MCC$s and free cells.

Thus, the last part of this section is devoted to actually find a sufficient statistic for a generic weakened independence model. The key idea is to start from the complete set of adjacent minors $C$ and to remove minors iteratively.
This approach is motivated by the fact that for the complete set $C$ a sufficient statistic is known to be formed by the row sums and the column sums, as extensively discussed in Section 2.

We begin our analysis from a simple case. Namely, we consider a set of binomials $\mathcal{B}$ with given sufficient statistic $A_\mathcal{B}$ and we investigate the behavior of the sufficient statistic when we remove one minor $m$ from $\mathcal{B}$, i.e., when the set of binomials is $\mathcal{B}' = \mathcal{B} \setminus \{m\}$. We separate two cases, depending on the number of double edges of the removed minor.

**Lemma 3.13.** Consider a weakened independence model obtained removing a binomial with four double edges by a given family of adjacent binomials $\mathcal{B}$, i.e. let $\mathcal{B}' = \mathcal{B} \setminus \{m\}$ where $m$ has four double edges. If we let $A_\mathcal{B}$ be the orthogonal to $Z_\mathcal{B}$, then the orthogonal to $Z_{\mathcal{B}'}$ is generated by the elements of $A_\mathcal{B}$ and by the indicator vector $Q$ of a quadrant centered on one of the indeterminates of the removed minor.

**Proof.** First notice that the elements of $A_\mathcal{B}$ are orthogonal to the columns of $Z_{\mathcal{B}'}$, i.e. $A_{\mathcal{B}'} \supseteq A_\mathcal{B}$, and clearly, by Lemma 3.2, one has
$$\dim(A_{\mathcal{B}'}) = \dim(A_\mathcal{B}) + 1,$$
where $A_{\mathcal{B}'}$ is the orthogonal to $Z_{\mathcal{B}'}$. Now let $Q$ be the indicator vector of a quadrant centered on one of the indeterminates of $m$. Then, $Q \notin A_\mathcal{B}$ as it is not orthogonal to the log-vector of $m$. But, $Q \in A_{\mathcal{B}'}$ as each binomial in $\mathcal{B}'$ either avoid the quadrant, or it is contained in the quadrant, or has exactly two elements on the border of the quadrant. This is enough to complete the proof.

The quadrant to be used in Example 3.10 is sketched Figure 6.

**Lemma 3.14.** Consider a weakened independence model obtained removing a binomial with not all the edges double by a given family of adjacent binomials $\mathcal{B}$, i.e. let $\mathcal{B}' = \mathcal{B} \setminus \{m\}$ where $m$ has not all the edges double. If we let $A_\mathcal{B}$ be the orthogonal to $Z_\mathcal{B}$, then the orthogonal to $Z_{\mathcal{B}'}$ is generated by: the elements of $A_\mathcal{B}$, the indicator vectors of the MCCs, of the MCRs and of the free cells.

**Proof.** Clearly, the elements of $A_\mathcal{B}$ are orthogonal to the column of $Z_{\mathcal{B}'}$, i.e. $A_{\mathcal{B}'} \supseteq A_\mathcal{B}$, and by Lemma 3.2 one has
$$\dim(A_{\mathcal{B}'}) = \dim(A_\mathcal{B}) + 1,$$
where $A_{\mathcal{B}'}$ is the orthogonal to $Z_{\mathcal{B}'}$. The removed binomial $m$, with not all the edges double, can be one of the following
and to complete the proof we only need to present, in each case, a vector $Q$ in $A_B'$ which is not in $A_B$. In case (a), either we have a new free cell or not. If we have, let $Q$ be the indicator vector of the free cell. Clearly, $Q \notin A_B$, but $Q \in A_B'$ has no minor is involving the variable corresponding to the free cell. If we do not have a new free cell, then we have a new MMC or a new MCR and its indicator vector is the required one. Repeating this kind of argument in cases (b) through (e) we complete the proof.

We are now ready to analyze the general case.

**Definition 3.15.** Let $\mathcal{B}$ be a set of adjacent minors and consider its complement $\overline{\mathcal{B}}$ in the set of all adjacent minors. Let $G_{\mathcal{B}}$ be the graph associated with $G_{\mathcal{B}}$. For each connected component of $G_{\mathcal{B}}$ not touching the border of the table, we consider the lex-smallest variable and we call it a corner.

**Remark 3.16.** We notice that the number of corners is just the number of holes one can find in the graph defined by the set of monomials.
Theorem 3.17. Let $\mathcal{B}$ be a set of adjacent minors. Then the orthogonal to $Z_{\mathcal{B}}$ is generated by the indicator vectors of the MCCs, of the MCRs, of the free cells and by quadrants centered in variables corresponding to corners.

Proof. $\mathcal{B}$ can be constructed by the set of all the adjacent minors by removing a minor at each time. Using Lemmas 3.13 and 3.14 we only need to show the result for the set of all the adjacent minors, but this is a straightforward consequence of Lemma 3.2 and Theorem 3.12.

Remark 3.18. In alternative to the straightforward use of Theorem 3.17 one can apply Lemmas 3.14 and 3.13 to determine a sufficient statistic for a weakened independence model with set of binomial $\mathcal{B}$. It is enough to start from the complete set of adjacent minors and remove one by one the minors not in $\mathcal{B}$. Notice that such an iterative procedure, and the theorem itself, yield a system of generators of the space orthogonal to $Z_{\mathcal{B}}$, but not a basis, i.e. some of the vectors we add are redundant.

We will show some examples and applications of Theorem 3.17 in the next sections.

4. Exponential models. In Section 3 we have carried out some computations to determine a sufficient statistic of a weakened independence model. We are now able to find a parametric representation of the model.

Let us introduce unrestricted positive parameters $\zeta_1, \ldots, \zeta_s$, where $s$ is the number of columns of the matrix $A_{\mathcal{B}}$. If $A_{\mathcal{B}}$ has full rank, then $s$ coincide with the dimension of the vector sub-space orthogonal to $Z_{\mathcal{B}}$.

The first step is to prove that weakened independence models belong to the class of toric models and therefore they are exponential (log-linear) models on the strictly positive simplex. The first result in this direction is a rewriting of a general theorem to be found in [20].

Remark 4.1. The main result in [20] can be applied to statistical models when the matrix representation $A_{\mathcal{B}}$ of the sufficient statistic has non-negative entries. Therefore, the theory developed in Section 3 is relevant not only to actually determine a sufficient statistic, but also to derive further theoretical properties of the weakened independence models.

Here we use again a vector notation in order to improve the readability and simplify the formulae.
Theorem 4.2 (Geiger, Meek, Sturmfels (2006), Th. 3.2). Given a $\mathcal{B}$-weakened independence model, it can be expressed as

\begin{equation}
    p(\zeta) = \zeta^{A_B}
\end{equation}

apart from the normalizing constant.

Clearly, the parametrization in Eq. (4.1) is not unique. Theorem 4.2 provides an easy way to switch from the implicit representation to its parametrization. It is enough to consider the matrix $A_B$, whose columns are orthogonal to the log-vectors of the binomials. As the columns of $A_B$ can be chosen with non-negative entries, then each binomial in $\mathcal{B}$ vanishes in all points of the form given in Eq. (4.1). This follows from a direct substitution. The converse part is less intuitive and the proof is not obvious.

As a corollary, Theorem 4.2 allows us to consider weakened independence models into the larger class of toric models, as described in [28] and [31]. In the following result, we summarize the main properties inherited from toric models.

Proposition 4.3. Consider a $\mathcal{B}$-weakened independence model $V_B$.

1. $V_B$ is a toric model;
2. With the constraint $p > 0$, $V_B$ is an exponential model;
3. In case of sampling, the sufficient statistic for the sample of size $n$ is the sum of the sufficient statistic of all components of the sample.

Proof. See Theorem 2 and the discussion in Section 3 of [31].

Remark 4.4. As noticed in [31], when we consider the general case $p \geq 0$ instead of $p > 0$, the toric model is not an exponential model. Nevertheless it can be described as the disjoint union of a suitable number of exponential models.

We conclude this section with two examples.

Example 4.5. As a first example, we consider a statistical model for $3 \times 3$ contingency tables defined through the binomials in Figure 7. Using the theory developed in the previous section, the $MCR$s, the $MCC$s and the free cells are sufficient to describe the orthogonal $Z_B$ and therefore the relevant matrices are in Table 1. Thus, a parametrization with parameters
Fig 7. Binomials for Example 4.5.

\[
[Z_B | A_B] = \begin{pmatrix}
1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
-1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\
1 & 1 & 0 & 1 & 0 & 0 & 1 & 0 \\
0 & -1 & 0 & 1 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & -1 & 0 & 0 & 1 & 0 & 1 & 0
\end{pmatrix}
\]

Table 1
Matrices $Z_B$ and $A_B$ for Example 4.5.

$\zeta_1, \ldots, \zeta_8$ is:

\[
\begin{align*}
    p_{1,1} &= \zeta_1 \zeta_4 \\
    p_{1,2} &= \zeta_1 \zeta_5 \\
    p_{1,3} &= \zeta_7 \\
    p_{2,1} &= \zeta_2 \zeta_4 \\
    p_{2,2} &= \zeta_2 \zeta_5 \\
    p_{2,3} &= \zeta_2 \zeta_6 \\
    p_{3,1} &= \zeta_8 \\
    p_{3,2} &= \zeta_3 \zeta_5 \\
    p_{3,3} &= \zeta_3 \zeta_6 \\
    p_{4,1} &= \zeta_4 \zeta_5 \\
    p_{4,2} &= \zeta_4 \zeta_6 \\
    p_{4,3} &= \zeta_4 \zeta_7 \zeta_9 \\
    p_{4,4} &= \zeta_4 \zeta_8 \zeta_9
\end{align*}
\]

Example 4.6. Let us consider the weakened independence model for $4 \times 4$ defined in Example 3.10. In that model, a minor with four double edges has been removed and consequently the MCRs, MCCs and free cells are not sufficient to describe the orthogonal $Z_B$. A vector must be added according to Theorem 3.13. Following the same approach as in the previous example one can easily write down the matrices $Z_B$ and $A_B$. A parametrization with parameters $\zeta_1, \ldots, \zeta_9$ is:

\[
\begin{align*}
    p_{1,1} &= \zeta_1 \zeta_5 \\
    p_{1,2} &= \zeta_1 \zeta_6 \\
    p_{1,3} &= \zeta_1 \zeta_7 \\
    p_{1,4} &= \zeta_1 \zeta_8 \\
    p_{2,1} &= \zeta_2 \zeta_5 \\
    p_{2,2} &= \zeta_2 \zeta_6 \\
    p_{2,3} &= \zeta_2 \zeta_7 \\
    p_{2,4} &= \zeta_2 \zeta_8 \\
    p_{3,1} &= \zeta_3 \zeta_5 \\
    p_{3,2} &= \zeta_3 \zeta_6 \\
    p_{3,3} &= \zeta_3 \zeta_7 \zeta_9 \\
    p_{3,4} &= \zeta_3 \zeta_8 \zeta_9 \\
    p_{4,1} &= \zeta_4 \zeta_5 \\
    p_{4,2} &= \zeta_4 \zeta_6 \\
    p_{4,3} &= \zeta_4 \zeta_7 \zeta_9 \\
    p_{4,4} &= \zeta_4 \zeta_8 \zeta_9
\end{align*}
\]
5. Inference and examples. In the previous sections we have defined and studied the weakened independence models. When the statistical model is given through a set of adjacent minors \( \mathcal{B} \), we are now able to compute a sufficient statistic for a sample of size 1 (see Proposition 4.3) and to find a parametrization of the statistical model \( V_{\mathcal{B}} \) (see Theorem 4.2.) In this section we give some ideas on how to compute maximum likelihood estimates (MLE) and to perform exact inference through Algebraic Statistics.

In the independence model defined by the set \( \mathcal{C} \) of all adjacent minors, the maximum likelihood estimate can be expressed in closed form in terms of the observed value of the sufficient statistic \( T \). In the weakened independence models this is no longer true, but numerical algorithms for log-linear models can be used. As pointed out in Section 4, at least in the strictly positive case, a weakened independence model is log-linear and thus modified Newton-Raphson methods, Iterative Proportional Fitting or EM methods can be used, see e.g. [3]. To compute the MLEs of the cell probabilities for the examples in this paper, we have used the \( \mathbb{R} \) software, see [29], together with the package \texttt{gllm} (generalized log-linear models), see [14]. This package allows to define a generic matrix for the sufficient statistic. This is the main advantage of the \texttt{gllm} package with respect to other available procedures in different software systems.

Another theoretical result which highlights once again the interplay between statistical models and polynomial algebra is the Birch’s Theorem (see e.g. [6]). It states that the MLE is the unique point \( \hat{p} \) of the model \( V_{\mathcal{B}} \) which satisfies the constraints \( A_{\mathcal{B}} \hat{p} = A_{\mathcal{B}} p_{\text{obs}} \), where \( p_{\text{obs}} \) are the observed frequencies. We will have the opportunity to apply such result later in Example 5.3.

Once the MLE is available, the goodness-of-fit can be evaluated through a chi-squared test. The Pearson test statistic

\[
C^2 = n \sum_{i,j} \frac{(p_{i,j} - \hat{p}_{i,j})^2}{\hat{p}_{i,j}}
\]

or the log-likelihood ratio test statistic

\[
G^2 = 2n \sum_{i,j} p_{i,j} \log \left( \frac{p_{i,j}}{\hat{p}_{i,j}} \right)
\]

are evaluated and compared with the chi-square distribution with \#\( \mathcal{B} \) degrees of freedom, where \#\( \mathcal{B} \) is the cardinality of \( \mathcal{B} \), see [22] or [6].

Alternatively, one can run the goodness-of-fit test within Algebraic Statistics, using a Markov Chains Monte Carlo (MCMC) algorithm. A number of
papers have shown the relevance of this approach, see [13], and e.g. [30], [4], and [8]. The algebraic MCMC algorithm was first described in [13], and it is by now widely used to compute non-asymptotic $p$-values for goodness-of-fit tests in contingency tables problems.

Let $h$ be the observed contingency table for a sample of size $n$, written as a vector in $\mathbb{N}^{IJ}$. The MCMC algorithm is useful to efficiently sample from the reference set $\mathcal{F}_t$ of a contingency table $h$ given a sufficient statistic with matrix representation $A_B$, i.e., from the set

$$\mathcal{F}_t = \left\{ h' \in \mathbb{N}^{IJ} \mid A_B^t h' = A_B^t h \right\}.$$

The algorithm samples tables from $\mathcal{F}_t$ with the appropriate hypergeometric distribution $\mathcal{H}$ through a Markov chain based on a suitable set of moves making the chain connected. Such set of moves is called a Markov basis. With more details, a Markov basis is a set of tables $\{m_1, \ldots, m_L\}$ with integer entries such that:

- $A_B^t m_k = 0$ for all $k = 1, \ldots, L$.
- if $h_1$ and $h_2$ are tables in $\mathcal{F}_t$, there exist moves $m_{k_1}, \ldots, m_{k_A}$ and signs $\epsilon_1, \ldots, \epsilon_A$ ($\epsilon_a = \pm 1$) such that

$$h_2 = h_1 + \sum_{a=1}^A \epsilon_a m_{k_a} \quad \text{and} \quad h_1 + \sum_{a=1}^l \epsilon_a m_{k_a} \geq 0 \quad \text{for all} \ l = 1, \ldots, A.$$

These conditions ensure the irreducibility of the Markov chain defined by the algorithm below:

- Start from a table $h_1 \in \mathcal{F}_t$;
- Choose a move $m_k$ uniformly in $\{m_1, \ldots, m_L\}$ and a sign $\epsilon$ uniformly in $\{-1, 1\}$. Define $h_2 = h_1 + \epsilon m_k$;
- Choose $u$ uniformly distributed in the interval $[0, 1]$. If $h_2 \geq 0$ and $
\min(1, H(h_2)/H(h_1)) > u$ then move from $h_1$ to $h_2$, otherwise stay at $h_1$.

In the general case, the computation of a Markov basis needs symbolic computations (the Diaconis-Sturmfels algorithm). Nevertheless, a Markov basis for the weakened independence models can be derived theoretically. In the following, we will determine a Markov basis for the weakened independence models.

Given the set $B$ of binomials defining the $B$-weakened independence model, let $A_B$ be the matrix representation of the sufficient statistic. Moreover, we denote by $I_B$ the polynomial ideal in $\mathbb{R}[p]$ generated by the binomials in $B$. Diaconis and Sturmfels ([13], Theorem 3.1) proved that a Markov basis is
formed by the log-vectors of a set of generators of the toric ideal associated to $A_B$, i.e. the ideal

$$J_B = \{ p^a - p^b \mid a, b \in \mathbb{R}^{I,J}, A_B^t(a) = A_B^t(b) \}.$$ 

Therefore, the computation of a Markov basis translates into the computation of a set of generators of a toric ideal.

Bigatti et al. [5] showed that the toric ideal associated to $A_B$ is the saturation of $I_B$ with respect to the product of the indeterminates. Such ideal is defined as:

$$I_B : (p_{1,1} \cdots p_{I,J})^\infty = \{ f \in \mathbb{R}[p] \mid (p_{1,1} \cdots p_{I,J})^n f \in I_B \text{ for some } n \}.$$ 

In order to compute a set of generators of this ideal, one can use symbolic algebra packages, e.g. the function Toric of CoCoA. For further details on ideals and their operations, see e.g. [10] and [25].

**Example 5.1.** The data we present as a first example in this section have been collected by one of the authors in his Biostatistics course. Each of the 34 students must submit a homework before the exam and this report is evaluated by two instructors on a scale with levels $\{1, 2, 3\}$. The final grade is the maximum of the two evaluations. The data are in the Table 2.

The model we use to analyze such data is the model defined by the adjacent minors in Example 4.5. Using the gllm package, we obtain the MLEs written in parentheses in the table. The Pearson statistic is 0.9863. Running a MCMC algorithm with a Markov basis consisting of 2 moves, we find a $p$-value of 0.6665 for the goodness-of-fit test, showing a good fit. The Monte Carlo computations are based on a sample of 10,000 tables, with a burn-in phase of 50,000 tables and sampling every 50 steps.

| Second instructor | First instructor | Total |
|-------------------|-----------------|-------|
|                   | 1   | 2   | 3   |       |
| 1                 | 7   | 5   | 0   | 12    |
| (6.52)            | (5.48) | (0) |     |
| 2                 | 4   | 5   | 2   | 11    |
| (4.48)            | (3.76) | (2.76) |     |
| 3                 | 1   | 5   | 5   | 11    |
| (1)               | (5.76) | (4.24) |     |
| Total             | 12  | 15  | 7   | 34    |

Table 2

*Evaluation of 34 homeworks by two instructors. In parentheses are the MLE estimates for the weakened independence model.*
Models of this kind are used in [7] to detect category indistinguishability both in intra-rater and in inter-rater agreement problems. The model we used shows that categories 1 and 2 are confused, as well as categories 2 and 3. This lack of distinguishability can be ascribed to a relevant non-homogeneity of the marginal distributions.

**Example 5.2.** The data in Table 3 show the cross-classification of 103 subjects with respect to 2 ordinal variables: the smoking level, 4 categories from “No Smoking” to “More than 10 cigarettes”, and the quantity of High-Density Lipoprotein Cholesterol (HDLC) in the blood, 4 categories from “Normal” to “Abnormal”. The data are presented in [24] and analyzed by the authors under both the independence model and the RC (Row Column effects) model. The authors compute the exact p-values for the independence model (0.049) and for the RC model (0.657) using the log-likelihood ratio test statistic.

We use a weakened independence model with binomials in Figure 8. According to Theorem 3.17, a sufficient statistic is formed by 4 $MCR$s, 4 $MCC$s and 3 free cells. Moreover, the relevant Markov basis has 14 binomials.

With our model we find a p-value of 0.7205. Therefore, this weakened independence model fits better than the independence model and it is as good as the RC model. In particular, removing only three adjacent minors from the complete configuration with 9 minors, we obtain a model whose fit is dramatically improved. Moreover, the removed minors allow us to identify quickly the cells which cause the departure from independence.

**Example 5.3.** To conclude this section, we show how the models defined in the present paper have some relationships with a recent problem, first stated by Bernd Sturmfels in 2005 and known as the “100 Swiss Francs
Fig 8. Weakened independence model for the cholesterol data.

Problem”, see [32]. Such problem is related to the modelling of DNA sequence alignments. We briefly describe the probabilistic experiment. For a plain description, the reader can refer to [27], Example 1.15.

A DNA sequence is a sequence of symbols in the alphabet \{A, T, C, G\}. A major problem in molecular biology is to compare two DNA sequences. In [32], the following observed sequences were considered:

\[
\begin{align*}
ATCACCAAAACATTGGGATGCCCTGTCATTGCAAGCGGCT \\
ATGAGTCTTTAACACGCTGGCCATGTCCATCTTAGACAGCG
\end{align*}
\]

leading to the observed table below:

\[
\begin{pmatrix}
4 & 2 & 2 & 2 \\
2 & 4 & 2 & 2 \\
2 & 2 & 4 & 2 \\
2 & 2 & 2 & 4
\end{pmatrix}
\]

The hypothesis of the author is that such two DNA sequences are generated through a (biased) coin and four tetrahedral dice \(D_1, D_2, D_3, D_4\) with the letters A, T, C, G on the facets. When the coin outcome is “Head”, then the dice \(D_1\) and \(D_2\) are rolled. The outcome of \(D_1\) is registered in the first sequence and the outcome of \(D_2\) in the second one. When the coin outcome is “Tail”, then the dice \(D_3\) and \(D_4\) are rolled.

Denote by \(q_1, \ldots, q_4\) the probability vectors of the four dice and by \(\alpha\) the probability of “Head” in the coin. Then, the probability distribution of the final outcome is

\[
\alpha q_1 q_2^T + (1 - \alpha) q_3 q_4^T.
\]

Therefore, the construction of this experiment leads us to consider the statistical model of \(4 \times 4\) matrices of probabilities whose rank is less than or
The author conjectured that the maximum likelihood estimate of the probabilities under the model of matrices with rank at most 2 is:

\[
\hat{P}_g = \frac{1}{40} \begin{pmatrix}
3 & 3 & 2 & 2 \\
3 & 3 & 2 & 2 \\
2 & 2 & 3 & 3 \\
2 & 2 & 3 & 3 
\end{pmatrix}
\]

Further analyses to be found in [16] show that the model is non-identifiable and that numerical methods are able to identify 3 global maxima and 4 local maxima for the likelihood function. Apart from the simultaneous permutation of the row and column labels, the global maximum is reached for the matrix in Eq. (5.5) and the local maximum is obtained by the matrix:

\[
\hat{P}_l = \frac{1}{40} \begin{pmatrix}
8/3 & 8/3 & 8/3 & 2 \\
8/3 & 8/3 & 8/3 & 2 \\
8/3 & 8/3 & 8/3 & 2 \\
2 & 2 & 2 & 4 
\end{pmatrix}
\]

Now, consider the following probability models for 4 × 4 contingency tables:

- the model \( M \) of the matrices with rank at most 2;
- the weakened independence models \( M_1 \) and \( M_2 \) whose binomials are presented in Figure 9.

One can easily check that both \( M_1 \) and \( M_2 \) are proper subsets of \( M \). In fact, in \( M_1 \) the first row is proportional to the second row and so are the third and the fourth, while in \( M_2 \), the first three rows are proportional.

Now it is easy to check by direct substitution that the matrix \( \hat{P}_g \) of global maximum in Eq. (5.5) belongs to \( M_1 \), while the matrix \( \hat{P}_l \) of local maximum
in Eq. (5.6) belongs to $M_2$. Such matrices are the MLEs for the two models, respectively.

**Remark 5.4.** This is not a proof that the matrix $\hat{P}_g$ is the MLE for the model $M$. Nevertheless, it is interesting to notice that our models contain both the local and the global maxima. However, our model can not suffice to find the local extrema in $M$ as $M$ is not a toric model, e.g., it is not defined by binomials.

6. **Final remarks and future work.** In this paper we used the binomial representation of the independence model to introduce a new class of statistical models: these models are devised to weaken independence. We studied their sufficient statistic, we proved that they are log-linear models for strictly positive probabilities and we showed how to make inference on these models. Some numerical examples emphasized the importance and the wide applicability of our models.

We have in mind different ways to generalize this work. First, we want to find a procedure to characterize the relevant Markov bases to be used in the Diaconis-Sturmfels algorithm. Then, we plan to consider models defined by non-adjacent $2 \times 2$ minors and try to analyze them with similar techniques. Moreover, we are interested in the study of higher dimensional minors, e.g., $3 \times 3$ minors which appear in the definition of the models in Example 5.3. Finally, for large tables there will be many weakened independence models and model selection strategies must be studied. Further applications of this kind of models will be investigated, in particular in the field of computational biology. From a geometrical point of view, we would like to explore the structure of the varieties defined by some adjacent minors, as done in [23] when all adjacent minors are considered.

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