Geometry of diagonal-effect models for contingency tables

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Abstract
In this work we study several types of diagonal-effect models for two-way contingency tables in the framework of Algebraic Statistics. We use both toric models and mixture models to encode the different behavior of the diagonal cells. We compute the invariants of these models and we explore their geometrical structure.

Key words: toric models; mixture models; invariants; Markov bases

1 Introduction
A probability distribution on a finite sample space $\mathcal{X}$ with $k$ elements is a normalized vector of $k$ non-negative real numbers. Thus, the most general
probability model is the simplex

\[ \Delta = \left\{ (p_1, \ldots, p_k) : p_i \geq 0, \quad \sum_{i=1}^{k} p_i = 1 \right\}. \tag{1} \]

A statistical model \( \mathcal{M} \) is therefore a subset of \( \Delta \).

A classical example of finite sample space is the case of two-way contingency tables, where the sample space is usually written as a cartesian product of the form \( \mathcal{X} = \{1, \ldots, I\} \times \{1, \ldots, J\} \). We will consider this case extensively in the next sections.

When \( \mathcal{M} \) is defined through algebraic equations, the model \( \mathcal{M} \) is said to be an algebraic model. In such a case, algebraic and geometric techniques are useful to study the structure of the model and many statistical quantities such as sufficient statistics and maximum likelihood estimators. In recent literature this approach is known as “Algebraic Statistics”. For a survey on this field the reader can refer to Pistone et al. (2001a) and Pachter and Sturmfels (2005).

With this point of view, a statistical model is defined as the set of points in \( \Delta \) where certain polynomials \( f_1(p_1, \ldots, p_k), \ldots, f_\ell(p_1, \ldots, p_k) \) vanish. Notice that the non-negativity and normalization conditions increase the complexity of the geometrical study. In fact, Algebraic Geometry usually works in complex projective spaces, see e.g. Harris (1992), while in Algebraic Statistics we have to consider a real affine variety and we must intersect the variety with the simplex.

A description of the problems raised by non-negativity and normalization are described for instance in Pistone et al. (2001b) and Geiger et al. (2006), while the use of Algebraic Statistics in various applications is presented in Riccomagno (2009).

The difference between models with positive probabilities and models with non-negative probabilities has been deeply studied in Algebraic Statistics. When only positive probabilities are involved usually one takes the log-probabilities \( \log(p_1), \ldots, \log(p_k) \). Hence, many statistical models are defined by linear equations in the log-probabilities. The most widely used models for contingency tables are defined in this way and are called log-linear models, see e.g. Agresti (2002). The use of polynomial algebra instead of linear algebra has led to the study of models with non-negative probabilities. Therefore, the new class of toric models has been introduced and many geometric properties have been related to statistical properties, see e.g. Geiger et al. (2006). Toric models generalize the log-linear models to include models with structural zeros, see e.g. Rapallo (2007). Exact infer-
ence on toric model can be done through MCMC methods based on Markov bases. The difference between positivity and non-negativity is also a major issue in the computation of Markov bases, see Diaconis and Sturmfels (1998) and Chen et al. (2005) where the difference between lattice bases and Markov bases is shown to be essential.

In this paper we consider the diagonal-effect models, i.e., models encoding a special behavior of the diagonal cells of the table with respect to the independence model. It is a class of statistical models for square two-way contingency tables with a wide range of applications, from social mobility analysis in Psychometry to rater agreement analysis in medical and pharmaceutical sciences, see e.g. Agresti (1992), Schuster (2002). Some results in Algebraic Statistics for this kind of models have already been discussed in Rapallo (2005), Carlini and Rapallo (2009) and Krampe and Kuhnle (2007). Due to the variety of the applications, this type of statistical models has been approached in many different ways and several mathematical definitions have been introduced, often to describe the same objects. In this paper, we will concentrate especially on toric models and mixture models.

The main aim of this paper is to study the geometric structure of the diagonal-effect models, showing the differences between toric models and mixture models. In particular, we compute the invariants of these models. We recall that an invariant of a model is a polynomial function vanishing in the points of the model, see Garcia et al. (2005). We show that the toric and mixture models differ not only on the boundary of the simplex but also in its interior, also when the models have the same invariants.

In Section 2 we recall some basic definitions and results on toric models, with special emphasis on the independence model. In Section 3 we define the diagonal-effect models as both toric models and mixture models, we show that they have the same invariants, and we describe their structure, while in Section 4 we study in more details their geometry. Finally, in Section 5 we study a special class of diagonal effect models which encodes a common behavior of the diagonal cells, i.e., all diagonal cells give the same contribution.

The results presented here also suggest future works on these topics as such as: the comparison of two or more diagonal effect models; the study of the geometry of more complex models, such as diagonal models for multi-way tables or non-square tables; a better understanding of the notion of maximum likelihood estimates for this kind of models.
2 Basic facts on toric models and independence

In this paper we consider a two-way contingency table as the joint observed counts of two categorical random variables $X$ and $Y$. Let us suppose that the random variable $X$ has $I$ levels, and $Y$ has $J$ levels. Therefore, the sample space is the cartesian product $\mathcal{X} = \{1, \ldots, I\} \times \{1, \ldots, J\}$ and the observed contingency table is a point $f \in \mathbb{N}^{IJ}$.

A probability distribution for an $I \times J$ contingency table is a matrix $P = (p_{i,j})$ such that $p_{i,j} = \mathbb{P}(X = i, Y = j)$. Clearly the matrix $P$ is such that $p_{i,j} \geq 0$ for all $i = 1, \ldots, I$ and $j = 1, \ldots, J$, and $\sum_{i,j} p_{i,j} = 1$. In other words, the matrix $P$ is a point of the closed simplex

$$\Delta = \left\{ P = (p_{i,j}) : p_{i,j} \geq 0, \sum_{i,j} p_{i,j} = 1 \right\}.$$  

(2)

A statistical model is a subset of $\Delta$. In most cases, the statistical model is defined through algebraic equations and the model is said to be algebraic. A wide class of algebraic statistical models is the class of toric models, see Pistone et al. (2001a), Pistone et al. (2001b) and Rapallo (2007).

In a toric model, the raw probabilities of the cells are defined in parametric form as power products through a map $\phi: \mathbb{R}^{s}_{\geq 0} \rightarrow \mathbb{R}^{IJ}_{\geq 0}$:

$$p_{i,j} = \prod_{h=1}^{s} \zeta^{A_{(i,j),h}}.$$

(3)

Therefore, the structure of the toric model is encoded in an $IJ \times s$ non-negative integer matrix $A$ which extends $\phi$ to a vector space homomorphism, see [Pistone et al. (2001a)], Chapter 6. Notice that, in the open simplex

$$\Delta_{>0} = \left\{ P = (p_{i,j}) : p_{i,j} > 0, \sum_{i,j} p_{i,j} = 1 \right\}$$

(4)

the power product representation leads to a vector-space representation by taking the log-probabilities. Moreover, it is known that eliminating the $\zeta$ parameters from Equations in (3) one obtains the toric ideal $\mathcal{I}_A$ associated to the statistical model. The ideal $\mathcal{I}_A$ is a polynomial ideal in the ring $\mathbb{R}[p] = \mathbb{R}[p_{1,1}, \ldots, p_{I,J}]$ generated by pure binomials. We recall that a binomial $p^a - p^b$ is pure if $\text{gcd}(p^a, p^b) = 1$. The notation $p^a - p^b$ is a vector notation for $\prod_{i,j} p_{i,j}^{a_{i,j}} - \prod_{i,j} p_{i,j}^{b_{i,j}}$. 

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A move for the toric model defined by the matrix $A$ is a table $m \in \mathbb{Z}^{IJ}$ with integer entries such that $A^t(m) = 0$. The move $m$ is represented in the ring $\mathbb{R}[p]$ by the pure binomial $p^m^+ - p^m^-$, where $m^+$ and $m^-$ are the positive and negative part of $m$.

A Markov basis for the statistical toric model defined by the matrix $A$ is a finite set of tables $m_1, \ldots, m_\ell \in \mathbb{Z}^{IJ}$ that connects any two contingency tables $f_1$ and $f_2$ in the same fiber, i.e. such that $A^t(f_1) = A^t(f_2)$, with a path of elements of the fiber. The path is therefore formed by tables of non-negative counts with constant image under $A^t$.

The relation between the notion of Markov basis and the toric ideal $I_A$ is given in the theorem below.

**Theorem 2.1** (Diaconis and Sturmfels (1998), Theorem 3.1). The set of moves \{\(m_1, \ldots, m_\ell\}\} is a Markov basis if and only if the set \{\(p^{m_i^+} - p^{m_i^-}\), \(i = 1, \ldots, \ell\}\} generates the ideal $I_A$.

In many applications this theorem has been used in its “if” part to deduce Markov bases from the computation of a system of generators of a toric ideal, see e.g. Rapallo (2003) and Chen et al. (2006). On the contrary, in the next section we will make use of Theorem 2.1 in its “only if” implication.

In this paper the independence model will play a special role. It can be considered as the simplest toric model. The variables $X$ and $Y$ are independent if $P(X = i, Y = j) = P(X = i)P(Y = j)$, i.e., the joint distribution is the product of the marginal distributions. The independence condition can be written as:

$$p_{i,j} = \zeta_{(r)}^i \zeta_{(c)}^j \quad \text{for all } i, j$$

(5)

for suitable $\zeta_{(r)}^i$’s and $\zeta_{(c)}^j$’s. The non-negativity constraint reflects into non-negativity of the parameters. Namely, we suppose $\zeta_{(r)}^i \geq 0$ for all $i = 1, \ldots, I$, and $\zeta_{(c)}^j \geq 0$ for all $j = 1, \ldots, J$. Using Equation (3), the independence model is then defined as the set

$$\mathcal{M} = \{P = (p_{i,j}) : p_{i,j} = \zeta_{(r)}^i \zeta_{(c)}^j, \ 1 \leq i \leq I, \ 1 \leq j \leq J\} \cap \Delta,$$

(6)

for non-negative $\zeta_{(r)}^i$’s and $\zeta_{(c)}^j$’s.

Notice that Equation (5) implies that the matrix $P$ has rank 1 and therefore a probability matrix $P$ in the independence model must have all $2 \times 2$ minors equal to zero. In formulae, it is therefore easy to write the independence model in implicit form as:

$$\mathcal{M}' = \{P = (p_{i,j}) : p_{i,j}p_{k,h} - p_{i,k}p_{j,h} = 0, \ 1 \leq i < k \leq I, \ 1 \leq j < h \leq J\} \cap \Delta.$$

(7)
In [Diaconis and Sturmfels (1998)], the authors have studied this set to find Markov bases for the independence model, while the corresponding polynomial ideal has been considered in Algebraic Geometry in the framework of determinantal ideals, see [Hosten and Sullivant (2004)].

As the independence model is toric, Lemma 2 in [Rapallo (2007)] says that the model $M$ in parametric form and the corresponding model $M'$ in implicit form coincide in the open simplex $\Delta_{>0}$.

**Proposition 2.2.** With the notation above, in $\Delta_{>0}$ we have that $M = M'$.

**Proof.** Using the same notation as above, consider the sets

$$
\{ P = (p_{i,j}) : p_{i,j} = \zeta^r_i \zeta^c_j, \ 1 \leq i \leq I, \ 1 \leq j \leq J \}
$$

and

$$
\{ P = (p_{i,j}) : p_{i,j}p_{k,h} - p_{i,h}p_{k,j} = 0, \ 1 \leq i < k \leq I, \ 1 \leq j < h \leq J \}.
$$

Taking the log-probabilities, both sets are defined as a linear system and it is immediate to show that they define two vector sub-spaces with the same dimension. \qed

It is known that $M$ and $M'$ are in general different on the boundary $\Delta \setminus \Delta_{>0}$. A complete description of this issue can be found in Section 4 of [Rapallo (2007)].

### 3 Diagonal-effect models

As mentioned in the Introduction, diagonal-effect models for square $I \times I$ tables can be defined in at least two ways. In the field of toric models, one can define these models in monomial form as follows.

**Definition 3.1.** The diagonal-effect model $M_1$ is defined as the set of probability matrices $P \in \Delta$ such that:

$$
p_{i,j} = \zeta^r_i \zeta^c_j \quad \text{for} \quad i \neq j \quad (8)
$$

and

$$
p_{i,j} = \zeta^r_i \zeta^c_j \zeta^{(\gamma)}_i \quad \text{for} \quad i = j \quad (9)
$$

where $\zeta^r$, $\zeta^c$ and $\zeta^{(\gamma)}$ are non-negative vectors with length $I$.  

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In literature, such a model is also known as quasi-independence model, see Agresti (2002). As the model in Definition 3.1 is a toric model, it is relatively easy to find the invariants. Eliminating the parameters \( \zeta^{(r)}, \zeta^{(c)} \) and \( \zeta^{(\gamma)} \) one obtains the following result.

**Proposition 3.2.** The invariants of the model \( M_1 \) are the binomials

\[
p_{i,j}p_{i',j'} - p_{i,j'}p_{i',j}
\]

for \( i, i', j, j' \) all distinct, and

\[
p_{i,i'}p_{i',i''}p_{i''} - p_{i,i'}p_{i'',i'}p_{i''}
\]

for \( i, i', i'' \) all distinct.

**Proof.** In Aoki and Takemura (2005), it is shown that a minimal Markov basis for the model \( M_1 \) is formed by:

- The basic degree 2 moves:

\[
\begin{array}{c|cc}
    & j & j' \\
  \hline
  i & +1 & -1 \\
  i' & -1 & +1 \\
\end{array}
\]

with \( i, i', j, j' \) all distinct, for \( I \geq 4 \);

- The degree 3 moves of the form:

\[
\begin{array}{c|ccc}
    & i & i' & i'' \\
  \hline
  i & 0 & +1 & -1 \\
  i' & -1 & 0 & +1 \\
  i'' & +1 & -1 & 0 \\
\end{array}
\]

with \( i, i', i'' \) all distinct, for \( I \geq 3 \).

Thus, using Theorem 2.1, the binomials in Equations 10 and 11 form a set of generators of the toric ideal associated to the model \( M_1 \).

**Remark 3.3.** To study the geometry of the model with structural zeros on the main diagonal it is enough to consider the variety defined by the polynomials in Proposition 3.2 and intersect it with the hyperplanes \( \{p_{i,i} = 0\} \) for all \( i \).
In the framework of the mixture models, the diagonal-effect models have an alternative definition as follows.

**Definition 3.4.** The diagonal-effect model $M_2$ is defined as the set of probability matrices $P$ such that
\[
P = \alpha cr^t + (1 - \alpha)D
\]
where $r$ and $c$ are non-negative vectors with length $I$ and sum 1, $D = \text{diag}(d_1, \ldots, d_I)$ is a non-negative diagonal matrix with sum 1, and $\alpha \in [0, 1]$.

**Remark 3.5.** Notice that while in Definition 3.1 the normalization is applied once, in Definition 3.4 the normalization is applied twice as we require that both $cr^t$ and $D$ are probability matrices. This difference will be particularly relevant in the study of the geometry of the models.

First, we study the invariants and some geometrical properties of these models, then we will give some results on their sufficient statistics.

**Theorem 3.6.** The models $M_1$ and $M_2$ have the same invariants.

**Proof.** Writing explicitly the polynomials in Equations (8) and (9) it is easy to check that each $\zeta_i^{(r)}$ appears in only one polynomial. The same for each $d_i$ in Equations (12). Thus, following Theorem 3.4.5 in Kreuzer and Robbiano (2000), such polynomials are deleted when we eliminate the indeterminates $\zeta_i^{(r)}$'s and $d_i$'s.

As the remaining polynomials, corresponding to off-diagonal cells, are the same in both models, the models $M_1$ and $M_2$ have the same invariants. \(\square\)

In order to study in more details the connections between $M_1$ and $M_2$ we further investigate their geometric structure. The non-negativity conditions imposed in the definitions imply that $M_1 \neq M_2$ and neither $M_2 \subset M_1$ nor $M_1 \subset M_2$. We can show this by two easy examples.

First, let $\zeta^{(r)}$ and $\zeta^{(c)}$ respectively the vectors, of length $I$, $(\frac{1}{I}, \frac{1}{I}, \ldots, \frac{1}{I})$ and $(\frac{1}{I-1}, \frac{1}{I-1}, \ldots, \frac{1}{I-1})$ and define $\zeta^{(r)}$ as the zero vector. Thus, the probability table we obtain in toric form is:
\[
P = \begin{pmatrix}
0 & \frac{1}{I-I} & \frac{1}{I-I} & \cdots & \frac{1}{I-I} \\
\frac{1}{I-I} & 0 & \frac{1}{I-I} & \cdots & \frac{1}{I-I} \\
\frac{1}{I-I} & \frac{1}{I-I} & 0 & \cdots & \frac{1}{I-I} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\frac{1}{I-I} & \frac{1}{I-I} & \frac{1}{I-I} & \cdots & 0
\end{pmatrix}.
\]
Such probability matrix belongs to $\mathcal{M}_1$ by constructions, while it does not belong to $\mathcal{M}_2$. In fact, $p_{1,1} = 0$ in Equation \((12)\) would imply either $\alpha = 0$ (a contradiction, as $P$ is not a diagonal matrix), or $\zeta_1^{(r)} = 0$ (a contradiction, as $P$ has not the first row with all 0’s), or $\zeta_1^{(c)} = 0$ (a contradiction, as $P$ has not the first column with all 0’s).

On the other hand, let $P$ be the diagonal matrix

$$
P = \begin{pmatrix}
\frac{1}{I} & 0 & 0 & \ldots & 0 \\
0 & \frac{1}{I} & 0 & \ldots & 0 \\
0 & 0 & \frac{1}{I} & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \ldots & \frac{1}{I}
\end{pmatrix}.
$$

Such probability matrix belongs to $\mathcal{M}_2$ by setting $\alpha = 0$ and $D = \text{diag}(\frac{1}{I}, \ldots, \frac{1}{I})$, while it does not belong to $\mathcal{M}_1$. To prove this it is enough to note that $p_{1,2} = 0$ would imply either $\zeta_1^{(r)} = 0$ (a contradiction, as the first row of $P$ is not zero), or $\zeta_2^{(c)} = 0$ (a contradiction, as the second column of $P$ is not zero).

Nevertheless, in the open simplex we can prove one of the inclusions.

**Proposition 3.7.** In the open simplex $\Delta_{>0}$,

$$
\mathcal{M}_2 \subset \mathcal{M}_1
$$

**Proof.** In fact, let us consider a probability table in $\mathcal{M}_2$, given by $P = \alpha cr^t + (1 - \alpha)D$. As $P \in \Delta_{>0}$, $\alpha \neq 0$, $r_i \neq 0$ for all $i = 1, \ldots, I$ and $c_j \neq 0$ for all $j = 1, \ldots, I$. Then we can describe $P$ as an element of $\mathcal{M}_1$ in the following way. We define $\zeta_i^{(r)} = r_i$ for all $i$ and $\zeta_j^{(c)} = \alpha c_j$, for all $j$. After that, it is enough to find the diagonal parameters by solving the equations

$$
\alpha r_i c_i \zeta_i^{(\gamma)} = \alpha r_i c_i + (1 - \alpha) d_i
$$

that is, as $\alpha \neq 0$, $r_i \neq 0$, and $c_i \neq 0$, we have

$$
\zeta_i^{(\gamma)} = 1 + \frac{(1 - \alpha) d_i}{\alpha r_i c_i}.
$$

Moreover, in the open simplex $\Delta_{>0}$, the inclusion in Proposition 3.7 is strict. Let us analyze the probability matrices in the difference $\mathcal{M}_1 \setminus \mathcal{M}_2$. 

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Consider three vectors $\zeta^{(r)} = (\zeta_1^{(r)}, \ldots, \zeta_I^{(r)})$, $\zeta^{(c)} = (\zeta_1^{(c)}, \ldots, \zeta_I^{(c)})$ and $\zeta^{(\gamma)} = (\zeta_1^{(\gamma)}, \ldots, \zeta_I^{(\gamma)})$. Using these vectors, we define the probability table $P$ as in Definition 3.1 and then we normalize it, i.e. dividing by $N_T = \sum_{i \neq j} \zeta_i^{(r)} \zeta_j^{(c)} + \sum_{i=j} \zeta_i^{(r)} \zeta_i^{(c)} \zeta_i^{(\gamma)}$. Define also $N = \sum_{i,j} \zeta_i^{(r)} \zeta_j^{(c)}$ (which can be seen as the normalization of the toric model when $\zeta^{(\gamma)}$ is the unit vector, i.e., it is the vector with all components equal to one).

We want to find three vectors $c = (c_1, \ldots, c_I)$, $r = (r_1, \ldots, r_I)$, $d = (d_1, \ldots, d_I)$, with $\sum r_i = \sum c_i = \sum d_i = 1$ and a scalar $0 \leq \alpha \leq 1$ such that

$$
\begin{bmatrix}
\zeta_1^{(r)} \zeta_1^{(c)} & \zeta_1^{(r)} \zeta_2^{(c)} & \cdots & \zeta_1^{(r)} \zeta_I^{(c)} \\
\zeta_2^{(r)} \zeta_1^{(c)} & \zeta_2^{(r)} \zeta_2^{(c)} & \cdots & \zeta_2^{(r)} \zeta_I^{(c)} \\
\cdots & \cdots & \cdots & \cdots \\
\zeta_I^{(r)} \zeta_1^{(c)} & \zeta_I^{(r)} \zeta_2^{(c)} & \cdots & \zeta_I^{(r)} \zeta_I^{(c)}
\end{bmatrix} = \alpha \begin{pmatrix}
r_1 c_1 & r_1 c_2 & r_1 c_3 & \cdots & r_1 c_I \\
r_2 c_1 & r_2 c_2 & r_2 c_3 & \cdots & r_2 c_I \\
r_3 c_1 & r_3 c_2 & r_3 c_3 & \cdots & r_3 c_I \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
r_I c_1 & r_I c_2 & r_I c_3 & \cdots & r_I c_I
\end{pmatrix} + (1-\alpha) \begin{pmatrix}
d_1 & 0 & 0 & \cdots & 0 \\
0 & d_2 & 0 & \cdots & 0 \\
0 & 0 & d_3 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & d_I
\end{pmatrix}
$$

(14)

We start studying the off-diagonal elements. Consider first the case $N_T > N$. Thus we have $\frac{\zeta_i^{(r)} \zeta_i^{(c)}}{N_T} < \frac{\zeta_i^{(r)} \zeta_i^{(c)}}{N}$ and $\frac{N}{N_T} < 1$. In this situation the only possible choice is given by

$$
\alpha = \frac{N}{N_T} \quad r_i = \frac{\zeta_i^{(r)}}{\sum \zeta_i^{(r)}} \quad c_j = \frac{\zeta_j^{(c)}}{\sum \zeta_j^{(c)}}.
$$

(15)

In fact, recalling the definition of $N$, we have

$$
\alpha r_i c_j = \frac{N}{N_T} \frac{\zeta_i^{(r)}}{\sum \zeta_i^{(r)}} \frac{\zeta_j^{(c)}}{\sum \zeta_j^{(c)}} = \frac{N}{N_T} \frac{\zeta_i^{(r)} \zeta_j^{(c)}}{\frac{N}{N_T}} = \frac{\zeta_i^{(r)} \zeta_j^{(c)}}{N_T}
$$

(16)

for all $i, j$ with $i \neq j$. Taking the log-probabilities, we obtain a linear system. It is easy to prove, as in Chapter 6 of *Pistone et al. (2001a)*, that the rank of this system is equal to $(2I-1)$. Hence, considering the normalizing equations for $r$ and $c$, we see that the solution in (15) is unique.
Let us consider the generic equation of the $i$-th diagonal element:

$$
\zeta_i^{(r)} \zeta_i^{(c)} \zeta_i^{(\gamma)} = \alpha r_i c_i + (1 - \alpha) d_i.
$$

After substituting the previous values for $r_i$, $c_i$ and $\alpha$ we get

$$
\zeta_i^{(r)} \zeta_i^{(c)} \zeta_i^{(\gamma)} = \frac{N}{N_T} \zeta_i^{(r)} \zeta_i^{(c)} + \frac{N_T - N}{N_T} d_i.
$$

As we consider matrices in $\Delta_{>0}$, the quantity $\zeta_i^{(r)} \zeta_i^{(c)}$ is different from zero. Therefore, after multiplying for $N_T$ and dividing by $\zeta_i^{(r)} \zeta_i^{(c)}$ we obtain

$$
\zeta_i^{(\gamma)} = 1 + \frac{N_T - N}{\zeta_i^{(r)} \zeta_i^{(c)}} d_i,
$$

that is

$$
d_i = \frac{\zeta_i^{(r)} \zeta_i^{(c)}}{N_T - N} \left( \zeta_i^{(\gamma)} - 1 \right)
$$

Thus we see that the $P \in M_1 \setminus M_2$ when $N_T > N$ and there exists at least an index $i$ such that $\zeta_i^{(\gamma)} < 1$.

When $N_T = N$, from Equations (10) we obtain $\alpha = 1$. Therefore in Equation (14) the matrix on the right hand side has rank 1, and this implies that $P \in M_2$ if and only if $\zeta_i^{(\gamma)} = 1$ for all $i$.

Consider now the case $N_T < N$. Hence we have $\frac{\zeta_i^{(r)} \zeta_i^{(c)}}{N_T} > \frac{\zeta_i^{(r)} \zeta_i^{(c)}}{N}$ and $\frac{N}{N_T} > 1$. Again the only possible choice for the off-diagonal elements would be given by

$$
\alpha = \frac{N}{N_T}, \quad r_i = \frac{\zeta_i^{(r)}}{\sum_i \zeta_i^{(r)}}, \quad c_i = \frac{\zeta_i^{(c)}}{\sum_i \zeta_i^{(c)}}
$$

but in this case $\alpha = \frac{N}{N_T} > 1$. Thus we conclude that all $P \in M_1$ with $N_T < N$ are in $M_1 \setminus M_2$. This leads to the following result.

**Theorem 3.8.** Let $P \in M_1 \cap \Delta_{>0}$ be a strictly positive probability table given by the vectors $\zeta^{(r)} = (\zeta_1^{(r)}, \ldots, \zeta_{I}^{(r)})$, $\zeta^{(c)} = (\zeta_1^{(c)}, \ldots, \zeta_{I}^{(c)})$ and $\zeta^{(\gamma)} = (\zeta_1^{(\gamma)}, \ldots, \zeta_{I}^{(\gamma)})$. Define $N_T = \sum_{i \neq j} \zeta_i^{(r)} \zeta_j^{(c)} + \sum_{i=j} \zeta_i^{(r)} \zeta_j^{(c)} \zeta_i^{(\gamma)}$ and $N = \sum_{i,j} \zeta_i^{(r)} \zeta_j^{(c)}$. Then $P \in M_1 \setminus M_2$ if one of the following situations holds:

(i) $N_T < N$;

(ii) $N_T = N$ and there exists at least an index $i$ such that $\zeta_i^{(\gamma)} \neq 1$;
(iii) $N_T > N$ and there exists at least an index $i$ such that $\zeta_i^{(\gamma)} < 1$.

We conclude this section with a result on the sufficient statistics for the models $\mathcal{M}_1$ and $\mathcal{M}_2$.

**Proposition 3.9.** For an independent sample of size $n$, the models $\mathcal{M}_1$ and $\mathcal{M}_2$ have the same sufficient statistic.

**Proof.** In fact, let $f = (f_{i,j})$ be the table of counts for the sample. The likelihood function for the model in toric form is

$$L_1(\xi^{(r)}, \xi^{(c)}, \xi^{(\gamma)}; f) = \prod_{i,j} p_{i,j}^{f_{i,j}} = \prod_{i \neq j} (\xi_i^{(r)} \xi_j^{(c)})^{f_{i,j}} \prod_i (\xi_i^{(r)} \xi_i^{(c)} \xi_i^{(\gamma)})^{f_{i,i}} = \prod_i (\xi_i^{(r)})^{f_{i,+}} \prod_j (\xi_j^{(c)})^{f_{+,j}} \prod_i (\xi_i^{(\gamma)})^{f_{i,i}},$$

where $f_{i,+}$ and $f_{+,j}$ are the row and column marginal totals, respectively. This proves that the marginal totals together with the counts on the main diagonal are a sufficient statistic. With the same statistic we can also write the likelihood under the mixture model $\mathcal{M}_2$:

$$L_2(r, c, d, \alpha; f) = \prod_{i,j} p_{i,j}^{f_{i,j}} = \prod_{i \neq j} \left((\alpha r_i c_j)^{f_{i,j}} \prod_i (\alpha r_i c_i + (1 - \alpha)d_i)^{f_{i,i}} \right) = \alpha^{(n - \sum_i f_{i,i})} \prod_i (f_{i,+} - f_{i,i}) \prod_j (f_{+,j} - f_{j,j}) \prod_i (\alpha r_i c_i + (1 - \alpha)d_i)^{f_{i,i}}.$$

$\square$

### 4 A geometric description of the diagonal-effect models

In this section, we try to describe the models we studied using some geometric flavor. This analysis will also shed some light on the elements in $\mathcal{M}_1 \setminus \mathcal{M}_2$. We use very basic and classic geometric ideas and facts. As references, we suggest [Harris (1992)] and [Hartshorne (1977)].

We start with the model $\mathcal{M}_1$. The basic object we need is the variety $V$ describing all $I \times I$ matrices having rank at most one. When we fix $\xi_i^{(\gamma)} = 1, i = 1, \ldots, I$ the parametrization in (8) and (9) is just describing $V$. Hence, fixing values for all the $\xi_i^{(c)}$'s and the $\xi_i^{(r)}$'s and setting $\xi_j^{(\gamma)} = 1, j = 1, \ldots, I$ we obtain a point $M \in V$. Now, if we let $\xi_i^{(\gamma)}$ to vary we
are describing a line passing through $M$ and moving in the direction of the vector $(0, \ldots, 1, \ldots, 0)$, where the only non-zero coordinate is the $(l, l)$-th; the set of all these lines is a cylinder. Now we set $\zeta_l^{(\gamma)} = a\zeta$ and $\zeta_m^{(\gamma)} = b\zeta$ for fixed reals $a$ and $b$. When we let $\zeta$ vary, we are now describing a cylinder with directrix parallel to the line of equations $bp_{i,l} - ap_{m,m}$, $p_{i,j} = 0$ for $(i, j) \neq (l, l), (m, m)$. The same argument can be repeated fixing linear relations among the diagonal elements. In conclusion, we can describe $M_1$ as the intersection of the simplex with the union of cylinders having base $V$ and directrix parallel to the directions given by diagonal elements.

We now use the join of two varieties, i.e. the closure of the set of all the lines joining a point of any variety with any point of another variety. In order to do this, we also need to consider $W$ the variety of diagonal matrices. Then $M_2$ is the union of the segment joining a point of $V \cap \Delta$ with a point of $W \cap \Delta$, i.e. a subvariety of the join of $V$ and $W$. Each of this segment lies on a line contained in one of the cylinders we used to construct $M_1$. Hence we get again the inclusion $M_2 \subset M_1$ in $\Delta$.

5 Common-diagonal-effect models

A different version of the diagonal-effect models are the so-called common-diagonal-effect models. The definitions are as in the models above but:

- The vector $\zeta^{(\gamma)}$ is constant in the toric model definition;
- The matrix $D$ is diag$(\frac{1}{I}, \ldots, \frac{1}{I})$ in the mixture model definition.

This kind of models is much more complicated than the models in Section 3. Just to have a first look at these models, we note that for $I = 3$ the diagonal-effect models have only one invariant. For the common-diagonal-effect models, we have computed the invariants with CoCoA, see CoCoATeam (2007), for $I = 3$ and we have obtained the following lists of invariants.

For the toric model we obtain 9 binomials:

\[
P_{1,2}P_{2,3}P_{3,1} - P_{1,3}P_{2,1}P_{3,2},
\]
\[
P_{1,3}P_{2,2}P_{3,1} - P_{1,1}P_{2,3}P_{3,2},
\]
\[
-P_{1,1}P_{2,3}P_{3,2} + P_{1,2}P_{2,1}P_{3,3},
\]
\[
-P_{2,2}P_{3,1}^2 + P_{2,1}^2P_{3,2}P_{3,3},
\]
\[
P_{1,2}P_{2,2}P_{3,1}^2 - P_{1,1}P_{2,1}P_{3,2}^2,
\]

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\[-p_{1,1}p_{1,3}p_{3,2}^2 + p_{1,2}p_{3,1}p_{3,3},\]
\[-p_{1,3}p_{2,2}p_{3,2} + p_{1,2}p_{2,3}p_{3,3},\]
\[-p_{1,1}p_{2,3}p_{3,1} + p_{1,3}p_{2,1}p_{3,3},\]
\[p_{1,3}p_{2,1}p_{2,2} - p_{1,1}p_{1,3}p_{2,3}^2.\]

For the mixture model we obtain:

- 1 binomial

\[p_{1,2}p_{2,3}p_{3,1} - p_{1,3}p_{2,1}p_{3,2};\]

- 12 polynomials with 4 terms

\[p_{1,3}p_{2,1}p_{2,2} - p_{1,2}p_{2,1}p_{2,3} + p_{1,3}p_{2,3}p_{3,1} - p_{1,3}p_{2,1}p_{3,3},\]
\[+p_{1,2}p_{1,3}p_{2,2} + p_{1,2}p_{2,3} - p_{1,3}p_{3,2} + p_{1,2}p_{1,3}p_{3,3},\]
\[p_{1,3}p_{2,1}p_{3,1} - p_{1,1}p_{2,3}p_{3,1} + p_{2,2}p_{2,3}p_{3,1} - p_{2,1}p_{2,3}p_{3,2},\]
\[p_{1,2}p_{1,3}p_{3,1} - p_{1,1}p_{3,2}p_{3,2} + p_{1,3}p_{2,2}p_{3,2} - p_{1,2}p_{3,2}p_{3,2},\]
\[p_{1,2}p_{2,1}p_{2,3} - p_{2,3}p_{3,1} + p_{2,1}p_{3,3}p_{3,3},\]
\[p_{1,2}p_{2,1}p_{3,2} - p_{1,2}p_{2,3}p_{3,2} + p_{1,2}p_{2,3}p_{3,3},\]
\[+p_{1,2}p_{2,2}p_{3,1} - p_{2,3}p_{3,1} + p_{2,1}p_{3,3}p_{3,3},\]
\[p_{1,2}p_{2,2}p_{3,1} - p_{1,2}p_{2,3}p_{3,2} - p_{1,3}p_{3,1}p_{3,3} + p_{1,2}p_{3,1}p_{3,3},\]
\[p_{1,2}p_{3,1}^2 - p_{1,1}p_{1,3}p_{3,1} - p_{2,3}p_{3,1} + p_{1,2}p_{3,1}p_{3,2} - p_{2,1}p_{3,1}p_{3,2},\]
\[p_{1,2}p_{3,1} - p_{1,1}p_{2,3}p_{3,2} - p_{1,3}p_{3,1}p_{3,3} + p_{1,2}p_{3,2}p_{3,3};\]

- 6 polynomials with 8 terms

\[p_{1,1}p_{1,3}p_{2,2} - p_{1,3}p_{2,2} + p_{1,1}p_{1,2}p_{2,3} + p_{1,2}p_{2,2}p_{2,3} +\]
\[+ p_{1,3}p_{3,1} - p_{1,3}p_{2,3}p_{3,2} - p_{1,1}p_{1,3}p_{3,3} + p_{1,3}p_{2,2}p_{3,3},\]
\[p_{1,1}p_{1,3}p_{2,1} - p_{1,1}p_{2,3} - p_{1,2}p_{2,1}p_{2,3} + p_{1,1}p_{2,2}p_{2,3} +\]
\[+ p_{2,3}p_{3,2} - p_{1,3}p_{2,1}p_{3,3} + p_{1,1}p_{2,3}p_{3,3} - p_{2,2}p_{2,3}p_{3,3} ;\]
\[-p_{1,1}p_{2,2}p_{3,1} + p_{2,2}^2p_{3,1} - p_{1,3}p_{3,1}^2 + p_{1,1}p_{2,1}p_{3,2}^+ \\
- p_{2,1}p_{2,2}p_{3,2} + p_{2,3}p_{3,1}p_{3,2} + p_{1,1}p_{3,1}p_{3,3} - p_{2,2}p_{3,1}p_{3,3},\]
\[p_{1,1}p_{1,2}p_{3,1} - p_{1,1}p_{3,2}^+ - p_{1,2}p_{2,1}p_{3,2} + p_{1,1}p_{2,2}p_{3,2}^+ \\
+ p_{2,3}p_{3,1} - p_{1,2}p_{3,1}p_{3,3} + p_{1,1}p_{3,2}p_{3,3} - p_{2,2}p_{3,2}p_{3,3},\]
\[p_{1,2}p_{2,1}^2 - p_{1,1}p_{2,1}p_{2,2} - p_{1,1}p_{2,3}p_{3,1} - p_{2,1}p_{2,3}p_{3,2}^+ \\
+ p_{1,2}p_{1,2}p_{3,3} + p_{2,1}p_{2,2}p_{3,3} + p_{2,3}p_{3,1}p_{3,3} - p_{2,1}p_{3,3}^2,\]
\[p_{1,2}p_{2,1} - p_{1,1}p_{1,2}p_{2,2} - p_{1,1}p_{1,3}p_{3,2} - p_{1,2}p_{2,3}p_{3,2}^+ \\
+ p_{1,1}p_{2,3}p_{3,3} + p_{1,2}p_{2,3}p_{3,3} + p_{1,3}p_{3,2}p_{3,3} - p_{1,2}p_{3,3}^2;\]

- 1 polynomial with 12 terms

\[-p_{1,1}p_{1,2}p_{2,1} - p_{1,1}p_{2,2} - p_{1,2}p_{2,1}p_{2,2} + p_{1,1}p_{2,2}^2 + \\
- p_{1,1}p_{1,3}p_{3,1} + p_{2,2}p_{2,3}p_{3,2} + p_{1,1}p_{3,3}^2 - p_{2,2}p_{3,3} + \\
+ p_{1,3}p_{3,1}p_{3,3} - p_{2,3}p_{3,2}p_{3,3} - p_{1,1}p_{3,3}^2 + p_{2,2}p_{3,3}^2.\]

In the case of toric models, the invariants can be characterized theoretically. In fact, also in this case a Markov basis is known. In \cite{Hara et al. (2008)} it is shown that a Markov basis for this toric model is formed by 6 different types of moves. We need the 2 types of moves for the diagonal-effect model plus the moves below:

- The degree 3 moves of the form:

\[
\begin{array}{ccccccccc}
  i & i' & i'' & i & i' & i'' & i & i' & i'' \\
  +1 & 0 & -1 & +1 & -1 & 0 & 0 & -1 & +1 \\
  0 & -1 & +1 & 0 & -1 & +1 & 0 & -1 & +1 \\
  -1 & +1 & 0 & +1 & -1 & +1 & 0 & -1 & +1 \\
\end{array}
\]

with \(i, i', i''\) all distinct, for \(I \geq 3\);  

- The degree 3 moves of the form:
\[
\begin{array}{ccc}
  i & i' & j \\
  i & +1 & 0 & -1 \\
  i' & 0 & -1 & +1 \\
  j' & -1 & +1 & 0 \\
\end{array}
\]

with \(i, i', j, j'\) all distinct, for \(I \geq 4\).

- The degree 4 moves of the form:

\[
\begin{array}{ccc}
  i & i' & j \\
  i & +1 & +1 & -2 \\
  i' & -1 & -1 & +2 \\
\end{array}
\]

with \(i, i', j\) all distinct, for \(I \geq 3\), and their transposed.

- The degree 4 moves of the form:

\[
\begin{array}{cccc}
  i & i' & j & j' \\
  i & +1 & +1 & -1 & -1 \\
  i' & -1 & -1 & +1 & +1 \\
\end{array}
\]

with \(i, i', j, j'\) all distinct, for \(I \geq 4\), and their transposed.

Therefore, as in Proposition 3.2, we can easily derive the invariants. We do not write explicitly the analog of Proposition 3.2 for common-diagonal-effect models in order to save space.

The study of the common-diagonal-effect models in mixture form is much more complicated. In fact, notice that in the computations above, the mixture model present invariants which are not binomials. However, some partial results can be stated.

**Theorem 5.1.** (a) For \(i, j, k, l\) all distinct we define

\[b_{ijkl} = p_{i,j}p_{k,l} - p_{i,l}p_{k,j};\]

(b) For \(i, j, k\) all distinct we define

\[t_{ijk} = p_{i,j}p_{k,i} - p_{i,k}p_{j,i};\]

(c) For \((i, j)\) and \((k, l)\) two distinct pairs in \(\{1, \ldots, I\}\) with \(i \neq j\), and \(k \neq l\) and \(m \in \{1, \ldots, I\} \setminus \{i, j\}\) and \(n \in \{1, \ldots, I\} \setminus \{k, l\}\) with \(m \neq n\) we define

\[f_{ijklmn} = p_{i,j}p_{k,l}p_{n,m} - p_{i,j}p_{n,l}p_{k,m} - p_{i,j}p_{p_{k,l}p_{m,n}} + p_{k,l}p_{p_{m,n}}p_{i,m};\]
(d) for two distinct indices $i$ and $j$ in $\{1, \ldots, I\}$ and for $k \in \{1, \ldots, I\} \setminus \{i, j\}$ we define

$$g_{ijk} = p_{i,j}p_{i,k}p_{k,k} + p_{i,j}p_{j,j}p_{k,k} - p_{i,j}p_{i,j}p_{j,j} + p_{i,j}p_{k,k}p_{k,k} + p_{k,k}p_{i,k}p_{k,j} - p_{i,i}p_{i,k}p_{k,j} + \frac{a^2}{2}p_{i,j}p_{j,i} - p_{i,j}p_{j,j}p_{j,j};$$

(e) For $i, j, k$, all distinct we define

$$h_{ijk} = p_{i,i}p_{j,j}^2 + p_{i,i}p_{k,k}^2 + p_{j,j}p_{k,k}^2 - p_{i,i}p_{j,j}^2 - p_{j,j}p_{k,k}^2 - p_{i,i}p_{k,k}^2 + p_{i,i}p_{i,j}p_{j,i} +$$

$$- p_{i,i}p_{i,k}p_{k,i} + p_{j,j}p_{j,k}p_{k,j} - p_{j,j}p_{j,j}p_{i,j} + p_{k,k}p_{i,i}p_{i,k} - p_{k,k}p_{k,j}p_{j,k}.$$

Then the previous polynomials are invariants for the common-diagonal-effect models in mixture form.

**Proof.** Cases (a) and (b) follow from Proposition 3.2 since the off-diagonal elements of the probability table are described, up to scalar, in the same monomial form as for the elements of $\mathcal{M}_1$.

For case (c), consider the term $g_1 = p_{i,j}p_{k,l}p_{l,n}$ in $f_{ijklmn}$. This gives two monomials: $\alpha^3 r_{ij} r_{lk} c_{ln} c_n$ and $\alpha^2 r_{ij} r_{lk} c_{l} (1 - \alpha) d$, where $d = 1/I$. The term $-g_2 = -p_{i,j}p_{k,n}p_{n,l}$ of $f_{ijklmn}$ cancels the first monomial of $g_1$. In fact $-p_{i,j}p_{k,n}p_{n,l} = \alpha^3 r_{ij} r_{lk} c_{l} c_{ln} c_n$. Since in $g_2$ there are not diagonal variables, we need another term in order to cancel the second monomial of $g_1$. Thus we subtract, to $g_1 - g_2$, a term of the form $g_3 = p_{i,j}p_{k,l}p_{m,m}$ which gives the monomials $-\alpha^2 r_{ij} r_{lk} c_{l} (1 - \alpha) d$ and $-\alpha^3 r_{ij} r_{lk} c_{l} c_{m} c_m$. To cancel this last monomial it is enough to add the term $g_4 = p_{k,l}p_{m,j}p_{l,m} = \alpha^3 r_{ij} r_{lk} c_{l} c_{m} c_m$. Thus $f_{ijklmn} = g_1 - g_2 - g_3 + g_4$ vanishes on the entries of a probability table of the mixture model with common diagonal effect.

For case (d), consider first the terms with pairs of variables on the diagonal.

$$p_{i,j}p_{i,k}p_{k,k} = \alpha^3 r_{ij} r_{lk} c_{j} c_k + \alpha^2 r_{ij} r_{lk} c_j d - \alpha^3 r_{ij} r_{lk} c_j d + \boxed{\alpha^2 r_{ij} r_{lk} c_j c_k d} +$$

$$+ \alpha r_{ij} c_j d^2 - 2 \alpha^2 r_{ij} c_j d^2 - \alpha^2 r_{ij} r_{lk} c_j c_k d + \alpha^3 r_{ij} c_j d^2;$$

$$p_{i,j}p_{j,k}p_{k,k} = \alpha^3 r_{ij} r_{jk} c_j c_k + \alpha^2 r_{ij} r_{jk} c_j d - \alpha^3 r_{ij} r_{jk} c_j d + \boxed{\alpha^2 r_{ij} r_{jk} c_j c_k d} +$$

$$+ \alpha r_{ij} c_j d^2 - 2 \alpha^2 r_{ij} c_j d^2 - \alpha^2 r_{ij} r_{jk} c_j c_k d + \alpha^3 r_{ij} c_j d^2;$$

$$p_{i,j}p_{i,j}p_{j,j} = \alpha^3 r_{ij} r_{ij} c_j c_j + \alpha^2 r_{ij} r_{ij} c_j d - \alpha^3 r_{ij} r_{ij} c_j d + \boxed{\alpha^2 r_{ij} r_{ij} c_j c_j d} +$$

$$+ \alpha r_{ij} c_j d^2 - 2 \alpha^2 r_{ij} c_j d^2 - \alpha^3 r_{ij} r_{ij} c_j d + \alpha^3 r_{ij} c_j d^2;$$

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\[ p_{i,j}p_{k,k}^2 = \alpha^3 r_i r_k^2 c_j c_k^2 + 2\alpha^2 r_i r_k c_j c_k d - 2\alpha r_i r_k^2 c_j c_k d + \alpha r_i c_j d^2 + \alpha^3 r_i c_j d^2. \]

It is easy to see that while some terms, such as \( \alpha^3 r_i c_j d^2 \), are simply cancelled considering the difference of two monomials, other terms, such as the boxed ones, appear in different monomials. However, they appear with the appropriate coefficients and considering \( p_{i,j}p_{i,k}p_{k,k} + p_{i,j}p_{j,j}p_{k,k} - p_{i,j}p_{i,j} - p_{i,j}p_{k,k}^2 \) we cancel most of them. In fact we obtain

\[ \alpha^3 r_i^2 r_k c_j c_k - \alpha^3 r_i r_k^2 c_j c_k^2 - \alpha^3 r_i^2 r_j c_j c_i + \alpha^3 r_i r_j r_k c_j c_k. \]

The only way to cancel the term \(-\alpha^3 r_i r_k^2 c_j c_k^2\) is to add the monomial \( p_{i,k}p_{j,j}p_{j,j} = \alpha^3 r_i r_k^2 c_j c_k^2 + \alpha^2 r_i r_k c_j c_k d - \alpha^3 r_i r_k c_j c_k d. \) However, this monomial adds two more terms that can be cancelled by using another monomial with a variable in the diagonal, that is \( p_{i,i}p_{i,k}p_{j,j} = \alpha^3 r_i^2 r_k c_j c_k + \alpha^2 r_i r_k c_j c_k d - \alpha^3 r_i r_k c_j c_k d. \) After that, the only two missing terms are \(-\alpha^3 r_i^2 r_j c_j c_i + \alpha^3 r_i r_j r_k c_j c_k\) which can be cancelled by adding \( p_{i,j}^2 + p_{j,i}^2 - p_{i,j}p_{j,i} \).

For the case (e), we omit the complete details of the proof. One has to proceed as in cases (c) and (d) considering separately \( p_{i,j}p_{j,j}^2 + p_{i,j}p_{i,j}^2 + p_{j,k}p_{k,k}^2 - p_{i,j}p_{i,j}^2 - p_{i,j}p_{j,k}^2 - p_{j,k}p_{k,k}^2 \) and the contributions of \( p_{i,i}p_{i,j}p_{j,i} - p_{i,i}p_{i,k}p_{k,i} + p_{j,k}p_{k,k}p_{j,i} - p_{j,j}p_{j,k}p_{i,j} + p_{k,k}p_{k,k}p_{i,j} - p_{k,k}p_{k,k}p_{j,i} \).

With some computations with CoCoA, we have found that the polynomials defined in Theorem 5.2 define the model \( M_2 \) for \( I = 3, 4, 5 \). We conjecture that this fact is true in general.

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