Probability matrices, non-negative rank, and parameterizations of mixture models

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November 9, 2009

Abstract

In this paper we parameterize non-negative matrices of sum one and rank at most two. More precisely, we give a family of parameterizations using the least possible number of parameters. We also show how these parameterizations relate to a class of statistical models, known in Probability and Statistics as mixture models for contingency tables.

Key words: parametrization; determinantal varieties; non-negative rank; contingency tables.

AMS 2000: 15A51, 62H17.

1 Introduction

The study of non-negative matrices with fixed rank has recently attracted a great deal of work both theoretical and applied. One of the main problems in this field is the so-called “non-negative matrix factorization problem”, which can be shortly stated as follows. Given a non-negative matrix $A \in \mathbb{R}^{I \times J}_+$ (where $\mathbb{R}_+$ denotes the set of real non-negative numbers), one has to find
an approximation of \( A \) as a linear combination of \( k \) dyadic products \( c_i r_i \), where the \( c_i \)'s and \( r_i \)'s are vectors with non-negative entries, i.e. \( c_i \in \mathbb{R}_+^I \) and \( r_i \in \mathbb{R}_+^J \).

The rank of a matrix gives the numbers of rank one matrices, i.e. dyadic products, needed to write the matrix as a sum of dyads. But there are no non-negative conditions on the vectors of the dyads. The non-negativity constraints make the situation more complex and one has to work with the non-negative rank of the matrix (see e.g. [Cohen and Rothblum (1993)]), which is in general bigger than the ordinary rank. Therefore, it is not possible in general to decompose a rank \( k \) matrix into the sum of exactly \( k \) dyadic products \( c_i r_i \) where \( c_i \) and \( r_i \) are non-negative vectors. We will review the main results about non-negative rank in the next section.

In recent literature, a number of results and algorithms for non-negative matrix factorization have been published, see e.g. [Lee and Seung (2000)]. In [Catral et al. (2004)] special techniques for symmetric tables are presented, while in [Ho and Van Dooren (2008)] the case of fixed row and column sums is analyzed, with applications to stochastic matrices. In [Finesso and Spreij (2006)], the authors discuss some connections between the factorization problem and the notion of I-divergence, which has a well known statistical role, see e.g. [Dacunha-Castelle and Duflo (1986) and Pardo (2005)].

From the point of view of Probability, non-negative matrices are a natural tool in the analysis of two-way contingency tables. A two-way contingency table \( A = (a_{i,j}) \) collects data from two categorical random variables measured on \( n \) subjects. Let us suppose that the first variable \( X \) has \( I \) levels \( 1, \ldots, I \) and the second variable \( Y \) has \( J \) levels \( 1, \ldots, J \). The element \( a_{i,j} \) is the count of subjects with \( X = i \) and \( Y = j \). Therefore, \( A \) is an \( I \times J \) matrix with non-negative integer entries.

A joint probability distribution for the pair \((X, Y)\) is a probability matrix with \( I \) rows and \( J \) columns \( P = (p_{i,j}) \) of non-negative real numbers such that \( \sum_{i,j} p_{i,j} = 1 \). A statistical model \( \mathcal{M} \) for \( I \times J \) contingency tables is a set of probability distributions, i.e. a subset of the simplex

\[
\Delta = \left\{ P = (p_{i,j}) : p_{i,j} \geq 0, \sum_{i,j} p_{i,j} = 1 \right\} \subset \mathbb{R}_+^{I \times J}.
\]

One of the most widely used models for two-way contingency tables is the independence model, see e.g. [Agresti (2002)]. It is defined through the vanishing of all \( 2 \times 2 \) minors of the generic matrix, i.e. by the equations

\[
p_{i,j}p_{l,h} - p_{i,h}p_{l,j} = 0 \quad 1 \leq i < l \leq I, \ 1 \leq j < h \leq J;
\]
Thus, the points of the independence model are rank 1 matrices. Recent developments in Statistics have shown the relevance of probability models whose points are matrices of rank at most 2. One example in this direction, based on a special symmetric matrix, is the so-called “100 Swiss francs problem”, see Sturmfels (2008). This problem comes from Computational Biology, where it is useful to analyze the alignment of DNA sequences, see Pachter and Sturmfels (2005). Although this particular problem has been solved in Gao et al. (2008), the study of fixed-rank probability matrices is mainly unexplored.

As the sum of \( k \) matrices with rank 1 has rank at most \( k \), the matrices which can be written as the sum of \( k \) dyadic products encode the notion of mixture of \( k \) distributions from independence models.

In Probability and Statistics it is interesting not only to study the approximation problem mentioned above, but also to have a parametrization of the models. While for rank 1 matrices the parametrization is easy, see e.g. Agresti (2002), the problem becomes difficult in the case of higher non-negative ranks. Already for \( k = 2 \), in Fienberg et al. (2010) it is shown that the model is not identifiable, meaning that different parameter values lead to the same probability distribution.

This issue is a well known problem in statistical modelling called “parameter redundancy”, see Catchpole and Morgan (1997) and Catchpole et al. (1998). The detection of parameter redundancy has a major relevance in maximum likelihood estimation, where the parameters of a statistical models are estimated through the maximization of a real-valued function called “likelihood function”, see e.g. Agresti (2002). In the papers mentioned above, the authors propose a purely analytical technique to detect the parameter redundancy of a statistical model, by computing the rank of the Jacobian matrix of a specific function. The redundancy is checked through Symbolic Algebra computations and the problem of redundancy is overcome via additional linear constraints on the parameters.

In this paper, we propose a method which uses linear algebra to make the maximization problem simpler by reducing the number of parameters involved. Then the usual analytic techniques can be used in a more effective way.

The paper is organized as follows: in Section 2 we introduce some definition and we recall some basic facts. In Section 3 we study the problem of parameters redundancy form a geometric point of view. In Section 4 we show a possible application of our results.
2 Definition and background material

Let $P = (p_{i,j})$ be a probability matrix with $I$ rows and $J$ columns, i.e. $P \in \Delta$. In order to simplify the formulae, let us suppose that $I \leq J$. Let $k$ be an integer, $1 \leq k \leq I$.

Definition 2.1. A probability matrix $P$ is the mixture of $k$ independence models if it can be written in the form:

$$P = \alpha_1 c_1 r_1^t + \ldots + \alpha_k c_k r_k^t$$

(3)

where for all $h = 1, \ldots, k$

- $\alpha_h \in \mathbb{R}^+$ and $\sum \alpha_h = 1$;
- $r_h \in \mathbb{R}^J_+$ and $\sum_i r_h(i) = 1$;
- $c_h \in \mathbb{R}^I_+$ and $\sum_j c_h(j) = 1$.

Definition 2.1 contains a simple parametric form of the probability distribution which has an intuitive probabilistic counterpart. Let us suppose that we have $k$ pairs of dice, say $(D_{1,r}, D_{1,c}), \ldots, (D_{k,r}, D_{k,c})$, where $D_{h,r}$ has $J$ facets and distribution $r_h$ and $D_{h,c}$ has $I$ facets and distribution $c_h$. We choose a pair of dice with probability distribution $\alpha = (\alpha_1, \ldots, \alpha_k)$ and we roll the selected pair of dice. The resulting distribution is just a mixture distribution as in Eq. (3).

As a Linear Algebra counterpart, the definition above is strictly related with the notion of non-negative rank of a matrix. For more on non-negative rank see, e.g., Cohen and Rothblum (1993). We recall here some useful facts.

Definition 2.2. Given a matrix $P$ with real non-negative elements, the non-negative rank of $P$ is the smallest number of non-negative column vectors $v_1, \ldots, v_k$ of $P$ such that each column of $P$ has a representation as a linear combination of $v_1, \ldots, v_k$ with non-negative coefficients. The non-negative rank of a matrix $P$ is denoted with $rk_+(P)$.

The definition above has an equivalent formulation in terms of linear combinations of row vectors. In the following proposition we summarize the main properties of the non-negative rank. The reader can refer to Cohen and Rothblum (1993) for proofs and further details. The non-negative rank is of special relevance for Probability and Statistics. In fact, $rk_+(A)$ is the number of dyadic products of non-negative vectors that we can use to represent $A$. 

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Proposition 2.3. Let $P$, $Q$ be two non-negative matrices with $I$ rows and $J$ columns.

(a) $\text{rk}(P) \leq \text{rk}_+(P) \leq \min\{I, J\}$;
(b) $\text{rk}_+(P) = \text{rk}_+(P^t)$;
(c) $\text{rk}_+(P + Q) \leq \text{rk}_+(P) + \text{rk}_+(Q)$.

Moreover, if $P$ has dimensions $I \times K$ and $Q$ has dimensions $K \times J$, then $\text{rk}_+(PQ) \leq \min\{\text{rk}_+(P), \text{rk}_+(Q)\}$.

Items (b) – (d) in Proposition 2.3 show that the non-negative rank has properties similar to the classical rank. In general, the rank and non-negative rank are different, as shown by the following matrix

$$
\begin{pmatrix}
1 & 0 & 1 & 0 \\
1 & 0 & 0 & 1 \\
0 & 1 & 1 & 0 \\
0 & 1 & 0 & 1
\end{pmatrix}
$$

which has rank 3 but non-negative rank 4.

Among the cases where the rank and the non-negative rank coincide, there are the following special classes of matrices Cohen and Rothblum (1993).

Proposition 2.4. Let $P$ be a non-negative matrix with $I$ rows and $J$ columns.

(a) If $\text{rk}(P) \leq 2$ then $\text{rk}_+(P) = \text{rk}(P)$;
(b) If $P$ is diagonal, then $\text{rk}_+(P) = \text{rk}(P)$.

In what follows we will heavily use part (a) of Proposition 2.4. Hence, for the convenience of the reader, we produce a self contained proof of this fact for probability matrices.

Lemma 2.5. Let $P$ be a probability matrix. If $\text{rk}(P) \leq 2$, then $\text{rk}_+(P) = \text{rk}(P)$.

Proof. If $\text{rk}(P) = 1$ then the proof is trivial; thus we will assume $\text{rk}(P) = 2$. Denote with $C_i, i = 1, \ldots, J$ the columns of $P$. We will show that there exist two columns, say $\tilde{C}$ and $\tilde{C}$, such that $C_i = t_i\tilde{C} + s_i\tilde{C}$ for all $i$ and the coefficients $t_i$’s and $s_i$’s are non-negative.

Clearly, as $P$ has rank at most two, all columns are linear combinations of two fixed ones. Without loss of generality, we may assume that $C_1$ and $C_2$ are
linearly independent. Thus for any other column we have \( C_i = t_iC_1 + s_iC_2 \). If all the pairs \((t_i, s_i)\) are non-negative we are done. Otherwise, consider in the plane \( \mathbb{R}^2 \) the rays spanned by the pairs \((t_i, s_i)\) and let \((\bar{t}, \bar{s})\) and \((\tilde{t}, \tilde{s})\) be the extremal rays and denote by \( \bar{C} \) and \( \tilde{C} \) the corresponding columns. We recall that the extremal rays are the minimal generators of the convex cone spanned by the the pairs \((t_i, s_i)\). Now consider the angle \( \phi \) between the extremal rays containing at least one positive semi-axis. If \( \phi < \pi \) radiants then we are done by using the addition rule for vectors in the plane and all the columns are non-negative linear combinations of \( \bar{C} \) and \( \tilde{C} \). If \( \phi = \pi \) radiants we get the contradiction as \( \bar{C} + \tilde{C} = 0 \) and hence \( C_1 \) and \( C_2 \) would be proportional. If \( \phi > \pi \) we get again a contradiction. In fact, a non-negative combination of the extreme rays would be in the negative quadrant. Hence, a non-negative linear combination of \( \bar{C} \) and \( \tilde{C} \) would be non-positive and hence equal to zero being \( P \) non-negative. Thus, \( C_1 \) and \( C_2 \) would be proportional again. 

3 Parameters and parameterizations

Often in Probability and in Statistic models are described using parameters. This description can be easily expressed in geometric terms. Given the variety representing the model we look for a surjective function into it. More precisely, if \( M \) is the model, a surjective function \( U \subseteq \mathbb{R}^n \rightarrow M \) gives a parametrization of \( M \). If the function we found is described by rational functions and its image is dense in the model, we say that the map is dominant and we describe the model up to a measure zero set.

Given a model \( M \) there are two basic questions: Does there exist a dominant map \( \mathbb{R}^n \rightarrow M \)? What is the smallest \( n \) for which such a map exists? Answering the first question is a deep and difficult problem in Geometry called “the unirationality problem”, see [Harris, 1992, page 87]. The second question is difficult too, but we can easily give a bound on \( n \) using the dimension of \( M \), namely we must have \( n \geq \dim M \).

When we have a parametrization of a model \( M \) such that \( n = \dim M \) we say that the parametrization is non-redundant, or that the parameters are non-redundant. It is not always possible to find a non-redundant parametrization. But, in some interesting situations, it is possible to decompose the model \( M \) as union of subvarieties and for each of this one can find a non-redundant parametrization. We will give examples of these phenomena in the case of rank \( k \) and rank 2 mixture models.
3.1 A parametrization for the rank $k$ matrices

Given natural numbers $I \leq J$ we consider the following family of matrices with rank at most $k$:

\[ \mathcal{M}_k = \left\{ P = (p_{i,j}) \in \mathbb{R}^{I \times J} : \text{rk}(P) \leq k , \sum_{i,j} p_{i,j} = 1 \right\}. \]

As the elements of $\mathcal{M}_k$ have rank at most $k$, they can be written as a linear combination of at most $k$ rank one probability matrices. More precisely, if $P \in \mathcal{M}_k$ then

\[ P = \alpha_1 c_1 r_1^t + \ldots + \alpha_k c_k r_k^t \tag{4} \]

for a choice of scalars $\alpha_i$’s and of column vectors $c_i$’s and $r_i$’s. Hence, we can represent elements of $\mathcal{M}_k$ using $k(I + J) + k$ parameters. In other words, (4) gives a surjective polynomial map

\[ \mathbb{R}^{k(I+J)+k} \rightarrow \mathcal{M}_k. \]

We recall that a map between algebraic varieties, say $V_1 \rightarrow V_2$, can be a parametrization, only if dim $V_1 \geq$ dim $V_2$. To know whether the parameters we are using are necessary or redundant, we need to know the dimension of $\mathcal{M}_k$ and compare it with $k(I + J) + k$.

**Proposition 3.1.** With the notation above, we have

\[ \dim \mathcal{M}_k \leq k(I + J) - k^2 - 1. \]

**Proof.** The dimension of the family of complex $I \times J$ matrices of rank at most $k$ is well known to be $k(I + J) - k^2$, see [Harris (1992)]. Imposing that the sum of all the entries is 1 and taking real matrices give the bound. □

Proposition 3.1 shows that the parametrization (4) is redundant and we are using more parameters than the best possible value. Actually, it is not possible to use $k(r + s) - k^2 - 1$ parameters to get all the elements of $\mathcal{M}_k$. In the case of $k = 2$ we will show how to decompose $\mathcal{M}_k$ in open subsets which can each be described using the optimal number of parameters.
3.2 Non-redundant parameterizations of probability models for \( k = 2 \)

In this section we only deal with matrices of rank at most two. Hence we fix \( k = 2 \) and we set

\[
\mathcal{M} = \mathcal{M}_2^+ = \left\{ P \in \mathbb{R}_+^{I \times J}, \text{rk}_+(P) = 2 \right\} \cap \Delta.
\]

In this situation, \( \dim \mathcal{M} \leq 2I + 2J - 5 \) and we will use this number of parameters to describe \( \mathcal{M} \), hence finding a non-redundant parametrization. Set \( D = 2I + 2J - 5 \). We will construct maps

\[
f_{j_1,j_2} : U_{j_1,j_2} \subset \mathbb{R}^D \rightarrow \mathcal{M}
\]

for \( 1 \leq j_1 < j_2 \leq J \), with the property that the union of the images of the \( f_{j_1,j_2} \) is the whole \( \mathcal{M} \), i.e. \( \bigcup \text{Im}(f_{j_1,j_2}) = \mathcal{M} \).

Each map is constructed in such a way that \( \text{Im}(f_{j_1,j_2}) \) is contained in the open subset of the matrices with the \( j_1 \)-th and the \( j_2 \)-th columns linearly independent. We give an explicit description only for \( f_{1,2} \), the other cases being completely analogous. We set

\[
f_{1,2}(a_1, \ldots, a_{I-1}, b_3, \ldots, b_J, c_1, \ldots, c_{I-1}, d_3, \ldots, d_J, \alpha) = \alpha \left( \begin{array}{c} a_1 \\ a_2 \\ \vdots \\ a_{I-1} \\ 1 - \sum a_i \end{array} \right) \left( \begin{array}{cccc} 1 - \sum b_i & 0 & b_3 & \ldots & b_J \end{array} \right) +
+(1 - \alpha) \left( \begin{array}{c} c_1 \\ c_2 \\ \vdots \\ c_{I-1} \\ 1 - \sum c_i \end{array} \right) \left( \begin{array}{cccc} 0 & 1 - \sum d_i & d_3 & \ldots & d_J \end{array} \right),
\]

defined on

\[
U'_{1,2} = \left\{ (a_1, \ldots, a_{I-1}, b_3, \ldots, b_J, c_1, \ldots, c_{I-1}, d_3, \ldots, d_J, \alpha) \in \mathbb{R}^D : 0 \leq a_i, b_i, c_i, d_i, \alpha \leq 1 \text{ and } 0 \leq \sum a_i, \sum b_i, \sum c_i, \sum d_i \leq 1 \right\}.
\]

To define \( f_{j_1,j_2} \) one simply moves element in the row vectors. In the first row vector the \( 1 - \sum b_i \) element is moved in position \( j_1 \) and the 0 is moved in position \( j_2 \); similarly for the second row vector.
Remark 3.2. With standard computations one can easily check that
\[ \text{Im}(f_{j_1,j_2}) \subset \mathcal{M} \]
for all \( j_1 \) and \( j_2 \), \( j_1 < j_2 \).

Now we analyze the functions \( f_{j_1,j_2} \) in order to derive some useful properties. We work with \( f_{1,2} \) and all the results trivially extend to the other functions.

Lemma 3.3. Let \( P \in \mathcal{M} \) be the following matrix
\[
P = \begin{pmatrix}
x_1 & y_1 & \ldots & t_1x_1 + s_1y_1 & \ldots & t_Jx_1 + s_Jy_1 \\
\vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\
x_1 & y_1 & \ldots & t_1x_J + s_1y_J & \ldots & t_Jx_J + s_Jy_J
\end{pmatrix}
\]
where the coefficients \( x_i, y_i, s_i \) and \( t_i \) are non-negative.
If the first two columns of \( P \) are non-zero, we set
\[
a_i = \frac{x_i}{\sum x_i}, \quad c_i = \frac{y_i}{\sum y_i}, \quad b_i = \frac{t_i}{1 + \sum t_i}, \quad d_i = \frac{s_i}{1 + \sum s_i}
\]
and also \( \alpha = (\sum t_i + 1) \sum x_i = 1 - (\sum s_i + 1) \sum y_i \).
If \( \sum y_i = 0 \), we set
\[
a_i = \frac{x_i}{\sum x_i}, \quad b_i = \frac{t_i}{1 + \sum t_i}
\]
and also \( \alpha = 1 \), and \( c_i = d_i = 0 \) for all \( i \).
If \( \sum x_i = 0 \), we set
\[
c_i = \frac{y_i}{\sum y_i}, \quad d_i = \frac{s_i}{1 + \sum s_i}
\]
and also \( \alpha = 0 \) and \( a_i = b_i = 0 \) for all \( i \).

If we set \( P' = (a_1, \ldots, a_{I-1}, b_3, \ldots, b_J, c_1, \ldots, c_{I-1}, d_3, \ldots, d_J, \alpha) \), then \( P' \in U_{1,2}' \) and
\[
f_{1,2}(P') = P.
\]
Prove. The definition of \( P' \) and the condition on the entries of \( P \) yield that \( P' \in U_{1,2}' \). A straightforward computation shows that \( f_{1,2}(P') = P \). The two expressions for the parameter \( \alpha \) coincide as \( P \) is a matrix with sum one.
\[ \Box \]
Finally we can show that the maps $f_{j_1,j_2}$ give a parametrization of $\mathcal{M}$.

**Corollary 3.4.** The variety $\mathcal{M}$ is covered by the images of the functions $f_{j_1,j_2}$, more precisely $\bigcup \text{Im}(f_{j_1,j_2}) = \mathcal{M}$.

**Proof.** Let $P \in \mathcal{M}$, by Lemma 2.5 we know that $P$ can be written as in the statement of Lemma 3.3 for some columns $C_{j_1}$ and $C_{j_2}$ and hence $P \in \text{Im}(f_{j_1,j_2})$.

### 4 An application

It is often interesting to find maxima and minima of a function over a variety. As an example consider the well known likelihood function. We will use the parametrization we found in the previous sections to propose a strategy to study extremal points on $\mathcal{M}$. The advantage of this approach is that we are going to study functions involving the least possible number of variables as the parametrization we found is non-redundant.

**Remark 4.1.** Given a function $F : \mathcal{M} \rightarrow \mathbb{R}$ we consider the composite functions $F \circ f_{j_1,j_2}$. Consider a point $P = f_{j_1,j_2}(P') \in \mathcal{M}$ such that $P$ is in the interior of $\text{Im}(f_{j_1,j_2})$. Then $P$ is a maximum/minimum for $F$ if and only if $P'$ is a maximum/minimum for $F \circ f_{j_1,j_2}$.

Using Remark 4.1 we can apply the usual gradient and Hessian matrix approach to detect extremal points of $F$ lying in the interior of one of the $\text{Im}(f_{j_1,j_2})$. Hence it useful to have the following:

**Lemma 4.2.** If $P'$ is in the interior of $U'_{j_1,j_2}$ then $f_{j_1,j_2}(P')$ is in the interior of $\text{Im}(f_{j_1,j_2})$.

**Proof.** We produce a proof for $j_1 = 1$ and $j_2 = 2$ but a completely analogous argument works in the general situation. Given $P'$ we compute $P = f_{1,2}(P')$ and thus we write $P$ as in the statement of Lemma 3.3. Moreover, as $P'$ is in the interior of $U'_{1,2}$ the coefficients $t_i$ and $s_i$ in $P$ are strictly positive. Now consider a neighborhood $U$ of $P$. Given a matrix $Q \in U$ we can write it in the form of Lemma 3.3 by computing the coefficients $t_i$ and the $s_i$. This is done by solving linear systems of equations having the elements of $Q$ as coefficients. Hence, it is possible to choose a suitable $U$ such that for all the matrices in $U$ the coefficients $t_i$ and $s_i$ are strictly positive. In conclusion, the formulae of Lemma 3.3 produce a map $g_{1,2} : U \rightarrow U'_{1,2}$. It is straightforward to see that $g_{1,2}$ is a continuous map on $U$ and that the map

$$f_{1,2} \circ g_{1,2}$$
is the identity map. Now we take a neighborhood of $P'$, say $U' \subset f_{1,2}^{-1}(U)$. Then we get a neighborhood of $P$

$$g_{1,2}^{-1}(U') \subset \text{Im}(f_{1,2})$$

and we are done. \hfill \square

Lemma 4.2 shows that we only have to worry about points of $M$ which are images of boundary points of $U_{j_1,j_2}$. Thus it is useful to have the following description:

**Lemma 4.3.** Let $P' \in U'_{j_1,j_2}$ be the point

$$P' = (a_1, \ldots, a_{I-1}, b_3, \ldots, b_J, c_1, \ldots, c_{I-1}, d_3, \ldots, d_J, \alpha)$$

and let $P = f_{j_1,j_2}(P')$. Then the following hold:

1. if any of the coefficients $a_i$ or $c_i$ is zero then $P$ is a point of the boundary of $M$;
2. if $\sum a_i = 1$ or $\sum b_i = 1$ then $P$ is a point of the boundary of $M$;
3. if $\alpha = 0$ or $\alpha = 1$ then $P$ is a rank one matrix;
4. if any of the coefficients $b_i$ or $d_i$ is zero then $P$ has at least two proportional columns;
5. if $\sum a_i = 1$ or $\sum b_i = 1$ then $P$ has at least two proportional columns.

**Proof.** For (1) and (2) it is enough to notice that $P$ has some zero element. Hence a neighborhood of $P$ contains matrices with negative entries. Thus $P$ is on the boundary of $M$. The other cases are obtained by direct computations. \hfill \square

By Lemma 4.3 we see that the composite map $F \circ f_{j_1,j_2}$ will detect maxima and minima of $F$ if these extremal points do not have rank one or if they have rank two and do not have two proportional columns. In many situation of interest rank one matrices can be efficiently treated, e.g. for the likelihood function. Rank two matrices with proportional columns can be treated using our parametrization in a subtler way.

**Lemma 4.4.** Let $P = f_{j_1,j_2}(P'_{j_1,j_2})$ be a rank two matrix with at least two proportional columns. Then a neighborhood of $P$ in $M$ can be covered using images of neighborhoods of $P'_{j_1,j_2}$ in $U'_{j_1,j_2}$ for different pairs $(j_1,j_2)$.
Proof. Given $P$, choose two independent columns, say the $j_1$-th and the $j_2$-th. As $P$ has proportional columns, when written as in Lemma 3.3 some of the coefficients $t_i$ and $s_i$ vanish. Hence, in each neighborhood of $P$ there will be matrices requiring negative values of the coefficients $t_i$ or $s_i$. Then there is no neighborhood where the formulae of the Lemma can be applied to get and inverse on $f_{j_1,j_2}$ and hence we can not reproduce the argument of Lemma 4.2. But we can find a neighborhood of $P'$, say $W'_{j_1,j_2} \subset U'_{j_1,j_2}$, such that there exists an inverse of $f_{j_1,j_2}$ on $f_{j_1,j_2}(W'_{j_1,j_2})$, but this is not a neighborhood of $P$. By Lemma 2.5 we see that the $f_{j_1,j_2}(W'_{j_1,j_2})$ cover a neighborhood of $P$ as $(j_1, j_2)$ varies and we are done. \hfill \qed

We can now describe our strategy. Given a function $F : \mathcal{M} \rightarrow \mathbb{R}$ we can look for maxima and minima of $F$ in following way:

1. study $F$ on rank one matrices using an ad hoc method. When $F$ is the likelihood function, the problem is quite simple, see e.g. Agresti (2002);

2. consider the functions $F \circ f_{j_1,j_2}$ and compute their maxima and minima on $U'_{j_1,j_2}$ for all $1 \leq j_1 < j_2 \leq J$ (notice that these computation are as simple as they could be as the least number of variable is involved); let $Q$ be one of the point we found;

3. if $Q$ is in the interior of one of the $U'_{j_1,j_2}$ then $f_{j_1,j_2}(Q)$ is a maximum or minimum of $F$;

4. if $Q$ lies on the boundary of one of the $U'_{j_1,j_2}$ and $f_{j_1,j_2}(Q)$ is on the boundary of $\mathcal{M}$, then $f_{j_1,j_2}(Q)$ is a maximum or minimum of $F$;

5. if $Q$ lies on the boundary of one of the $U'_{j_1,j_2}$ and $f_{j_1,j_2}(Q)$ has rank one we already treated this case in the first step;

6. if $Q$ lies on the boundary of one of the $U'_{j_1,j_2}$ and $f_{j_1,j_2}(Q)$ has two proportional columns, then $Q$ will lie on the boundary of at least two of the $U'_{j_1,j_2}$; for each each pair $(j_1, j_2)$ such that $Q$ is on the boundary of $U'_{j_1,j_2}$ we have to compare the extremal behavior of the functions $F \circ f_{j_1,j_2}$, if these behavior agree then $f_{j_1,j_2}(Q)$ is a maximum/minimum of $F$ otherwise it is not.

In this paper we only considered matrices of rank at most two. For higher values of the rank the situation gets much more involved and almost impossible to treat. For example, it is not even known how to effectively compute the non-negative rank of a matrix. But, some preliminary results
in [Dong et al. (2009)](#) suggest that matrices with non-negative rank different from the ordinary rank are exceptional, i.e. they form a zero-measure set. This observation can be of some help to try and extend our approach.

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