Characterization of multivariate Bernoulli
distributions with given margins

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Abstract

We express each Fréchet class of multivariate Bernoulli distributions with given margins as the convex hull of a set of densities, which belong to the same Fréchet class. This characterisation allows us to establish whether a given correlation matrix is compatible with the assigned margins and, if it is, to easily construct one of the corresponding joint densities. We reduce the problem of finding a density belonging to a Fréchet class and with given correlation matrix to the solution of a linear system of equations. Our methodology also provides the bounds that each correlation must satisfy to be compatible with the assigned margins. An algorithm and its use in some examples is shown.

Keywords: Algebraic statistics; Correlation; Fréchet class; Multivariate binary distribution; Simulation.
1 Introduction

Dependent binary variables play a key role in many important scientific fields such as clinical trials and health studies. The problem of the simulation of correlated binary data is extensively addressed in the statistical literature, e.g. [3], [6], [15] and [9]. Simulation studies are a useful tool for analysing extensions or alternatives to current estimating methodologies, such as generalised linear mixed models, or for the evaluation of statistical procedures for marginal regression models ([13]). The simulation problem consists of constructing multivariate distributions for given Bernoulli marginal distributions and a given correlation matrix $\rho$. Frequently, assumptions are made about the correlation structure. Probably the most common is equicorrelation, e.g. [3]. A popular approach also uses working correlation matrices ([10] and [16]), such as first order moving average correlations or first order autoregressive correlations ([12] and references therein). An important issue for these simulation procedures is the compatibility of marginal binary variables and their correlations, since problems may arise when the margins and the correlation matrix are not compatible ([4], [14] and [3]). The range of admissible correlation matrices for binary variables is well known in the bivariate case. This problem has been widely identified in the literature, but, to the best of our knowledge no effective solution exists for multivariate binary distributions with more than three variables ([3]).

We propose a new but simple methodology to characterise Bernoulli variables belonging to a given Fréchet class, i.e. with given marginal distributions. This characterisation allows us to establish whether a given correlation matrix is compatible with the assigned margins and, if it is, to easily construct one of the corresponding joint densities. It also provides the bounds that each correlation must satisfy to be compatible with the assigned margins. Furthermore, if the correlation structure and the margins are not compatible, we can find a new correlation matrix which is close to the desired one but compatible with the given margins. It is worth noting that this methodology puts no restriction either on the number of variables or on the correlation structure. It also provides a new computational procedure to simulate multivariate distributions of binary variables with assigned margins and given moments.

The proposed methodology is based on a polynomial representation of all the multivariate Bernoulli distributions of a given Fréchet class, i.e. of all the distributions with fixed Bernoulli margins. This representation is linked to the Farlie-Gumbel-Morgesten copula ([11]). It allows us to write each Fréchet class as the convex hull of the ray densities, which are densities that belong to the Fréchet class under consideration. By so doing, the problem of finding one distribution with given moments in a Fréchet class is reduced to the solution of a linear system of equations.
2 Preliminaries

Let $\mathbb{F}_m$ be the set of $m$-dimensional distributions which have Bernoulli univariate marginal distributions. Let us consider the Fréchet class $\mathcal{F}(p_1, \ldots, p_m) \subseteq \mathbb{F}_m$ of distribution functions in $\mathbb{F}_m$ which have the same Bernoulli marginal distributions $B(p_i), 0 < p_i < 1, i = 1, \ldots, m$. If $X = (X_1, \ldots, X_m)$ is a random vector with joint distribution in $\mathcal{F}(p_1, \ldots, p_m)$, we denote

- its cumulative distribution function by $F_p$ and its density function by $f_p$ where $p = (p_1, \ldots, p_m)$;

- the column vector which contains the values of $F_p$ and $f_p$ over $S_m := \{0, 1\}^m$, with a small abuse of notation, still by $F_p = (F_p(x) : x \in S_m)$ and $f_p = (f_p(x) : x \in S_m)$ respectively; we make the non-restrictive hypothesis that $S_m$ is ordered according to the reverse-lexicographical criterion;

- the marginal cumulative distribution function and the marginal density function of $X_i$ by $F_{p,i}$ and $f_{p,i}$ respectively, $i = 1, \ldots, m$;

- the values $f_{p,i}(0) \equiv F_{p,i}(0)$ and $f_{p,i}(1)$ by $q_i$ and $p_i$ respectively, $i = 1, \ldots, m$.

We observe that $q_i = 1 - p_i$ and that the expected value of $X_i$ is $p_i$, $E[X_i] = p_i$, $i = 1, \ldots, m$.

Given two matrices $A \in \mathcal{M}(n \times m)$ and $B \in \mathcal{M}(d \times l)$ the matrix $A \otimes B \in \mathcal{M}(nd \times ml)$ indicates their Kronecker product and $A^\otimes n$ is $\underbrace{A \otimes \ldots \otimes A}_{n \text{ times}}$.

If we consider a Bernoulli variable $B(\tau), 0 < \tau < 1$, with $F_\tau$ and $f_\tau$ as cumulative and density function respectively, the following holds

$$
\begin{pmatrix}
    f_\tau(0) \\
    f_\tau(1)
\end{pmatrix} = D \cdot 
\begin{pmatrix}
    F_\tau(0) \\
    F_\tau(1)
\end{pmatrix}
$$

where $D = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}$ is the difference matrix.

It follows that given $F_p$ and $f_p$ in $\mathcal{F}(p_1, \ldots, p_m)$ we have

$$
f_p = D^\otimes m F_p. \quad (2.1)
$$

Finally we can write $f_p \in \mathcal{F}(p_1, \ldots, p_m)$, $F_p \in \mathcal{F}(p_1, \ldots, p_m)$ and $X \in \mathcal{F}(p_1, \ldots, p_m)$. 
3 Construction of multivariate Bernoulli distributions with given margins

We give a polynomial and matrix representation of all the \( F_p \in \mathcal{F}(p_1, \ldots, p_m) \). We make the non-restrictive hypothesis that \( \{q_1, 1\} \times \ldots \times \{q_m, 1\} \) is ordered according to the reverse-lexicographical criterion. We denote \( \{q_1, 1\} \times \ldots \times \{q_m, 1\} \) by \( Q_m \).

**Theorem 3.1.** Any distribution \( F_p \in \mathcal{F}(p_1, \ldots, p_m) \) admits the following representation over \( Q_m \)

\[
F_p = \Lambda_p U_p \theta
\]

where \( \Lambda_p = \text{diag}(q_1^{(1-\alpha_1)}, \ldots, q_m^{(1-\alpha_m)}), (\alpha_1, \ldots, \alpha_m) \in S_m \), \( U_p = U_{p_1} \otimes \ldots \otimes U_{p_m}, U_{p_i} = \begin{pmatrix} 1 & 1 - q_i \\ 1 & 0 \end{pmatrix}, i = 1, \ldots, m \) and \( \theta = (\theta_0, \theta_m, \theta_{m-1}, \theta_{m,m-1}, \ldots, \theta_{12\ldots m}) \).

**Proof.** Given \( u = (u_1, \ldots, u_m) \in Q_m \) let us define

\[
g(u) = \left( \prod_{i=1}^m u_i \right) \left( \theta_0 + \sum_{j=1}^m \theta_j (1-u_j) + \sum_{1 \leq k < j \leq m} \theta_{jk} (1-u_j) (1-u_k) + \cdots + \theta_{12\ldots m} \prod_{i=1}^m (1-u_i) \right)
\]

and the row vectors \( a_i = (1, 1 - u_i), i = 1, \ldots, m \). We can write \( g(u) \in \mathbb{R} \) as

\[
g(u) = \left( \prod_{i=1}^n u_i \right) \left( a_1 \otimes \ldots \otimes a_m \right) \begin{pmatrix} \theta_0 \\ \theta_m \\ \theta_{m-1} \\ \vdots \\ \theta_{12\ldots m} \end{pmatrix}
\]

Considering all the \( u \in Q_m \) we get the \( 2^m \)-vector \( (g(u), u \in Q_m) = \Lambda_p U_p \theta \).

We observe that the determinant of \( U_{p_i} = \begin{pmatrix} 1 & 1 - q_i \\ 1 & 0 \end{pmatrix} \) is \( \det(U_{p_i}) = -p_i \neq 0 \).

It follows that the determinant of \( U_p \), which is \( (p_1 \cdot \ldots \cdot p_m)^2 \), is also different from zero. Being the determinant of \( \Lambda_p \neq 0 \) we get that the determinant of \( \Lambda_p U_p \) is different from zero. It follows that the rank of \( \Lambda_p U_p \) is \( 2^m \) and then any vector \( y \in \mathbb{R}^{2^m} \) and in particular any distribution \( F_p \) can be written as \( F_p = \Lambda_p U_p \theta \).

If \( F_p \) is a distribution in \( \mathcal{F}(p_1, \ldots, p_m) \), the vector parameter \( \theta \) must satisfy the following necessary conditions:

1. \( \theta_0 = 1 \). The condition \( F_p(1, \ldots, 1) = 1 \) implies \( \theta_0 = 1 \), since \( F_p(1, \ldots, 1) = \theta_0 \);
2. \( \theta_i = 0, i = 1, \ldots, m \). The condition \( F_p(1, \ldots, 1, 0, 1, \ldots, 1) = q_i \) implies \( \theta_i = 0, i = 1, \ldots, m \), since \( F_p(1, \ldots, 1, 0, 1, \ldots, 1) = q_i (1 + \theta_i (1 - q_i)) \).
Remark 1. Under the necessary assumptions $\theta_0 = 1$ and $\theta_i = 0$, $i = 1, \ldots, m$, the polynomial function $g(u)$ in Theorem 3.1 is the restriction of the well-known Farlie-Gumbel-Morgesten copula $C(u)$ to $Q_m$:

$$C(u) := \left(\prod_{i=1}^{m} u_i\right) \left(1 + \sum_{1 \leq j < k \leq n} \theta_{jk} (1-u_j)(1-u_k) + \cdots + \theta_{12 \ldots m} \prod_{i=1}^{m} (1-u_i)\right), \quad u \in [0,1]^m.$$  

Notice that the condition $\theta_0 = 1$ derives from $C(1, \ldots, 1) = 1$ and the condition $\theta_i = 0$ is necessary since a requirement to be a copula is that $C(1, \ldots, 1, q_i, 1, \ldots, 1) = q_i$, $i = 1, \ldots, m$. Our representation shows that the restriction to $Q_m$ of the Farlie-Gumbel-Morgesten copula allows us to represent all the binary distributions with given margins, and therefore to model all the possible dependence structures of multivariate Bernoulli distributions.

As a consequence of Theorem 3.1 and Equation 2.1 any density $f_p \in \mathcal{F}(p_1, \ldots, p_m)$ admits the following representation over $S_m$:

$$f_p = D^m \Lambda_p U_p \Theta$$  

(3.1)

We observe that given $f_p \in \mathcal{F}(p_1, \ldots, p_m)$ we can write it as in Eq.(3.1). Vice versa Theorem 3.1 does not provide any condition on $\theta_{i_1 \ldots i_k}$ for $k \geq 2$ such that $D^m \Lambda_p U_p \Theta$ represents a density function $f_p$ over $S_m$.

In the remaining part of this section we will provide a representation of all the densities $f_p \in \mathcal{F}(p_1, \ldots, p_m)$.

Theorem 3.2. Let $f_p \in \mathcal{F}(p_1, \ldots, p_m)$. It holds that

$$f_p = \sum_{i=1}^{n_F} \lambda_i R_p^{(i)},$$  

(3.2)

where $R_p^{(i)} = (R_p^{(i)}(x), x \in S_m) \in \mathcal{F}(p_1, \ldots, p_m)$, $\lambda_i \geq 0$, $i = 1, \ldots, n_F$ and $\sum_{i=1}^{n_F} \lambda_i = 1$.

Proof. Let us define $Y_p = D^m \Lambda_p U_p$. From Eq.(3.1) it holds that

$$f_p = Y_p \Theta,$$

with the conditions $\theta_0 = 1$ and $\theta_i = 0$, $i = 1, \ldots, m$. We can write

$$\Theta = Y_p^{-1} f_p.$$  

The conditions $\theta_i = 0$, $i = 1, \ldots, m$ can be written as

$$H f_p = 0,$$  

(3.3)
where $H$ is the $m \times 2^m$ sub-matrix of $Y_p^{-1}$ obtained by selecting the rows corresponding to $\theta_i$, $i = 1 \ldots , m$.

The condition $\theta_0 = 1 \iff F_p(1, \ldots , 1) = 1$ is ensured by requiring that $f_p$ is a density, i.e.

1. $f_p(x) \geq 0$;
2. $\sum_x f_p(x) = 1$

where $x \in S_m$.

All the positive solutions $f_p$ of (3.3) have the following form:

$$f_p = \sum_{i=1}^{n_F} \lambda_i R_p^{(i)}, \quad \lambda_i \geq 0,$$

where $R_p^{(i)} = (\bar{R}_p^{(i)}, j = 1, \ldots , 2^m) \in \mathbb{R}^{2^m}$, $\bar{R}_p^{(i)} \geq 0$ and $H \bar{R}_p^{(i)} = 0$, $i = 1, \ldots , n_F$ are the extremal rays of the cone defined by $H f_p = 0$ (11 and 7).

By dividing $\bar{R}_p^{(i)}$ by the sum of its elements $R_{p+} = \sum_{j=1}^{2^m} \bar{R}_p^{(i)}$ we can write

$$f_p = \sum_{i=1}^{n_F} \lambda_i R_p^{(i)},$$

where $\lambda_i = \bar{\lambda}_i R_{p+}^{(i)}$ and $R_p^{(i)} = \frac{\bar{R}_p^{(i)}}{R_{p+}}$, $i = 1, \ldots , n_F$. It follows that $\sum_{j=1}^{2^m} R_p^{(i)} = 1$ and that the ray density defined as $R_p^{(i)}(x) := R_{p+}^{(i)}$ being $x$ the $j$-th element of $S_m$ belongs to $\mathcal{F}(p_1, \ldots , p_m)$, $i = 1, \ldots , n_F$.

Finally the condition $\sum_x f_p(x) = 1$ implies $\sum_{i=1}^{n_F} \lambda_i (\sum_{j=1}^{2^m} R_p^{(i)}) = \sum_{i=1}^{n_F} \lambda_i = 1$. Then we have $\lambda_i \geq 0$, $i = 1, \ldots , m$ and $\sum_{i=1}^{n_F} \lambda_i = 1$ and the assert is proved.

Notice that Theorem 3.2 makes extremely easy to generate any density $f_p$ of the Fréchet class $\mathcal{F}(p_1, \ldots , p_m)$. It is enough to take a positive vector $\lambda = (\lambda_1, \ldots , \lambda_{n_F})$, such that $\sum_{i=1}^{n_F} \lambda_i = 1$, and build $f_p = \sum_{i=1}^{n_F} \lambda_i R_p^{(i)}$.

The constraints $E[X_i] = p_i$, $i = 1, \ldots , m$ allow us to obtain an interesting interpretation of the matrix $H$ of (3.3). We have $E[X_i] = \sum_{(x_1, \ldots , x_m) \in S_m} x_i f_p(x_1, \ldots , x_m)$. It follows that

$$x_i^T f_p = p_i$$
$$\quad (1 - x_i)^T f_p = q_i$$

where $x_i$ is the vector which contains the $i$-th element of $x \in S_m$, $i = 1, \ldots , m$. If we consider the odds of the event $X_i = 1$, $\gamma_i = p_i/q_i$ we have $\gamma_i q_i - p_i = 0$. We can write

$$(\gamma_i (1 - x_i)^T - x_i^T) f_p = 0.$$
Then $H$ is simply the $m \times 2^m$ matrix whose rows, up to a non-influential multiplicative constant, are $(\gamma_i(1 - x_i)^T - x_i^T)$, $i = 1, \ldots, m$.

Using Theorem 3.2 we represent each Fréchet class $F(p_1, \ldots, p_m)$ as the convex hull of the ray densities. We observe that the ray densities depend only on the marginal distributions $F_1, \ldots, F_m$.

Building the ray matrix $R_p$

$$R_p = \begin{pmatrix} R_{p,1}^{(1)} & \ldots & R_{p,1}^{(n_F)} \\ \vdots & \ddots & \vdots \\ R_{p,2^m}^{(1)} & \ldots & R_{p,2^m}^{(n_F)} \end{pmatrix}$$

whose columns are the ray densities $R_p^{(i)}$, $i = 1, \ldots, n_F$ we write Eq. (3.2) simply as

$$f_p = R_p \lambda$$

with $\lambda = (\lambda_1, \ldots, \lambda_{n_F}), \lambda_i \geq 0$ and $\sum_{i=1}^{n_F} \lambda_i = 1$.

In practical applications the rays $\tilde{R}_p^{(i)}$ and therefore the ray densities $R_p^{(i)}$ can be found using the software 4ti2, [1]. In Section 5 we will use SAS and 4ti2 to show some numerical examples.

In the next sections we will see that the representation of $f_p$ as in Theorem 3.2 plays a key role in determining the densities with given moments.

### 3.1 Moments of multivariate Bernoulli variables

We observe that, given the Bernoulli variable $X \sim B(\tau), 0 < \tau < 1$ with density function $f_\tau$ we can compute the moments $E[X^\alpha], \alpha \in \{0, 1\}$ as

$$E[X^\alpha] = \begin{pmatrix} E[1] \\ E[X] \end{pmatrix} = M \begin{pmatrix} f_\tau(0) \\ f_\tau(1) \end{pmatrix}$$

where $M = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$.

It follows that given $X = (X_1, \ldots, X_m) \in F(p_1, \ldots, p_m)$ with multivariate joint density $f_p$, we can compute the vector of its moments $E[X^\alpha] = E[X_1^{\alpha_1} \cdot \ldots \cdot X_m^{\alpha_m}], \alpha = (\alpha_1, \ldots, \alpha_m) \in S_m$ as

$$E[X^\alpha] = M^{\otimes m} f_p.$$ 

We also observe that the correlation $\rho_{ij}$ between two Bernoulli variables $X_i \sim B(p_i)$ and $X_j \sim B(p_j)$ is related to the second-order moment $E[X_i X_j]$ as follows

$$E[X_i X_j] = \rho_{ij} \sqrt{p_i q_i p_j q_j} + p_i p_j. \quad (3.4)$$
3.2 Second-order moments of multivariate Bernoulli variables with given margins

From Theorem 3.2 we get
\[ E[X^\alpha] = M^\otimes m f_p = M^\otimes m R_p \lambda. \]

In particular for the second-order moments \( \mu_2 = E[X^\alpha : \|\alpha\|_0 = 2] \), where \( \|\alpha\|_0 = \sum_{i=1}^m \alpha_i \) we get the following result, which is crucial for the solution of the problem of simulating multivariate binary distributions with a given correlation matrix.

**Proposition 3.1.** It holds that
\[ \mu_2 = A_{2p}^\lambda \]  
(3.5)

where \( A_{2p} = (M^\otimes m)_2 R_p \) and \( (M^\otimes m)_2 \) is the sub-matrix of \( M^\otimes m \) obtained by selecting the rows corresponding to the second-order moments, \( R_p \) is the ray matrix and \( \lambda = (\lambda_1, \ldots, \lambda_{n_F}) \), \( \lambda_i \geq 0, i = 1, \ldots m \) and \( \sum_{i=1}^{n_F} \lambda_i = 1 \).

It follows that the target second-order moments are compatible with the means if they belong to the convex hull generated by the points which are the columns of the \( A_{2p} = (M^\otimes m)_2 R_p \) matrix. As a direct consequence of Proposition 3.1 we also get the univariate bounds for the second-order moments and the correlations.

**Proposition 3.2.** For each \( \alpha, \|\alpha\|_0 = 2 \), the second-order moment \( \mu_2^{(\alpha)} \) must satisfy the following bounds
\[ \min A_{2p}^{(\alpha)} \leq \mu_2^{(\alpha)} \leq \max A_{2p}^{(\alpha)} \]  
(3.6)

and the correlations \( \rho_S(\alpha) \) must satisfy the following bounds
\[ \frac{\min A_{2p}^{(\alpha)} - p_ip_j}{\sqrt{p_ip_jq_ip_jq_j}} \leq \rho_{ij} \leq \frac{\max A_{2p}^{(\alpha)} - p_ip_j}{\sqrt{p_ip_jq_ip_jq_j}} \]  
(3.7)

where \( A_{2p}^{(\alpha)} \) is the row of the matrix \( A_{2p} \) such that \( \mu_2^{(\alpha)} = A_{2p}^{(\alpha)} \lambda \) and \( \{i, j\} = \{k : \alpha_k = 1\} \).

**Proof.** From Proposition 3.1 using the the proper row of \( A_{2p} \) we get
\[ \mu_2^{(\alpha)} = A_{2p}^{(\alpha)} \lambda. \]

To prove (3.6) it is enough to observe that

1. being \( \lambda_i \geq 0 \) and \( \sum_{i=1}^{n_F} \lambda_i = 1 \) it follows that the minimum (maximum) value of \( \mu_2^{(\alpha)} \) will be obtained choosing \( \lambda \) equal to one of the \( e_i \)'s, where \( e_i \in \{0, 1\}^{n_F} \) is the binary vector with all the elements equal to zero apart from the \( i \)-th which is equal to one, \( i = 1, \ldots, n_F \);
2. the product $A_{2p}^a e_i$ gives the $i$-th element of $A_{2p}^a$.

To prove (3.7) we simply observe that using equation (3.4) the bounds in (3.6) can be transformed to those suitable for correlations.

Now we solve the problem of constructing a multivariate Bernoulli density $f_p \in \mathcal{F}(p_1, \ldots, p_m)$ with given correlation matrix $\rho = (\rho_{ij})_{i,j=1,\ldots,m}$. Using Equation (3.4) we transform the desired correlations $\rho_{ij}$ into the corresponding desired second-order moments $E[X_i X_j], i, j = 1, \ldots, m, i < j$. In this way the density $f_p$ with means $p_1, \ldots, p_m$ and correlation matrix $\rho$ can be built as $R_p \lambda$, where $\lambda = (\lambda_1, \ldots, \lambda_n), \lambda_i \geq 0, \sum_{i=1}^n \lambda_i = 1$ is a solution, if it exists, of the system of equations (3.5).

The space of solutions $\lambda$ of the system (3.5) defines the set of distributions in the Fréchet class with correlation matrix $\rho$. The choice of a particular solution does not modify the distributions of the sample means and of the sample second-order moments, which depend only on $p_1, \ldots, p_m$ and $\rho$ respectively. To explain this point let us consider a random sample $\{(X_{k1}, \ldots, X_{km}), k = 1, \ldots, N\}$ extracted from a randomly selected $m$-dimensional Bernoulli variable belonging to the Fréchet class $\mathcal{F}(p_1, \ldots, p_m)$ and with given second-order moments $\mu_{ij} := E[X_i X_j], i, j = 1, \ldots, n$. The sample means $\overline{X}_i, i = 1, \ldots, m$, are $\frac{1}{N} \text{Binomial}(N, p_i)$ and the sample second-order moments $\overline{X_i X_j} := \frac{1}{N} \sum_{k=1}^N X_{ki} X_{kj}, i, j = 1, \ldots, n, i < j$ are $\frac{1}{N} \text{Binomial}(N, \mu_{ij})$.

In general different distributions which belong to the same Fréchet class and which have the same correlation matrix $\rho$ (or equivalently the same vector of second-order moments $\mu_2$), will have different $k$-order moments, with $k \geq 3$. This methodology offers the opportunity to choose the best distribution according to a certain criterion. For example, as the moments of multivariate Bernoulli are always positive, it could be of interest to find one of the distributions with the smallest sum of all the moments with order greater than 2. This problem can be efficiently solved using linear programming techniques ([2]). It can be simply stated as

$$\min_{f \in \mathcal{F}_m} (1^T (M^m)_{3...m} f)$$

subject to

$$\left\{ \begin{array}{l}
H f = 0 \\
(M^m)_{2} f = \mu_2
\end{array} \right.$$ 

where $1$ is the vector with all the elements equal to 1 and $(M^m)_{3...m}$ is the sub-matrix of $M^m$ obtained by selecting the rows corresponding to the $k$-moments, with $k \geq 3$.

As we already mentioned, from a geometrical point of view a solution of the system of equations (3.5) exists if and only if a point whose coordinates are the desired second-order moments belongs to the convex hull generated by the points which are the columns of the $A_{2p} = (M^m)_2 R_p$ matrix. If the margins and the correlation matrix are not compatible,
the system (3.5) does not have any solution. In this case it is possible to search for a feasible $\rho^*$ which is the correlation matrix closest to the desired $\rho$, according to a chosen distance.

Finally it is worth noting that the method can be applied to the moments of order greater than 2 or to any selection of moments by simply replacing the $(M^\otimes m)_2$ matrix with the proper one.

3.3 Margins of multivariate Bernoulli variables with given second-order moments

In Section 3.2 we studied second-order moments of multivariate Bernoulli variables with given margins. The methodology can be easily generalised to solve the problem of studying $h$-order moments of multivariate Bernoulli variables with given $k$-order moments, $h, k \in \{1, \ldots, m\}, h \neq k$. We show this point by studying the $h = 1, k = 2$ case, i.e. studying margins of multivariate Bernoulli variables $f_{\mu_2}$ with given 2-order moments $\mu_2 = (\mu_{ij} : i, j = 1, \ldots, m, i < j)$.

We observe that $E[X_iX_j] = \sum_{(x_1, \ldots, x_m) \in S_m} x_ix_j f_{\mu_2}(x_1, \ldots, x_m)$, that is

$$x_{ij}^T f_{\mu_2} = \mu_{ij}$$
$$ (1 - x_{ij})^T f_{\mu_2} = 1 - \mu_{ij}$$

where $x_{ij}$ is the vector which contains the product $x_i x_j$ of the $i$-th and the $j$-th element of $x \in S_m$. If we consider the odds of the event $X_iX_j = 1$, $\gamma_{ij} = \mu_{ij}/(1 - \mu_{ij})$, we have $\gamma_{ij}(1 - \mu_{ij}) - \mu_{ij} = 0$ that is

$$(\gamma_{ij}(1 - x_{ij})^T - x_{ij}^T)f_{\mu_2} = 0.$$  

Building the matrix $H_2$ whose rows are $(\gamma_{ij}(1 - x_{ij})^T - x_{ij}^T)$, all the densities $f_{\mu_2}$ must satisfy the system of equations $H_2 f_{\mu_2} = 0$. The following proposition is the equivalent of Theorem 3.2 Proposition 3.1 and Proposition 3.2 for the case under study.

**Proposition 3.3.** Let $f_{\mu_2}$ a multivariate Bernoulli density with second-order moments $\mu_2 = (\mu_{ij} : i, j = 1, \ldots, m, i < j)$:

1. all the densities $f_{\mu_2}$ can be written as

$$f_{\mu_2} = \sum_{i=1}^{n_F} \lambda_i R_{\mu_2}^{(i)}; \tag{3.8}$$

where $R_{\mu_2}^{(i)} = (R_{\mu_2}^{(i)}(x), x \in S_m) i = 1, \ldots, n_F$ are multivariate Bernoulli densities with second-order moments $\mu_2$, $\lambda_i \geq 0, i = 1, \ldots, m$ and $\sum_{i=1}^{n_F} \lambda_i = 1$.  

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2. The vector \( p = (p_1, \ldots, p_m) \) is
\[
p = A_{1\mu_2} \lambda
\]  
where \( A_{1\mu_2} = (M \otimes m)_1 R_{\mu_2} \) and \((M \otimes m)_1\) is the sub-matrix of \( M \otimes m \) obtained by selecting the rows corresponding to the first-order moments, \( R_{\mu_2} \) is the ray matrix and \( \lambda = (\lambda_1, \ldots, \lambda_n) \), \( \lambda_i \geq 0, i = 1, \ldots, m \) and \( \sum_{i=1}^n \lambda_i = 1 \).

3. For each \( \alpha, \|\alpha\|_0 = 1 \), the first-order moment \( \mu_1^{(\alpha)} \equiv p_i \) must satisfy the following bounds
\[
\min A_{1\mu_2}^{(\alpha)} \leq p_i \leq \max A_{1\mu_2}^{(\alpha)}
\]  
where \( A_{1\mu_2}^{(\alpha)} \) is the row of the matrix \( A_{1\mu_2} \) such that \( p_i = A_{1\mu_2}^{(\alpha)} \lambda \) and \( \{i\} = \{k : \alpha_k = 1\} \).

4. **Bivariate Bernoulli density with given margins**

In this section we consider bivariate distributions, i.e. the class \( \mathcal{F}(p_1, p_2) \) of 2-dimensional random variables \((X_1, X_2)\) which have Bernoulli marginal distributions \( F_i \sim B(p_i), i = 1, 2 \). In the bivariate case two key distributions are \( F_L \) and \( F_U \), the lower and upper Fréchet bound of \( \mathcal{F}(p_1, p_2) \) respectively:
\[
F_L(x) = \max \{F_1(x_1) + F_2(x_2) - 1\} \tag{4.1}
\]
\[
F_U(x) = \min \{F_1(x_1), F_2(x_2)\} \tag{4.2}
\]
where \( x = (x_1, x_2) \in \{0, 1\}^2 \).

For any \( F_p \in \mathcal{F}(p_1, p_2) \) it holds that
\[
F_L(x) \leq F_p(x) \leq F_U(x), \ x \in \{0, 1\}^2. \tag{4.3}
\]
For an overview of Fréchet classes and their bounds see [5].

We now analyse Theorem 3.2 in the bivariate case. The number of rays is independent of the Fréchet class \( \mathcal{F}(p_1, p_2) \). We have two ray densities, which are the lower and upper Fréchet bound of each class.

**Proposition 4.1.** Let \( f \in \mathcal{F}(p_1, p_2) \), then
\[
f_p = \lambda f_L + (1 - \lambda) f_U, \ \lambda \in [0, 1],
\]
where \( f_L \) and \( f_U \) are the discrete densities corresponding to \( F_L \) and \( F_U \), respectively.

**Proof.** We observe that in \( x = (0, 0) \) the distribution function and the density function take the same value. Then using (4.3) we can write
\[
f_L(0, 0) \leq f_p(0, 0) \leq f_U(0, 0). \tag{4.4}
\]
It follows that \( f_p(0,0) = \lambda f_L(0,0) + (1 - \lambda) f_U(0,0) \) with \( \lambda = \frac{f_p(0,0) - f_U(0,0)}{f_L(0,0) - f_U(0,0)} \). It holds that \( 0 \leq \lambda \leq 1 \).

Now we observe that for any density function \( f \in \mathcal{F}(p_1, p_2) \) we have \( f(0,1) = q_1 - f(0,0) \). Then using \( (4.4) \) we can write

\[
q_1 - f_L(0,0) \geq q_1 - f_p(0,0) \geq q_1 - f_U(0,0)
\]

that is

\[
f_U(1,0) \leq f_p(1,0) \leq f_L(1,0).
\]

We can write \( f_p(1,0) = \lambda f_L(1,0) + (1 - \lambda) f_U(1,0) \). It is easy to verify that \( \lambda_1 = \lambda \). We proceed in an analogous way for \( f_p(0,1) = q_2 - f_p(0,0) \) and \( f_p(1,1) = 1 - q_1 - q_2 + f_p(0,0) \) and we get \( f_p(x) = \lambda f_L(x) + (1 - \lambda) f_U(x), \ x \in \{0,1\}^2 \) and \( 0 \leq \lambda \leq 1 \). \( \square \)

Proposition 4.1 states that \( \mathcal{F}(p_1, p_2) \) is the convex hull of the upper and lower Fréchet bound.

In the bivariate case we can also find the domain of \( \theta_{12} \) expressed as a function of the margins \( p_1, p_2 \). From Eq. (3.1) we get

\[
f_p(0,0) = q_1 q_2 (1 + \theta_{12} p_1 p_2).
\]

and consequently

\[
\theta_{12} = \frac{f_p(0,0) - q_1 q_2}{q_1 q_2 p_1 p_2}.
\]

Using \( (4.4) \) it follows

\[
\frac{f_L(0,0) - q_1 q_2}{q_1 q_2 p_1 p_2} \leq \theta_{12} \leq \frac{f_U(0,0) - q_1 q_2}{q_1 q_2 p_1 p_2}
\]

Now without loss of generality we assume \( q_2 \geq q_1 \). From Eq. (4.1) and (4.2) we get

1. if \( q_1 + q_2 \leq 1 \) then \( -\frac{1}{p_1 p_2} \leq \theta_{12} \leq \frac{1}{p_1 q_2} \);

2. if \( q_1 + q_2 > 1 \) then \( \frac{q_1 + q_2 - 1 - q_2 q_2}{q_1 q_2 p_1 p_2} \leq \theta_{12} \leq \frac{1}{p_1 q_2} \).

Finally (see also Theorem 1 in [8]) we obtain the bounds for the correlation coefficient

\[
\rho_{12} = \frac{\mathbf{E}[X_1 X_2] - p_1 p_2}{\sqrt{p_1 q_1 p_2 q_2}}.
\]

Being \( \mathbf{E}[X_1 X_2] = f_p(1,1), f_L(1,1) \leq f_p(1,1) \leq f_U(1,1) \) and \( f(1,1) = 1 - q_1 - q_2 + f(0,0) \) for any density function \( f \in \mathcal{F}(p_1, p_2) \) we obtain:

1. if \( q_1 + q_2 \leq 1 \) then \( -\frac{1 - q_1 - q_2 - p_1 p_2}{\sqrt{p_1 q_1 p_2 q_2}} \equiv -\sqrt{\frac{q_1 q_2}{p_1 p_2}} \leq \rho_{12} \leq -\frac{1 - q_1 - p_1 p_2}{\sqrt{p_1 q_1 p_2 q_2}} \equiv \sqrt{\frac{p_2 q_1}{p_1 q_2}} \);

2. if \( q_1 + q_2 > 1 \) then \( -\frac{p_1 p_2}{\sqrt{p_1 q_1 p_2 q_2}} \equiv -\sqrt{\frac{p_1 p_2}{q_1 q_2}} \leq \rho_{12} \leq -\frac{1 - q_1 - p_1 p_2}{\sqrt{p_1 q_1 p_2 q_2}} \equiv \sqrt{\frac{p_2 q_1}{p_1 q_2}} \).
5 Examples

In this section we show some results corresponding to different multivariate Bernoulli distributions. The algorithm is described in Section 5.4.

5.1 Trivariate Bernoulli distributions

Let us consider the case \( m = 3 \) and \( p = \left( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right) \). From Theorem 3.2 solving the system of equations (3.3), we get 6 ray densities. The ray matrix \( R_p \) is

\[
R_p = \begin{pmatrix}
0 & 0 & 0 & 0 & 0.5 & 0.25 \\
0 & 0 & 0.5 & 0.25 & 0 & 0 \\
0 & 0.5 & 0 & 0.25 & 0 & 0 \\
0.5 & 0 & 0 & 0 & 0 & 0.25 \\
0.5 & 0 & 0 & 0.25 & 0 & 0 \\
0 & 0.5 & 0 & 0 & 0 & 0.25 \\
0 & 0 & 0.5 & 0 & 0 & 0.25 \\
0 & 0 & 0 & 0.25 & 0.5 & 0 
\end{pmatrix}
\]

and the matrix \( A_{2p} \) as defined in Proposition 3.1 is

\[
A_{2p} = \begin{pmatrix}
0.5 & 0 & 0 & 0.25 & 0.5 & 0.25 \\
0 & 0.5 & 0 & 0.25 & 0.5 & 0.25 \\
0 & 0 & 0.5 & 0.25 & 0.5 & 0.25 
\end{pmatrix}
\]

Using Eq. (3.10) we get

\[-1 \leq \rho_{ij} \leq 1, \ i, j = 1, 2, 3, i < j.\]

Let us consider the case in which the \( X_i, i = 1, \ldots, 3 \) must be not correlated. We want to find a distribution \( F_p \in \mathcal{F}(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \) such that \( \rho_{12} = \rho_{13} = \rho_{23} = 0 \). From Eq. (3.5) we obtain \( \lambda_1 = \lambda_2 = \lambda_3 = \lambda_5 = 0.25 \) and \( \lambda_4 = \lambda_6 = 0 \). The corresponding density is uniform, \( f_p(x) = \frac{1}{8}, x \in S_3 \) as expected.

If we choose \( \rho_{12} = 0.2, \rho_{13} = -0.3 \) and \( \rho_{23} = 0.4 \), we obtain \( \lambda_1 = 0.275, \lambda_2 = 0.025, \lambda_3 = 0.375, \lambda_4 = 0, \lambda_5 = 0.325 \) and \( \lambda_6 = 0 \) as one of the solutions of Eq. (3.5). The corresponding density is

\[
f_p^T = (0.1625, 0.1875, 0.0125, 0.1375, 0.1375, 0.0125, 0.1875, 0.1625).
\]

If we choose \( \rho_{12} = 0.9, \rho_{13} = -0.3 \) and \( \rho_{23} = 0.6 \), we do not find any \( f_p \) with such correlations, even if each \( \rho_{ij} \) satisfies the constraints found for bivariate distributions, which, as we said before, in this case are \(-1 \leq \rho_{ij} \leq 1, \ i, j = 1, 2, 3, i < j.\)
If we search for a feasible $\rho^*$ which is the correlation matrix closest\(^1\) to the desired $\rho$ we obtain $\rho^*_{12} = 0.63, \rho^*_{13} = 0.33$ and $\rho^*_{23} = -0.03$. The corresponding density is

$$(f^*_p)^T = (0.2416, 0, 0.0916, 0.1666, 0.1666, 0.0916, 0, 0.2416).$$

Let us now consider the case $p = \left(\frac{1}{4}, \frac{3}{7}, \frac{1}{2}\right)$. The ray matrix $R_p$ contains 6 margins

$$R_p = \begin{pmatrix}
0 & 0 & 0 & 0 & 0.25 & 0.25 \\
0.25 & 0.25 & 0.5 & 0.5 & 0 & 0.25 \\
0 & 0.25 & 0 & 0 & 0 \\
0.25 & 0 & 0 & 0 & 0.25 & 0 \\
0.25 & 0 & 0.25 & 0 & 0 & 0 \\
0.25 & 0.5 & 0.25 & 0 & 0.5 & 0.25 \\
0 & 0.25 & 0 & 0 & 0 \\
0 & 0 & 0.25 & 0 & 0.25
\end{pmatrix}$$

and the $A_{2p}$ matrix is

$$A_{2p} = \begin{pmatrix}
0.25 & 0 & 0.25 & 0.25 & 0.25 \\
0.25 & 0.5 & 0.25 & 0.25 & 0.5 & 0.5 \\
0 & 0.25 & 0.25 & 0 & 0.25
\end{pmatrix}.$$

Using Eq. (3.10) we get

$$-1 \leq \rho_{12} \leq 0.333 \text{ and } -0.577 \leq \rho_{13}, \rho_{23} \leq 0.577.$$

If we choose $\rho_{12} = 0.3, \rho_{13} = 0.25$ and $\rho_{23} = -0.1$, we obtain $\lambda_1 = 0.2835, \lambda_2 = 0.025, \lambda_3 = 0, \lambda_4 = 0, \lambda_5 = 0.2781$ and $\lambda_6 = 0.4134$. The corresponding density is

$$f_p^T = (0.1729, 0.1805, 0.0063, 0.1404, 0.0709, 0.3258, 0, 0.1033).$$

As the last example of trivariate Bernoulli distribution we consider $p = \left(\frac{1}{4}, \frac{1}{7}, \frac{1}{2}\right)$. The ray matrix $R_p$ (rounded to the third decimal digit) has 11 ray densities

$$R_p = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.06 & 0.143 & 0.143 & 0.143 \\
0 & 0 & 0 & 0 & 0.083 & 0.143 & 0.143 & 0.113 & 0.083 & 0 & 0 \\
0 & 0 & 0.107 & 0.25 & 0.25 & 0 & 0.19 & 0.22 & 0.19 & 0 & 0.107 \\
0.333 & 0.333 & 0.226 & 0.083 & 0 & 0.19 & 0 & 0 & 0.19 & 0.083 \\
0.143 & 0.143 & 0 & 0 & 0 & 0.03 & 0 & 0 & 0 & 0 \\
0.143 & 0.143 & 0.143 & 0.06 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.25 & 0.107 & 0 & 0 & 0.25 & 0.06 & 0 & 0.107 & 0 & 0.107 \\
0.274 & 0.417 & 0.524 & 0.524 & 0.607 & 0.417 & 0.607 & 0.637 & 0.667 & 0.56 & 0.667
\end{pmatrix}.$$

\(^1\)The distance can be freely chosen. In this example we used the Euclidean distance.
Using Eq. (3.10) we get
\[-0.236 \leq \rho_{12} \leq 0.707, -0.408 \leq \rho_{13} \leq 0.816 \text{ and } -0.289 \leq \rho_{23} \leq 0.577.\]

If we choose \(\rho_{12} = 0.3, \rho_{13} = 0.25\) and \(\rho_{23} = -0.2\), we obtain
\[f_p^T = (0.0146, 0, 0.1197, 0.1990, 0.0665, 0.0617, 0.0491, 0.4893).\]

### 5.2 Multivariate \(m = 5\) Bernoulli distributions

Let us consider the case \(p = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)\). We obtain 2,712 ray densities. If we choose \(\rho_{12} = 0.3, \rho_{13} = 0.2, \rho_{14} = 0.2, \rho_{15} = 0.1, \rho_{23} = -0.2, \rho_{24} = 0.3, \rho_{25} = 0.2, \rho_{34} = 0.2, \rho_{35} = 0.1\) and \(\rho_{45} = -0.2\), we obtain
\[f_p = \begin{pmatrix}
0.025 \\
0.0625 \\
0.0125 \\
0 \\
0.025 \\
0.05 \\
0.1 \\
0.25 \\
0 \\
0.05 \\
0.0875 \\
0.0375 \\
0 \\
0.1 \\
0.05 \\
0.0125 \\
0.0625 \\
0 \\
0.05 \\
0.025 \\
0 \\
0.025 \\
0 \\
0.0125 \\
0.0375 \\
0.025 \\
0.125
\end{pmatrix}.
\]

### 5.3 Multivariate \(m \geq 6\) Bernoulli distributions

For \(m = 6\) and \(p = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)\) we obtain 707,264 ray densities. In general we observe that if the number of rays is too large with respect to the available computer power and if the objective can be reduced to the problem of finding just one density \(f \in \mathcal{F}_m\) with given margins \(p\) and second order moments \(\mu_2\), it is enough to solve the system
\[
\begin{align*}
(M^{\otimes m})_1 f &= p \\
(M^{\otimes m})_2 f &= \mu_2
\end{align*}
\]
using standard linear programming tools (e.g. [2]).
5.4 The algorithm

In this section we briefly describe the algorithm that we used in Section 5. Given $m$, $p$ and $\rho$ as input the algorithm returns the ray matrix $R_p$ and, if it exists, the density $f_p$, which has Bernoulli $B(p_i), i = 1, \ldots, m$ as marginal distribution and pairwise correlations $\rho = (\rho_{ij}, i, j = 1, \ldots, m, i < j)$. The algorithm has the following main steps:

1. the construction of the matrix $H$, see (3.3) of Theorem 3.2
2. the generation of the ray matrix $R_p$;
3. the construction of the density $f_p$ as the solution of the system (3.5) of Theorem 3.2

The construction of the matrix $H$ and of the density $f_p$ is implemented in SAS/IML. In particular, the system (3.5) is solved using the Proc Lpsolve that is part of SAS/QC. The rays are generated using 4ti2 ([1]). The software code is available on request. We performed the analysis using a standard laptop (CPU Intel core I7-2620M CPU 2.70GHz 2.70GHz, RAM 8GB).

6 Discussion

The proposed approach can be applied to any given set of moments, even of different orders. All the results given for moments and correlations can be easily adapted to other widely-used measures of dependence, such as Kendall’s $\tau$ and Spearman’s $\rho$. Furthermore, the polynomial representation of the distributions of any Fréchet class provides a link to copulas, which are a powerful instrument to model dependence.

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