On parametric families for sampling binary data with specified mean and correlation

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We discuss a class of binary parametric families with conditional probabilities taking the form of generalized linear models and show that this approach allows to model high-dimensional random binary vectors with arbitrary mean and correlation. We derive the special case of logistic conditionals as an approximation to the Ising-type exponential distribution and provide empirical evidence that this parametric family indeed outperforms competing approaches in terms of feasible correlations.

Keywords Binary parametric families · Sampling correlated binary data

1 Introduction

The need to sample random vectors of correlated binary variables arises in various statistical application; examples are estimation of the posterior mean in Bayesian variable selection (George and McCulloch, 1997), small-sample properties of estimators in longitudinal studies (Farrell and Rogers-Stewart, 2008, for a recent review), stochastic binary optimization in combinatorics (Rubinstein, 1999), simulation of ferromagnetic materials (Swendsen and Wang, 1987), performance of neural networks (Lebbah et al., 2008) and market segmentation analysis (Dolnicar and Leisch, 2001) among others.

Let $\mathbb{B} := \{0, 1\}$ denote the binary space. In some cases, such as small-sample analysis in longitudinal studies, we need a parametric family $q$ explicitly for sampling data on $\mathbb{B}^d$ with specified mean and correlations. In other cases, the parametric family serves as a proxy for a more complex distribution we cannot directly sample from. Suppose we have two functions $\tilde{\pi} : \mathbb{B}^d \to \mathbb{R}_+$ and $f : \mathbb{B}^d \to \mathbb{R}$ and we want to compute the expected value $E_\pi (f(\Gamma)) = h^{-1} \sum_{\gamma \in \mathbb{B}^d} f(\gamma) \tilde{\pi}(\gamma)$ with $h := \sum_{\gamma \in \mathbb{B}^d} \tilde{\pi}(\gamma)$.

If $d$ is too large for enumeration of the state space we have to rely on Monte Carlo algorithms, the vast majority of which involve sampling Markov transitions with invariant measure $\pi$, the standard approach being the Metropolis-Hastings kernel (Robert and Casella, 2004, ch. 7). For a transition from $X \sim \pi := \tilde{\pi}/h$, we sample $\Gamma \sim q(\cdot \mid X)$ from an auxiliary kernel $q$ and accept the step to $\Gamma$ with probability

$$\lambda_q(\Gamma, X) := \min\{1, [\tilde{\pi}(\Gamma)q(X \mid \Gamma)]/[\tilde{\pi}(X)q(\Gamma \mid X)]\}$$

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or return $X$ otherwise. Random walks on $B^d$ are easy to implement but often suffer from slow mixing; independent proposals $\Gamma \sim q$ provide fast-mixing if $\lambda_q(\Gamma, X)$ is reasonably high on average, in other words if $q$ is sufficiently close to $\pi$ (Schäfer and Chopin, 2011; Schäfer, 2012). This rationale complements other approaches to fast mixing such as parallel chains (Bottolo and Richardson, 2010, among others) or self-avoiding dynamics (Hamze et al., 2011).

The vast field of potential applications in Monte Carlo algorithms encourages the study of families with $d(d+1)/2$ parameters which, like the multivariate normal, accommodate all valid combinations of means and correlations. This paper elaborates some theoretical background on random binary vectors, proves the range of possible correlations for a particular class of parametric families, connects to existing work in the literature and provides broad numerical insight concerning the range of dependencies achievable in practice. It is structured as follows.

In Section 2, we introduce suitable notation and review results relating binary distributions to its moments. Section 3 elaborates on parametric families which have, by definition, conditional distributions that are generalized linear regressions. We show that they accommodate the whole range of possible correlations. Section 4 motivates the use of the logistic link function as an approximation to the Ising-type exponential quadratic family. In Section 5, we discuss how to adjust the parametric families to specified marginals. Finally, in Section 6 we perform numerical experiments to compare competing approaches for sampling correlated binary data in high dimensions.

2 Preliminaries on random binary vectors

We write $B := \{0, 1\}$ for the binary space and denote by $d \in \mathbb{N}$ the generic dimension. Given a vector $\gamma \in B^d$ and an index set $I \subseteq D := \{1, \ldots, d\}$, we write $\gamma_I \in B^{|I|}$ for the sub-vector indexed by $I$ and $\gamma_{-I} \in B^{d-|I|}$ for its complement. For $I = \{i, \ldots, j\}$ we use the more explicit notation $\gamma_{i:j}$. Unless otherwise defined, $\pi$ denotes an arbitrary probability mass function on $B^d$. We denote by $E_{\pi}(f(\Gamma))$ the expected value with respect to $\Gamma \sim \pi$ and write $P_{\pi}(A) := E_{\pi}(1_A(\Gamma))$ for an event $A \subseteq B^d$.

**Definition** Let $m \in (0, 1)^d$ be a mean vector. We call $\pi_m(\gamma) := \prod_{i \in D} m_i^\gamma_i (1 - m_i)^{1-\gamma_i}$ the product family or the mass function of $d$ independent Bernoulli variables.

2.1 Absolute cross-moments

**Definition** For a set $I \subseteq D$, we refer to $m^\pi_I := E_{\pi}(\prod_{i \in I} \Gamma_i) = \sum_{\gamma \in B^d} \pi(\gamma) \prod_{i \in I} \gamma_i$ as the cross-moment indexed by $I$.

Note that $m^\pi_I = P_{\pi}(\Gamma_I = 1)$ which means that cross-moments and marginal probabilities indexed by $I \subseteq D$ are identical. Higher order cross-moments coincide with first order cross-moments. The range of possible cross-moments is limited by the following constraints.

**Proposition 2.1.** The cross-moments of binary data fulfill the sharp inequalities

$$\max\{\sum_{i \in I} m_i - |I| + 1, 0\} \leq m_I \leq \min\{m_K : K \subseteq I\}.$$  (2)
Proof. The lower bound follows from
\[ |I| - 1 = \sum_{\gamma \in \mathbb{B}^d} (|I| - 1) \pi(\gamma) \geq \sum_{\gamma \in \mathbb{B}^d} \left( \sum_{i \in I} \gamma_i - \prod_{i \in I} \gamma_i \right) \pi(\gamma) = \sum_{i \in I} m_i - m_I, \]
the upper bound is the monotonicity of the measure. \( \square \)

For the special case \(|I| = 2\), Proposition 2 is a well-known result and has been invoked in several articles dealing with correlated binary data. For the general case, we remark that a mapping \( f: [0, 1]^{|I|} \to [0, 1], \ f((m_{i_1}, \ldots, m_{i_d})) = m_I \), which assigns a cross-moment \( m_I \) for \( I \subseteq D \) as function of the marginals \( m_i \) for \( i \in I \), is quite similar to a \(|I|\)-dimensional copula and the inequalities (2) are exactly the Fréchet-Hoeffding bounds (Nelsen, 2006, ch. 2).

**Definition** We say a \( d \times d \) symmetric matrix \( M := (m_{ij}) \) with entries in \((0, 1)\) is a cross-moment matrix of binary data if \( M - \text{diag}(M) \text{diag}(M)^\top \) is positive definite and condition (2) holds for all \( I \subseteq D \) with \(|I| = 2\).

We derive the family of distributions which, under the constraints that \( \pi \) has given cross-moments, maximizes the entropy \( H(\pi) = -\sum_{\gamma \in \mathbb{B}^d} \pi(\gamma) \log[\pi(\gamma)] \). The following proposition is just a special case of a more general concept (Soofi, 1994).

**Proposition 2.2.** Let \( I \subseteq 2^D \) be a family of index sets such that \( \{m_I: I \in \mathcal{I}\} \) is a valid set of cross-moments. The maximum entropy distribution having the specified cross-moments has the form \( q(\gamma) = \exp(\sum_{I \in \mathcal{I}} a_I \prod_{i \in I} \gamma_i) / [\sum_{\gamma \in \mathbb{B}^d} \exp(\sum_{I \in \mathcal{I}} a_I \prod_{i \in I} \gamma_i)] \).

**Proof.** Define the Lagrange multipliers \( \mathcal{L}(\pi, a) = \sum_{I \in \mathcal{I}} a_I [\sum_{\gamma \in \mathbb{B}^d} \pi(\gamma) \prod_{i \in I} \gamma_i - m_I] \) and differentiate \( \partial[H(\pi) + \mathcal{L}(\pi, a)] / \partial \pi(\gamma) = -\log[\pi(\gamma)] - 1 + \sum_{I \in \mathcal{I}} a_I \prod_{i \in I} \gamma_i \). Solving the first order condition and normalizing completes the proof. \( \square \)

### 2.2 Standardized cross-moments

**Definition** For a set \( I \subseteq D \), we define \( u_I^\pi(\gamma) := \prod_{i \in I} (\gamma_i - m_i^\pi) [m_i^\pi (1 - m_i^\pi)]^{-1/2} \) and refer to \( c_I^\pi := \mathbb{E}_\pi(u_I^\pi(\Gamma)) \) as the (generalized) correlation coefficient indexed by \( I \).

A \( d \times d \) positive definite matrix \( C \) with entries in \([-1, 1]\) and \( \text{diag}(C) = 1 \) is not the correlation matrix of a binary distribution for every mean vector \( \mathbf{m} \in (0, 1)^d \). In fact, \( C \) is a correlation matrix if and only if \( M = C \cdot \mathbf{s}s^\top + \mathbf{m} \mathbf{m}^\top \) is valid in the sense of Definition 2.1, where the dot means point-wise multiplication and \( s_i^2 := m_i(1 - m_i) \). Chaganty and Joe (2006) elaborate alternative conditions for compatibility between correlations and means, but these do not seem easier to express or to check.

In the context of binary data, the notion of “strong correlations” refers to correlation coefficients which are at the boundary of the feasible range with respect to the mean vector. Note that the absolute value of the correlation coefficient does, in itself, not tell whether the correlation is easy or difficult to model. The following statement relates the notions of uncorrelated and independent variables.

**Proposition 2.3.** Let \( X \) be a \( d \)-dimensional binary random vector. For \( d = 2 \), entries are uncorrelated if and only if they are independent. For \( d \geq 3 \), entries might be mutually uncorrelated but not independent.
Proof. Let $p_{x_1x_2} := \mathbb{P}(\Gamma_1 = x_1, \Gamma_2 = x_2)$. By definition $p_{11} = m_{12} = m_{1} m_{2}$. Further, we obtain $p_{10} = m_{1} - m_{12} = m_{1}(1 - m_{2})$ and, analogously, $p_{01} = (1 - m_{1})m_{2}$. Finally, we have $p_{00} = 1 + m_{12} - m_{1} - m_{2} = (1 - m_{1})(1 - m_{2})$. For $d \geq 3$, let for instance $p_{000} = p_{001} = p_{100} = p_{010} = p_{011} = 0$. The entries are mutually uncorrelated, but not independent since $p_{111} = 0 \neq 1/8 = m_{1} m_{2} m_{3}$. \hfill $\square$

The following representation by Bahadur (1961) allows to write a binary distribution in terms of its generalized correlation coefficients.

**Proposition 2.4.** Let $\pi$ be a binary distribution with mean $\mathbf{m} \in (0,1)^d$. Then,

$$
\pi(\gamma) = q^{\mathbf{m}}(\gamma) \left[ \sum_{I \subseteq D} c^I u^I(\gamma) \right].
$$

Proof. We give the proof by Bahadur (1961) using the notation introduced above. The set $\{u^I: I \subseteq D\}$ forms an orthonormal basis on $\mathcal{F} := \{ f: \mathbb{B}^d \to \mathbb{R} \}$ with respect to the inner product $(f,g) = \mathbb{E}_{q^{\mathbf{m}}}(f(\Gamma)g(\mathbf{X})) = \sum_{\gamma \in \mathbb{B}^d} f(\gamma)g(\gamma)q^{\mathbf{m}}(\gamma)$. Therefore, every function $f \in \mathcal{F}$ has a unique representation $f(\gamma) = \sum_{I \subseteq D}(f, u^I)u^I(\gamma)$. Compute the inner products $(f, q^{\mathbf{m}} u^I) = \sum_{\gamma \in \mathbb{B}^d} q^{\mathbf{m}}(\gamma)(f(\gamma)q^{\mathbf{m}}(\gamma) = \mathbb{E}_{\pi}(u^I(\Gamma)) = c^I$ to obtain the desired form $\pi(\gamma)/q^{\mathbf{m}}(\gamma) = \sum_{I \subseteq D} c^I u^I(\gamma)$. \hfill $\square$

Using Proposition 2.4, we may bound the $l^p$ distance between two binary distribution with the same mean in terms of nearness of their correlation coefficients.

**Proposition 2.5.** Let $\pi$ and $\omega$ be binary distributions with mean $\mathbf{m} \in (0,1)^d$. For $p \geq 1$,

$$
\sum_{\gamma \in \mathbb{B}^d} |\pi(\gamma) - \omega(\gamma)|^p \leq \sum_{I \subseteq D} 2^{(1-\min(p,2))|I|} |c^I - c^I|^p \leq (1 + r)^d - dr - 1
$$

where $r = 2^{1-\min(p,2)} \max_{I \subseteq D} |c^I - c^I|^p/|I|$.\hfill $\square$

Proof. Since $u^I = u^I$ for all $I \subseteq D$, applying Proposition 2.4 yields

$$
\sum_{\gamma \in \mathbb{B}^d} |\pi(\gamma) - \omega(\gamma)|^p = \sum_{\gamma \in \mathbb{B}^d} \left| q^{\mathbf{m}}(\gamma) \sum_{I \subseteq D} u^I(\gamma)(c^I - c^I) \right|^p \leq \sum_{I \subseteq D} |c^I - c^I|^p \mathbb{E}_{q^{\mathbf{m}}}(|u^I(\Gamma)|^p).
$$

Using that $x^{p-1} + (1 - x)^{p-1} \leq 2^{2-\min(p,2)}$ for all $x \in (0,1)$, we obtain the bound

$$
\mathbb{E}_{q^{\mathbf{m}}}(|u^I(\Gamma)|^p) \leq \prod_{i \in I}[m_i(1 - m_i)]^{1/2}[m_i^{p+1} + (1 - m_i) p^{-1}] \leq 2^{1-\min(p,2)}|I|.
$$

Finally, we have $\sum_{I \subseteq D} 2^{(1-\min(p,2))|I|} |c^I - c^I|^p \leq \sum_{I \subseteq D, |I| \geq 2} |I| = (1 + r)^d - dr - 1$, since by definition $c^I = c^I$ for all $I \subseteq D$ with $|I| \leq 2$. \hfill $\square$

**Corollary 2.6.** Let $\pi$ and $q$ be binary distributions with cross-moment matrix $\mathbf{M}$. Then we have $\sum_{\gamma \in \mathbb{B}^d} |\pi(\gamma) - q(\gamma)|^p \leq (1 + r)^d - \frac{1}{2} d(d - 1)r^2 - dr - 1$.

With regard to the Metropolis-Hastings kernel mentioned in the introductory section, the factor $\frac{1}{2} d(d - 1)r^2$ in Corollary 2.6 is the gain of a more complex proposal distribution $q_{\mathbf{M}}$ with $\mathbf{M} = \mathbf{M}^p = \mathbf{M}^q$ over a simple product model $q^{\mathbf{m}}$ with $\mathbf{m} = \mathbf{m}^p = \mathbf{m}^q$.

The following result shows how the cross-moments of the proposal distribution affect the auto-covariance of the independent Metropolis-Hastings sampler.
Proposition 2.7. Let \( \pi \) and \( q \) be binary distributions with mean \( m \in (0,1)^d \) and denote by \( \kappa(\gamma \mid x) := q(\gamma)\lambda_q(\gamma, x) + \delta_x(\gamma)[1 - \sum_{y \in \mathbb{B}^d} q(y)\lambda_q(y, x)] \) the Metropolis-Hastings kernel with invariant measure \( \pi \) and proposal distribution \( q \) where \( \lambda_q(\cdot, x) \) is defined in (1). The auto-covariance between \( X \sim \pi \) and \( \Gamma \sim \kappa(\cdot \mid X) \) is

\[
\mathbb{E}_{\kappa, \pi}(\Gamma^\top X) - mm^\top = \frac{1}{2}(M^\pi - M^q) + R^c
\]

with \( R^c = (r^c_{ij}) \) where \( |r^c_{ij}| \leq \sum_{\gamma \in \mathbb{B}^d} |\pi(\gamma) - q(\gamma)| \).

Proof. We plug the definition of the kernel into the expected value and obtain

\[
\mathbb{E}_{\kappa, \pi}(\Gamma^\top X) = \sum_{\gamma, x \in \mathbb{B}^d} \gamma_i x_j \kappa(\gamma \mid x) \pi(x)
\]

\[
= \sum_{\gamma, x \in \mathbb{B}^d} \gamma_i x_j q(\gamma)\lambda_q(\gamma, x)\pi(x) + \sum_{x \in \mathbb{B}^d} x_i x_j[1 - \sum_{y \in \mathbb{B}^d} q(y)\lambda_q(y, x)]\pi(x)
\]

\[
= m_i m_j + \sum_{\gamma, x \in \mathbb{B}^d} (\gamma_i x_j - x_i x_j)q(\gamma)\pi(x)\lambda_q(\gamma, x)
\]

\[
= m_i m_j + \frac{1}{2}(m_i^\pi - m_j^\pi) + \frac{1}{2} \sum_{\gamma, x \in \mathbb{B}^d} (\gamma_i x_j - x_i x_j)\left|q(\gamma)\pi(x) - q(x)\pi(\gamma)\right|
\]

where we used \( 2q(\gamma)\pi(x)\lambda_q(\gamma, x) = q(\gamma)\pi(x) + q(x)\pi(\gamma) - |q(\gamma)\pi(x) - q(x)\pi(\gamma)| \). The triangle inequality

\[
\sum_{\gamma, x \in \mathbb{B}^d} \left|q(\gamma)\pi(x) - q(x)\pi(\gamma)\right| = \sum_{\gamma, x \in \mathbb{B}^d} \left|q(\gamma)\pi(x) - \pi(\gamma)\pi(x) + \pi(\gamma)\pi(x) - q(x)\pi(\gamma)\right|
\]

\[
\leq \sum_{\gamma, x \in \mathbb{B}^d} \left(\left|q(\gamma) - \pi(\gamma)\right|\pi(x) + \left|\pi(x) - q(x)\right|\pi(\gamma)\right) = 2 \sum_{\gamma \in \mathbb{B}^d} \left|\pi(\gamma) - q(\gamma)\right|
\]

yields the bound on \( r^c_{ij} := \frac{1}{2} \sum_{\gamma, x \in \mathbb{B}^d} (\gamma_i x_j - x_i x_j)\left|q(\gamma)\pi(x) - q(x)\pi(\gamma)\right| \).

\[
\square
\]

2.3 Structured correlations

For some applications, it suffices to model structured dependencies, such as exchangeable \((c_{ij} = c)\), moving average \((c_{ij} = c_{i-1,j-1})\) or autoregressive \((c_{ij} = c_{i-j})\) correlations for \( i \neq j \in D \). There is a long series of articles concerned with efficient approaches to sampling binary vectors for structured correlations (Farrell and Sutradhar, 2006; Qaqish, 2003; Oman and Zucker, 2001; Lunn and Davies, 1998; Park et al., 1996). In this paper, we focus on the problem of sampling binary data with arbitrary cross-moment matrix.

3 Parametric families based on generalized linear models

We want to construct a parametric family \( q \) for sampling independent random vectors with specified mean and correlations. Sampling in high dimensions, however, requires the computation of conditional distributions \( q(\gamma_i \mid \gamma_{i-1-1}) \), and it is therefore convenient to define the parametric family directly in terms of its conditionals.
Definition Let \( \mu: \mathbb{R} \to [0, 1] \) be a monotonic function and \( A := (a_{ij}) \) a \( d \times d \) real-valued lower triangular matrix. We refer to
\[
q_A(\gamma) = \prod_{i=1}^d \left[ \mu(a_{ii} + \sum_{j=1}^{i-1} a_{ij} \gamma_j) \right]^{\gamma_i} \left[ 1 - \mu(a_{ii} + \sum_{j=1}^{i-1} a_{ij} \gamma_j) \right]^{1-\gamma_i},
\]
as the \( \mu \)-conditionals family.

**Proposition 3.1.** Let \( \mu: \mathbb{R} \to [0, 1] \) be a monotonic bijection and \( m \in (0, 1)^d \) a mean vector. For \( A = \text{diag}^{-1}(m) \) we have \( q_A = q_m \).

By construction, it is straightforward to sample \( x \sim q_A \) and evaluate \( q_A(x) \) pointwise as summarized in Procedure 1. Alternatively, one could sample from an auxiliary distribution \( \varphi \) on \( \mathbb{R}^d \) which allows to compute \( \varphi(x_i \mid x_{1:i-1}) \) and define a parametric family \( q_{\varphi, \omega}(\gamma) = \int_{\tau^{-1}(\gamma)} \varphi(x)dx \) through the mapping \( \tau: \mathbb{R}^d \to \mathbb{B}^d \). We come back to this idea in Section 5.2.

**Procedure 1** Sampling from a \( \mu \)-conditionals family

\[
x = (0, \ldots, 0), \ p \leftarrow 1
\]
for \( i = 1, \ldots, d \) do
\[
c \leftarrow q_A(x_i = 1 \mid x_{1:i-1}) = \mu(a_{ii} + \sum_{j=1}^{i-1} a_{ij} x_j), \ u \leftarrow U \sim U_{[0,1]}
\]
if \( u < c \) then \( x_i \leftarrow 1 \)
\[
p \leftarrow \begin{cases} p \cdot c & \text{if } x_i = 1 \\ p \cdot (1 - c) & \text{if } x_i = 0 \end{cases}
\]
end for
return \( x, p \)

Qaqish (2003) discusses the \( \mu \)-conditionals family with a truncated linear link function \( \mu(x) = \min(\max(x, 0), 1) \). The linear structure allows to compute the parameters by simple matrix inversion; on the downside, the linear function is truncated and fails to accommodate complicated correlation structures. Therefore, Qaqish (2003) elaborates on conditions that guarantee the linear conditionals family to be valid for special correlation structures.

Farrell and Sutradhar (2006) propose a \( \mu \)-conditionals family with a logistic link function \( \mu(x) = 1/[1 + \exp(-x)] \). However, they only analyze the special case of autoregressive correlation structure. In Section 4, we further motivate the use of the logistic link function which indeed allows to model any feasible correlation structure as states the following theorem.

**Theorem 3.2.** Let \( \mu: \mathbb{R} \to [0, 1] \) be a monotonic, differentiable bijection and \( M \) a \( d \times d \) cross-moment matrix. There is a unique \( d \times d \) real-valued lower triangular matrix \( A \) such that \( \sum_{\gamma \in \mathbb{B}^d} q_A(\gamma) \gamma \gamma^T = M \).

Besides the logistic function invoked above, popular link functions include the complementary log-log function with \( \mu(x) = 1 - \exp[-\exp(x)] \) and the probit function with \( \mu(x) = (2\pi)^{-1/2} \int_{-\infty}^x \exp(-y^2/2)dy \) (McCullagh and Nelder, 1989, sec. 4.3). We derive two auxiliary results to structure the proof of Theorem 3.2.

**Lemma 3.3.** For a cross-moment matrix \( M \) with mean vector \( m = \text{diag}(M) \), we have
\[
\begin{pmatrix} M & m \\ m^T & 1 \end{pmatrix} > 0.
\]
Proof. Note that \( m^\top M^{-1} m - (m^\top M^{-1} m)^2 = (M^{-1} m)(M - mm^\top)M^{-1} m > 0 \) because the covariance matrix \( M - mm^\top \) is positive definite. Dividing by \( m^\top M^{-1} m > 0 \) we obtain \( 1 - m^\top M^{-1} m > 0 \) which yields

\[
\det \begin{pmatrix} M & m \\ m^\top & 1 \end{pmatrix} = \det \begin{pmatrix} M & 0 \\ 0^\top & 1 \end{pmatrix} \begin{pmatrix} I & M^{-1} m \\ m^\top & 1 \end{pmatrix} = \det(M) \det \begin{pmatrix} I & M^{-1} m \\ 0^\top & (1 - m^\top M^{-1} m) \end{pmatrix} = \det(M)(1 - m^\top M^{-1} m) > 0.
\]

Therefore, all principal minors are positive. \(\square\)

**Lemma 3.4.** Let \( \mu: \mathbb{R} \to [0, 1] \) be a monotonic, differentiable bijection, and denote by \( B_r^n = \{ x \in \mathbb{R}^n \mid x^\top x < r^2 \} \) the open ball with radius \( r > 0 \). Let \( \pi \) be a binary distribution with cross-moment matrix \( M \). We write \( m = \text{diag}(M) \) and \( m^* = (m^\top, 1)^\top \) for the mean vector. There is \( \varepsilon_r > 0 \) such that the function

\[
f: B_r^{d+1} \to \bigtimes_{i=1}^{d+1} (\varepsilon_r, m_i^* - \varepsilon_r), \quad f(a) = \sum_{\gamma \in B^d} \pi(\gamma) \mu(a_{d+1} + \sum_{k=1}^d a_k \gamma_k) \begin{pmatrix} \gamma \\ 1 \end{pmatrix}
\]

is a differentiable bijection.

**Proof.** We set \( \varepsilon_r := \max \bigcup_{i \in D \cup \{d+1\}} \left\{ \min_{a \in B_r^{d+1}} f_i(a), m_i^* - \max_{a \in B_r^{d+1}} f_i(a) \right\} \). For \( i, j \in D \cup \{d+1\} \), the partial derivatives of \( f \) are

\[
\frac{\partial f_i}{\partial a_j} = \sum_{\gamma \in B^d} \pi(\gamma) \mu'(a_{d+1} + \sum_{k=1}^d a_k \gamma_k) \times \begin{cases} 
\gamma_i \gamma_j & (i, j \in \{1, \ldots, d\}) \\
\gamma_i & (j = d+1) \\
\gamma_j & (i = d+1) \\
1 & (i = j = d+1).
\end{cases}
\]

We have \( \eta_r := \min_{a \in B_r^{d+1}} \min_{\gamma \in B^d} \mu'(a_{d+1} + \sum_{i=1}^d a_i \gamma_i) > 0 \) since \( \mu \) is strictly monotonic. Then the Jacobian is positive for all \( a \in B_r^d \),

\[
\det f'(a) = \det \left[ \sum_{\gamma \in B^d} \pi(\gamma) \mu'(a_{d+1} + \sum_{i=1}^d a_i \gamma_i) \begin{pmatrix} \gamma \gamma^\top \\ \gamma \end{pmatrix} \right] \geq \eta_r^{d+1} \det \begin{pmatrix} M & m \\ m^\top & 1 \end{pmatrix} > 0,
\]

where we applied Lemma 3.3 in the last inequality. \(\square\)

**Theorem 3.2.** We proceed by induction over \( d \). For \( d = 1 \), \( A(1) \) is a scalar and we define the \( \mu \)-conditionals family \( q_{A(1)}^d \) via Corollary 3.1. Suppose that we have already constructed a \( \mu \)-conditionals family \( q_{A(d)}^d \) with \( d \times d \) lower triangular matrix \( A(d) \) and cross-moment matrix \( M(d) \). We can add a new dimension to the \( \mu \)-conditionals model
$q_{\Lambda(d)}^k$ without changing $M(d)$, since

$$
\sum_{x \in \mathbb{B}^{d+1}} q_{\Lambda(d+1)}^k(x) x x^T = \sum_{x \in \mathbb{B}^{d+1}} q_{\Lambda(d)}^k(x) x x^T \left[ \mu(a_{d+1,d+1} + \sum_{j=1}^{d} a_{d+1,j} x_j) \right]^{d+1} \times
$$

$$
\left[ 1 - \mu(a_{d+1,d+1} + \sum_{j=1}^{d} a_{d+1,j} x_j) \right]^{1-x_{d+1}}
$$

$$
= \sum_{\gamma \in \mathbb{B}^d} q_{\Lambda(d)}^k(\gamma) \left\{ \mu(a_{d+1,d+1} + \sum_{j=1}^{d} a_{d+1,j} \gamma_j) \left( \gamma \gamma^T \gamma \right) \right\}
$$

$$
= \sum_{\gamma \in \mathbb{B}^d} q_{\Lambda(d)}^k(\gamma) \mu(a_{d+1,d+1} + \sum_{j=1}^{d} a_{d+1,j} \gamma_j) \begin{pmatrix} \gamma^T 0 0 \\ 0 \gamma^T \gamma \end{pmatrix}
$$

$$
\begin{pmatrix} M(d) & 0 \\ 0 & 0 \end{pmatrix}
$$

For reasons of symmetry, it suffices to show that there is $a \in \mathbb{R}^{d+1}$ such that

$$f(a) = \sum_{\gamma \in \mathbb{B}^d} q_{\Lambda(d)}^k(\gamma) \mu(a_{d+1} + \sum_{i=1}^{d} a_i \gamma_i) \begin{pmatrix} \gamma^T 1 \\ 1 \end{pmatrix} = M(d+1) \ast_{d+1},
$$

where the r.h.s. denotes the $(d+1)$th column of the augmented cross-moment matrix. There is $\varepsilon > 0$ so that $M(d+1) \ast_{d+1} \in \times_{i=1}^{d+1}(\varepsilon, m_\ast^\varepsilon - \varepsilon)$ with $m_\ast^\varepsilon = (\text{diag}[M(d)]^T, 1)$ which implies that a solution is contained in a sufficiently large open ball $\mathbb{B}^{d+1}_\varepsilon$. We apply Lemma 3.4 to complete the inductive step and the proof.

4 The logistic conditionals family

We denote by $q_{\Lambda}$ the logistic conditionals family, that is the $\mu$-conditionals family with logistic link function $\ell(x) := 1/[1 + \exp(-x)]$. This parametric family has been proposed by Farrell and Sutradhar (2006), and in more general terms suggested by Arnold (1996). In this section, we motivate why the logistic link function arises somewhat naturally in the context of $\mu$-conditional families.

Definition Let $A$ be a $d \times d$ real-valued lower triangular matrix. We refer to

$$q_{\Lambda}(\gamma) = \exp(h + \gamma^T A \gamma),$$

as the exponential quadratic family with $h := -\log[\sum_{x \in \mathbb{B}^d} \exp(x^T A x)]$.

Proposition 4.1. If $A = \text{diag}(a)$, then $a_{ii} = \ell^{-1}(m_{ii})$ and $q_{\Lambda}^m = q_{\Lambda}^* = q_{\Lambda}^m$.

The exponential quadratic family is a natural way to design a parametric family and plays a central role in physics and life science being the well-studied Ising model on a weighted complete graph. It links to information theory (Soofi, 1994), log-linear theory for contingency tables (Bishop et al., 1975, ch. 5) and graphical models (Cox and Wermuth, 1996, ch. 2). Finding its mode is an NP-hard problem and intensively studied in the field of operation research (Boros et al., 2007, for a recent review).
Proposition 2.2 states that the exponential quadratic family is the maximum entropy distribution on $\mathbb{R}^d$ having a given cross-moment matrix. It appears to be the binary analogue of the multivariate normal distribution which is the maximum entropy distribution on $\mathbb{R}^d$ having a given covariance matrix (Kapur, 1989, sec. 5.1.1). We can read the parameters $a_{ij}$ as Lagrange multipliers or, if $i \neq j$, as conditional log odd-ratios since

$$a_{ij} = \log \frac{P_{R_A}(I_i = 1, I_j = 1 | \Gamma_{-i,j}) P_{R_A}(I_i = 0, I_j = 0 | \Gamma_{-i,j})}{P_{R_A}(I_i = 0, I_j = 1 | \Gamma_{-i,j}) P_{R_A}(I_i = 1, I_j = 0 | \Gamma_{-i,j})}.$$

We might interpret the constant conditional log odd-ratios as analogue of the constant conditional correlations of the multivariate normal distribution (Wermuth, 1976).

Despite these similarities to the multivariate normal distribution, we cannot easily sample from the exponential quadratic family nor explicitly relate the parameter $\mathbf{A}$ to the cross-moment matrix $\mathbf{M}$. The reason is that the lower dimensional marginal distributions are difficult to compute (Cox, 1972, (iii)).

**Proposition 4.2.** The marginal distribution of the exponential quadratic family is

$$q^*_\mathbf{A}(\gamma_{-d}) = \exp \left( h + \gamma^\top \mathbf{A}_{-d} \gamma_{-d} + \log \left[ 1 + \exp(a_{dd} + \sum_{j=1}^{d-1} a_{ij} \gamma_j) \right] \right). \tag{3}$$

We cannot repeat the marginalization since the multi-linear structure is lost. In fact, the following result shows that the logistic conditionals family is precisely constructed such that the non-linear term in the above expression vanishes.

**Proposition 4.3.** Let $\mathbf{A}$ be a $d \times d$ lower triangular matrix. The logistic conditionals family can be written as

$$q^\mathbf{A}(\gamma) = \exp \left( \gamma^\top \mathbf{A} \gamma - \sum_{i=1}^d \log \left[ 1 + \exp(a_{ii} + \sum_{j=1}^{i-1} a_{ij} \gamma_j) \right] \right).$$

**Proof.** Straightforward calculations yield

$$\log q^\mathbf{A}(\gamma) = \sum_{i=1}^d \log \left( [\ell(a_{ii} + \sum_{j=1}^{i-1} a_{ij} \gamma_j)]\gamma_i [1 - \ell(a_{ii} + \sum_{j=1}^{i-1} a_{ij} \gamma_j)]^{1-\gamma_i} \right)$$

$$= \sum_{i=1}^d \left( \gamma_i \log(\ell(a_{ii} + \sum_{j=1}^{i-1} a_{ij} \gamma_j)) + (1 - \gamma_i) \log(1 - \ell(a_{ii} + \sum_{j=1}^{i-1} a_{ij} \gamma_j)) \right)$$

$$= \sum_{i=1}^d \left( \gamma_i \ell(a_{ii} + \sum_{j=1}^{i-1} a_{ij} \gamma_j) + \log(1 - \ell(a_{ii} + \sum_{j=1}^{i-1} a_{ij} \gamma_j)) \right)$$

$$= \sum_{i=1}^d \left( \gamma_i (a_{ii} + \sum_{j=1}^{i-1} a_{ij} \gamma_j) - \log(1 + \exp(a_{ii} + \sum_{j=1}^{i-1} a_{ij} \gamma_j)) \right)$$

$$= \sum_{i=1}^d \sum_{j=1}^i a_{ij} \gamma_i \gamma_j - \sum_{i=1}^d \log[1 + \exp(a_{ii} + \sum_{j=1}^{i-1} a_{ij} \gamma_j)]$$

$$= \gamma^\top \mathbf{A} \gamma - \sum_{i=1}^d \log[1 + \exp(a_{ii} + \sum_{j=1}^{i-1} a_{ij} \gamma_j)],$$

where we used $\log[1 - \ell(x)] = -\log[1 + \exp(x)]$ in the third line. \qed

The full conditional probability of the $d$-dimensional exponential quadratic family is a logistic regression term.

**Proposition 4.4.** The conditional distribution of the exponential quadratic family is

$$q^\mathbf{A}(\gamma_i = 1 | \gamma_{-i}) = \ell(a_{ii} + \sum_{j=1}^{i-1} a_{ij} \gamma_j + \sum_{j=i+1}^d a_{ij} \gamma_j).$$
Since we cannot repeat the marginalization for lower dimensions, we cannot assess the lower dimensional conditional probabilities which are necessary for sampling. We can, however, derive a series of approximate marginal probabilities that produce a logistic conditionals family which is, for low correlations, close to the original exponential quadratic family. This idea goes back to Cox and Wermuth (1994).

**Proposition 4.5.** Let \( c_1 + c_2 x + c_3 x^2 \approx \log[\cosh(x)] \) be a second order approximation. We may approximate the marginal distribution \( q_\mathbf{A}^* (\gamma_{-d}) \) by an exponential quadratic family \( \exp(h_\mathbf{A} + \gamma_{-d}^\top \mathbf{A}_* \gamma_{-d}) \) with parameters

\[
    h_\mathbf{A} := h + \log(2) + c_1 + \frac{1}{2} a_{dd}, \quad \mathbf{A}_* := \mathbf{A}_{-d} + (c_2 + \frac{1}{2}) \text{diag}(\mathbf{a}_*), \quad \mathbf{a}_* := (a_{d1}, \ldots, a_{d,d-1})^\top
\]

where \( \mathbf{a}_* := (a_{d1}, \ldots, a_{d,d-1})^\top \) denotes the \( d \)th column of \( \mathbf{A} \) without \( a_{dd} \).

**Proof.** We write the marginal distribution of the exponential quadratic family as

\[
    q_\mathbf{A}^* (\gamma_{-d}) = \exp \left[ h + \gamma_{-d}^\top \mathbf{A}_{-d} \gamma_{-d} + \frac{1}{2} (a_{dd} + \mathbf{a}_*^\top \mathbf{a}_* \gamma_{-d}) + \log \left( 2 \cosh \left[ \frac{1}{2} (a_{dd} + \mathbf{a}_*^\top \mathbf{a}_* \gamma_{-d}) \right] \right) \right].
\]

Using the identity

\[
    \log[1 + \exp(x)] = \log \left( \exp(\frac{1}{2} x) \left[ \exp(-\frac{1}{2} x) + \exp(\frac{1}{2} x) \right] \right) = \frac{1}{2} x + \log \left[ 2 \cosh\left(\frac{1}{2} x\right)\right]
\]

and approximate the non-quadratic term by the second order polynomial

\[
    \log[\cosh\left(\frac{1}{2} a_{dd} + \frac{1}{2} \mathbf{a}_*^\top \mathbf{a}_* \gamma_{-d}\right)] \approx c_1 + c_2 a_{dd}^1 + c_3 (a_{dd}^1 \gamma_{-d})^2.
\]

We rewrite the inner products \( \mathbf{a}_*^\top \gamma_{-d} + (\mathbf{a}_* \gamma_{-d})^2 = \gamma_{-d}^\top [\text{diag}(\mathbf{a}_*) + \mathbf{a}_* \mathbf{a}_*^\top] \gamma_{-d} \) and rearrange the quadratic terms.

We can iterate the procedure to construct a logistic conditionals family which is close to the original exponential quadratic family. However, the function \( \log[\cosh(x)] \) behaves like a quadratic function around zero and like the absolute value function for large \( x \). Thus, a quadratic polynomial can only approximate \( \log[\cosh(x)] \) well for small values of \( x \) which means that exponential quadratic families with strong dependencies is hard to approximate. Cox and Wermuth (1994) propose a Taylor approximation which fits well around \( \frac{1}{2} a_{dd} \) and works for weak correlations. The parameters are \( \mathbf{c} = (\log[\cosh(\frac{1}{2} a_{dd})]), \frac{1}{2} \tanh(\frac{1}{2} a_{dd}), \frac{1}{2} \sech^2(\frac{1}{2} a_{dd}) \).

### 5 Sampling binary data with specified cross-moment matrix

If \( 2^d - 1 \) full probabilities are known, we easily sample from the corresponding multinomial distribution (Walker, 1977). For a valid set of cross-moments \( m_\mathcal{I}, I \in \mathcal{I} \), Gange (1995) proposes to compute the full probabilities using a variant of the Iterative Proportional Fitting algorithm (Haberman, 1972). While there are no restrictions on the range of dependencies, we have to enumerate the entire state space which limits this versatile approach to low dimensions.

In the sequel, we do not consider methods for structured correlations nor approaches which require enumeration of the state space. First, we show how to compute the parameter \( \mathbf{A} \) of a \( \mu \)-conditionals model for a given cross-moment matrix \( \mathbf{M} \). Secondly, we review an alternative approach to sampling binary data based on the multivariate normal distribution (Emrich and Piedmonte, 1991).
5.1 Fitting the conditionals family

The proof of Theorem 3.2 suggests an iterative procedure to adjust the parameter $A$ to a given cross-moment matrix $M$. We add new cross-moments $m \in (0,1)^{d+1}$ to the $d \times d$ lower triangular matrix $A$ by solving the non-linear equation $f(a) = m$ via Newton-Raphson iterations $a^{(k+1)} = a^{(k)} - [f'(a^{(k)})]^{-1}[f(a^{(k)}) - m]$ where

$$f(a) = \sum_{\gamma \in B_d} q_{k}^{\gamma} \mu((\gamma^\top, 1)a)(\gamma^\top, 1)^\top$$
$$f'(a) = \sum_{\gamma \in B_d} q_{k}^{\gamma} \mu'((\gamma^\top, 1)a)(\gamma^\top, 1)^\top(\gamma^\top, 1)$$

For dimensions $d > 10$, the exact computation of the expectations becomes expensive, and we replace $f$ and $f'$ by their Monte Carlo estimates

$$\hat{f}(a) = \sum_{k=1}^{n} q_{k}^{\gamma} \mu((x_k^\top, 1)a)(x_k^\top, 1)$$
$$\hat{f}'(a) = \sum_{k=1}^{n} q_{k}^{\gamma} \mu'((x_k^\top, 1)a)(x_k^\top, 1)^\top(x_k^\top, 1)$$

where $x_1, \ldots, x_n$ are drawn from $q_{k}^{\gamma}$. Some remarks are in order.

- If the smallest eigenvalue of $M - \text{diag}(M)\text{diag}(M)^\top$ approaches zero or a cross-moment $m_{ij}$ approaches the bounds (2), the parameter $a_{ij}$ may become very large in absolute value. The limited numerical accuracy available on a computer inhibits sampling from such extreme cases.

- We might encounter numerical trouble in the course of the fitting procedure. In order to circumvent problems, we set

$$m_{ij}(\lambda_k) := \lambda_k m_{ij} + (1 - \lambda_k)m_{ii}m_{jj}$$

for all $j = 1, \ldots, i - 1$ and compute a sequence of solutions $a(\lambda_k)$ to the cross-moments $m(\lambda_k)$. We stop if the parameters fail to converge which ensures that the mean of the $\mu$-conditionals family is always diag($M$).

- If we have data available instead of cross-moments, we would rather fit the family via component-wise likelihood maximization which is usually faster than the method of moments and can even be parallelized (Schäfer and Chopin, 2011).

- For the linear link function $\mu(x) = x$, we obtain

$$f(a) = \left[\sum_{\gamma \in B_d} q_{k}^{\gamma}((\gamma^\top, 1)^\top(\gamma^\top, 1))\right] a = \begin{pmatrix} M & m \\ m^\top & 1 \end{pmatrix} a$$

which always has a solution by virtue of Lemma 3.3; to construct a mass function, however, we have to fall back to the truncated version $\mu(x) = \min\{\max\{x, 0\}, 1\}$, and the range of feasible cross-moments is hard to assess (Qaqish, 2003).

5.2 Fitting the Gaussian copula family

Emrich and Piedmonte (1991) propose to dichotomize a multivariate Gaussian distribution for sampling multivariate binary data.
Definition For a vector $a \in \mathbb{R}^d$ and a $d \times d$ correlation matrix $\Sigma$ we define the Gaussian copula family

$$g_a^{\Sigma}(\gamma) = \int_{\tau_a^{-1}(\gamma)} \varphi(\xi) d\xi, \quad \varphi(\xi) = (2\pi)^{-d/2} |\Sigma|^{-1/2} \exp \left(-\frac{1}{2} \xi^\top \Sigma^{-1} \xi \right),$$

where $\tau_a(x) := \left( \mathbb{I}_{(-\infty,a)}(x_1), \ldots, \mathbb{I}_{(-\infty,a_d)}(x_d) \right)$.

For all $I \subseteq D$, the marginals are

$$m_I = \sum_{\gamma \in \mathbb{B}^d} g_a^{\Sigma}(\gamma) \prod_{i \in I} \gamma_i = \sum_{\gamma \in \mathbb{B}^d, \gamma_i = 1} \int_{\tau_a^{-1}(\gamma)} \varphi(\xi) d\xi = \int_{\bigcup_{\gamma \in \mathbb{B}^d, \gamma_i = 1} \tau_a^{-1}(\gamma)} \varphi(\xi) d\xi = \Phi^{(I)}(\sigma(I)),
$$

where $\Phi^{(I)}$ is the marginal cumulative distribution function of the multivariate Gaussian. We set $a_i = \Phi^{-1}(m_{ij})$ for $i \in D$ to adjust the mean. In order to compute the parameter $\Sigma$ that yields the desired cross-moments $M$, we may use a fast series approximations (Drezner and Wesolowsky, 1990) to solve $m_{ij} = \Phi_{\sigma_{ij}}(a_i, a_j)$ for $\sigma_{ij}$ via Newton-Raphson iterations $\sigma_{ij}^{r+1} = \sigma_{ij}^r - \left[ \Phi_{\sigma_{ij}}(a_i, a_j) - m_{ij} \right] / \varphi_{\sigma_{ij}}(a_i, a_j)$; Modarres (2011) suggests the bivariate Plackett (1965) distribution as a proxy for $\varphi_{\sigma_{ij}}$ which might provide a good starting value $\sigma_{ij}^0 \in (-1, 1)$.

While we always obtain a solution in the bivariate case, it is well-known that the resulting matrix $\Sigma$ is not necessarily positive definite due to the range of the Gaussian copula which allows to attain the bounds (2) for $d \leq 2$, but not for higher dimensions. In that case, we can replace $\Sigma$ by

$$\Sigma^* = (\Sigma + |\lambda| \mathbf{I})/(1 + |\lambda|) > 0$$

where $\lambda$ is smaller than any eigenvalue of $\Sigma$. Alternatively, we can project $\Sigma$ into the set of correlation matrices; see Higham (2002) and follow-up papers for algorithms that compute the nearest correlation matrix in Frobenius norm.

The point-wise evaluation of $g_a^{\Sigma}(\gamma)$ requires the computation of multivariate normal probabilities, that is high-dimensional integrals with the respect to the density of the multivariate normal distribution. This is a computationally challenging task in itself (see e.g. Genz and Bretz, 2009), and the Gaussian copula family is therefore not easily incorporated into the Markov chain Monte Carlo algorithms briefly discussed in the introduction.

6 Numerical experiments

In this section, we compare the $\mu$-conditionals family with truncated linear and logistic link function to the Gaussian copula family. We draw random cross-moment matrices of varying dimension and difficulty, fit the parametric families and record how well the desired correlation structure can be reproduced on average.

6.1 Random cross-moments

We first sample the mean $m = \text{diag}(M) \sim U_{(0,1)^d}$. For the off-diagonal elements, we have to ensure that the covariance matrix $M - mm^\top$ is positive definite and that the constraints (2) are all met. We alternate the following two steps.
- Permutations $m_{ij} = m_{\sigma(i)\sigma(j)}$ for $i, j \in D$ with uniform $\sigma \sim \mathcal{U}_{S(D)}$ where we denote by $S(D) := \{\sigma: D \rightarrow D, \sigma \text{ is bijective}\}$ the set of all permutations on $D$.

- Replacements $m_{id} = m_{di} \sim \mathcal{U}_{[a_i, b_i]}$ for all $i = \sigma(1), \ldots, \sigma(d - 1)$ with uniform $\sigma \sim \mathcal{U}_{S(D \setminus \{d\})}$ where the bounds $a_i, b_i$ are subject to the constraints $\det(M) > 0$ and $\min\{m_{ii} + m_{dd} - 1, 0\} \leq m_{id} \leq \max\{m_{ii}, m_{dd}\}$.

The replacement step needs some consideration. We denote by $N$ the inverse of the $(d - 1) \times (d - 1)$ upper sub-matrix of $M$ and define $\tau_i := m_{di} \sum_{j \in D \setminus \{d\}} m_{dj} n_{ij}$ such that $\det(M) = [1/\det(N)] (m_{dd} - \sum_{i \in D \setminus \{d\}} \tau_i)$. If we replace $m_{di} = m_{id}$ by $x_i$ we have to ensure that $\det[M(x_i)] = \det(M) + m_{di}(m_{di} n_{ii} + 2\tau_i) - x_i(x_i n_{ii} + 2\tau_i) > 0$ which means $(x_i + \tau_i/n_{ii}) \in (-c_i, c_i)$ with $c_i := [\tau_i^2/n_{ii}^2 + \det(M) + m_{di}(m_{di} n_{ii} + 2\tau_i)]^{-1/2}$. Therefore, the lower and upper bounds, $a_i := \max\{m_{ii} + m_{dd} - 1, 0, -\tau_i/n_{ii} - c_i\}$ and $b_i := \min\{m_{ii}, m_{dd}, -\tau_i/n_{ii} + c_i\}$, respect all constraints on $x_i$. We rapidly update the value of the determinant $\det[M(x_i)]$ and proceed with the next entry.

We perform $10 \cdot d$ permutation steps and run 500 sweeps of replacements between permutations. The result is approximately a uniform draw from the set of feasible cross-moments matrices. However, sampling according to these cross-moments might not be possible in higher dimensions because the cross-moment matrix is likely to contain extreme cases which are beyond the scope of the parametric family or not workable for numerical reasons. We introduce a parameter $\varrho \in [0, 1]$ which governs the difficulty of the sampling problem by shrinking the upper and lower bounds $a$ and $b$ of the uniform distributions to $a^\varrho := [(1+\varrho)a + (1-\varrho)b]/2$ and $b^\varrho := [(1-\varrho)a + (1+\varrho)b]/2$, respectively.

### 6.2 Figure of merit

Let $M$ be a cross-moments matrix and let $M^\theta$ denote the cross-moment matrix with mean $m = \text{diag}(M)$ and uncorrelated entries $m^\theta_{ij} = m_{ij} m_{jj}$ for all $i \neq j \in D$. For a parametric family $q_\varrho$, we define the figure of merit

$$
\tau_q(M) := \frac{\|M - M^\varrho\| - \|M - M^\theta\|}{\|M - M^\varrho\|},
$$

where $M^\theta$ denotes the sampling cross-moment matrix of the parametric family with parameter $\theta$ adjusted to the desired cross-moment matrix $M$. The norm $\| \cdot \|$ might be any non-trivial matrix norm; in our numerical experiments we use the spectral norm $\|A\|_2 := \lambda_{\max}(A^T A)$, where $\lambda_{\max}$ delivers the largest eigenvalue, but we found the Frobenius norm $\|A\|_F := \text{tr}(A A^T)$ to provide qualitatively the very same picture.

### 6.3 Computational results

For fitting the logistic conditionals family when $d > 10$, we replace the exact terms by Monte Carlo estimates (4) where we use $n = 10^4$ random samples. We estimate the cross-moment matrix of the parametric family $q$ by $M^q \approx n^{-1} \sum_{k=1}^n x_k x_k^T$ where we use $n = 10^6$ samples from $q$. This concerns only the logistic and linear conditionals families; for the Gaussian copula family, we can explicitly compute the sampling cross-moments as $m^q_{ij} = \Phi_2(\mu_i, \mu_j; \sigma_{ij})$, where $\Sigma$ is the adjusted correlation matrix of the underlying multivariate normal distribution made feasible via (5).

We loop over 15 levels of difficulty $\varrho \in [0, 1]$ in 3 dimensions $d = 10, 25, 50$, and generate at each time 200 cross-moments matrices. We denote by $\tau_1 \leq \cdots \leq \tau_{200}$ the ordered figures of merit of the random cross-moment matrices. We report the median and the
quantiles \((\tau_{(0.5-\omega)n}, \tau_{(0.5+\omega)n})\), depicted as underlying gray areas for 20 equidistant values of \(\omega \in [0,0,0.5]\). Figures 1-3 show the results grouped by parametric families; the \(y\)-axis with the scale on the left represents the figure of merit \(\tau \in [0,1]\), the \(x\)-axis represents the level of difficulty \(\varrho \in [0,1]\), and the \([0,0,0.5]\)-gray-scale on the right refers to the level of the quantiles.

Figure 1: Logistic conditionals family

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{logistic_family.png}
\caption{Logistic conditionals family}
\end{figure}

Figure 2: Gaussian copula family

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{gaussian_copula_family.png}
\caption{Gaussian copula family}
\end{figure}

Figure 3: Truncated linear conditionals family

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{truncated_linear_family.png}
\caption{Truncated linear conditionals family}
\end{figure}

6.4 Discussion

While Theorem 3.2 suggests that the scope of the logistic conditionals family is far beyond competing approaches, we cannot, in practice, expect a binary parametric family with \(d(d-1)/2\) dependency parameters to produce just any desired correlation structure. However, the practical scope of the logistic family is limited only by the available numerical accuracy while the scope of competing methods is also limited by their mathematical structure.

The truncated linear conditionals family is fast to compute but its quality deteriorates rapidly with growing complexity. The Gaussian copula family is guaranteed to have the correct mean but it is less flexible than the logistic conditionals family; besides, it does not allow for point-wise evaluation of its mass function. The logistic conditionals family is computationally demanding but by far the most versatile option. These findings confirm similar comparisons carried out against the backdrop of particular applications (Farrell and Rogers-Stewart, 2008; Schäfer, 2012).
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