A Set of Efficient Methods to Generate High-Dimensional Binary Data With Specified Correlation Structures

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\textbf{ABSTRACT}

High-dimensional correlated binary data arise in many areas, such as observed genetic variations in biomedical research. Data simulation can help researchers evaluate efficiency and explore properties of different computational and statistical methods. Also, some statistical methods, such as Monte Carlo methods, rely on data simulation. Lunn and Davies proposed linear time complexity methods to generate correlated binary variables with three common correlation structures. However, it is infeasible to specify unequal probabilities in their methods. In this article, we introduce several computationally efficient algorithms that generate high-dimensional binary data with specified correlation structures and unequal probabilities. Our algorithms have linear time complexity with respect to the dimension for three commonly studied correlation structures, namely exchangeable, decaying-product and $K$-dependent correlation structures. In addition, we extend our algorithms to generate binary data of specified nonnegative correlation matrices satisfying the validity condition with quadratic time complexity. We provide an R package, CorBin, to implement our simulation methods. Compared to the existing packages for binary data generation, the time cost to generate a 100-dimensional binary vector with the common correlation structures and general correlation matrices can be reduced up to $10^5$ folds and $10^3$ folds, respectively, and the efficiency can be further improved with the increase of dimensions. The R package CorBin is available on CRAN at https://cran.r-project.org/.

\textbf{1. Introduction}

Binary data are commonly observed in many research areas, such as social survey responses, marketing data concerning specific issues with “yes/no” questions, responses to treatments in clinical trials, and measurements of genetic or epigenetic variations among individuals. Usually, multiple variables are collected from an individual in these studies, and correlations among these variables are ubiquitous. Instead of considering each variable individually, it is essential to model the correlated variables together as a multidimensional vector (Cox 1972; Carey, Zeger, and Diggle 1993).

With the improvements of technologies over the past decade, more and more variables are collected, yielding high-dimensional data. One example is the genomic data from biomedical research. Through high-throughput genotyping (Kennedy et al. 2003) and sequencing technologies (Metzker 2010), millions of genetic variants of an individual can be collected simultaneously. It is well known that nearby genetic variants are often highly correlated, which is known as linkage disequilibrium (Pritchard and Przeworski 2001). Hence, we cannot simply regard each variant as an independent variable, and the variants constitute a high-dimensional correlated binary vector. Other examples of high-dimensional data include community DNA fingerprints data (Wilbur et al. 2002), binary questionnaire data (Fieuws et al. 2006), consumer financial history data (Diwakar and Vaidya 2009), and consumer behavior data (Naik et al. 2008).

Data simulation can help researchers evaluate the performance of a specific method when real data are difficult to access and/or there is no ground truth about the underlying model/mechanism. We can explore the properties of the method through analyzing simulated data, such as exploring the small sample properties of generalized estimating equations (GEE) (Hardin and Hilbe 2002). In addition, many statistical estimation methods rely on the generation of random numbers, such as Monte Carlo methods. With an ever increasing dimension in real world problems, it is essential to develop efficient simulation methods to generate high-dimensional data. In this article, we focus on how to efficiently generate high-dimensional binary data with specified marginal probabilities and correlation structures.

To generate random numbers, a direct method is to compute the probability moment function and generate random samples with probabilities equal to the function values. Bahadur established a parametric model expressing the joint mass function of binary variables with high-order correlations, but...
the distribution becomes computationally infeasible when the dimension is high (Bahadur 1959). During the 1990s, a number of more efficient methods were proposed to simulate multi-dimensional binary data. Emrich and Piedmonte first identified a multivariate normal distribution whose pairwise copulas are linked with the specified correlation matrix (Emrich and Piedmonte 1991). Binary variables satisfying marginal and correlation conditions can be subsequently obtained by dichotomizing the identified distribution. This algorithm has been implemented in an R package, bindata (Leisch, Weingessel, and Hornik 1998). One drawback of this method is that the multivariate normal distribution for a given correlation structure may not exist. In addition, a large number of nonlinear equations with numerical integrations need to be solved in the algorithm. Lee proposed two algorithms based on linear programming to generate binary data with the exchangeable correlation structure (Lee 1993). However, even with the structure assumption, a large number of nonlinear equations are still needed. Gange proposed to use iterative proportional fitting approach to generate multidimensional categorical variables, which is more general than binary variables (Gange 1995). The extra iterative procedure makes the method computationally inefficient. This method has been implemented in the R package MultiOrd (Demirtas 2006). Similar to Emrich and Piedmonte’s idea, Park et al. proposed to generate correlated binary data by dichotomizing correlated Poisson variables (Park, Park, and Shin 1996). The Poisson variables can be generated efficiently by summing independent Poisson variables. Park et al.’s method is very efficient when the dimension is low. Nevertheless, when the dimension grows high, it performs slower than the Emrich and Piedmonte’s method. All the methods above are computationally inefficient when the dimension gets high.

Instead of generating binary data with correlations specified by an arbitrary positive semidefinite matrix, Lunn and Davies proposed algorithms to generate binary data with three common correlation structures, including exchangeable, decaying-product and 1-dependent (Lunn and Davies 1998). The algorithms have linear time complexity with respect to the dimension. However, these algorithms only work when all the marginal probabilities are equal, which limits the applicability of these algorithms.

Efficiently simulating binary variables with unequal probabilities is critical in many applications. For example, let us assume we want to simulate single nucleotide polymorphism (SNP) data, most of which are biallelic (Sachidanandam et al. 2001), to study some statistical behavior of a certain genomic method under different correlation structures. Since the allele frequencies (marginal probabilities) of different SNPs are naturally unequal, it will be unrealistic for us to model them with equal allele frequencies. Therefore, we may need to generate correlated binary data with a certain correlation structure and unequal marginal probabilities. Binary variables with unequal probabilities and specified correlation structures are also common in longitudinal studies. A study on comparing two treatments for a common toenail infection is provided in Section 1.5.3 (pp. 11–12) and Section 7.1 (pp. 142–149) of Shults and Hilbe (2014), where 294 patients were randomized to one of two treatments, and measured at various time points (baseline, 1, 2, 3, 6, 9, and 12 months post baseline) to determine the presence or absence of a severe toenail infection. Hence, the outcome variables are dichotomous. They assumed an exchangeable correlation structure in each treatment group, and the probabilities of each time points are obviously unequal. In addition, this kind of data are commonly used in the GEE method, where the working correlation matrix are often specified as the forms we mentioned in the article, and the probabilities are not necessarily equal.

In this article, we generalize Lunn and Davies’ algorithms to generate high-dimensional correlated binary data with varied marginal probabilities. In line with their work, we first focus on three commonly used correlation structures including exchangeable, decaying-product, as well as 1-dependent correlations. Our algorithms have linear time complexity with respect to the dimension. In addition, we generalize the method to K-dependent structure and extend the applicability to general nonnegative correlation matrices. Although the time complexity becomes to quadratic with general non-negative correlation matrices, the algorithm is still extremely efficient compared to existing approaches. We combine and implement these algorithms in an R package CorBin, which is publicly available on the Comprehensive R Archive Network (CRAN). Compared with existing binary data generation packages, our package spends around \( \frac{1}{700,000} \) of the time used in bindata and \( \frac{1}{120,000} \) of MultiOrd when generating 100-dimensional binary data with exchangeable structure. The ratios reach around \( \frac{1}{350,000} \) and \( \frac{1}{2,060,000} \) when the dimension increases to 500. Similar speed up is also observed for the other two correlation structures. For generating data with general correlation matrices, the ratios become around \( \frac{1}{859} \) and \( \frac{1}{320} \) of bindata and MultiOrd, respectively. The package is easy to use, and a pdf document (CorBin-manual.pdf, supplementary materials) is provided to illustrate the usage for readers.

2. Models and Algorithms

In this section, we propose algorithms for generating an \( m \)-dimensional random binary vector \( \mathbf{X} = (X_1, X_2, \ldots, X_m)' \) with several correlation structures, where \( X_i \) follows the Bernoulli distribution with marginal probability \( p_i, \ i = 1, 2, \ldots, m \). In contrast to the algorithms proposed in Lunn and Davies (1998), here we do not require all marginal probabilities to be equal, which extends the applicability of the algorithms. In the following, we denote the correlation between \( X_i \) and \( X_j \) as \( r_{ij} (1 \leq i \leq j \leq n) \). We assume the correlations are nonnegative, that is, \( r_{ij} \geq 0 \), and use \( \mathbf{R} \) to represent the correlation matrix constituted from \( r_{ij} \). We also assumed all of the Bernoulli random variables used in each algorithm are generated independently.

2.1. Natural Restrictions for Correlated Binary Variables

In this subsection, we present the natural restrictions for any correlated binary variables must satisfy. First, the correlation matrix \( \mathbf{R} \) should be positive definite. This imposes restrictions on the correlation coefficients within \( \mathbf{R} \) matrices. Taking the \( \mathbf{R} \)
matrix presented in Equation (30) (Section 2.4) as an example, \( \rho_i \) must take values in \((-\frac{1}{r_m}, \frac{1}{r_m})\) to satisfy the positive definite restriction, where \( c_m = 2\sin(\pi(m-1)/(2m+1)) \) (Shults and Hilbe 2014). When \( m \to +\infty \), the constraints will approach \((-0.5, 0.5)\).

Second, natural constraints of \( R \) are also imposed by the marginal expectations. Let’s consider a simple bivariate example, in which \( p_1, p_2 = 0.1, 0.4 \), and \( \rho = 0.9 \). The corresponding correlation matrix is obviously positive definite. However, \( P(Y_1 = 1, Y_2 = 1) = 0.1 \times 0.4 + 0.9 \cdot 0.1 \times 0.4 \times (1-0.1) \times (1-0.4) = 0.172; P(Y_1 = 1, Y_2 = 0) = P(Y_1 = 1) - P(Y_1 = 1, Y_2 = 1) = 0.1 - 0.172 = -0.072 < 0 \), which leads to an invalid probability. Prentice formulated the constraints imposed for marginal expectations and correlation coefficients, which are known as the Prentice constraints (Prentice 1988). Specifically, under multivariate binary distribution, the correlation between any two dimensions \( i, j \) should satisfy
\[
\max \left\{ -\frac{p_i(1-p_i)}{\sqrt{p_i(1-p_i)}}, -\frac{p_j(1-p_j)}{\sqrt{p_j(1-p_j)}} \right\} \leq r_{ij} \leq \min \left\{ \frac{p_i(1-p_i)}{\sqrt{p_i(1-p_i)}}, \frac{p_j(1-p_j)}{\sqrt{p_j(1-p_j)}} \right\}.
\]

For the nonnegative correlation structure, each element of the correlation matrix should satisfy \( r_{ij} \in [0, \min \left\{ \frac{p_i(1-p_i)}{\sqrt{p_i(1-p_i)}}, \frac{p_j(1-p_j)}{\sqrt{p_j(1-p_j)}} \right\}] \), based on the Prentice constraints. In our R package, we will first check whether the input parameters satisfy the Prentice constraints. If not, we will print out a warning message with exact values of the Prentice constraints for users.

Please note that the Prentice constraints and the positive definiteness are necessary but not sufficient conditions to guarantee the existence of multivariate binary distributions with the specified correlation structures. Actually, as we later presented in Section 2.2 and 2.3, for exchangeable and decaying-product correlation structure, the Prentice constraints are sufficient to guarantee the existence of the distributions. However, it is not true for all correlation structures. For example, Chaganty and Joe (2006) presented a simple example with a 1-dependent correlation structure (detailed in Section 2.4), in which the Prentice constraints were satisfied but the corresponding distribution is not valid. Further, Shults and Hilbe provided a brief review on additional constraints for correlated binary data (Shults and Hilbe 2014).

In following subsections, we provide implementation details and related properties of algorithms to generate binary data with different correlation structures.

### 2.2. Exchangeable Correlation Structure

The exchangeable correlation structure is one of the most commonly used structures in data simulation, and is regarded as the default setting in most binary data generation packages. In this case, every pair of observations on a specific unit has the same correlation, that is,
\[
r_{ij} = \begin{cases} \rho, & i \neq j, \\ 1, & i = j. \end{cases}
\]

The correlation matrix of the exchangeable correlation structures is
\[
R = \begin{pmatrix} 1 & \rho & \cdots & \rho \\ \rho & 1 & \cdots & \rho \\ \vdots & \vdots & \ddots & \vdots \\ \rho & \rho & \cdots & 1 \end{pmatrix}.
\]

We use \( p_{\min} \) and \( p_{\max} \) to denote the minimal and maximal values in the desired marginal probabilities, that is,
\[
p_{\min} = \min_{k \in \{1, \ldots, m\}} p_k, \quad p_{\max} = \max_{k \in \{1, \ldots, m\}} p_k.
\]

An intuitive thinking to generate binary data with exchangeable structure is to make each variable \( X_i \) taking the linear combination form \((1 - U_i)Y_i + U_iZ_i\), where \( U_i \sim \text{Bern}(\alpha_i) \), \( Y_i \sim \text{Bern}(\beta_i) \), \( Z \sim \text{Bern}(\gamma) \), and all of the random variables are mutually independent. A careful selection of \( \alpha_i, \beta_i, \gamma \) is needed to make the constructed variables having specified marginal probabilities and correlations. We describe the constructions in detail in Algorithm 1.

In the following, we first show the justification of the algorithm, that is, if \( \alpha_i, \beta_i, \gamma \) lies in \([0, 1]\), the binary data generated from Algorithm 1 have specified marginal expectations and exchangeable correlation structure. After that, we prove that if the data to be generated satisfy the necessary condition of their existence, namely the Prentice constraints, the construction of Algorithm 1 can guarantee that the parameters lie in \([0, 1]\).

### Algorithm 1 Generate binary data under the exchangeable correlation structure.

**Input:** The expected values of the Bernoulli random variables \( p_1, p_2, \ldots, p_m \); and the correlation coefficient \( \rho \)

**Output:** The correlated binary variables \( X_1, X_2, \ldots, X_m \)

0: Check whether the input satisfies the Prentice constraints.
1: \( \gamma = \frac{\sqrt{p_{\min}p_{\max}}}{\sqrt{p_{\min}p_{\max}} + \sqrt{(1 - p_{\min})(1 - p_{\max})}} \)
2: Generate \( Z \sim \text{Bern}(\gamma) \)
3: for \( i = 1, 2, \ldots, m \) do
4: \( \alpha_i = \frac{\sqrt{p_i(1-p_i)}}{\sqrt{(1-\gamma)}} \)
5: \( \beta_i = \frac{p_i - \alpha_i\gamma}{1 - \alpha_i} \)
6: Generate \( U_i \sim \text{Bern}(\alpha_i) \)
7: Generate \( Y_i \sim \text{Bern}(\beta_i) \)
8: \( X_i = (1 - U_i)Y_i + U_iZ \)
9: return \( X_1, X_2, \ldots, X_m \)

**Theorem 2.1.** If intermediate variables \( \alpha_1, \ldots, \alpha_m, \beta_1, \ldots, \beta_m, \gamma \in [0, 1] \), Algorithm 1 returns binary data \( X_1, \ldots, X_m \) with marginal probabilities \( p_1, \ldots, p_m \) and common correlation \( \rho \).
Proof. $X_i$ is a binary variable with the support $\{0,1\}$. For any $i \in \{1, 2, \ldots, m\}$,
$$EX_i = E((1 - U_i)Y_i + U_iZ) = E(1 - U_i)EY_i + EU_iEZ$$
$$= (1 - \alpha_i)\beta_i + \alpha_i\gamma = (1 - \alpha_i)\frac{p_i - \alpha_i\gamma}{1 - \alpha_i} + \alpha_i\gamma = p_i.$$  
(5)

For any $i \neq j \in \{1, 2, \ldots, m\}$
$$r_{ij} = \frac{\text{cov}(X_i, X_j)}{\sqrt{\text{var}(X_i)\text{var}(X_j)}}$$
$$= \frac{\text{cov}((1 - U_i)Y_i + U_iZ, (1 - U_j)Y_j + U_jZ)}{\sqrt{p_ip_j(1 - p_i)(1 - p_j)}}$$
$$= \frac{\alpha_i\alpha_j\gamma(1 - \gamma)}{\sqrt{p_ip_j(1 - p_i)(1 - p_j)}} = \rho.$$  
(6)

Thus, the algorithm returns binary variables satisfying the required marginal and correlation conditions we provide. 

In the following theorem, we show that if the specified binary data with nonnegative exchangeable structure satisfies the Prentice constraints, the probability parameters $\alpha_i$, $\beta_i$, and $\gamma$ will automatically lie in the range of $[0,1]$.

Theorem 2.2. If the specified binary data with nonnegative exchangeable correlation structure satisfy the Prentice constraints, the constructions in Algorithm 1 guarantee that $\alpha_1, \ldots, \alpha_m, \beta_1, \ldots, \beta_m, \gamma$ lie in the range of $[0, 1]$.

Proof. By definition,
$$\gamma = \frac{\sqrt{p_{\min}p_{\max}}}{\sqrt{p_{\min}p_{\max}} + \sqrt{(1 - p_{\min})(1 - p_{\max})}}.$$  
(7)

Since $0 \leq \sqrt{p_{\min}p_{\max}} \leq \sqrt{p_{\min}p_{\max}} + \sqrt{(1 - p_{\min})(1 - p_{\max})}$, we have $0 < \gamma < 1$.

Meanwhile,
$$\gamma(1 - \gamma) = \frac{\sqrt{p_{\min}p_{\max}}(1 - p_{\min})(1 - p_{\max})}{(\sqrt{p_{\min}p_{\max}} + \sqrt{(1 - p_{\min})(1 - p_{\max})})^2}.$$  
(8)

From Cauchy–Schwarz inequality,
$$\left(\sqrt{p_{\min}p_{\max}} + \sqrt{(1 - p_{\min})(1 - p_{\max})}\right)^2 \leq (p_{\min} + 1 - p_{\min})(p_{\max} + 1 - p_{\max}) = 1.$$  
(9)

According to (8) and (9), we have $\gamma(1 - \gamma) \geq \sqrt{p_{\min}p_{\max}}(1 - p_{\min})(1 - p_{\max})$. 

For any $i \in \{1, 2, \ldots, m\}$, $\alpha_i$ is obviously nonnegative. With the Prentice constraints, we have
$$\rho \leq \frac{\sqrt{p_{\min}(1 - p_{\max})}}{p_{\max}(1 - p_{\min}).}$$  
(10)

Therefore,
$$\rho p_i(1 - p_i) \leq \rho p_{\max}(1 - p_{\min})$$
$$\leq \frac{\sqrt{p_{\min}(1 - p_{\max})}}{p_{\max}(1 - p_{\min})} p_{\max}(1 - p_{\min})$$
$$= \sqrt{p_{\min}p_{\max}(1 - p_{\min})(1 - p_{\max})} \leq \gamma(1 - \gamma).$$  
(11)

Hence, we have
$$\alpha_i = \frac{\rho p_i(1 - p_i)}{\gamma(1 - \gamma)} \leq 1.$$  
(12)

On the other hand, due to the fact that $p_{\min} \leq p_i \leq p_{\max}$,
$$1 - \frac{p_{\max}}{p_i} \leq \frac{1 - p_i}{p_i} \leq \frac{1 - p_i}{\sqrt{p_{\min}p_{\max}}(1 - p_{\min})(1 - p_{\max})} \leq \frac{1 - p_i}{p_i} \frac{\sqrt{p_{\min}p_{\max}}}{1 - \gamma} = \frac{p_i}{p_i} 1 - \gamma - \frac{\sqrt{p_{\min}p_{\max}}}{1 - \gamma},$$
and
$$\rho_{\min} \leq \frac{p_i}{p_i} 1 - \gamma \leq \frac{p_i}{p_i} 1 - \gamma - \frac{\sqrt{p_{\min}p_{\max}}}{1 - \gamma},$$
that is,
$$\frac{\sqrt{p_{\min}(1 - p_{\max})}}{p_{\max}(1 - p_{\min})} \leq \min \left\{ \frac{1 - p_i}{p_i} 1 - \gamma, \frac{1 - p_i}{p_i} 1 - \gamma \right\}.$$  
(13)

Combined with inequality (10),
$$\rho \leq \frac{\sqrt{p_{\min}(1 - p_{\max})}}{p_{\max}(1 - p_{\min})} \leq \min \left\{ \frac{1 - p_i}{p_i} 1 - \gamma, \frac{1 - p_i}{p_i} 1 - \gamma \right\}.$$  
(14)

Then we can derive that
$$\rho \leq \frac{1 - p_i}{p_i} 1 - \gamma \leq \frac{\rho p_i(1 - p_i)}{\gamma(1 - \gamma)} \leq \frac{1 - p_i}{\gamma(1 - \gamma)} \leq \alpha_i$$
$$= \frac{\rho p_i(1 - p_i)}{\gamma(1 - \gamma)} \leq \frac{1 - p_i}{\gamma(1 - \gamma)} \leq \frac{p_i - \alpha_i \gamma}{1 - \alpha_i} \leq 1.$$  
(15)

Similarly,
$$\rho \leq \frac{p_i}{1 - \gamma} \leq \frac{\rho p_i(1 - p_i)}{\gamma(1 - \gamma)} \leq \frac{p_i^2}{\gamma^2} \leq \alpha_i$$
$$= \frac{\rho p_i(1 - p_i)}{\gamma(1 - \gamma)} \leq \frac{p_i}{\gamma(1 - \gamma)} \leq \frac{p_i - \alpha_i \gamma}{1 - \alpha_i} \geq 0 \leq \beta_i \geq 0.$$  
(16)

Combining (7), (12), (16), and (17), we finish the proof.  

2.3. Decaying-Product Correlation Structure

The commonly used first-order autoregressive (AR(1)) correlation structure is a special case of the decaying-product correlation structure, where the correlations are highest for adjacent variables and decrease in the power of the distance between dimension indices. The correlation matrix of AR(1) is as follows:
$$R = \begin{pmatrix}
1 & \rho & \rho^2 & \cdots & \rho^{n-1} \\
\rho & 1 & \rho & \cdots & \rho^{n-2} \\
\rho^2 & \rho & 1 & \cdots & \rho^{n-3} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\rho^{n-1} & \rho^{n-2} & \rho^{n-3} & \cdots & 1
\end{pmatrix}.$$  
(18)
Here, we consider the more general decaying-product correlation structure. We allow the marginal probabilities to be freely specified. Given the elements on the minor diagonal of the correlation matrix \( \rho = (\rho_1, \ldots, \rho_{m-1}) \), the correlation between any two variables under this structure can be expressed as

\[
r_{jk} = \prod_{l=j}^{k-1} \rho_l, \quad j < k,
\]

that is,

\[
R = \begin{pmatrix}
1 & \rho_1 & \rho_1 \rho_2 & \rho_1 \rho_2 \rho_3 & \cdots & \prod_{l=1}^{m-1} \rho_l \\
\rho_1 & 1 & \rho_2 & \rho_2 \rho_3 & \cdots & \prod_{l=2}^{m-1} \rho_l \\
\rho_1 \rho_2 & \rho_2 & 1 & \rho_3 & \cdots & \prod_{l=3}^{m-1} \rho_l \\
\rho_1 \rho_2 \rho_3 & \rho_2 \rho_3 & \rho_3 & 1 & \cdots & \prod_{l=4}^{m-1} \rho_l \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
\prod_{l=1}^{m-1} \rho_l & \prod_{l=2}^{m-1} \rho_l & \prod_{l=3}^{m-1} \rho_l & \prod_{l=4}^{m-1} \rho_l & \cdots & 1
\end{pmatrix}.
\]  

(20)

Similarly to the construction method in the previous subsection, we also assume the variable, \( X_i \) takes the linear combination form \( (1 - U_i)Y_i + U_iX_{i-1} \), where \( U_i \sim \text{Bern}(\alpha_i) \), \( Y_i \sim \text{Bern}(\beta_i) \), and all of the random variables are mutually independent. Here the construction of \( X_i \) uses the information of \( X_{i-1} \), bringing the correlation between adjacent elements. Similar to the exchangeable correlation structure, we make a suitable construction of \( \alpha_i \) and \( \beta_i \) in order that the constructed variables have specified marginal probability and correlations. We describe the constructions in detail in Algorithm 2. In the following, we will first show the justification of the algorithm in Theorem 2.3 and prove that the Prentice constraints are enough to guarantee the intermediate parameters in the interval \([0, 1]\) in Theorem 2.4.

**Algorithm 2** Generate binary data under decaying-product correlation structure.

**Input:** The expected values of the Bernoulli random variables \( p_1, p_2, \ldots, p_m \); and the off-diagonal correlation vector \( \rho \)

**Output:** The correlated binary variables \( X_1, X_2, \ldots, X_m \)

1. Check whether the input satisfies the Prentice constraints.
2. Generate \( X_1 \sim \text{Bern}(p_1) \)
3. for \( i = 2, \ldots, m \) do
4. \( \alpha_i = p_{i-1} \sqrt{\frac{p_i(1-p_i)}{p_{i-1}(1-p_{i-1})}} \)
5. \( \beta_i = \frac{p_i - \alpha_i p_{i-1}}{1 - \alpha_i} \)
6. Generate \( U_i \sim \text{Bern}(\alpha_i) \)
7. Generate \( Y_i \sim \text{Bern}(\beta_i) \)
8. \( X_i = (1 - U_i)Y_i + U_iX_{i-1} \)
9. return \( X_1, X_2, \ldots, X_m \)

**Theorem 2.3.** If intermediate variables \( \alpha_2, \ldots, \alpha_m, \beta_2, \ldots, \beta_m \in [0, 1] \), Algorithm 2 returns binary data with the specified marginal probabilities and decaying-product correlation.

**Proof.** In Algorithm 2, \( EX_i = p_i \) is naturally satisfied. Now we prove \( EX_i = p_i \) for \( i = 2, \ldots, m \) by induction. For any \( i \in \{2, \ldots, m\} \), assuming that \( EX_{i-1} = p_{i-1} \), then

\[
EX_i = E((1 - U_i)Y_i + U_iX_{i-1}) = (1 - \alpha_i)\beta_i + \alpha_iEX_{i-1}
\]

\[
= p_i - \alpha_ip_{i-1} + \alpha_ip_{i-1} = p_i.
\]

(21)

For any \( k \in \{1, 2, \ldots, m - 1\} \) and \( i \in \{1, 2, \ldots, m - k\} \),

\[
r_{i+k} = \frac{\text{cov}(X_i, X_{i+k})}{\text{var}(X_i)\text{var}(X_{i+k})} = \frac{\text{cov}(X_i, U_{i+k}U_{i+k-1} \cdots U_{i+1}X_i)}{\sqrt{p_i(1-p_i)}(1 - p_{i+k})}
\]

\[
= \alpha_{i+k} \cdots \alpha_{i+1} \sqrt{p_i(1-p_i)}(1 - p_{i+k})
\]

\[
= \rho_0 \rho_1 \cdots \rho_{i+k-1}.
\]

Thus, the decaying-product correlation structure holds.

**Theorem 2.4.** If the specified binary data with nonnegative decaying-product correlation structure satisfy the Prentice constraints, the constructions in Algorithm 2 guarantee that \( \alpha_2, \ldots, \alpha_m, \beta_2, \ldots, \beta_m \) lie in the range of \([0, 1]\).

**Proof.** For each \( i \in \{2, \ldots, m\} \), we show \( 0 \leq \alpha_i, \beta_i \leq 1 \) in two complementary cases:

When \( p_{i-1} \leq p_i \), according to the Prentice constraints, we have

\[
0 \leq \alpha_i = p_{i-1} \sqrt{\frac{p_i(1-p_i)}{p_{i-1}(1-p_{i-1})}} \leq \sqrt{\frac{p_{i-1} - p_i}{p_{i-1}(1-p_{i-1})}} \cdot \frac{p_i - p_{i-1}}{p_i(1-p_i)} = \frac{1 - p_i}{1 - p_{i-1}} \leq 1. \quad (23)
\]

Thus,

\[
(1 - p_{i-1})\alpha_i \leq 1 - p_i \iff p_i - \alpha_ip_{i-1} \leq 1 - \alpha_i \iff \beta_i = \frac{p_i - \alpha_ip_{i-1}}{1 - \alpha_i} \leq 1. \quad (24)
\]

At the same time,

\[
\beta_i = \frac{p_i - \alpha_ip_{i-1}}{1 - \alpha_i} \geq \frac{p_i - \alpha_ip_{i-1}}{1 - \alpha_i} = p_i \geq 0. \quad (25)
\]

Then we have \( 0 \leq \beta_i \leq 1 \).

In the other case, that is, \( p_{i-1} > p_i \), according to the Prentice constraints,

\[
0 \leq \alpha_i = p_{i-1} \sqrt{\frac{p_i(1-p_i)}{p_{i-1}(1-p_{i-1})}} \leq \sqrt{\frac{p_{i-1} - p_i}{p_{i-1}(1-p_{i-1})}} \cdot \frac{p_i - p_{i-1}}{p_i(1-p_i)} = \frac{p_i}{p_{i-1}} \leq 1. \quad (26)
\]

Then we have

\[
p_i \geq \alpha_ip_{i-1} \iff \beta_i = \frac{p_i - \alpha_ip_{i-1}}{1 - \alpha_i} \geq 0. \quad (27)
\]

Meanwhile,

\[
\beta_i = \frac{p_i - \alpha_ip_{i-1}}{1 - \alpha_i} \leq \frac{p_i - \alpha_ip_{i-1}}{1 - \alpha_i} = p_i \leq 1. \quad (28)
\]

At this point, we have proved that, with the Prentice constraints satisfied, \( 0 \leq \alpha_i, \beta_i \leq 1 \) hold for any binary data with nonnegative decaying-product correlation structure, indicating they can be generated by Algorithm 2.
2.4. 1-Dependent Correlation Structure

Under the stationary K-dependent structure, there is a band of stationary correlations, such that each of the correlation is truncated to zero after the Kth order band (Hardin and Hilbe 2002). The correlation coefficient is

\[ r_{ij} = \begin{cases} 
\rho_{|i-j|}, & \text{if } i \neq j \text{ and } |i-j| \leq K, \\
0, & \text{if } |i-j| > K, \\
1, & \text{if } i = j.
\end{cases} \]  

(29)

As the most common case, the stationary 1-dependent correlation matrix can be expressed as

\[ R = \begin{pmatrix} 
1 & \rho_1 & 0 & \cdots & 0 & 0 \\
\rho_1 & 1 & \rho_2 & \cdots & 0 & 0 \\
0 & \rho_1 & 1 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 1 & \rho_1 \\
0 & 0 & 0 & \cdots & 0 & 1
\end{pmatrix}, \]  

(30)

where the elements on the minor diagonal are equal. To expand the applicability of our method, we design the algorithms on a more general 1-dependent case, allowing the elements on the minor diagonal to vary, that is, \( \rho_1 = (\rho_{11}, \rho_{12}, \ldots, \rho_{1m-1}) \). For simplicity, we use \( \rho \) to represent \( \rho_1 \) in this section.

In the main context, we focus on the generation of binary data with 1-dependent correlation structure. We introduce two algorithms with different applicable conditions. Both algorithms allow marginal probabilities to vary. We will describe the details of applicable conditions separately after introducing the corresponding algorithms.

Intuitively, we intend to construct variables that have correlation between adjacent elements, but independent with those not adjacent, to satisfy the 1-dependent correlation structure. Our Algorithm 3 uses the form of \( X_i = U_iY_{i-1} \) to guarantee the independence of \( X_i \) and \( X_j \) when \( |i-j| \geq 2 \). In addition, the intermediate parameters are also important to make sure that the correlation coefficients, and the marginal probabilities are satisfied. We present the details in Algorithm 3.

**Theorem 2.5.** If intermediate variables \( \alpha_1, \ldots, \alpha_m, \beta_1, \ldots, \beta_m \in [0,1] \), Algorithm 3 returns the binary data with given marginal expectation and 1-dependent correlation structure.

**Proof.** For each \( i \in \{1,2,\ldots,m-1\} \),

\[ EX_i = EU_iY_{i-1} = \alpha_i\beta_i\beta_{i-1} = \frac{\beta_i}{\beta_i\beta_{i-1}} = \beta_i = \beta_{i+1} = p_i. \]

(31)

Meanwhile,

\[ EX_m = EU_mY_mY_{m-1} = \alpha_m\beta_m\beta_{m-1} = \sqrt{p_m\beta_m\beta_{m-1}} = p_m. \]

(32)

**Algorithm 3** Generate binary data under the 1-dependent correlation structure. (Method I)

**Input:** The expected binary data under the 1-dependent correlation structure. (Method I)

**Output:** The correlated binary variables \( X_1, X_2, \ldots, X_m \)

0: Check whether the input satisfies the Prentice constraints.
1. \( \beta_0 = 1 \)
2. \( Y_0 \sim Bern(1) \)
3: for \( i = 1,2,\ldots,m-1 \) do
4: \( \beta_i = \sqrt{p_i\beta_{i+1}} \sqrt{(1-p_i)(1-p_{i+1})} \)
5: \( \alpha_i = \frac{\beta_i}{\beta_{i+1}} \)
6: if \( \alpha_i > 1 \) Indicate that the algorithm fails; break
7: Generate \( U_i \sim Bern(\alpha_i) \)
8: Generate \( Y_i \sim Bern(\beta_i) \)
9: \( X_i = U_iY_{i-1} \)
10: \( \alpha_m = \sqrt{p_m} \)
11: \( \beta_m = \sqrt{p_{m-1}} \)
12: Generate \( U_m \sim v(\alpha_m) \)
13: Generate \( Y_m \sim Bern(\beta_m) \)
14: \( X_m = U_mY_mY_{m-1} \)
15: return \( X_1, X_2, \ldots, X_m \)

From the generation process, it is obvious that \( r_{ij} = 0 \) when \( |j-i| > 1 \). Then for \( i \in \{1,2,\ldots,m-1\} \),

\[ r_{i,i+1} = \frac{cov(X_i, X_{i+1})}{\sqrt{var(X_i)var(X_{i+1})}} = \frac{cov(U_iY_{i-1}, U_{i+1}Y_{i+1}Y_i)}{\sqrt{p_i\beta_{i+1}(1-p_i)(1-p_{i+1})}} = \frac{E(U_iU_{i+1}Y_{i-1}Y_iY_{i+1}) - E(U_iY_{i-1}E(Y_i)E(U_{i+1}Y_{i+1}Y_i))}{\sqrt{p_i\beta_{i+1}(1-p_i)(1-p_{i+1})}} = \frac{(\alpha_i\beta_i\beta_{i+1})(1-\beta_i)}{\beta_i\sqrt{p_i\beta_{i+1}(1-p_i)(1-p_{i+1})}} = \frac{(1-\beta_i)(1-p_i)}{\beta_i} = \rho_i. \]

(33)

Similar to the previous algorithms, the data generated by Algorithm 3 require intermediate parameters \( \alpha_i \) and \( \beta_i \) to be in the range of \([0,1]\). Otherwise, intermediate variables \( U_i \) and \( Y_i \) cannot be generated, nor can \( X_i \). In the following theorem, we show the restriction for \( \rho \) such that the intermediate parameter requirement is satisfied.

**Theorem 2.6.** Only binary data with nonnegative 1-dependent structure satisfying the following inequalities can be generated from Algorithm 3:

\[ A_i\rho_{i-1}\rho_i + B_{i+1}\rho_{i+1} \leq C_i, \quad i = 2, \ldots, m-1, \]  

(34)

where \( A_i = \sqrt{(1-p_i)(1-p_{i+1})} \), \( B_{i+1} = \sqrt{(1-p_i)(1-p_{i+1})p_{i+1}} \), \( B_{i+1} = \sqrt{p_{i+1}(1-p_{i+1})} \), and \( C_i = \sqrt{p_{i+1}(1-p_{i+1})} \). When \( \rho_1 = \rho_2 = \cdots = \rho_m = \rho \), we denote \( A = A_i, B = B_{i+1} + B_{i+1}, \) and \( C = C_i \); then the inequality (34) can
be simplified to

$$0 \leq \rho_i \leq \frac{-B + \sqrt{B^2 + 4AC}}{2A}. \tag{35}$$

Further, in the special case when \(p_1 = p_2 = \cdots = p_m = \rho\), the applicable condition is \(0 \leq \rho \leq \frac{\sqrt{\rho}}{1 + \sqrt{\rho}}\).

**Proof.** Since \(\rho \geq 0\), it is obvious that \(\alpha_i \geq 0\) and \(0 \leq \beta_i \leq 1\) based on the definitions of \(\alpha_i\) and \(\beta_i\). Now we study the applicable condition for \(\rho\) such that the intermediate parameter \(\alpha_i \leq 1\). For each \(i \in \{1, 2, \ldots, m-1\}\), we have

$$\alpha_i = \frac{p_i}{\beta_i \beta_{i-1}} = \frac{(\sqrt{p_i p_{i+1}} + \rho_i \sqrt{(1-p_i)(1-p_{i+1})})}{\sqrt{\beta_i \beta_{i-1} (1-p_i)(1-p_{i+1})}} \leq 1,$$

which is equivalent to inequality (34).

When \(\rho_1 = \rho_2 = \cdots = \rho_m = \rho\), denote A, B, and C as above, and we get

$$\alpha_i \leq 1 \iff A\rho^2 + B\rho - C \leq 0 \iff \rho \leq \frac{-B + \sqrt{B^2 + 4AC}}{2A}. \tag{37}$$

Thus, given the marginal probabilities of a variable as well as its neighbors, we can derive the constraint for the corresponding correlation in **Algorithm 3**.

In the special case when \(p_1 = p_2 = \cdots = p_m = \rho\), the above constraint can be reduced to \(\rho \leq \frac{\sqrt{\rho}}{1 + \sqrt{\rho}}\), which does not involve the dimension \(m\) but only the marginal probability \(\rho\). **Figure 1** shows the relationship between the maximal allowed correlation \(\rho_{\text{max}}\) and the marginal probability \(p\). The maximal allowed correlation increases monotonically with \(p\) and converge to 0.5, which is consistent with the natural restrictions for positive definiteness discussed in **Section 2.1**.

For **Algorithm 4**, we used the form \(W_i = (1 - U_i)Y_i + U_iY_{i-1}\) to generate variables with 1-dependent correlation structure, and then multiply \(W_i\) by an \(A_i\) to adjust the probability. Actually, the idea of multiplying by an \(A_i\) has been discussed in Lunn and Davies’ article. As they discussed in the article, this strategy can only be applied in 1-dependent correlation structure. Nevertheless, we provide the details of this strategy for generating binary data with 1-dependent correlation structure in **Algorithm 4**. In the following, we provide the proof of related properties for **Algorithm 4**.

**Algorithm 4** Generate binary data under the 1-dependent correlation structure. (Method II)

**Input:** The expected values of the Bernoulli random variables \(p_1, p_2, \ldots, p_m\), and the correlation coefficient vector \(\rho = (\rho_1, \rho_2, \ldots, \rho_{m-1})\)

**Output:** The correlated binary variables \(X_1, X_2, \ldots, X_m\)

0: Check whether the input satisfies the Prentice constraints.
1: \(p_{\text{max}} = \max\{p_1, \ldots, p_m\}\)
2: Denote \(\alpha_i = \frac{p_i}{p_{\text{max}}}, i = 1, \ldots, m\)
3: Denote \(\rho'_i = \rho \sqrt{\frac{(1 - p_i)(1 - p_{i+1})}{p_i p_{i+1}(1 - p_{\text{max}})}}, i = 1, \ldots, m - 1\)
4: \(Y_1 \sim \text{Bern}(p_{\text{max}})\)
5: \(W_1 = Y_1\)
6: \(r_1 = 0\)
7: for \(i = 2, \ldots, m\) do
8: \(r_i = \frac{1}{1 + p_i}\)
9: if \(r_i > 1\) indicate the algorithm fails; **break**
10: Generate \(U_i \sim \text{Bern}(r_i)\)
11: Generate \(Y_i \sim \text{Bern}(p_{\text{max}})\)
12: \(W_i = (1 - U_i)Y_i + U_iY_{i-1}\)
13: for \(i = 1, \ldots, m\) do
14: Generate \(A_i \sim \text{Bern}(\alpha_i)\)
15: \(X_i = A_iW_i\)
16: **return** \(X_1, X_2, \ldots, X_m\)

**Theorem 2.7.** If intermediate variables \(a_2, \ldots, a_m, r_2, \ldots, r_m \in [0, 1]\), **Algorithm 4** returns binary data with given marginal expectation and 1-dependent correlation structure.

**Proof.** From the definition, \(EX_1 = p_1\). For \(i \in \{2, \ldots, m\}\), we have

$$EX_i = EA_iW_i = \alpha_i((1 - r_i)p_{\text{max}} + r_ip_{\text{max}}) = \frac{p_i}{p_{\text{max}}}, \tag{39}$$

Then for each \(i \in \{1, 2, \ldots, m - 1\}\), we can obtain that

$$r_{i,i+1} = \frac{\text{cov}(X_i, X_{i+1})}{\sqrt{\text{var}(X_i)\text{var}(X_{i+1})}} = \frac{\alpha_i a_{i+1}\text{cov}((1 - U_i)Y_i, U_{i+1}Y_i)}{\sqrt{p_i p_{i+1}(1 - p_i)(1 - p_{i+1})}}$$

$$= \frac{\alpha_i a_{i+1}(E((1 - U_i)Y_i U_{i+1}Y_i^2) - E((1 - U_i)Y_i)E(U_{i+1}Y_i))}{\sqrt{p_i p_{i+1}(1 - p_i)(1 - p_{i+1})}}$$

$$= \frac{\rho'_i(1 - p_{\text{max}})\sqrt{p_i p_{i+1}}}{p_{\text{max}}\sqrt{(1 - p_i)(1 - p_{i+1})}} = \frac{p_i}{p_{\text{max}}} \frac{\rho_i \sqrt{p_i p_{i+1}}}{p_{\text{max}} \sqrt{\alpha_i a_{i+1}}}$$

$$= \frac{p_i}{p_{\text{max}}} = \rho_i,$$
Theorem 2.8. Only binary data with nonnegative 1-dependent correlation structure satisfying the following inequalities can be generated from Algorithm 4:

\[ 0 \leq \rho_i \leq \frac{\sqrt{\rho_i p_{i+1}}}{\sqrt{(1-p_i)(1-p_{i+1})}} \frac{1-p_{\text{max}}}{p_{\text{max}}} (1-r_i), \]  \hspace{1cm} (40)

where \( r_i = \frac{\rho_{i-1}}{1-r_{i-1}} \sqrt{\frac{(1-p_{i-1})(1-p_i)}{p_{i-1}p_i}} \frac{1-p_{\text{max}}}{p_{\text{max}}} \) is a function of previous correlation \( \rho_{i-1} \). In the special case when \( p_1 = p_2 = \cdots = p_m = p \) and \( \rho_1 = \rho_2 = \cdots = \rho_m = \rho \geq 0 \), the validity condition is \( \frac{1}{\sqrt{4p}} \left[ (1 + \sqrt{1 - 4\rho})^{m+1} - (1 - \sqrt{1 - 4\rho})^{m+1} \right] \geq 0 \).

\textbf{Proof.} In Algorithm 4, \( A_i \) and \( Y_i \) can always be generated since their corresponding probabilities \( \alpha_i \) and \( p_{\text{max}} \) are in the range of \([0, 1]\). Hence, we only need to consider the generation of \( U_i \).

Based on the definition of \( U_i \)'s marginal probability \( r_i \), it is obvious that \( r_i \geq 0 \) if \( r_{i-1} \leq 1 \) holds. Therefore, the only requirement of Algorithm 4 is \( r_i \leq 1 \) \((i = 1, \ldots, m)\). Thus, we have the validity condition:

\[ r_i = \frac{\rho_{i-1}}{1-r_{i-1}} \sqrt{\frac{(1-p_{i-1})(1-p_i)}{p_{i-1}p_i}} \frac{1-p_{\text{max}}}{p_{\text{max}}} \leq 1 \iff \rho_i \leq \frac{\sqrt{\rho_i p_{i+1}}}{\sqrt{(1-p_i)(1-p_{i+1})}} \frac{1-p_{\text{max}}}{p_{\text{max}}} (1-r_i). \] \hspace{1cm} (41)

In practice, we can obtain the condition for each \( \rho_i \) by iteration.

In the special case when \( p_1 = \cdots = p_m = p \), \( \rho_1 = \cdots = \rho_m = \rho \), the requirement becomes the following series of inequalities:

\[ r_1 = 0 \leq 1 \]
\[ r_2 = \frac{\rho}{1-r_1} = \rho \leq 1 \]
\[ r_3 = \frac{\rho}{1-r_2} = \frac{\rho}{1-\rho} \leq 1 \implies \rho \leq \frac{1}{2} \]
\[ r_4 = \frac{\rho}{1-r_3} = \frac{\rho}{1-\frac{\rho}{1-\rho}} = \frac{\rho(1-\rho)}{1-2\rho} \leq 1 \implies \rho \leq \frac{3 - \sqrt{5}}{2} \]
\[ \cdots \]

The general term formula of \( r_i \) is \( r_i = \frac{2\rho}{\sqrt{4\rho}} \left[ \frac{(1+\sqrt{1-4\rho})^{i+1} - (1-\sqrt{1-4\rho})^{i+1}}{(1+\sqrt{1-4\rho})^{i+1} - (1-\sqrt{1-4\rho})^{i+1}} \right] \). The series of inequalities can be reduced to

\[ \frac{1}{\sqrt{1-4\rho}} \left[ (1 + \sqrt{1 - 4\rho})^{i+1} - (1 - \sqrt{1 - 4\rho})^{i+1} \right] \geq 0, \] \hspace{1cm} (43)

where \( i = 1, \ldots, m \).

From the inequalities above we see that as \( i \) increases, the restriction of \( \rho \) becomes more and more strict. Hence, we only need to satisfy the last inequality in Algorithm 4, that is,

\[ \frac{1}{\sqrt{1-4\rho}} \left[ (1 + \sqrt{1 - 4\rho})^{m+1} - (1 - \sqrt{1 - 4\rho})^{m+1} \right] \geq 0. \] \hspace{1cm} (44)

Compared to the conditions for validity of Algorithm 3, the restriction of Algorithm 4 is only related with the dimension \( m \) and not the marginal probability \( p \). Figure 2 describes the relationship between the maximal allowed correlation \( \rho_{\text{max}} \) and the dimension \( m \). The \( \rho_{\text{max}} \) monotonically decreases as \( m \) increases, and converges to 0.25. Therefore, if \( \rho \leq 0.25 \), this algorithm is suitable to generate binary data with an arbitrary dimension \( m \).

To conclude, both algorithms have their own specialities and validity conditions for generating binary data with 1-dependent correlation structure. In Algorithm 3, the limitation for each entry of correlation vector is only related with nearby marginal probabilities. In Algorithm 4, the limitation is also related with previous entries of correlation vector. It is difficult to distinguish which algorithm has more general validity conditions. We give a detailed analysis when \( p_1 = p_2 = \cdots = p_m = p \) and \( \rho_1 = \rho_2 = \cdots = \rho_m = \rho \). In this situation, Algorithm 3 has no limitation on the dimension, meaning that the dimension can be arbitrarily large with feasible marginal probabilities. Thus, this algorithm is perfect for the situation when high dimension is required. On the other hand, Algorithm 4 is more flexible when the dimension is not too high, since it is not restricted by the marginal probabilities.

To incorporate the two methods, we provide a function cBern1dep in our R package CorBin, which can automatically choose the suitable algorithm based on the given \( p \) and \( \rho \). In our function, we will first derive \( r_i \) \((i = 1, 2, \ldots, m)\) in Algorithm 4.

\[ \text{Figure 2. Relationship between the maximal allowed correlation \( \rho_{\text{max}} \) and the dimension \( m \) in Algorithm 4, when } p_1 = \cdots = p_m = p \text{ and } \rho_1 = \rho_2 = \cdots = \rho_m = \rho. \text{ As } m \text{ increases, the maximum of } \rho \text{ will decrease, and gradually converges to 0.25.} \]
If all the $r_i$ lie in the interval $[0, 1]$, we will use Algorithm 4 to generate the binary data. If not, the function will automatically call function rhoMaxIdep to calculate the largest entries of $\rho$ allowed in Algorithm 3. If all the entries of given $\rho$ lies in the interval, the binary data will be generated using Algorithm 3.

### 2.5. K-Dependent Correlation Structure and General Correlation Matrices

In Section 2.4, we provide two algorithms to generate binary data with 1-dependent correlation structure. Here we discuss the generation of binary data with $K$-dependent ($K > 1$) correlation structure by extending Algorithm 3. Specifically, if we set $K = m - 1$, we can obtain binary data with the general nonnegative correlation matrices. Based on the intuition of Algorithm 3, we provide the details of the binary data generation algorithm under the $K$-dependent correlation structure (and also a general correlation matrix) in Algorithm 5.

We first denote $Y = (Y_1, \ldots, Y_m)$ as a $K \times m$ matrix:

$$Y = \begin{pmatrix} Y_{11} & Y_{12} & \cdots & Y_{1m} \\ Y_{21} & Y_{22} & \cdots & Y_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ Y_{K1} & Y_{K2} & \cdots & Y_{Kn} \end{pmatrix}. \quad (45)$$

In the algorithm, we use $\rho_i$ to denote the $m - i$ elements on the $i$th diagonal of the correlation matrix, that is,

$$\rho_i = (\rho_{i1}, \rho_{i2}, \ldots, \rho_i(m-i)) = (r(i+1), r(i+2), \ldots, r(m-i)m). \quad (46)$$

**Algorithm 5 Generate binary data under $K$-dependent correlation structure (and general correlation matrix if $K = m - 1$).**

**Input:** The expected values of the Bernoulli random variables $p_1, p_2, \ldots, p_m$; and the correlation coefficient vector $\rho_1, \rho_2, \ldots, \rho_K$

**Output:** The correlated binary variables $X_1, X_2, \ldots, X_m$

1. Check whether the input satisfies the Prentice constraints.
2. Let $p_{m+1} = p_{m+2} = \cdots = p_{m+k} = p_m$
3. for $i = 1, 2, \ldots, K$ do
   - Let $\rho_i = \rho_i(m-(i-1)) = \rho_i(m-(i-1)+1) = \cdots = \rho_i m = 0$
4. for $j = 1, 2, \ldots, m$ do
   - Let $\beta_j = \frac{p_j}{\beta_j} \beta_j = \frac{p_j}{\beta_j} \beta_j \frac{1}{1 - p_{j+1}}$
5. $Y_{ij} \sim \text{Bern} (\beta_j)$
6. Generate $U_i \sim \text{Bern} (\alpha_i)$
7. $X_i = U_i \prod_{l=1}^{K_i} Y_{il}$
8. if $\alpha_i > 1$: Indicate that the algorithm fails.
9. Generate $U_i \sim \text{Bern} (\alpha_i)$
10. Denote $K_i = \min(i-1, K)$
11. if $\alpha_i > 1$: Indicate that the algorithm fails;
12. Generate $U_i \sim \text{Bern} (\alpha_i)$
13. $X_i = U_i \prod_{l=1}^{K_i} Y_{il}$
14. return $X_1, X_2, \ldots, X_m$

In the following, we show the justification of Algorithm 5 in Theorem 2.9.

**Theorem 2.9.** If intermediate variables $\alpha_1, \ldots, \alpha_m$, $\beta_1, \ldots, \beta_km \in [0, 1]$, Algorithm 5 returns the corresponding binary data with given marginal probabilities and $K$-dependent correlation structure.

**Proof.** For $i = 1$, we have

$$E_X = E_U \prod_{l=1}^{K} Y_{il} = \alpha_1 \prod_{l=1}^{K} \beta_{il} = p_1. \quad (47)$$

For each $i \in \{2, \ldots, m\}$,

$$E_X = E_U \prod_{l=1}^{K} Y_{il} \prod_{l=1}^{K_{i-1}} Y_{i(l-\ell)} = \alpha_1 \prod_{l=1}^{K} \beta_{il} \prod_{l=1}^{K_{i-1}} \beta_{i(l-\ell)} = \prod_{l=1}^{K} \beta_{il} \prod_{l=1}^{K_{i-1}} \beta_{i(l-\ell)} = p_i. \quad (48)$$

From the generation process, it is obvious that $r_{ij} = 0$ when $|j - i| > K$. Considering $i = 1, j \in \{1, 2, \ldots, m-1\}$,

$$r_{i+1,1} = \frac{\text{cov}(X_i, X_{i+1})}{\sqrt{\text{var}(X_i) \text{var}(X_{i+1})}} = \frac{\text{cov}(U_1 \prod_{l=1}^{K_i} Y_{il}, U_{i+1} \prod_{l=1}^{K_{i-1}} Y_{i(l+1)})}{\sqrt{p_1 p_{i+1} (1 - p_1) (1 - p_{i+1})}} = \frac{p_1 p_{i+1} (1 - p_1) (1 - p_{i+1})}{\beta_j} = \beta_j. \quad (49)$$

For $i \in \{2, \ldots, m-1\}$, $j \in \{1, 2, \ldots, m-i\}$, we have

$$r_{i+1,j} = \frac{\text{cov}(X_i, X_{i+j})}{\sqrt{\text{var}(X_i) \text{var}(X_{i+j})}} = \frac{\text{cov}(U_1 \prod_{l=1}^{K_i} Y_{il}, U_{i+j} \prod_{l=1}^{K_{i-j}} Y_{i(l+j)})}{\sqrt{p_1 p_{i+j} (1 - p_1) (1 - p_{i+j})}} = \frac{p_1 p_{i+j} (1 - p_1) (1 - p_{i+j})}{\beta_j} = \beta_j. \quad (50)$$

Here, we have finished the proof.

Due to the increased model complexity, it is difficult to derive the conditions for validity of Algorithm 5 theoretically. However, given marginal probabilities and a general correlation matrix, we can still check whether the binary data can be generated using the algorithm by examining whether all intermediate parameters $\alpha_1, \ldots, \alpha_m$, $\beta_1, \ldots, \beta_km$ lie in the range of $[0, 1]$. 

3. Performance

We implemented and integrated the above mentioned algorithms in an R package CorBin. In this section, we demonstrate the effectiveness and computational efficiency of our package. If a dataset is generated from the desired distribution, the sample mean should converge to the specified marginal probabilities when sample size increases. Meanwhile, the sample correlation matrix should also converge to the specified correlation matrix. Here, we demonstrate the effectiveness of our package by checking the consistency of sample mean and correlation matrix from the generated data. After that, we demonstrate the computational efficiency of our package by calculating the time needed for generating large-scale high-dimensional datasets. We further compare computational time with two commonly used binary data-generation packages: bindata (Leisch, Weingessel, and Hornik 1998) and MultiOrd (Demirtas 2006).

3.1. Effectiveness

To check the consistency of sample mean and correlation matrix, we generate datasets with different sample sizes in which the dimension $m$ is fixed to 100. For sample mean, we use the $l_2$ norm of the difference between the sample mean and the specified marginal probabilities as the error. For correlation matrix, we calculate the Frobenius norm of the residual matrix between sample and desired correlation matrix as the error. We randomly sampled the marginal expectations from a uniform distribution $U(0.5, 0.8)$. The upper bound of correlation coefficients based on the Prentice constraints is $\sqrt{0.5 \times 0.2 / 0.5 \times 0.8} = 0.5$. Then we generated a correlation coefficient from a uniform distribution $U(0, 0.5)$ for exchangeable and AR(1) correlation structures. As the constraints for 1-dependent correlation structures are more stringent, we simulated the correlation coefficient from $U(0, 0.2)$. Although Algorithm 5 can be applied to general cases, randomly generating the correlation coefficients cannot always satisfy the natural restrictions. Thus, we fixed the structures to AR(1), and the settings were the same with simulations of Algorithm 2. For each choice of a sample size $n$ and a correlation structure, we randomly generated 10 sets of $n$ vectors, and calculated the average of errors for each distribution and verify the effectiveness of the algorithms. Figure 3 shows that under the four correlation structures we have considered and a specified general correlation matrix, both errors gradually approached to 0 as sample size increased, indicating that the sample mean and correlation matrix of the generated data converged to the true settings we specified. These results demonstrate the effectiveness of our methods.

In addition, we provide five simple examples to illustrate the constructions of the algorithms and the choices for the parameters for better demonstration. For each scenario, we list out all possible binary vectors that can occur under the particular algorithm, and find the probability that each such vector occurs. Then we verify the algorithm by matching the resulting expected value and correlation structure for the random vector to what is desired. The specified marginal probabilities and the specified correlation for each algorithms are summarized in Table 1. The details of the data generation process for each example are attached in the supplementary materials (Example1-5.csv). In addition, we also provide their reproducing code in the supplementary materials (Example-code.R).

3.2. Computational Efficiency

In this section, we demonstrate the superiority of our package in computational efficiency. All experiments performed here were based on a single processor of an Intel(R) Core(TM) 2.20GHz PC. For comparison, we also considered two commonly used packages bindata and MultiOrd to generate high-dimensional binary data in the experiments.

It is easy to find that all algorithms presented in Section 2.2–2.4 involve only one layer of iterative process. Hence, the time complexity of our algorithms generating binary data with exchangeable, decaying-product and 1-dependent correlation
Table 1. Examples for illustration of the algorithms.

| Algorithm | Structure     | $m$ | $p$              | $R$                          | Supplementary file |
|-----------|---------------|-----|-----------------|------------------------------|--------------------|
| 1         | Exchangeable  | 3   | (0.1, 0.2, 0.3) | $\begin{pmatrix} 1 & 0.3 & 0.3 \\ 0.3 & 1 & 0.3 \\ 0.3 & 0.3 & 1 \end{pmatrix}$ | Example1.csv       |
| 2         | AR(1)         | 3   | (0.1, 0.2, 0.3) | $\begin{pmatrix} 1 & 0.2 & 0.1 \\ 0.2 & 1 & 0.5 \\ 0.1 & 0.5 & 1 \end{pmatrix}$ | Example2.csv       |
| 3         | 1-Dependent   | 3   | (0.80, 0.82, 0.83) | $\begin{pmatrix} 1 & 0.3 & 0 \\ 0.3 & 1 & 0.5 \\ 0 & 0.5 & 1 \end{pmatrix}$ | Example3.csv       |
| 4         | 1-Dependent   | 3   | (0.80, 0.82, 0.83) | $\begin{pmatrix} 1 & 0.3 & 0 \\ 0.3 & 1 & 0.5 \\ 0 & 0.5 & 1 \end{pmatrix}$ | Example4.csv       |
| 5         | Generalized   | 3   | (0.6, 0.7, 0.8)  | $\begin{pmatrix} 1 & 0.3 & 0.1 \\ 0.3 & 1 & 0.2 \\ 0.1 & 0.2 & 1 \end{pmatrix}$ | Example5.csv       |

NOTE: The table summarized specified marginal probabilities and correlation matrices for each example, the details of data generation process for each example were presented in the corresponding file.

Figure 4. The relationship between the computational time (in seconds) and the dimension when simulating binary data using our package. The time is the average of 10 runs.

The calculation efficiency is impressive when generating the high-dimensional binary data. It takes only 0.2, 4.0, and 2.0 sec to generate a $10^6$-dimensional binary data with exchangeable correlation structure, decaying-product and 1-dependent correlation structures, respectively. This dimension scale is too high for other data generation packages, such as bindata and MultiOrd. Table 2 shows the time of different packages for generating binary data in a relative small scale ($m = 100–500$). The time recorded is based on experiments of 10 runs. For data generation with general correlation matrix, our algorithm is still very efficient compared to other packages.

It can be seen from Table 2 and Figure 4, our method CorBin scales linearly with the dimension under three correlation structures and scales quadratically with general correlation matrix. As a comparison, the computational time increases rapidly with the growth of dimensions for the other two packages. Taking the exchangeable correlation structure as an example, it takes bindata around 14.2 sec to generate a 100-dimensional data and 360.3 sec to generate a 500-dimensional data, which is around...
Table 2. Computational times (in seconds) needed for three algorithms under different correlation structures.

| Structure   | m     | CorBin | bindata | MultiOrd |
|-------------|-------|--------|---------|----------|
| Exchangeable ($\rho = 0.5$) | 100   | 2e − 5 (6e − 6) | 14.19 (0.07) | 6.517 (0.06) |
|             | 100   | 4e − 5 (5e − 6) | 57.13 (0.38) | 26.24 (0.63) |
|             | 500   | 8e − 5 (7e − 6) | 360.3 (2.46) | 164.9 (0.47) |
| AR(1) ($\rho = 0.4$) | 100   | 3e − 4 (4e − 5) | 14.36 (0.06) | 5.783 (0.05) |
|             | 200   | 1e − 3 (7e − 5) | 56.27 (0.93) | 18.18 (0.21) |
|             | 500   | 3e − 3 (3e − 4) | 358.3 (2.24) | 123.5 (0.31) |
| 1-Dependent ($\rho = 0.2$) | 100   | 3e − 4 (2e − 5) | 14.30 (0.05) | 5.977 (0.06) |
|             | 200   | 6e − 4 (1e − 4) | 56.83 (0.28) | 18.81 (0.33) |
|             | 500   | 1e − 3 (9e − 5) | 366.2 (3.27) | 112.3 (0.13) |

NOTE: The least time under each condition is highlighted in boldface. Standard deviations are in the bracket.

Figure 5. The relationship between the computational time (in seconds) and the dimension when simulating binary data with general correlation structure using CorBin, bindata, and MultiOrd. The time is the average of 10 runs.

Compared with Lunn and Davies’ method, we generalize the algorithms so that the unequal probability settings can be satisfied. Concretely speaking, Lunn and Davies actually generated clusters of binary variables, and specified fixed the marginal probability and correlation coefficient in each independent cluster. Thus, it is not feasible to specify unequal probabilities in their method. Specifically, for exchangeable correlation structures, we generated each variable by $X_i = (1 - U_i) Y_i + U_i Z$, while Lunn and Davies generated $Y_i \sim \text{Bern}(p)$ and $U_i \sim \text{Bern}(\sqrt{p})$. To generate variables with unequal probabilities, an intuitive way is to simply fix a $\gamma$ and generate $Z \sim \text{Bern}(\gamma)$, and adjust the expectation of $Y_i$ so that the probability of $X_i$ is $p_i$. It is infeasible because there is no way to guarantee the expectation of $Y_i$ exactly lies in $[0, 1]$. A suitable construction of $\gamma$, $\alpha_i$ and $\beta_i$ is important in our algorithm, which can obtain proper $\alpha_i$’s $\in [0, 1]$, and derive the desired result (as proved in Theorems 2.1 and 2.2).

There are still some limitations with our methods. First, our package is applicable only when the correlations are non-negative, because in our algorithms we need to generate some variables following Bernoulli distribution with marginal probabilities related to the correlations. Negative correlations will lead to negative marginal probabilities, making it infeasible to generate corresponding binary vectors. Although in most situations, the capacity to generate binary data with positive correlations will suffice (Preisser and Qaqish 2014), negative correlations may still arise in some special situations. For these situations, Guerra and Shults (2014) proposed an alternative algorithms and uploaded on CRAN for readers to use. Compared with two state-of-the-art binary data generation packages bindata and MultiOrd (Leisch, Weingessel, and Hornik 1998; Demirtas 2006), our algorithms require no complicated numerical procedures such as equation-solving or numerical integration and have linear time complexity with respect to the dimension when generating binary data with common correlation structures, leading to significant improvement in computational efficiency. In our simulations, CorBin needs less than 0.002 sec to generate a $10 \times 1000$-dimensional binary data with exchangeable correlation structure, while generating such data takes more than 14,000 sec and 6400 sec for bindata and MultiOrd, respectively.

4. Discussion and Conclusions

In this article, we have proposed several efficient algorithms to generate high-dimensional correlated binary data with varied marginal expectations and correlation structures. We first focus on three common correlation structures including exchangeable, decaying-product as well as 1-dependent correlation structures, and then generalize the method to $K$-dependent structure and extend the applicability to the general nonnegative correlation matrices. An R package CorBin is also built based on these
way to simulate discrete random vectors with decaying product structure, in which negative correlations are allowed.

We further derived validity conditions for Algorithms 1–4, and surprisingly found that if the Prentice constraints are satisfied, with nonnegative exchangeable and decaying-product structures, our algorithms will be able to generate any specified binary data by using Algorithms 1 and 2. But this is not the case for the K-dependent stationary structure. Therefore, we proposed two algorithms with different validity conditions to generate binary data for K = 1 and an algorithm with K > 1. Our package will automatically select the suitable algorithm according to the input parameters, but an algorithm with more general validity conditions is still needed for K-dependent structure.

Appendix A

Table A.1. The computational time (in sec) consumed in CorBin for generating binary data with different correlation structures.

| m   | 1e + 2 | 1e + 3 | 1e + 4 | 1e + 5 | 1e + 6 |
|-----|--------|--------|--------|--------|--------|
| Exchangeable | 2e − 5 | 2e − 4 | 2e − 3 | 2e − 2 | 2e − 1 |
| (5e − 6) | (5e − 5) | (5e − 4) | (5e − 3) | (5e − 2) |
| AR(1) | 5e − 4 | 3e − 3 | 4e − 2 | 4e − 1 | 4e + 0 |
| (4e − 5) | (7e − 4) | (8e − 3) | (1e − 2) | (1e − 0) |
| 1-Dependent | 2e − 4 | 2e − 3 | 2e − 2 | 2e − 1 | 2e + 0 |
| (2e − 5) | (1e − 4) | (3e − 3) | (2e − 2) | (4e − 2) |

NOTE: The time is the average of 10 runs. Standard deviations are in the brackets.

Supplementary Materials

CorBin: R-package CorBin containing code to implement the algorithms described in the article. (GNU zipped tar file)

CorBin-manual: User manual for R package CorBin. (.pdf file)

Examples: The demonstration data contain five CSV files (Example1-5.csv), corresponding to five examples in described in Section 3.1 (Table A.1), which illustrate the constructions of the algorithms and the choices for the parameters. (.csv file)

Example-code: The reproducing code for demonstration data. (.R file)

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