JMASM3: A Method for Simulating Systems of Correlated Binary Data

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An efficient algorithm is derived for generating systems of correlated binary data. The procedure allows for the specification of all pairwise correlations within each system. Intercorrelations between systems can be specified qualitatively. The procedure requires the simultaneous solution of a system of equations for obtaining the threshold probabilities to generate each system of binary data. A numerical example is provided to demonstrate that the procedure generates correlated binary variables that yield correlations in close agreement with the specified population correlations.

Keywords: Correlated binary variables, Simulation, Uniform random deviates

Introduction

The availability of the desktop computer has made simulation and Monte Carlo techniques widely applicable in statistical research. For example, Monte Carlo methods may be used to compare the small sample properties of a test statistic with its competitors or whether these properties are consistent with the statistic's asymptotic approximation (Headrick & Rotou, 2001). Markov chain Monte Carlo methods (e.g., the Gibbs or slice sampler, Robert & Casella, 1999) are also commonly used to generate posterior distributions to carry out Bayesian analyses. Further, these techniques are now applicable to many areas of research interest. Some examples include: bootstrap tilting (Hesterberg, 2001); conditional logistic regression (Mehta, Patel, & Senchaudhuri, 2000); and likelihood inference with missing data (Gilks, Richardson, & Spiegelhalter, 1998).

There may be occasions when it is desirable to investigate the properties of statistics that involve correlated binary data. Most procedures that generate correlated binary variables are based on an underlying joint distribution that is multivariate normal (e.g., Bahadur, 1961; Emirch & Piedmonte, 1991; Leisch, 2001). This approach presents a problem because correlated binary variables with normal covariance structures may not provide a realistic simulation (Oman & Zucker, 2001). Further, the popular Bahadur (1961) method requires the specification of higher order correlations. These higher order correlations are nuisance parameters that make the Bahadur (1961) procedure arduous (Parzen, Bellamy, Lipsitz, & Fitzmaruice, 2001).

Thus, the purpose of this study is to derive a simple procedure that generates correlated binary variables. The proposed method simulates systems of multivariate binary data using *a priori* specified marginal probabilities and only requires a uniform random number generator.

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Notation and a theoretical derivation of the proposed method are first provided. A numerical example is subsequently worked to demonstrate the procedure. *Mathematica* (Wolfram, Version 4.0, 1999) notebooks are available from the author that simultaneously solves systems of equations that provide the probability threshold points for implementing the procedure. Fortran 77 source code is also provided in the Appendix to demonstrate the algorithm.

Methodology

Let π_i be a pre-specified constant such that $\pi_i \in (0,1)$ and U be a $K \times 1$ vector of uniform random deviates on the interval $(0, 1)$ where $i = 1, ..., T$. Let Y_i represent a $K \times 1$ vector of a sequence of independent Bernoulli trials defined by

$$
Y_1 = \begin{cases} 1 & U_1 < \pi_1 \\ 0 & U_1 > \pi_1 \end{cases} . \tag{1}
$$

It follows that

$$
E[Y_1] = \mu_{Y_1} = \pi_1, \text{ and } \tag{2}
$$

$$
Var[Y_1] = \mu_{Y_1}(1 - \mu_{Y_1}) = \pi_1(1 - \pi_1).
$$
 (3)

For subscripts $i = 2, \ldots, T$, let Y_i represent the *i*th $K \times 1$ vector of binary variables resulting from a sequence of independent trials defmed by

$$
Y_{i} = \begin{cases} Y_{1} & U_{i} < \pi_{i} \\ Y_{1} + 1 & U_{i} > \pi_{i} \text{ and } Y_{1} = 0 \\ 1 - Y_{1} & U_{i} > \pi_{i} \text{ and } Y_{1} = 1 \end{cases}
$$
(4)

Thus, we have

$$
E[Y_i] = \mu_{Y_i} = \pi_1 \pi_i + (1 - \pi_1)(1 - \pi_i), \qquad (5)
$$

$$
E[Y_1 Y_i] = \mu_Y \pi_i = \pi_1 \pi_i \text{, and}
$$
 (6)

$$
Var[Y_i] = \mu_{Y_i} (1 - \mu_{Y_i}), \ \forall_{i>1}.
$$
 (7)

Given the definitions of Y_1 and Y_i in (1) and

(4), let their measure of correlation, denoted as $P_{Y_1Y_i}$, be defined as

$$
\rho_{Y,Y_1} = \frac{\text{Cov} \left[Y_1, Y_1 \right]}{\sqrt{\text{Var}[Y_1]} \sqrt{\text{Var}[Y_1]}}
$$
\n
$$
= \frac{\text{E}[Y_1Y_1] - \text{E}[Y_1]\text{E}[Y_1]}{\left\{ \text{E}[Y_1^2] - \text{E}[Y_1]\right\}^2 \times \text{E}[Y_1^2] - \left\{ \text{E}[Y_1]\right\}^2 \right\}^{1/2}}
$$
\n
$$
= \frac{\text{E}[Y_1Y_1] - \text{E}[Y_1]\text{E}[Y_1]}{\left\{ \text{E}[Y_1](1 - \text{E}[Y_1])(1) \times \text{E}[Y_1](1 - \text{E}[Y_1])(1) \right\}^{1/2}}.
$$
\n(8)

where $E[Y_i^2] = E[Y_i]$ and $E[Y_i^2] = E[Y_i]$ because Y_i and Y_i are binary realizations of either 1 or 0. Substituting equations (2) , (3) , (5) , (6) , and (7) into (8) yields:

$$
\rho_{Y_{i}Y_{i}} = \frac{\pi_{1}\pi_{i} - \mu_{Y_{i}}\mu_{Y_{i}}}{\sqrt{\mu_{Y_{i}}(1 - \mu_{Y_{i}})}\sqrt{\mu_{Y_{i}}(1 - \mu_{Y_{i}})}}
$$
(9)

Given T vectors of Y_i , define X_{ij} as the j-th $K \times 1$ vector of binary variables generated from Y_i as follows:

$$
X_{ij} = \begin{cases} Y_i & U_{ij} < \pi_{ij} \\ Y_i + 1 & U_{ij} > \pi_{ij} \text{ and } Y_i = 0 \\ 1 - Y_i & U_{ij} > \pi_{ij} \text{ and } Y_i = 1 \end{cases}
$$

$$
Var[X_{1k}] = \mu_{X_{1k}}]
$$

$$
Var[X_{1k}] = \mu_{X_{1k}}
$$

 Taking expected

with $j = 1, ..., k, ..., N$ (10)

where the second index
$$
(j)
$$
 runs faster than the first. As such, there are *NT* vectors of X_{ij} . Note that the *NT* vectors of X_{ij} are independent of the *T* vectors of U_i and the constants of π_{ij} are not necessarily equal π_{ij} .

Taking expectations with respect to X_u and the product term of $X_{1i}X_{1k}$ gives

$$
E[X_{1i}] = \mu_{X_{1i}} = \pi_1 \pi_{1i} + (1 - \pi_1)(1 - \pi_{1i}), \qquad (11)
$$

$$
E[X_{1k}] = \mu_{X_{1k}} = \pi_1 \pi_{1k} + (1 - \pi_1)(1 - \pi_{1k}),
$$
\n(12)

$$
E[X_{1j}X_{1k}] = \pi_1 \pi_{1j} \pi_{1k} + (1 - \pi_1)(1 - \pi_{1j})(1 - \pi_{1k}), \qquad (13)
$$

and hence

$$
Var[X_{1j}] = \mu_{X_{1j}}(1 - \mu_{X_{1j}}), \qquad (14)
$$

$$
Var[X_{1k}] = \mu_{X_{1k}} (1 - \mu_{X_{1k}}). \tag{15}
$$

tions with respect to X_{ij} and the product term $X_{ii}X_{ik}$ for $i = 2,...,T$ yields

$$
E[X_{ij}] = \mu_{X_{ij}} = \pi_{ij}(\pi_1 \pi_i + (1 - \pi_1)(1 - \pi_i)) + (1 - \pi_{ij})(1 - (\pi_1 \pi_i + (1 - \pi_1)(1 - \pi_i)))
$$
\n(16)

$$
E[X_{ik}] = \mu_{X_{ik}} = \pi_{ik}(\pi_1 \pi_i + (1 - \pi_1)(1 - \pi_i)) + (1 - \pi_{ik})(1 - (\pi_1 \pi_i + (1 - \pi_1)(1 - \pi_i)))
$$
\n(17)

$$
E[X_{ij}X_{ik}] = \pi_{ij}\pi_{ik}(\pi_i\pi_i + (1 - \pi_1)(1 - \pi_i)) + (1 - \pi_{ij})(1 - \pi_{ik})(1 - (\pi_i\pi_i + (1 - \pi_1)(1 - \pi_i)))
$$
\n(18)

$$
Var[X_{ij}] = \mu_{X_{ij}} (1 - \mu_{X_{ij}}), \text{ and} \tag{19}
$$

$$
Var[X_{ik}] = \mu_{X_{ik}} (1 - \mu_{X_{ik}}). \tag{20}
$$

The correlations $\rho_{X_{1j}X_{1k}}$ and $\rho_{X_{ij}X_{ik}}$ can be determined by substituting the expressions in (11) through (15) and (16) through (20) into analogous definitions of (8) expressed in terms of the X_{ii} .

Given specified constants of π , an efficient number of correlated X_{ii} vectors for each integer of $i = 1$, the

selection of $N = 3$ yields a system of three equations (for three pairwise correlations $\rho_{X_{11}X_{12}}$, $\rho_{X_{11}X_{13}}$, $\rho_{X_{12}X_{13}}$) solvable in terms of three unknowns (probability threshold points of π_{11} , π_{12} , π_{13}). This system is constructed by first substituting the right-hand sides of (11) and (12) into (14) and (15) . Subsequently substituting (11) through (15) into three equations of the form in (8) yields

$$
\rho_{X_{11}X_{12}} =
$$

$$
\frac{\left[\pi_1\pi_{11}\pi_{12} + (1-\pi_1)(1-\pi_{11})(1-\pi_{12})\right] - \left[\pi_1\pi_{11} + (1-\pi_1)(1-\pi_{11})\right]\left[\pi_1\pi_{12} + (1-\pi_1)(1-\pi_{12})\right]}{\sqrt{\left[\pi_1\pi_{11} + (1-\pi_1)(1-\pi_{11})\right]\left(1 - \left[\pi_1\pi_{11} + (1-\pi_1)(1-\pi_{11})\right]\right)\sqrt{\left[\pi_1\pi_{12} + (1-\pi_1)(1-\pi_{12})\right]\left(1 - \left[\pi_1\pi_{12} + (1-\pi_1)(1-\pi_{12})\right]\right]}}}
$$
(21)

 $\rho_{x_{11}x_{13}} =$

$$
\frac{\left[\pi_1\pi_{11}\pi_{13} + (1-\pi_1)(1-\pi_{11})(1-\pi_{13})\right] - \left[\pi_1\pi_{11} + (1-\pi_1)(1-\pi_{11})\right]\left[\pi_1\pi_{13} + (1-\pi_1)(1-\pi_{13})\right]}{\sqrt{\left[\pi_1\pi_{11} + (1-\pi_1)(1-\pi_{11})(1-\pi_1\pi_{11} + (1-\pi_1)(1-\pi_{11}))\right]\sqrt{\left[\pi_1\pi_{13} + (1-\pi_1)(1-\pi_{13})\right]\left[1-\left[\pi_1\pi_{13} + (1-\pi_1)(1-\pi_{13})\right]\right]}}\n\tag{22}
$$

 $\rho_{\scriptscriptstyle X_{12}X_{13}}$

$$
\frac{\left[\pi_1\pi_{12}\pi_{13} + (1-\pi_1)(1-\pi_{12})(1-\pi_{13})\right] - \left[\pi_1\pi_{12} + (1-\pi_1)(1-\pi_{12})\right]\left[\pi_1\pi_{13} + (1-\pi_1)(1-\pi_{13})\right]}{\sqrt{\left[\pi_1\pi_{12} + (1-\pi_1)(1-\pi_{12})\right]\left(1-\left[\pi_1\pi_{13} + (1-\pi_1)(1-\pi_{12})\right]\right)\sqrt{\left[\pi_1\pi_{13} + (1-\pi_1)(1-\pi_{13})\right]\left(1-\left[\pi_1\pi_{13} + (1-\pi_1)(1-\pi_{13})\right]\right)}}}
$$
\n(23)

Specifying π_1 and selecting positive values for ρ_{X_1, X_2} , ρ_{X_1, X_3} , and ρ_{X_1, X_4} in (21), (22), and (23) and then simultaneously solving these equations gives the probability threshold points of π_{11} , π_{12} , π_{13} to generate X_{11} , X_{12} , and X_{13} with the desired intercorrelations for (10). Systems of equations analogous to (21), (22), and (23) can be created in the same manner for all $i = 2, \ldots, T$ from equations (16) through (20). As such, 3T vectors of X_i can be generated with three positive pairwise correlations within each system

Without loss of generality, feasible solutions (i.e., $0 \leq \pi_{ii} \leq 1$) are obtainable provided that the following conditions hold with respect to the left-hand sides of(21), (22), and (23)

$$
\frac{(\rho_{X_{11}X_{12}})(\rho_{X_{11}X_{13}})}{(\rho_{X_{12}X_{13}})} \le 1,
$$
\n(24a)

$$
\frac{(\rho_{x_1, x_2})(\rho_{x_1, x_3})}{(\rho_{x_1, x_3})} \le 1, \text{ and}
$$
 (24b)

$$
\frac{(\rho_{X_{11}X_{13}})(\rho_{X_{12}X_{13}})}{(\rho_{X_{11}X_{12}})} \le 1.
$$
 (24c)

These conditions must also hold with respect to the other *T -* 1 systems of equations.

Because all Y_i for $i = 2, ..., T$ are a function of Y_i from (4), intercorrelations between X_i belonging to *different* systems may also exist and can be analytically determined as follows:

$$
\rho_{X_{ij}X_{jj}} = (\rho_{X_{ij}Y_i}) (\rho_{Y_iY_j}) (\rho_{Y_jX_{jj}}). \qquad (25)
$$

Further, and by inspection of (5) and (9), correlations in equation (25) may be negative, zero, or positive. Specifically, correlations are respectively negative, zero, or positive when π_i < 0.5, π_i = 0.5, or π_i > 0.5 in equation (9) for all $i = 2, ..., T$. Note that the correlations ρ_{X_i,Y_i} and ρ_{Y_i,X_j} in (2.5) are derived analogously as $(21), \ldots, (23)$ from (8) .

Numerical Example

Suppose it is desired to generate two systems of correlated binary data with correlations $P_{X_{11}X_{12}} = 0.40$, $\rho_{X_{11}X_{13}} = 0.50$, $\rho_{X_{12}X_{13}} = 0.60$; and $\rho_{X_{21}X_{22}} = 0.75$, $P_{X_{21}X_{23}} = 0.80$, $P_{X_{22}X_{23}} = 0.90$ and where the variables between the systems are inversely related. The following steps are taken:

1. Ensure that three pairwise intercorrelations within the systems satisfy (24a), (24b), and (24c).

2. Specify values for π_1 and π_2 . Let $\pi_1 = 0.90$ and let $\pi_2 = 0.10$ to obtain the inverse relationships between the two systems.

3. Simultaneously solve the two systems of the form in

(21), (22) and (23) given the specified correlations and values of π_1 and π_2 . The numerical equation solver FindRoot *(Mathematica,* 1999) yields solutions of $\pi_{11} = 0.881247$, $\pi_{12} = 0.924095$, $\pi_{13} = 0.97245$ $\pi_{21} = 0.939341$, $\pi_{22} = 0.974722$, and $\pi_{23} = 0.993961$.

4. Use equation (25) to determine the correlations between the variables of the two systems. The correlations are: $\rho_{X_1|X_2} = -0.294484$, $\rho_{X_1|X_2} = -0.331295$, $\rho_{X_1|X_2} = -0.331295$ 0.353381, $\rho_{X_{12}X_{21}} = -0.353381, \ \rho_{X_{12}X_{22}} = -0.397554,$ $\rho_{X_{12}X_{23}} = -0.424057$, $\rho_{X_{13}X_{21}} = -0.441726$, $\rho_{X_{13}X_{22}} = -$ 0.496942, and $\rho_{X_{13}X_{23}} = -0.530071$.

5. Given the parameters and solutions from steps 2 and 3, generate the correlated binary data. Fortran 77 source code is presented in the Appendix to implement this example. Presented in Table 1 are population correlations and computed correlations for both within and between the two systems described in steps 1 and 4. Single samples of binary data with $K = 5000$ were generated for each of the six variables as described in step 5. Inspection of Table 1 indicates that the proposed method generated correlated binary data that yielded computed correlations that were in close agreement with the population correlations.

Conclusion

As previously mentioned the systems of equations of the form in (21), (22), and (23) solve for the probability threshold points (π_{ij}) for only positive correlations. However, it may be desirable to generate binary data with negative correlations. This can be accomplished by writing additional *if-else* structure statements in the Fortran 77 source code that simultaneously reversing the 1's and O's within each selected vector. Such reversals will allow for the construction of negative correlations within the system(s).

More specifically, suppose that it was desired that $\rho_{X_1|X_2} = -0.40$, and $\rho_{X_1|X_2} = -0.50$ in the numerical example. This can be accomplished by simultaneously reversing the 1's and 0's in the vectors X_{12} , and X_{13} . It should be noted that these changes would also create positive correlations between the systems of: $\rho_{x_1,x_2} = 0.353381$, $\rho_{X_{12}X_{22}} = 0.397554, \rho_{X_{12}X_{23}} = 0.424057, \rho_{X_{13}X_{21}} = 0.441726,$ $\rho_{X_{13}X_{22}} = 0.496942$, and $\rho_{X_{13}X_{23}} = 0.530071$.

It should also be pointed out that as the sample sizes become smaller the probability increases of obtaining vectors of either all 1's or all O's (i.e., standard deviations of zero). Thus, one way to circumvent this problem in a larger simulation would be to initialize the correlation computed in the subroutine (e.g., PCOR in the Appendix) to zero when either standard deviation is zero and

JMASM3: SIMULATING CORRELATED BINARY DATA (FORTRAN 77)

\cdots are the policies of called complete of called the System 1		System ₂	
Variables: X_{11} , X_{12} , X_{13}		Variables: X_{21} , X_{22} , X_{23}	
Pop. Correlations Within System 1	Computed Correlations	Pop. Correlations Within System 2	Computed Correlations
$\rho_{x_{11}x_{12}} = 0.40$	0.400780	$\rho_{x_{21}x_{22}} = 0.75$	0.745030
$\rho_{x_{11}x_{13}} = 0.50$	0.503307	$\rho_{\scriptscriptstyle X_{2l} \scriptscriptstyle X_{23}}=0.80$	0.790314
$\rho_{x_{12}x_{13}} = 0.60$	0.591606	$\rho_{x_{\rm n} x_{\rm n}}=0.90$	0.893551
Population Correlations		Computed Correlations	
Between System 1 and System 2			
$\rho_{x_{11}x_{21}} = -0.294484$		-0.290305	
$\rho_{x_{11}x_{22}} = -0.331295$		-0.330829	
$\rho_{x_{11}x_{22}} = -0.353381$		-0.351456	
$\rho_{X_{12}X_{21}} = -0.353381$		-0.347825	
$\rho_{x_{12}x_{22}} = -0.397554$		-0.390941	
$\rho_{x_{12}x_{23}} = -0.424057$		-0.407341	
$\rho_{X_{13}X_{21}} = -0.441726$		-0.449708	
$\rho_{x_{13}x_{22}} = -0.496942$		-0.504316	
$\rho_{x_{13}x_{23}} = -0.530071$		-0.526768	

Table 1. Two systems of correlated binary data generated using the Fortran source code provided in the Appendix. A single sample of size $K = 5000$ was drawn for each of the six variables.

keep count of the zero correlations throughout the simulation. Thus, the total real number of replications could be computed by subtracting the number of times a zero correlation occurs due to standard deviations of zero (e.g., 50 occurrences) from the initialized total number of replications (e.g. 10,000). That is, the total real number of replications would be 9950.

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APPENDIX

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10 CONTINUE

PROGRAM BINARY REAL *YI(5000), Y2(5000),* Xl *1(5000),* Xl 2(5000), XI3(5000), *X21(5000), X22(5000),* X23(5000), UI(SOOO),*U2(SOOO),*UII(SOOO), UI2(5000), UI3(5000), U2 1*(5000),* U22(5000), U23(5000), PI, P2, PII, P12, P13, P21, P22, P23, R112, RIl3, R123, R212, R213, R223, R1211, R1212, R1213, R1221, R1222, R1223, R1231, R1232, Rl233 INTEGERI,K DOUBLE PRECISION DSEEDI, PSEED2, DSEED3, DSEED4, DSEEDS, DSEED6, DSEED7, DSEED8 READ (.,.) K, PI, P2, PII, P12, P13, P21, P22, P23 .
The shortest started that the started of the started started by the started started started started that the started C··· . C INITIALIZE DSEED(I.8) AND CALL UNII TO GENERATE ARRAYS OF UI, U2, UII, C U12, U13, U21, U22, U23 C··· . CALL UNII (DSEEDI, K, UI) C··········~·························~················ . C CREATE CALL UNI1 STATEMENTS FOR U2,...,U23

CILLIALITY IN INTERFERENT PRODUCTS OF USE OF THE EXAMPLE AND INTERFERENT PRODUCTS. C···•................... DO 10 $I = 1, K$ IF ($UI(I)$.LE. $P1$) THEN $Y1(II) = 1.0$ ELSE IF $($ U1 (I) .GE. P1) THEN $Y1(I) = 0.0$ ENDIF IF ($U2(I)$.LE. P2) THEN $Y2(I) = Y1(I)$ ELSE IF (U2(I) \cdot GE. P2 \cdot AND. Y1(I) \cdot EQ. 0) THEN $Y2(I)=Y1(I) + 1$ ELSE IF (U2(I) \overline{AB} . GE, P2 \overline{AND} . Y1(I) \overline{EQ} . 1) THEN $Y2(I)=Y2(I) - 1$ ENDIF IF $($ U11 (I) .LE. P11 $)$ THEN $X11(II)=Y1(II)$ ELSE IF (U11(I) \overline{AB} . GE. P11 .AND. Y1(I) \overline{B} . EQ. 0) THEN $X11(I)=Y1(I) + 1$ ELSE IF (U11(I) \overline{AB} . GE. P11 \overline{AND} . Y1(I) \overline{EQ} . 1) THEN $X11(1)=Y1(1)-1$ **ENDIF** C··· . C CREATE IF-TIIEN STRVCTIJRESTO GENERATE VECTORS X12 AND X13 FROM Yl. C···• IF($U21(I)$.LE. P21) THEN $X21(I)=Y2(I)$ ELSE IF (U21(I) .GE. P21 .AND. Y2(I) .EQ. 0) THEN $X21(I)=Y2(I) + 1$ ELSE IF (U21(I) .GE. P21 .AND. Y2(I) .EQ. 1) TIIEN $X21(I)=Y2(I) -1$ ENDIF C··· . C CREATE IF.-TIIEN STRUCTURES TO GENERATE VECTORS X22 AND X23 FROM Y2. c··· .

c··· .

C CALL PCOR TO COMPUfE TIlE CORRELATIONS

c··· •.......•............... CALL PCOR (XII, XI2, K, RII2) CALLPCOR (XII, X13, K, Rl13) CALL PCOR (XI2, X13, K, R123) CALL PCOR (X21, X22, K, R212) CALL PCOR (X2I, X23, K, R213) CALL PCOR (X22, X23, K, R223) CALL PCOR (XII, X2I, K, RI2II) CALL PCOR (XII, X22, K, RI212) CALL PCOR (XII, X23, K, RI2l3) CALL PCOR (XI2, X2I, K, R122I) CALL PCOR (XI2, X22, K, R1222) CALL PCOR (X12, X23, K, RI223) CALL PCOR (X13, X21, K, R1231) CALL PCOR (Xl3, X22, K, RI232) CALL PCOR (X13, X23, K, R1233) STOP

END