

Minimum correlation in construction of multivariate distributions

Vanja M. Dukic

Department of Applied Mathematics, University of Colorado, Boulder, Colorado 80309, USA

Nevena Marić

Department of Mathematics and Computer Science, University of Missouri–St. Louis, St. Louis, Missouri 63121, USA

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In this paper we present an algorithm for exact generation of multivariate samples with prespecified marginal distributions and a given correlation matrix, based on a mixture of Fréchet-Hoeffding bounds and marginal products. In the bivariate case, the algorithm can accommodate any among the theoretically possible correlation coefficients, and explicitly provides a connection between simulation and the minimum correlation attainable for different distribution families. We calculate the minimum correlations in several common distributional examples, including in some that have not been looked at before. As an illustration, we provide the details and results of implementing the algorithm for generating three-dimensional negatively and positively correlated Beta random variables, making it the only noncopula algorithm for correlated Beta simulation in dimensions greater than two. This work has potential for impact in a variety of fields where simulation of multivariate stochastic components is desired.

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I. INTRODUCTION

The original question of generating multivariate probability distributions with prespecified margins has a long history, dating in part back to the work of Wigner [1] on thermodynamic equilibria. The general form of the problem was studied by Fréchet [2] and Hoeffding [3] in a body of work which grew out of the problem originally posed by Lévy [4]. Today, this work falls under the scope of Fréchet-Hoeffding classes. An excellent overview of the developments in this field can be found in Dall’Aglia *et al.* [5], Rüschendorf *et al.* [6], and Conway [7].

Today, algorithms for generation of correlated random variables with prespecified marginal distributions play an important role in simulation of stochastic processes and hybrid deterministic-stochastic systems. Such algorithms are encountered in a variety of fields—for example, statistics and applied probability [8–11], finance [12], environmental science [13], physics [14], engineering [15], and ecology where “demographic” or “weather” stochasticity is an increasingly more relevant component of species dynamics [16]. Much of the development of these algorithms has so far relied on coupling ideas—or antithetic coupling for negatively-correlated variables [17]—and copula-based methods [18,19].

Copula methods, in particular, have recently become widely used in generation of samples from multivariate distributions with prespecified marginals and a dependency function [19]. Copula methodology relies on the results of Sklar [18] who proved that a multivariate distribution can be characterized (uniquely in the case of continuous distributions) by the set of its marginal distributions and a “copula” function which describes the dependence between the components. The dependence among the original variables is then translated, via the copula function, into the dependence on the scale of uniform random variables. Consequently, the entire desired multivariate distribution is obtained via a transformation of these correlated uniform variables. Unfortunately, the correlation is not preserved under these transformations, and the sampling is not exact.

In this paper we present an alternative algorithm that generates *exact* multivariate samples with prespecified marginals

and a given correlation matrix. We note that specifying marginal distributions and a correlation matrix is in general not enough to completely determine the entire multivariate distribution. Nonetheless, specifying marginal distributions and a set of linear relationships (through a set of correlation coefficients) among the random variables is frequently done, perhaps due to the strong intuitiveness of the linear relationship.

The algorithm can be used for generating a realization of a set of random variables X_1, X_2, \dots, X_I such that each variable X_i has a specified marginal distribution F_i , and such that each pairwise correlation coefficient $\text{cor}(X_i, X_j)$ equals some set value ρ_{ij} . We take the correlation coefficient between two random variables X_i and X_j to be defined as

$$\text{cor}(X_i, X_j) = \frac{\text{cov}(X_i, X_j)}{\sigma_{X_i} \sigma_{X_j}},$$

where $\text{cov}(X_i, X_j)$ stands for covariance between X_i and X_j .

The paper is organized as follows: Section II introduces the basic idea of the algorithm, which allows for fast simulation and can accommodate any among the theoretically plausible correlation ranges. We discuss its implementation and performance, and present detailed examples for several bivariate distribution families (uniform, arcsine, Weibull, exponential, Erlang, Beta, and Gaussian) in Sec. II B. We also calculate the minimal correlations (or *maximum negative* correlations as they are called in Kotz *et al.* [20]) for these distributions, including some that have not been obtained before. In Sec. III we present a multivariate extension of the algorithm. Finally, Sec. IV concludes the paper with a brief summary of benefits and limitations of the proposed approach.

II. THE ALGORITHM FOR GENERATING BIVARIATE SAMPLES FROM PRESCRIBED MARGINALS WITH SPECIFIED CORRELATION

Perhaps not surprisingly, over the years the problem of generating bivariate distributions with fixed marginals and a specified correlation coefficient has gotten more attention from the simulation communities (e.g., [21]) than from the

probability community [22]. A notable exception is a work by Johnson and Tenenbein [23], who provide a bivariate generation algorithm based on a method different from the one presented in this paper. Moreover, bivariate distributions have been studied mostly for marginals with common distributional form, such as the normal, exponential, or Gamma (see, e.g., [20]). The case of exponential marginals is particularly well studied; however, providing a constructive algorithm that can produce all theoretically possible correlation coefficients still proved to be a significant theoretical advance [24]. For general marginals, Michael and Schucany [25] introduced a mixture-density based (hierarchical) approach, although this algorithm relies on finding a feasible mixture density for each example, which need not always be straightforward.

Trivariate reduction methods were introduced initially for construction of dependent Gamma random variable pairs (see, for example, [10,26,27]), as an alternative to once computationally costly *distribution inversion* based methods. The trivariate reduction idea relies on the use of three independent variables in order to obtain one pair of correlated variables. However, these methods are limited to additive families of distributions, such as Gamma or Poisson. The algorithm we present here will not have that limitation.

The algorithm in this paper is a hybrid version of the trivariate reduction method, as it relies on three uniformly distributed random variables to produce a pair, but it is not inversion-free. It is based on the following reasoning: With a certain probability we use the same source of randomness in the construction of the pair, and two independent sources otherwise. The probability used to determine which source is used will be closely related to the correlation coefficient.

To set notation, let F and G be cumulative distribution functions (CDFs) with finite positive variances, and let X and Y be random variables with distributions F and G , respectively, $X \sim F$ and $Y \sim G$. The first question to be asked is whether *any correlation* $\rho \in [-1, 1]$ can be attained for the pair (X, Y) . The answer to that question is negative, and dates back to the work of Hoeffding [3] and Fréchet [2], where the concept of *extremal distributions* was originally introduced: If we let $\Pi(F, G)$ be the set of all bivariate CDFs having F and G as marginals, then among the elements of $\Pi(F, G)$, there are CDFs H^* and H_* which have maximum and minimum correlation coefficient (ρ^* and ρ_*), respectively. Such extremal distributions are also called (upper and lower) *Fréchet-Hoeffding bounds*. They were later characterized by Whitt [28] who provides the following two equivalent statements.

Theorem 1 (Hoeffding [3]). For any F and G with finite positive variances,

$$H^*(x, y) = \min\{F(x), G(y)\},$$

$$H_*(x, y) = \max\{0, [F(x) + G(y) - 1]\},$$

for all $(x, y) \in \mathbb{R}^2$.

Theorem 2 (Hoeffding [3]). For any F and G with finite positive variances,

$$(F^{-1}(U), G^{-1}(U)) \text{ has CDF } H^*$$

$$\text{and } (F^{-1}(U), G^{-1}(1 - U)) \text{ has CDF } H_*,$$

where U has uniform distribution on $[0, 1]$ and F^{-1} and G^{-1} are inverse distribution functions, defined as $F^{-1}(y) = \inf\{x : F(x) \geq y\}$, and $G^{-1}(y) = \inf\{x : G(x) \geq y\}$, respectively.

Fréchet [2] suggested that any system of bivariate distributions with specified marginals F and G should include H_* and H^* as limiting cases [20]. The crux of our algorithm is precisely in this reasoning, as we construct multivariate distributions through careful blending of Fréchet-Hoeffding bounds and marginal products. This blending, although clearly apparent in the bivariate case, becomes less obvious in dimensions greater than two and in the presence of negative correlations.

A. The basics: Bivariate algorithm

Suppose F and G are desired marginal distributions, with finite positive variances. Then the main bivariate problem can be stated as follows: Construct X and Y such that $X \sim F$, $Y \sim G$, and correlation $\text{cor}(X, Y) = \rho$. Here, $\rho \in [\rho_*, \rho^*]$, where ρ_* and ρ^* are minimum and maximum theoretically possible correlation coefficients, respectively.

Let m_F, σ_F and m_G, σ_G be the first moments and standard deviations corresponding to F and G , respectively. Let ϕ be an algorithm such that $\phi(U) \sim F$, and let ψ be an algorithm such that $\psi(U) \sim G$, where U is a uniformly distributed random variable on $[0, 1]$. (It can be assumed, although it is not necessary, that $\phi = F^{-1}$ and $\psi = G^{-1}$). Let V also be a uniform random variable on $[0, 1]$ and define

$$c^{\phi, \psi}(U, V) = \frac{E[\phi(U)\psi(V)] - m_F m_G}{\sigma_F \sigma_G}, \quad (1)$$

where $E[\cdot]$ is used to denote the expected value of a random variable. To simplify notation, we will denote $c^{\phi, \psi}$ as c^ϕ . Also, observe that $c^\phi(U, U) = [E(X^2) - m_F^2]/\sigma_F^2 = 1$, for $X = \phi(U) \sim F$.

The following construction, presented as Algorithm 1 below, will yield a pair of variables (X, Y) , such that $X \sim F$, $Y \sim G$, and $\text{cor}(X, Y) = \rho$ for $\rho \in [\rho_*, \rho^*]$.

ALGORITHM 1: Construction of two random variables with prescribed marginal distributions F, G and correlation coefficient ρ .

```

1: sample  $U, V, W \sim U(0, 1)$ , independently
2: let  $X = \phi(U)$ 
3: if  $\rho > 0$  then
4:   let  $U' = U$ .
5: else
6:   let  $U' = 1 - U$ .
7: end if
8: if  $W < \rho / c^{\phi, \psi}(U, U')$  then
9:   let  $Y = \psi(U')$ 
10: else
11:   let  $Y = \psi(V)$ 
12: end if
13: RETURN  $(X, Y)$ 

```

Theorem 3. If (X, Y) is generated by Algorithm 1, then
(a) $X \sim F$, $Y \sim G$, and $\text{cor}(X, Y) = \rho$, if $\rho / c^{\phi, \psi}(U, U') \leq 1$.
(b) If $\phi = F^{-1}$, $\psi = G^{-1}$, then

(i) (X, Y) has the joint distribution $H(x, y)$, where

$$\begin{aligned} \text{for } \rho \geq 0 : H(x, y) &= \frac{\rho}{\rho^*} H^*(x, y) + \left(1 - \frac{\rho}{\rho^*}\right) F(x)G(y); \\ \text{for } \rho \leq 0 : H(x, y) &= \frac{\rho}{\rho_*} H_*(x, y) + \left(1 - \frac{\rho}{\rho_*}\right) F(x)G(y). \end{aligned}$$

(ii) Algorithm 1 is applicable for all $\rho_* \leq \rho \leq \rho^*$.

Proof: (a) By construction, $X \sim F$, $Y \sim G$. Using $\mathbf{1}(\cdot)$ to denote the indicator function, $E[\cdot]$ to denote expected value of a random quantity, and c in the place of $\rho/c^{\phi, \psi}(U, U')$, we have

$$\begin{aligned} E[XY] &= E[XY\mathbf{1}(W < c)] + E[XY\mathbf{1}(W > c)] \\ &= E[\phi(U)\psi(U')\mathbf{1}(W < c)] + E[\phi(U)\psi(V)\mathbf{1}(W > c)] \\ (U, V, W \text{ independent}) & \\ &= P(W < c)E[\phi(U)\psi(U')] + P(W > c)E\phi(U)E\psi(V) \\ &= cE[\phi(U)\psi(U')] + (1 - c)m_F m_G \\ &= c(E[\phi(U)\psi(U')] - m_F m_G) + m_F m_G. \end{aligned}$$

Then, from (1), it follows that $\text{cor}(X, Y) = \rho$. Observe also that when ϕ and ψ are nondecreasing functions, $\text{cov}(\phi(U), \psi(U))$ is always positive, while $\text{cov}(\phi(U), \psi(1 - U))$ is always negative. This can be verified easily using a coupling argument as in [17]. Inverse distribution functions $\phi = F^{-1}$, $\psi = G^{-1}$ are of course nondecreasing.

(b) For positive ρ , Algorithm 1 produces $(F^{-1}(U), G^{-1}(U))$ with probability $\rho/c^{F^{-1}, G^{-1}}(U, U)$. By Theorem 2, the pair $(F^{-1}(U), G^{-1}(U))$ has the CDF $H^*(x, y)$. With probability $1 - \rho/c^{F^{-1}, G^{-1}}(U, U)$, the outcome of Algorithm 1 is a pair of two independent variables $(F^{-1}(U), G^{-1}(V))$, with the CDF that is a product of the marginal CDFs $F(x)G(y)$. The argument works analogously for negative values of ρ .

When $\rho > 0$, by Theorem 2, the maximum correlation between F and G is attained with the coupling $(F^{-1}(U), G^{-1}(U))$, so that

$$\rho^* = \frac{E[F^{-1}(U)G^{-1}(U)] - m_F m_G}{\sigma_F \sigma_G} = c^{F^{-1}, G^{-1}}(U, U). \quad (2)$$

It follows that $\rho/c^{F^{-1}, G^{-1}}(U, U) \leq 1 \Leftrightarrow \rho \leq \rho^*$.

When $\rho < 0$, we again have, by Theorem 2, that the minimal correlation between F and G is attained with the coupling $(F^{-1}(U), G^{-1}(1 - U))$, and that then

$$\begin{aligned} \rho_* &= \frac{E[F^{-1}(U)G^{-1}(1 - U)] - m_F m_G}{\sigma_F \sigma_G} \\ &= c^{F^{-1}, G^{-1}}(U, 1 - U). \end{aligned} \quad (3)$$

In this case it follows that $\rho/c^{F^{-1}, G^{-1}}(U, 1 - U) \leq 1 \Leftrightarrow \rho \geq \rho_*$. As noted in the last paragraph of the proof of part (a), since $\phi = F^{-1}$, $\psi = G^{-1}$, we have that $\rho^* > 0$ and $\rho_* < 0$. Therefore the algorithm works for the entire range of possible correlations between F and G . ■

Remark. Note that we allow a possibility that ϕ and ψ are not inverse distribution functions, because the main idea of the algorithm is applicable to transformations that are not inverse

distribution functions. We will present Algorithm 4 in Sec. III as an example of using such transformations.

B. Examples: Finding minimum correlations

We now illustrate the implementation of Algorithm 1 using several common distributions as examples. We will assume identical marginal distributions, $F = G$, and that ϕ denotes an inverse distribution function in each case below. Since the correlation coefficient is not preserved under inverse distribution transformation—namely, in general $\text{cor}(F^{-1}(U), F^{-1}(V)) \neq \text{cor}(U, V)$ —the range of possible correlations for any individual distribution has to be derived separately. Once the range of feasible correlations is known, application of Algorithm 1 is very simple and requires only few lines of code.

It should be noted that determination of minimum (and maximum) possible correlation among two distributions has had a theoretical value in its own right. At the same time it is also of practical value, as knowing the maximum and minimum correlations allows us to place the correlation estimates in perspective, which is of great importance in empirical data analysis. Moran [29] showed that only symmetric bivariate distributions for which there exist η_0 and η_1 such that $\eta_0 + \eta_1 Y$ has the same distribution as X allow ρ to take any value in the entire range $[-1, 1]$. Some ranges for correlation coefficients for bivariate distributional families are provided in [7]; however, many ranges still remain to be computed.

When the marginals are equal, maximum correlation $\rho^* = 1$ since $\text{cor}(X, X) = 1$, and only ρ_* has to be determined. We present briefly several examples and derive the minimum correlation for each case. The first two cases, the uniform and arcsine, easily follow from Moran [29], so we show them only as illustrations.

(1) *Uniform.* In the case of uniform distribution on $[0, 1]$, we have that $\phi(U) = U$ and

$$\rho_* = \frac{E(U(1 - U)) - [E(U)]^2}{\text{Var}(U)} = \frac{1/6 - 1/4}{1/12} = -1.$$

(2) *Arcsine.* In the case of the arcsine distribution with density $1/(\pi\sqrt{1 - x^2})$ on $[-1, 1]$, $\phi(U) = \cos(\pi U)$ [22]. As the mean of this density is 0 and variance $1/2$, it follows that

$$\begin{aligned} \int_0^1 \cos(\pi x) \cos \pi(1 - x) dx &= \int_0^1 \cos^2(\pi x) dx \\ &= \frac{1}{2} \int_0^1 1 + \cos(2\pi x) dx = \frac{1}{2}. \end{aligned}$$

From here $\rho_* = -1$, and that the algorithm is applicable for all $\rho \in [-1, 1]$.

(3) *Exponential.* If the variables are exponentially distributed with mean 1 (density e^{-x}) then $\phi(U) = -\ln(U)$ and $\rho_* = 1 - \pi^2/6 \approx -0.6449$, since

$$E[\phi(U)\phi(1 - U)] = \int_0^1 \ln(x) \ln(1 - x) dx = 2 - \frac{1}{6}\pi^2.$$

The above integral can be solved using Maclaurin series representation of $\ln(x)$, using either double or single series, and we present this proof in the Appendix.

TABLE I. Minimal correlation of a bivariate distribution with marginals distributed as Weibull(k), for different values of parameter k .

k	4	3	2	1	0.9	0.8	0.5
ρ_*	-0.999	-0.996	-0.947	-0.645	-0.574	-0.492	-0.193

Consequently, since $S \sim \exp(\lambda)$ (for $\lambda > 0$) can be obtained as λT where $T \sim \exp(1)$, the same range of attainable correlation $\rho \geq \rho_* = 1 - \pi^2/6$ is valid for any choice of marginal exponential distribution. It is worth noting that many different bivariate exponential distribution algorithms have been studied, including a classic example by Gumbel [30] and many others mentioned in [20]. Another recent construction of bivariate exponential distribution that allows an arbitrary positive or negative correlation coefficient has been introduced by [24]. They use an elegant concept of multivariate phase-type distributions, and provide a constructive algorithm that achieves minimum correlation ρ_* through a limit of a sequence.

(4) *Erlang*. As a $\text{Gamma}(n, \lambda)$ distribution where n is an integer, an $\text{Erlang}(n, \lambda)$ random variable (density $x^{n-1}e^{-x/\lambda}/[(n-1)!\lambda^n]$) can be obtained as a sum of n independent exponential random variables with parameter λ . Let $(S_1^1, S_1^2), (S_2^1, S_2^2), \dots, (S_n^1, S_n^2)$ be n independent outputs of Algorithm 1, where each variable in the pair has an exponential marginal distribution (with parameter λ), and where $\text{cor}(S_i^1, S_i^2) = \rho$, for $i = 1, \dots, n$. (Notice also that for $j \neq i$, S_i^1 and S_j^1 are independent, as are S_i^1 and S_j^2 .) Let $X = S_1^1 + \dots + S_n^1$ and $Y = S_1^2 + \dots + S_n^2$. Then $X, Y \sim \text{Gamma}(n, \lambda)$ and $\text{cor}(X, Y) = \rho$. It follows that the minimal possible correlation of X and Y is $1 - \pi^2/6 \approx -0.6449$.

(5) *Weibull*. The Weibull distribution with density $kx^{k-1}e^{-x^k}$, for $x \geq 0$, and $k > 0$, has $\phi(U) = -\ln^{1/k}(U)$. Here, the minimal correlation, given in Eq. (3), for different values of k could only be evaluated numerically, and is given in Table I. Please notice that the case $k = 1$ corresponds to $\exp(1)$ distribution that we have already discussed.

(6) *Beta*. A random variable with $\text{Beta}(a, 1)$ distribution (density ax^{a-1} on $[0, 1]$) can be sampled as $U^{1/a}$ and, due to symmetry, $\text{Beta}(1, b)$ can be sampled as $1 - U^{1/b}$ [22]. We analyze the first case in which $\phi(U) = U^{1/a}$ and $E(\phi(U)\phi(1-U)) = \mathbf{B}(1/a + 1, 1/a + 1)$, where \mathbf{B} stands for the beta function $\mathbf{B}(x, y) = \int_0^1 t^{x-1}(1-t)^{y-1} dt$. For a special case when $a = 1/n$, where n is an integer, the minimum correlation can be obtained analytically by realizing that $\mathbf{B}(n+1, n+1) = \frac{(n!)^2}{(2n+1)!}$. If we let m and σ be the mean and standard deviation of $\text{Beta}(1/n, 1)$, then

$$\begin{aligned} \rho_* &= \frac{E(\phi(U)\phi(1-U)) - m^2}{\sigma^2} \\ &= \frac{\frac{(n!)^2}{(2n+1)!} - \frac{1}{(1+n)^2}}{\frac{n^2}{(1+n)^2(1+2n)}} = \frac{[(n+1)!]^2 - (2n+1)!}{n^2(2n)!}. \end{aligned}$$

For other values of a , minimal correlations can be obtained numerically, which we show in Table II.

TABLE II. Minimal correlation of a bivariate distribution with marginals distributed as $\text{Beta}(a, 1)$, for different values of a .

a	5	4	3	2	1	0.8	0.5	0.3
ρ_*	-0.795	-0.824	-0.867	-0.931	-1	-0.989	-0.875	-0.634

(7) Minimum correlations for the *Poisson* distribution are calculated by Shin and Pasupathy [31], while the *log-normal* case was studied in De Veaux [32], among others. We refer the readers to derivations in their papers.

III. MULTIVARIATE ALGORITHM

In this section we propose an extension of the above algorithm to the multivariate case. We start with the simplest case, where X_1, X_2, \dots, X_n is a set of n identically distributed random variables, each with F as the marginal distribution, and identical positive pairwise correlation coefficient for each pair, $\text{cor}(X_i, X_j) = \rho^2$.

As before, let ϕ be an algorithm such that $\phi(U) \sim F$, where U is a uniform random variable on $[0, 1]$. (Although not necessary, we can set ϕ to equal F^{-1} .) Then the construction given in Algorithm 2 below yields a set of n random variables, (X_1, \dots, X_n) , such that $X_i \sim F$ for each i , and $\text{cor}(X_i, X_j) = \rho^2$ for each $i \neq j$, $i, j \leq n$:

ALGORITHM 2: Construction of n random variables, X_1, X_2, \dots, X_n , identically distributed with a prescribed marginal distribution F and identical positive pairwise correlation coefficient ρ^2 .

```

1: sample  $U, V_1, V_2, \dots, V_n, W_1, W_2, \dots, W_n \sim U(0, 1)$ , independently
2: for  $i = 1 \rightarrow n$  do
3:   if  $W_i < |\rho|$  then
4:     let  $X_i = \phi(U)$ 
5:   else
6:     let  $X_i = \phi(V_i)$ 
7:   end if
8: end for
9: RETURN  $X_1, \dots, X_n$ 

```

Algorithm 2 will be applicable to a range of correlation values, which will depend not only on F as in the bivariate case, but also on the conditions required for positive semidefiniteness or positive definiteness of the correlation matrix. For example, a commonly used necessary and sufficient condition for positive definiteness of a matrix is Sylvester's criterion, which states that a matrix is positive definite if and only if all leading principal minors have positive determinants. In the case of a 3-dimensional "compound symmetry" correlation matrix—a matrix where all diagonal elements are equal to 1 and all off-diagonal elements are equal to $r \in (-1, 1)$ —Sylvester's criterion equates to the condition that the determinant, $1 - 3r^2 + 2r^3$, is positive, or equivalently that $-0.5 < r < 1$. The matrix structure assumed by Algorithm 2 above will thus be positive definite for any $\rho^2 < 1$. The topic of conditions for positive semidefiniteness of a correlation matrix can be found in [33], among others.

The next multivariate algorithm extension is to the case when X_1, X_2, \dots, X_n is again a set of n identically distributed random variables, each with F as the marginal distribution. However, now we allow the pairwise correlation coefficient to be different for every pair, $\text{cor}(X_i, X_j) = \rho_{ij}$, but only if each ρ_{ij} can be expressed as $\rho_i \rho_j$ where $\rho_i \in (\rho_*, \rho^*)$ for all $i = 1, \dots, n$. The construction given in Algorithm 3 below yields a set of n random variables, (X_1, \dots, X_n) , such that $X_i \sim F$ for each i , and $\text{cor}(X_i, X_j) = \rho_{ij} = \rho_i \rho_j$ for each $i \neq j, i, j \leq n$:

ALGORITHM 3: Construction of n random variables, X_1, X_2, \dots, X_n , identically distributed with a prescribed marginal distribution F , and pairwise correlation coefficients $\rho_{ij} = \rho_i \rho_j$.

```

1:  sample  $U, V_1, V_2, \dots, V_n, W_1, W_2, \dots, W_n \sim U(0, 1)$ ,
    independently
2:  for  $i = 1 \rightarrow n$  do
3:    if  $\rho_i > 0$  then
4:      let  $U' = U$ 
5:    else
6:      let  $U' = 1 - U$ 
7:    end if
8:    if  $W_i < \rho_i / c^\phi(U, U')$  then
9:      let  $X_i = \phi(U')$ 
10:   else
11:     let  $X_i = \phi(V_i)$ 
12:   end if
13: end for
14: RETURN  $X_1, \dots, X_n$ 

```

Algorithm 3 will also be applicable to a range of correlation values, which will depend not only on the choice of F , but also on the properties required of the correlation matrix. For example, for a general 3-dimensional correlation matrix, where the three correlation coefficients are p, q , and r , with $|p| < 1, |q| < 1, |r| < 1$, Sylvester's criterion for positive definiteness equates to the determinant being positive, $1 - p^2 - q^2 - r^2 + 2pqr > 0$.

In addition, while Algorithm 3 allows for negative correlation between variables, the correlation coefficient factorization requirement imposes an added restriction. For example, Algorithm 3 cannot accommodate cases such as independence between X_1 and X_2 , but dependence between X_1 and X_3 and between X_2 and X_3 ; nor can it accommodate correlation matrices with an odd number of negative correlation coefficients. This added restriction in the 3-dimensional case is shown in Fig. 1. In the top plot we see the general applicable 3-dimensional region for the 3 correlation coefficients p, q , and r required for positive definiteness. Two views of the subset of that region where Algorithm 3 is applicable are given the middle and bottom plots.

Only subsets of this region shown in the middle and bottom plots in Fig. 1 may be applicable to specific distributions. In the case of 3-dimensional random variable with uniform marginals, the region in the middle and bottom plots in Fig. 1 is fully attainable. However, in the case of a 3-dimensional Weibull(0.5), the region shown in the middle and bottom plots in Fig. 1 has to be further restricted via intersecting it with $[-0.1992, 1] \times [-0.1992, 1] \times [-0.1992, 1]$.

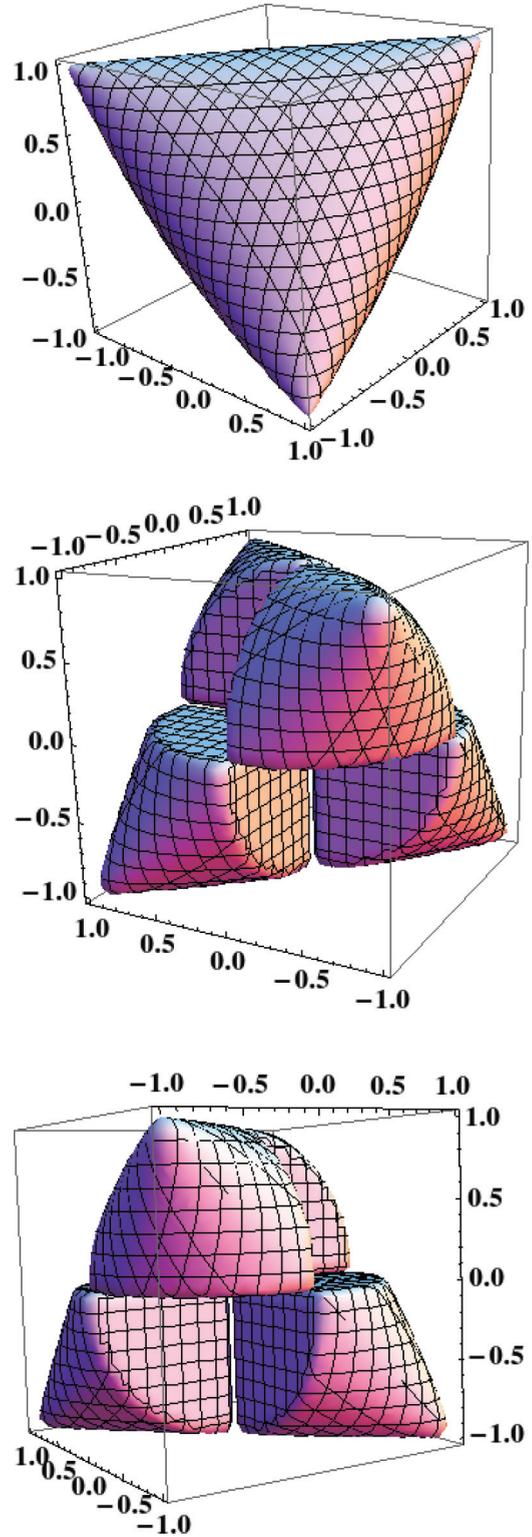


FIG. 1. (Color online) General applicable region for the 3-dimensional implementation of Algorithm 3. The top plot shows the full 3-dimensional domain of allowable correlation coefficients p, q , and r [shown as the range $(-1, 1)$ on the three coordinate axes], which support positive definiteness of a 3-dimensional correlation matrix. The middle and bottom plots are alternative views of that region further restricted by the factorization requirement in Algorithm 3; these plots are obtained by taking the region depicted in the top plot and removing the coordinate axes and subregions where $rpq < 0$.

Finally, we note that for any given set of correlation coefficients, ρ_{ij} , $i, j = 1, \dots, n$, the factorization into ρ_i terms will generally not be unique. In particular, the factorization can be obtained by solving a set of $\binom{n}{2}$ equations in n unknowns which will, in the case of all nonzero correlations, generally yield two sets of solutions with alternate signs. Algorithm 3 will work for any of the admissible factorizations, but choosing the factorization with the smaller number of negative ρ_i coefficients is recommended, to reduce the number of comparisons with $c^\phi(U, 1 - U)$. In the next section we will give a concrete example of an implementation of Algorithm 3 starting with a given correlation matrix.

A. Example: Algorithm for generating multivariate correlated Beta random variables

We conclude this section with an application of Algorithm 3 for sampling a 3-dimensional random variable, (X_1, X_2, X_3) , with $\text{Beta}(v_1, v_2)$ marginals and a set of pairwise correlation coefficients $\text{cor}(X_i, X_j) = \rho_{ij}$ for $i, j = 1, 2, 3$. Among other things, a Beta density is used in practice to describe concentrations of compounds in a chemical reaction. A multivariate Beta density can thus be used to jointly describe multiple compounds, where a negative correlation would exist between a compound and its inhibitors, and a positive one between a compound and its promoters.

Algorithm 4, given below, is the only non-copula-based algorithm for generating multivariate correlated Beta random variables for dimensions greater than 2. This algorithm is valid for integers v_1 and v_2 , and is based on generating two Gamma-distributed random variables, $G_1 \sim \text{Gamma}(v_1, 1)$ and $G_2 \sim \text{Gamma}(v_2, 1)$, and forming a new variable as $B = G_1 / (G_1 + G_2)$, which will be distributed as $\text{Beta}(v_1, v_2)$. As v_1 and v_2 are integers, G_1 and G_2 can be obtained via a sum of v_1 and v_2 exponential random variables with mean 1, respectively. This example illustrates two facts: (1) that $\phi(\cdot)$ need not be an inverse CDF and (2) that the source of randomness used in generation of a random variable need not be a scalar. Expanding the definition of the quantity $c^{\phi, \psi}$ defined by Eq. (1), we will let $\mathbf{U} = (U_1, \dots, U_{v_1+v_2})$ and define $\phi_{v_1, v_2}(\mathbf{U}) = \sum_{i=1}^{v_1} \ln U_i / \sum_{i=1}^{v_1+v_2} \ln U_i$.

The example with 10 000 simulated 3-dimensional variables with $\text{Beta}(4, 7)$ marginals, $\rho_{12} = 0.4$, $\rho_{13} = 0.3$, and $\rho_{23} = 0.2$, resulting from Algorithm 4, is shown in Fig. 2 (top). The bottom plot of Fig. 2 shows an example with 10 000 simulated 3-dimensional variables with the same marginals, but with $\rho_{12} = -0.4$, $\rho_{13} = -0.3$, and $\rho_{23} = 0.3$. Note that for $\text{Beta}(4, 7)$, $c^{\phi_{4,7}}(\mathbf{U}, \mathbf{1} - \mathbf{U}) \approx -0.71$, so only $\rho_{ij} \geq -0.71$ can be considered for generating $\text{Beta}(4, 7)$ using Algorithm 4.

IV. CONCLUSIONS

The algorithm presented in this paper is a simple generalization of the trivariate-reduction method for generation of multivariate samples with specified marginal distributions and correlation matrix. In comparison with the copulas it is simpler in that it is based only on marginal distributions and a correlation matrix and does not require a whole multivariate distribution specification. On the other hand it is exact and more transparent to implement than copulas. Additionally,

ALGORITHM 4: Construction of 3-dimensional $\text{Beta}(v_1, v_2)$ random variable, with $\text{Beta}(v_1, v_2)$ marginals and with correlation coefficients ρ_{12} , ρ_{13} , ρ_{23} .

```

1:  sample  $\mathbf{U} = \{U_1^1, \dots, U_1^{v_1}, U_2^1, \dots, U_2^{v_2}\}, W_1, W_2, W_3 \sim U(0, 1)$ ,
    independently
2:  if any of the eigenvalues of the given correlation matrix are
    negative then
3:    stop: matrix not positive semidefinite
4:  else
5:    if  $\rho_{12}\rho_{13}\rho_{23} < 0$ , only one of  $\rho_{12}$ ,  $\rho_{13}$ ,  $\rho_{23}$  is 0, or any
     $\rho_{ij} \leq c^{\phi_{v_1, v_2}}(\mathbf{U}, \mathbf{1} - \mathbf{U})$  then
6:      stop: algorithm not applicable.
7:    else
8:      if  $\rho_{12} = \rho_{13} = \rho_{23} = 0$  then
9:        let  $\rho_1 = \rho_2 = \rho_3 = 0$ 
10:       else
11:         if  $\rho_{ij} = 0$ ,  $\rho_{ik} = 0$  and  $\rho_{jk} \neq 0$  then
12:           let  $\rho_i = 0$ ,  $\rho_j = 1$  and  $\rho_k = \rho_{ik}$ 
13:         else
14:           let  $\rho_2 = \sqrt{\rho_{12}\rho_{23}/\rho_{13}}$ ,  $\rho_1 = \rho_{12}/\rho_2$ ,  $\rho_3 = \rho_{23}/\rho_2$ 
15:           if  $\rho_i \leq c^{\phi_{v_1, v_2}}(\mathbf{U}, \mathbf{1} - \mathbf{U})$  for any  $i$  then
16:             stop: negative correlations cannot be exact.
17:           else
18:             for  $i = 1 \rightarrow 3$  do
19:               if  $\rho_i > 0$  then
20:                 let  $\mathbf{U}' = \mathbf{U}$ 
21:               else
22:                 let  $\mathbf{U}' = \mathbf{1} - \mathbf{U}$ 
23:             end if
24:             if  $W_i < \rho_i / c^{\phi_{v_1, v_2}}(\mathbf{U}, \mathbf{U}')$  then
25:               let  $G_1 = \sum_{j=1}^{v_1} -\ln(U_1^j)$ 
26:               let  $G_2 = \sum_{j=1}^{v_2} -\ln(U_2^j)$ 
27:             else
28:               sample  $V_1^1, \dots, V_1^{v_1}, V_2^1, \dots, V_2^{v_2} \sim U(0, 1)$ ,
    independently
29:               let  $G_1 = \sum_{j=1}^{v_1} -\ln(V_1^j)$ 
30:               let  $G_2 = \sum_{j=1}^{v_2} -\ln(V_2^j)$ 
31:             end if
32:             let  $X_i = G_1 / (G_1 + G_2)$ 
33:           end for
34:         end if
35:       end if
36:     end if
37:   end if
38:   end if
39:   RETURN  $X_1, X_2, X_3$ 

```

we generate samples directly from uniform random variables, the immediate output from random number generators, which may be more desirable and faster than going through others distributions, such as Gaussians, as in many other methods.

The algorithm is applicable to all distributions with finite variances, and, in the bivariate case, can accommodate the entire range of theoretically feasible correlations. Its major computational difficulty is related to determination of exact pairwise correlation ranges, a question of theoretical and practical value *per se*, which has to be answered *once* for every set of marginal distributions. We emphasize that lower and

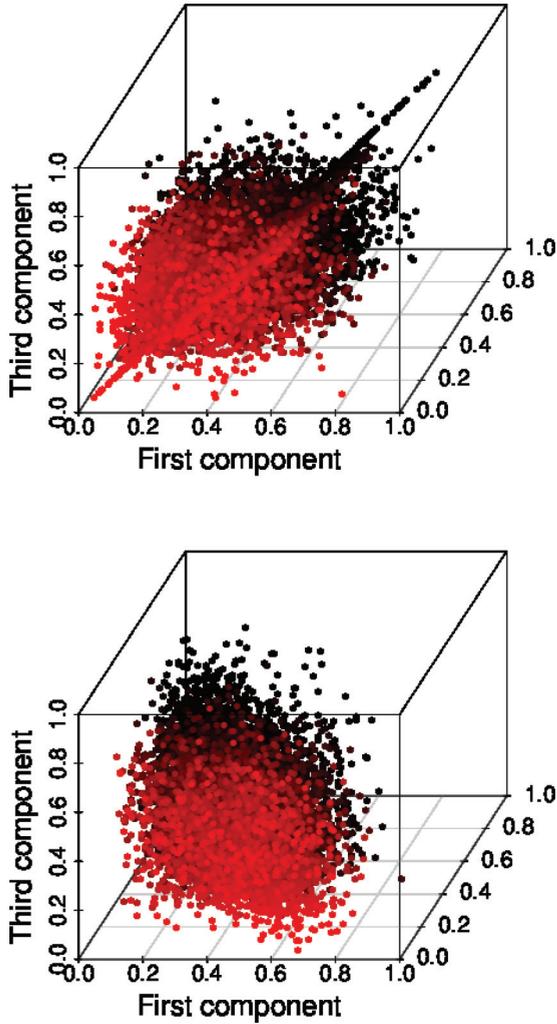


FIG. 2. (Color online) An example with 10 000 simulated 3-dimensional Beta(4,7) variables resulting from Algorithm 4. Top panel: $\rho_{12} = 0.4$, $\rho_{13} = 0.3$, $\rho_{23} = 0.2$. Bottom panel: $\rho_{12} = -0.4$, $\rho_{13} = -0.3$, and $\rho_{23} = 0.3$.

upper bounds for the correlation coefficient actually depend on the family of marginal distributions in question, and that the commonly used $[-1, 1]$ interval can be inappropriate in many applications. In this paper we have presented exact ranges for some common distributional examples so that the implementation of the algorithms is straight-forward.

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APPENDIX

To prove the exponential distribution result from Sec. II B,

$$\int_0^1 \ln(x) \ln(1-x) dx = 2 - \frac{1}{6} \pi^2,$$

we use a representation of $\ln(x)$ as a Maclaurin series for $x \in (0, 1)$:

$$\begin{aligned} \ln(x) \ln(1-x) &= - \sum_{i=1}^{\infty} \frac{x^i}{i} \sum_{j=1}^{\infty} (-1)^{j+1} \frac{(x-1)^j}{j} \\ &= \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \frac{x^i (1-x)^j}{ij}. \end{aligned}$$

Observe that $\lim_{x \rightarrow 0} \ln(x) \ln(1-x) = \lim_{x \rightarrow 1} \ln(x) \ln(1-x) = 0$, and the double sum equals $\ln(x) \ln(1-x)$ for all $x \in [0, 1]$. Furthermore,

$$\begin{aligned} \int_0^1 \ln(x) \ln(1-x) dx &= \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \frac{1}{ij} \beta(i+1, j+1) \\ &= \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \frac{1}{ij} \frac{i! j!}{(i+j+1)!} \\ &= \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \frac{(i-1)!(j-1)!}{(i+j+1)!} \\ &= \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \frac{(i-1)!}{(i+2)! \binom{i+j+1}{j-1}} \\ &= \sum_{i=1}^{\infty} \frac{1}{i(i+1)(i+2)} \sum_{j=1}^{\infty} \frac{1}{\binom{i+j+1}{j-1}}, \end{aligned} \tag{A1}$$

where $\beta(i+1, j+1) = \int_0^1 x^i (1-x)^j dx = \frac{i! j!}{(i+j+1)!}$ is a standard presentation of the beta function with i, j integers.

To proceed from here we use the Corollary 3.7 in [34],

$$\sum_{k=0}^{\infty} \frac{1}{\binom{n+k}{k}} = \frac{n}{n-1},$$

so the last j sum in Eq. (A1) equals $(i+2)/(i+1)$ and

$$\int_0^1 \ln(x) \ln(1-x) dx = \sum_{i=1}^{\infty} \frac{1}{i(i+1)^2}. \tag{A2}$$

To prove that the above series converges to $2 - \pi^2/6$ recall that $\sum_{i=1}^{\infty} 1/i^2 = \pi^2/6$. Now we add that series to Eq. (A2) and show that it adds up to 2:

$$\begin{aligned} \sum_{i=1}^{\infty} \frac{1}{i(i+1)^2} + \frac{\pi^2}{6} &= \sum_{i=1}^{\infty} \frac{1}{i(i+1)^2} + \sum_{i=1}^{\infty} \frac{1}{i^2} \\ &= 1 + \sum_{i=1}^{\infty} \frac{1}{(i+1)^2} \left(\frac{1}{i} + 1 \right) \\ &= 1 + \sum_{i=1}^{\infty} \frac{1}{i(i+1)} \\ &= 1 + \sum_{i=1}^{\infty} \left(\frac{1}{i} - \frac{1}{i+1} \right) = 1 + 1 = 2. \end{aligned}$$

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