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MODELING DEPENDENCIES IN STOCHASTIC SIMULATION INPUTS

James R. Wilson

Department of Industrial Engineering
North Carolina State University
Raleigh, NC 27695-7906, U.S.A.

ABSTRACT

We discuss some basic techniques for modeling dependence between the random variables that are inputs to a simulation model, with the main emphasis being continuous bivariate distributions that have flexible marginal distributions and that are readily extended to higher dimensions. First we examine the bivariate normal distribution and its advantages and drawbacks for use in simulation studies. To achieve a greater variety of distributional shapes while accurately reflecting a desired dependency structure, we discuss bivariate Johnson distributions. Although space limitations preclude inclusion in this article, the oral presentation of this tutorial will also include discussions of how to use (a) bivariate Bézier distributions as a means for achieving even greater flexibility in modeling the marginal distributions, and (b) ARTA (AutoRegressive To Anything) processes as a means for generating an entire stochastic process with specified marginals and a desired covariance structure.

1 INTRODUCTION

In most introductory discussions of stochastic simulation input modeling, little consideration is given to the dependencies between the different random variables that constitute the inputs to the simulation model. For example, a workpiece arriving at a manufacturing cell for processing at several workstations within the cell may exhibit strong dependencies between its processing times at those workstations. In particular, a workpiece that requires higher-than-average processing time at its first workstation is likely to require higher-than-average processing times at the other workstations visited; and the stochastic dependencies between these processing times can have a large effect on the overall flow time of the workpiece in the manufacturing cell. In the simulation model, however, the processing times at different workstations may be sampled independently simply because the variate-generation routines in the underlying simulation software system are limited to generating independent samples.

Another example of the importance of accounting for dependencies between stochastic simulation inputs occurs in reliability studies. The times to failure for several system components may be strongly related if those components tend to fail simultaneously because of a common shock to the system. A striking example of this type of joint failure was the near crash of an airliner several years ago when all three engines failed because of an error in maintenance that caused the loss of oil pressure in all three engines at the same time.

In this tutorial we present some basic techniques for modeling dependencies between the inputs to a stochastic simulation model, but we focus our main attention on techniques for modeling the joint behavior of a pair of continuous random variables. References are given for the extension of these techniques to higher dimensions. Section 2 contains the basic nomenclature that we use to describe the stochastic behavior of a pair of continuous random variables. In Section 3 we introduce the bivariate normal distribution. Bivariate Johnson distributions are discussed in Section 4. Finally in Section 5 we summarize the main points of this article.

2 PROPERTIES OF BIVARIATE DISTRIBUTIONS

Suppose a pair of random variables (X, Y) constitute one of the inputs to a stochastic simulation model. Thus for workpieces arriving at a repair and inspection facility, X might represent the item's repair time and Y might represent the associated inspection time. We are interested in the effect of the *joint* behavior of X and Y on some system performance measure of interest, such as the average flow time of workpieces through the fac ility—and in fact it is in precisely such situations that mathematical techniques frequently fail so that simulation is the analysis technique of choice. When we want to emphasize the dimensionality of the input-modeling task at hand, we will sometimes write (X_1, X_2) rather than (X, Y).

The probabilistic properties of the random vector (X, Y) is specified by a *joint cumulative distribution function* (c.d.f.)

$$F_{X,Y}(x, y) = \Pr\{X \le x, Y \le y\} \text{ for all } (x, y)$$

with the following properties:

1. It is a nondecreasing function of each argument x, y.
2. It is continuous from the right in each argument so that for all (x, y),
$$\left.\begin{array}{ll} \lim\limits_{\substack{x^* \to x \\ x^* > x}} & F_{X,Y}(x^*, y) \\ \lim\limits_{\substack{y^* \to y \\ y^* > y}} & F_{X,Y}(x, y^*) \end{array}\right\} = F_{X,Y}(x, y).$$
3. It satisfies the following relationships:
$$\left.\begin{array}{lll} \lim\limits_{\substack{x \to -\infty \\ y \to -\infty}} F_{X,Y}(x, y) & = & 0, \\ \lim\limits_{\substack{x \to +\infty \\ y \to +\infty}} F_{X,Y}(x, y) & = & 1. \end{array}\right\}$$
4. For any $x < x^*$ and $y < y^*$, we have
$$\begin{aligned} \Pr\{x < X \le x^*, y < Y \le y^*\} &= F_{X,Y}(x^*, y^*) \\ &\quad - F_{X,Y}(x, y^*) - F_{X,Y}(x^*, y) + F_{X,Y}(x, y) \\ &\ge 0. \end{aligned}$$

Requirements 1–4 emphasize the importance of selecting joint c.d.f.'s with great care.

We assume that the random vector (X, Y) possesses a *probability density function* (p.d.f.) so that for all x, y,

$$F_{X,Y}(x, y) = \int_{-\infty}^{x} \int_{-\infty}^{y} f_{X,Y}(u, v)\, dv\, du.$$

The existence of such a nonnegative, integrable function $f_{X,Y}(x, y)$ is sufficient to ensure requirements 1–4 of $F_{X,Y}(x, y)$ above.

Let $F_X(x) = F_{X,Y}(x, +\infty)$ denote the marginal c.d.f. of X with marginal p.d.f. $f_X(x)$, marginal mean

$$\mu_X = \mathrm{E}[X] = \int_{-\infty}^{\infty} x f_X(x)\, dx$$

and marginal variance

$$\begin{aligned} \sigma_X^2 = \mathrm{Var}(X) &= \mathrm{E}[(X - \mu_X)^2] \\ &= \int_{-\infty}^{+\infty} (x - \mu_X)^2 f_X(x)\, dx \\ &= \mathrm{E}[X^2] - \mu_X^2 = \int_{-\infty}^{+\infty} x^2 f_X(x)\, dx - \mu_X^2. \end{aligned}$$

The marginal p.d.f. and moments of Y are defined similarly.

The random variables X and Y are *stochastically independent* if and only if their joint c.d.f. can be factored into the product of the two marginal c.d.f.'s so that

$$F_{X,Y}(x, y) = F_X(x) F_Y(y) \text{ for all } x, y.$$

In terms of p.d.f.'s, X and Y are independent if and only if their joint p.d.f. can be factored into the product of the two marginal p.d.f.'s.

When X and Y are not stochastically independent, the most common characterizations of their dependence are (a) the *covariance of* X *and* Y,

$$\mathrm{Cov}(X, Y) = \mathrm{E}[(X - \mu_X)(Y - \mu_Y)],$$

and (b) the *product moment correlation of* X *and* Y,

$$\begin{aligned} \rho_{X,Y} = \mathrm{corr}(X, Y) &= \mathrm{Cov}(X, Y)/(\sigma_X \sigma_Y) \\ &= \mathrm{E}\left[\left(\frac{X - \mu_X}{\sigma_X}\right)\left(\frac{Y - \mu_Y}{\sigma_Y}\right)\right]. \end{aligned}$$

Notice that if X and Y are independent, then $\mathrm{Cov}(X, Y) = 0$ and $\rho_{X,Y} = 0$. On the other hand, zero covariance (or correlation) between X and Y does not generally imply that X and Y are independent.

Whereas the covariance $\mathrm{Cov}(X, Y)$ depends on the scale (units of measurement) of X and Y, the correlation coefficient $\rho_{X,Y}$ does not since the *standardized random variables* $(X - \mu_X)/\sigma_X$ and $(Y - \mu_Y)/\sigma_Y$ each have mean zero and variance one. It can be easily shown that $-1 \le \rho_{X,Y} \le +1$. If Y is a linear function of X so that $Y = a + bX$ with probability one, then $\rho_{X,Y} = +1$ if $b > 0$ and $\rho_{X,Y} = -1$ if $b < 0$. Thus the correlation $\rho_{X,Y}$ is a measure of the degree of linear dependence between X and Y with the following properties: (a) it is independent of the location and scale in which the quantities X and Y are expressed; (b) it is zero if X and Y are independent; (c) it ranges between -1 and $+1$ when X and Y are dependent, and its sign reflects the direction of the linear dependence; and (d) if its magnitude is 1, then a linear relationship between X and Y holds with probability one. Although there are other useful measures of the association or dependence between two random variables, the product moment correlation coefficient is the most widely used quantity; and as we shall see, this quantity enters naturally into the formulation of the bivariate input models discussed in this article.

3- BIVARIATE NORMAL DISTRIBUTION

The best known and most widely used bivariate distribution is the bivariate normal distribution. This state of affairs is partly because of the pervasive impact of the central limit theorem but mainly because of the lack of many suitable alternative multivariate distributions. When seeking to model the behavior of a bivariate random vector (X, Y), we often have information about the marginal means μ_X and μ_Y, the marginal standard deviations σ_X and σ_Y, and the correlation coefficient $\rho_{X,Y}$; and in this situation it is sometimes appropriate to assume that (X, Y) has the bivariate normal p.d.f.

$$f_{X,Y}(x, y) = \frac{\exp\left[-\frac{1}{2}Q(x-\mu_X, y-\mu_Y)\right]}{2\pi\sigma_X\sigma_Y(1-\rho^2)^{1/2}}\,, \tag{1}$$

where $Q(u, v)$ is the quadratic function

$$Q(u, v) = \frac{1}{1-\rho^2}\left(\frac{u^2}{\sigma_X^2} - 2\rho\frac{u}{\sigma_X}\cdot\frac{v}{\sigma_Y} + \frac{v^2}{\sigma_Y^2}\right). \tag{2}$$

It follows easily from (1) and (2) that the marginal distribution of X is univariate normal with mean μ_X and variance σ_X^2, so that $X \sim N(\mu_X, \sigma_X^2)$ with p.d.f.

$$f_X(x) = \frac{1}{(2\pi)^{1/2}\sigma_X}\exp\left[-\frac{1}{2}\left(\frac{x-\mu_X}{\sigma_X}\right)^2\right] \tag{3}$$

for all x; and a similar result applies to Y. Moreover, the parameter ρ is the coefficient of correlation between X and Y:

$$\mathrm{E}\left[\left(\frac{X-\mu_X}{\sigma_X}\right)\left(\frac{Y-\mu_Y}{\sigma_Y}\right)\right] = \rho.$$

Conditional distributions provide another means of characterizing the dependence between two random variables. Given $X = x$, it follows from (1) and (2) that the conditional p.d.f. of Y is normal

$$f_{Y|X}(y|x) = \frac{\exp\left\{-\dfrac{1}{2}\dfrac{(y-\mathrm{E}[Y|X=x])^2}{\mathrm{Var}[Y|X=x]}\right\}}{(2\pi)^{1/2}\sigma_Y(1-\rho^2)^{1/2}} \tag{4}$$

with conditional mean

$$\mathrm{E}[Y|X=x] = \mu_Y + \frac{\rho\sigma_Y}{\sigma_X}(x-\mu_X) \tag{5}$$

and conditional variance

$$\mathrm{Var}[Y|X=x] = \sigma_Y^2(1-\rho^2)\,. \tag{6}$$

Thus Y has a linear regression on X as specified by (5). Moreover, the marginal variance of Y, σ_Y^2, consists of two parts: (a) the component $\rho^2\sigma_Y^2$ that is "due to" to the variation in X; and (b) the component $(1-\rho^2)\sigma_Y^2$ that is independent of X and that represents the variation of Y about the regression line. Generally it is difficult in simulation applications to work with the conditional distributions associated with a given bivariate distribution. The simplicity of the conditional distributions associated with the multivariate normal p.d.f. is another reason for the popularity of this input model.

Figure 1 shows a three-dimensional plot of the normal density (1) for $\rho > 0$. Since we can express the joint p.d.f. (1) as the product of the marginal p.d.f. (3) and the conditional p.d.f. (4), we see that the curve formed by the intersection of the bivariate density's surface and a plane perpendicular to the x axis (say, $x = a$) is a "normal-like" curve, and the area under this curve is $f_X(a)$ rather than one. Moreover, the mean of this curve lies on the regression line (5); and every such curve has common variance (6). Clearly the tallest such "normal-like" curve is the one defined by the plane $x = \mu_X$, since this value of x maximizes the marginal p.d.f. $f_X(x)$. By symmetry, planes perpendicular to the y axis will intersect the surface in "normal-like" curves with similar properties.

It is also informative to consider the curves formed by the intersection of the bivariate normal surface with planes perpendicular to the (vertical) z axis (say, $z = c$). Each such curve has the form

$$Q(x-\mu_X, y-\mu_Y) = c^*. \tag{7}$$

It can be shown that (7) defines an ellipse centered at the point (μ_X, μ_Y) with principal axes rotated through the angle

$$\theta = \begin{cases} \frac{1}{2}\tan^{-1}[2\rho\sigma_X\sigma_Y/(\sigma_X^2-\sigma_Y^2)], & \text{if } \sigma_X \neq \sigma_Y, \\ \pi/4, & \text{if } \sigma_X = \sigma_Y. \end{cases} \tag{8}$$

From (8) we see that in general the principal axes of these contour ellipses are not parallel to the regression of Y on X or to the regression of X on Y as might be supposed. This should also be clear from Figure 1. For a complete discussion of the bivariate normal distribution, see Hald (1953)

Fitting a bivariate normal distribution to a random sample $\{(X_j, Y_j) : j = 1, \ldots, n\}$ is straightforward. The sample mean and variance

$$\bar{X} = \frac{1}{n}\sum_{j=1}^{n} X_j \quad \text{and} \quad S_X^2 = \frac{1}{n-1}\sum_{j=1}^{n}(X_j - \bar{X})^2$$

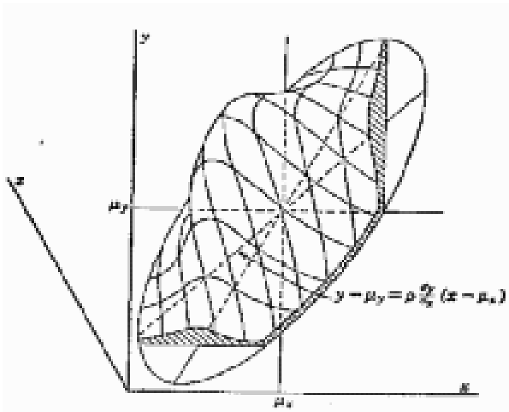

Figure 1: Plot of Bivariate Normal Density

estimate μ_X and σ_X^2, respectively; and similar results apply to the estimation of μ_Y and σ_Y^2. Finally ρ is estimated by the sample coefficient of correlation

$$r = \frac{1}{n-1}\sum_{j=1}^{n}\left(\frac{X_j-\bar{X}}{S_X}\right)\left(\frac{Y_j-\bar{Y}}{S_Y}\right).$$

Given estimates of its parameters, the bivariate normal distribution $N_2(\boldsymbol{\mu},\boldsymbol{\Sigma})$ with respective mean vector and covariance matrix

$$\boldsymbol{\mu} = \begin{bmatrix}\mu_X\\ \mu_Y\end{bmatrix} \text{ and } \boldsymbol{\Sigma} = \begin{bmatrix}\sigma_X^2 & \rho\sigma_X\sigma_Y\\ \rho\sigma_X\sigma_Y & \sigma_Y^2\end{bmatrix}$$

can be readily generated by exploiting the results (3)–(6). In particular, we may generate X from the univariate normal distribution $N(\mu_X,\sigma_X^2)$; then given the sampled value $X=x$, we generate Y from the univariate normal distribution with mean (5) and variance (6).

4 JOHNSON SYSTEM OF DISTRIBUTIONS

4.1 Univariate Johnson Distributions

Starting from a continuous random variable X whose distribution is unknown and is to be approximated and subsequently sampled, Johnson (1949a) proposed a set of four normalizing translations. These translations have the general form

$$Z = \gamma + \delta\cdot g\left(\frac{X-\xi}{\lambda}\right), \tag{9}$$

where Z is a standard normal random variate (that is, $Z\sim N(0,1)$), γ and δ are shape parameters, λ is a scale parameter, ξ is a location parameter, and $g(\cdot)$ is a function whose form defines the four distribution families in the Johnson translation system,

$$g(y) = \begin{cases}\ln(y), & \text{for } S_L \text{ (lognormal) family,}\\ \ln\left[y+\sqrt{y^2+1}\right], & \text{for } S_U \text{ (unbounded) family,}\\ \ln[y/(1-y)], & \text{for } S_B \text{ (bounded) family,}\\ y, & \text{for } S_N \text{ normal family.}\end{cases} \tag{10}$$

The translation (9) should approximately transform the continuous random variate X into a standard normal variate. The process of fitting a Johnson distribution to sample data involves first selecting a fitting method and the desired translation function $g(\cdot)$ and then obtaining estimates of the four parameters γ, δ, λ, and ξ. The fitting method utilized in this paper is moment matching. The Johnson translation system of distributions has the flexibility to match any feasible set of sample values for the mean, variance, skewness, and kurtosis. Additionally, the skewness and kurtosis uniquely identify the appropriate translation function $g(\cdot)$. As a result, fitting a data set using moment matching is reduced to the problem of finding the values of γ, δ, λ, and ξ which approximately transform X into a standardized normal variate. Although there are no closed-form expressions for the parameter estimates based on the method of moments, these parameter estimates can be accurately approximated using an iterative procedure of Hill, Hill, and Holder (1976). Moreover, other methods may used to fit each marginal distribution—for example, any of the estimation procedures implemented in the FITTR1 software package (Swain, Venkatraman, and Wilson 1988).

After the data set has been fitted with a Johnson distribution, variate generation is straightforward. First, a standardized normal variate Z should be generated. The corresponding realization of the Johnson variate X is found by applying to Z the inverse translation

$$X = \xi + \lambda\cdot g^{-1}\left(\frac{Z-\gamma}{\delta}\right), \tag{11}$$

where

$$g^{-1}(z) = \begin{cases}e^z, & \text{for } S_L \text{ (lognormal) family,}\\ \left(e^z-e^{-z}\right)/2, & \text{for } S_U \text{ (unbounded) family,}\\ 1/\left(1+e^{-z}\right), & \text{for } S_B \text{ (bounded) family,}\\ z, & \text{for } S_N \text{ (normal) family.}\end{cases} \tag{12}$$

If X is generated according to (11), then the p.d.f. of X is given by

$$f_X(x) = \frac{\delta}{\lambda(2\pi)^{1/2}} g'\left(\frac{x-\xi}{\lambda}\right) \times \exp\left\{-\frac{1}{2}\left[\gamma + \delta \cdot g\left(\frac{x-\xi}{\lambda}\right)\right]^2\right\} \tag{13}$$

for all $x \in \mathcal{H}$, where

$$g'(y) = \begin{cases} 1/y, & \text{for } S_L \text{ (lognormal) family,} \\ 1/\sqrt{y^2+1}, & \text{for } S_U \text{ (unbounded) family,} \\ 1/[y/(1-y)], & \text{for } S_B \text{ (bounded) family,} \\ 1, & \text{for } S_N \text{ normal family,} \end{cases} \tag{14}$$

and where the support $\mathcal{H}$ of the distribution is

$$\mathcal{H} = \begin{cases} [\xi, +\infty), & \text{for } S_L \text{ (lognormal) family,} \\ (-\infty, +\infty), & \text{for } S_U \text{ (unbounded) family,} \\ [\xi, \xi+\lambda], & \text{for } S_B \text{ (bounded) family,} \\ (-\infty, +\infty), & \text{for } S_N \text{ normal family,} \end{cases} \tag{15}$$

See Johnson (1949a) or Johnson (1987, pp. 31–33) for a graphs illustrating the broad diversity of distributional shapes that can achieved with the Johnson system of univariate probability distributions.

4.2 Bivariate Johnson Distributions

Johnson (1949b) proposed a bivariate distribution based on the univariate Johnson distributions. The parameterized model matches the first four moments for each marginal distribution and then attempts to approximate the correlation between component variates. As detailed below, the technique is easily extended to higher dimensions. Consider a continuous multivariate random vector $\mathbf{X}$ with 2 components,

$$\mathbf{X} = (X_1, X_2)^{\mathrm{T}},$$

which is to be modeled with some parameterized distribution. The Johnson bivariate modeling method determines a normalizing translation such that

$$\mathbf{Z} = \boldsymbol{\gamma} + \boldsymbol{\delta}\mathbf{g}\left[\boldsymbol{\lambda}^{-1}(\mathbf{X} - \boldsymbol{\xi})\right] \sim N_2(\mathbf{0}_2, \boldsymbol{\Sigma}), \tag{16}$$

the bivariate normal distribution with null mean vector $\mathbf{0}_2$ and covariance matrix of the form

$$\boldsymbol{\Sigma} = \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix}.$$

This is accomplished as follows:

1. Identify the transformation

   $$\mathbf{g}\left[(y_1, y_2)^{\mathrm{T}}\right] \equiv [g_1(y_1), g_2(y_2)]^{\mathrm{T}}$$

   such that the marginal distribution of X_i is approximated by an appropriate univariate Johnson distribution, where $i = 1, 2$ and $g_i(\cdot)$ is one of the translation functions in (10)

2. Estimate the matrices of shape parameters,

   $$\boldsymbol{\gamma} \equiv (\gamma_1, \gamma_2)^{\mathrm{T}}, \quad \boldsymbol{\delta} \equiv \mathrm{diag}(\delta_1, \delta_2),$$

   and the matrices of the respective location and scale parameters,

   $$\boldsymbol{\xi} \equiv (\xi_1, \xi_2)^{\mathrm{T}}, \quad \boldsymbol{\lambda} \equiv \mathrm{diag}(\lambda_1, \lambda_2),$$

   using the method of moments on each marginal distribution separately.

3. Estimate correlation matrix $\boldsymbol{\Sigma}$ by (a) inserting each sample value $\{\mathbf{X}_j : j = 1, \ldots, n\}$ into the estimated normalizing translation (16) to obtain the corresponding sample $\{\mathbf{Z}_j : j = 1, \ldots, n\}$ of estimated standard normal random vectors; and (b) computing the sample correlation matrix of the $\{\mathbf{Z}_j\}$ as the approximate moment-matching estimator of $\boldsymbol{\Sigma}$.

Random vector generation consists of generating $\mathbf{Z}$ from a two-dimensional multivariate normal distribution $N_2(\mathbf{0}_2, \boldsymbol{\Sigma})$ and then applying the inverse translation,

$$\mathbf{X} = \boldsymbol{\xi} + \boldsymbol{\lambda}\mathbf{g}^{-1}\left[\boldsymbol{\delta}^{-1}(\mathbf{Z} - \boldsymbol{\gamma})\right], \tag{17}$$

using the previously determined parameter vectors and the vector-valued inverse translation function

$$\mathbf{g}^{-1}\left[(z_1, z_2)^{\mathrm{T}}\right] \equiv \left[g_1^{-1}(z_1), g_2^{-1}(z_2)\right]^{\mathrm{T}}, \tag{18}$$

where $g_i^{-1}(\cdot)$ is defined by (12) for $i = 1, 2$. This method will generate random vectors with exactly the same marginal moments as the original sample data (at least to the limits of machine accuracy); and if each of the empirical marginal distributions of the original sample data is nearly symmetric about its mean, then the intercomponent correlations of the fitted multivariate Johnson distribution will nearly match the sample correlations of the original sample data. However, if some of the empirical marginal distributions of the original sample data (or the corresponding underlying theoretical marginals) possess marked skewness, then the correlation matrix of the fitted multivariate Johnson distribution will not match the sample correlation matrix of the original data set. See Stanfield et al. (1996) for an alternative approach to fitting bivariate Johnson distributions.

If the random vector $\mathbf{X}$ is generated according to (17) and (18), then the joint p.d.f. of $\mathbf{X}$ has the form

$$f_{X_1,X_2}(x_1,x_2) = \frac{1}{2\pi(1-\rho^2)} \prod_{i=1}^{2} \frac{\delta_i}{\lambda_i} g_i'\left(\frac{x_i - \xi}{\lambda_i}\right) \times \exp\left[-\frac{1}{2} \quad \frac{z_1^2 - 2\rho z_1 z_2 + z_2^2}{1-\rho^2}\right)\right] \quad (19)$$

for all $(x_1, x_2) \in \mathcal{H}_1 \times \mathcal{H}_2$, where for the ith coordinate ($i = 1, 2$), the following objects are defined: $\mathcal{H}_i$ is the appropriate support for X_i as specified in (15); $g_i'(x_i)$ is given by the appropriate function in (14) and $z_i = \gamma_i + \delta_i g_i[(x_i - \xi_i)/\lambda_i]$ as in (9). For an extensive set of contour plots of bivariate Johnson p.d.f.'s, see Johnson (1987). In the oral presentation of this article, three-dimensional plots of the selected bivariate Johnson p.d.f.'s will also be presented to illustrate the diversity of bivariate dependency structures that can be achieved with (19).

5- CONCLUSION

The bivariate Johnson distribution family provides substantially more flexibility than the bivariate normal distribution, and it is readily extended to higher dimensions. However, in some multivariate simulation input-modeling applications, even greater flexibility is required in the marginals and in mimicking a desired covariance structure. See Wagner and Wilson (1995, 1996a, 1996b) for an alternative approach to modeling dependencies in stochastic simulation inputs. Moreover, for situations in which it is desirable to model the covariance structure of an entire stochastic process, ARTA processes (AutoRegressive To Anything) (Cario and Nelson 1996) possess distinct advantages. These more advanced techniques will be covered in the oral presentation of this article.

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AUTHOR BIOGRAPHY

JAMES R. WILSON is Professor and Director of Graduate Programs in the Department of Industrial Engineering at North Carolina State University. He was *Proceedings* Editor for WSC '86, Associate Program Chair for WSC '91, and Program Chair for WSC '92. Currently he serves as a corepresentative of the INFORMS College on Simulation to the WSC Board of Directors. He is a member of ASA, ACM, IIE, and INFORMS.