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A Review Method for Simulating Multivariate Random Variables in Computational Geosciences

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Abstract
Environmental variables are known to be dependent in space and time. Detecting and modeling spatial and temporal dependencies of multivariate data are fundamental to many practical applications. Furthermore, simulation of multivariate random variables are commonly used in engineering applications such as uncertainty analysis, risk assessment, ensemble forecasting and decision making among others. By the current research a non-Gaussian copula is used by a non-monotonic transformations of the Gaussian copula for simulation of spatially dependent random variables. The non-monotonic transformation is performed using two parameters that express the anomaly from the Gaussianity. The asymmetry of dependence structures, if exists, can be described using the copula parameters. Application of this method in physical sciences is then briefly discussed.

Key Word and Phrases
Copula, Multivariate Simulation, Non-Gaussian, Spatial Dependence, Asymmetrical Dependence

1. Introduction

Environmental data, particularly weather variables, are known to be multidimensional and thus require multivariate analyses as well as conditional probability distributions of variables [1]. A reasonable description of spatio-temporal dependence structure is required for a variety of engineering applications such as data infilling, interpolation, multi-site weather generators, stochastic simulation. For example, spatial dependencies of extreme rainfall events over a given river basins is of paramount importance for predicting occurrence probability of simultaneous flood events and operational forecasting of river flows. Most engineering decisions are made based upon associations among environmental variables. Classical families of multivariate distributions are commonly used for modeling joint probability distributions of several random variables. Furthermore, classical multivariate distributions such as bivariate normal, log-normal and gamma are built with a number of model parameters that describe the behavior of each random variable as well as the joint probability distribution itself. The main disadvantage of such approaches is that modeling the dependence structure between variables is not independent of the choice of the marginal distributions [1] [2]. It is worth remembering that the multivariate distribution of multiple variables expresses not only how each variable behaves individually but also the way in which the variables behave jointly.

There are different parametric and nonparametric methods to describe the dependence structure [3].The most commonly used method is the well-known Pearson linear correlation coefficient (matrix). However, Embrechts et al. [4] argued that for reasonable representation of stochastic dependence, one may need to go beyond the simple linear correlation. As an alternative to the Pearson linear correlation, nonparametric methods such as Kendall, Spearman and Gamma correlation can be used [5] [6]. It should be noted that the Pearson correlation is based on normal assumption and thus, a representative measure of dependence for multivariate normally or elliptically distributed data [4]. However, environmental variables are not necessarily normally distributed and thus, linear measure of correlation may not be appropriate. Alternative methods are required to describe the departure from normality and asymmetric dependencies. The advent of copulas allows modelers to avoid this restriction. The application of copulas in simulation of multivariate data, extreme value analysis and modeling dependence structure has become popular in engineering applications [7] [8] [9] [10] [11] [12] [13] [14] [15] [16] [17] [18] [19] [20] [64] [22] [23]. In the subsequent sections, after a brief review on the theory of copulas, the v-copula family is discussed in more detail. Then, simulation using this copula family is explained step by step. Finally, example applications are briefly reviewed.

2. Copulas

A copula C of n random variables is defined as a multivariate distribution function on the n-dimensional unit cube with uniform marginals:

$$C : [0, 1]^n \rightarrow [0, 1] \tag{2.1}$$

In other words, copulas are joint cumulative distribution functions that describe dependencies among variables independent of their marginal [3] [26]:

$$C^n(u_1,..., u_n) = Pr(U_1 \leq u_1,..., U_n \leq u_n) \tag{2.2}$$

where C^n is an n-dimensional joint cumulative distribution function of a multivariate random vector $U(U1,..., Un)$ whose marginals are $u[0, 1]$. Note that throughout this document, a common statistical convention is used in which uppercase characters denote random variables and lowercase characters are their specified variables.

In the theory of copulas, Sklar's theorem is fundamental to many applications. Sklar [24] showed that each continuous multivariate distribution $F(F_1,..., F_n)$ can be represented with a unique copula C that can couple multivariate distribution functions to their corresponding marginal distribution functions:

$$F(x_1,..., x_n) = C^n(F_1(x_1),..., F_n(x_n)) \tag{2.3}$$

Note that the copula C^n is unique only if $F1,..., Fn$ are all continuous. Otherwise, the copula C^n is uniquely determined on $RandF_1,..., RandF_n$ [54] [27]. For proof and derivations, interested readers are referred to Sklar [54]. The Sklar theorem indicates that for multivariate distributions, the multivariate dependence structure and the univariate marginal distributions can be separated, and hence, the dependence structure can be represented by a copula independent of the marginals. Having described the dependencies using a copula, a transformation function can be applied to each variable in order to transform the marginal distribution into the desired marginal [26]:

$$C^n(u_1,..., u_n) = F(F^{-1}(u_1),..., F^{-1}(u_n)) \tag{2.4}$$

where $F(F_1,..., F_n)$ is the multivariate cumulative distribution function (CDF) with marginals $F_1,..., F_n$ belonging to different distribution families. In other words, using the Sklar theorem, one can simulate random variables with the same probability distribution as that of the input data while preserving the dependence structure of the variables. In the above Equation, for all x in $RandF$ the following relationship is valid: $F(F^{-1}(x)) = x$. It is noted that the independence of n random variable can also be recognized using copulas. Denote $X_1,..., X_n$ be continuous random variables with different or similar marginal distributions. The random variables $X_1,..., X_n$ are said to be independent if $C^n = \Pi^n (X_1,..., X_n)$ [26] [27].

It is important to remark that copulas are invariant to monotonic transformations of the variables. That is, if $X_1,..., X_n$ are continuous random variables with copula C^n and $F_1,..., F_n$ are increasing functions on $RandX_1,..., RandX_n$, then $F_1(X_1),..., F_n(X_n)$ have the same copula C^n. Hence, the copula C^n is said to be invariant under monotonic transformations. In the following, the aforementioned property of copulas is explored in more detail as it is fundamental to the discussion in the following chapters. Assume $F_1,..., F_n$ to be the distribution functions of $X_1,..., X_n$, respectively. Consider monotonic transformations of the random variables $\Psi(X_1),..., \Psi(X_n)$ with their corresponding marginals $G_1,..., G_n$. Let C^n and C^n be the copula Ψ of $X_1,..., X_n$ and $\Psi(X_1),..., \Psi(X_n)$, respectively. The strictly increasing property of Ψ indicates that for any $x \in R$ [27]:

$$G(x) = Pr\ (\Psi(X) \leq x) = PrX \leq \Psi^{-1}(x) = F\Psi^{-1}(x) \tag{2.5}$$

This is a great advantage in simulation as the Ψ variables may belong to different probability distributions and applying transformation functions may be required to obtain the right marginals. It is noted that for a joint distribution function of $F(F_1,..., F_n)$, for example in Equation 3, the density function f is obtained by differentiating with respect to all variables:

$$f(x_1,..., x_n) = c^n(F_1(x_1),..., F_n(x_n))(f_1(x_1),..., f_n(x_n)) \tag{2.6}$$

where $f_1,..., f_n$ are the density functions of the corresponding marginals $F_1,..., F_n$ and $f(x_1,..., x_n)$ is the density function of the joint distribution. c^n, which is termed as copula density, is basically the n-th partial derivative of an n-dimensional copula C^n (for derivations, the reader is pointed to [26] [27]:

$$c^n(u_1,..., u_n) = \partial n/ \partial u_1 \cdot \partial u_2 ...\partial u_n \quad C^n(u_1,..., u_n) \tag{2.7}$$

There are many families of copulas developed for different practical contexts. Each family of copulas has a number of parameters to describe the dependencies. The main difference associated with different copulas is in the detail of the dependence they represent. For instance, various copula families may differ in the part of their distributions (upper tail/lower tail) where the association is strongest/weakest. In this study, two elliptical copulas, namely a normal copula and t-copula, as well as a non-Gaussian (v-transformed) copula are used for simulations. In the following, the v-copula family is discussed in detail. For additional information regarding different copula families, the reader is referred to [26] [3].

3. V-Copula

As mentioned earlier, the v-copula is obtained through a non-monotonic transformation of the multivariate Gaussian copula. The multivariate Gaussian copula, derived from the multivariate normal distribution, is perhaps the most commonly used copula family mainly due to its simplicity. The n-dimensional multivariate Gaussian copula with correlation matrix $\rho n\times n$ can be expressed as [26]:

$$C\rho(u_1, ..., u_n) = F_\rho^n(F^{-1}(u_1), ..., F^{-1}(u_n)) \tag{3.1}$$

The v-copula can be derived with the following transformation of the multivariate Gaussian copula (N^n) with the mean of zero and unit standard deviation [12]:

$$X_i = K\,(N_i - m) \quad \text{if } N_i \geq m$$
$$X_i = m - N_i \quad \text{if } N_i < m \tag{3.2}$$

where : k and m = copula parameters. This type of copula family was first introduced by Bardossy and Li [12] for interpolation of groundwater quality parameters and uncertainty analysis. In the following, simulation of multivariate fields using this copula family is discussed.

4. Application to Geosciences

Simulation of random fields is important for uncertainty analysis of different data sets. For example, there are many satellite data sets [34] [56] that are subject to high errors and uncertainties [57] [21] [58] [39] [40] [65] [66] [38] [32] [30] [59] [48] [51] [63] [52]. This copula family can be used to generate spatially dependent random fields for uncertainty assessment (see example applications in [31] [25]. Currently, satellite data are frequently used for risk assessment, drought monitoring, precipitation estimation, temperature analysis, etc [62] [37] [45] [47] [35] [42] [36]. One of the main limitations of satellite data is lack of information on the underlying uncertainties. Providing uncertainty information can substantially improve the use of satellite data in practical applications.

Uncertainty in climate model simulations, hydrologic models and weather prediction models have been widely discussed in the literature. One potential application of simulated environmental variables would be their application for assessing uncertainties in climate, hydrological, weather prediction models. The simulated fields can be used as input into models to generate an ensemble of model simulations for uncertainty analysis (e.g., [53]).

In recent years, analyses of climate extremes have become popular in the literature [67] [60] [44] [55] [61] [29]. However, there exist spatial dependencies between environmental variables that are often ignored in simulation of extremes. The V-copula can potentially be used to describe the non-Gaussian dependence for spatial analysis of extremes. Furthermore, copulas provide the opportunity to model non-linear dependence between hydrology and climate variables.

In addition over the recent years, numerous models have been developed and presented for simulating weather variables known as weather generators (see [50] [28]). A common limitation of weather generators is that the point simulations are often independent of each other, and inconsistent with the natural behavior of environmental//physical variables. For example, temperature data from two nearby stations are not independent of each other. For this reason, one needs a model for linking the individual site simulations of weather variables. The presented copula in this study can be used a way to address this issue.

5. Summary and Remarks

This study aimed to discuss a non-Gaussian copula-based model for simulation of multivariate random fields. The model can be used to describe the dependence structure of environmental variables without the influence of the marginal distribution. The model can then be extended for conditional stochastic simulation. Unlike many copula families (e.g. Archimedean copulas), the v-copula exhibits theoretical strong dependence for high dimensions. That is, the v-copula gives the Frechet upper bound (full dependence) for fully dependent variables.

Modeling asymmetrical dependencies among variables is often necessary in practical applications. Elliptical copulas [41] which are based on elliptical distributions (e.g. normal distribution, t-distribution) cannot describe asymmetries in the dependence structure as their dependencies are fully symmetrical [33]. The v-copula, however, can be used to model asymmetrical dependencies through its model parameters. So far, the v-copula family is employed in only few engineering applications: interpolation [12] rainfall simulation [21]. Further research is required to evaluate the statistical robustness and reliability of this copula family for practical applications.

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