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ABSTRACT

A method for inducing a desired rank correlation matrix on a multivariate input random variable is introduced in this paper. This method is simple to use, is distribution free, preserves the exact form of the marginal distributions on the input variables, and may be used with any type of sampling scheme for which correlation of input variables is a meaningful concept. A small simulation study provides an estimate of the bias and variability involved in the method. Input variables used in a model for study of geologic disposal of radioactive waste provide an example of the usefulness of this procedure.

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1. INTRODUCTION

Computer models are used widely to simulate the intricate relationships between variables in economic, social, and physical environments, in order to estimate unknown quantities or predict future events. The ever expanding capability and capacity of computers has allowed the complexity of these models to increase dramatically. It is not uncommon to find models which have perhaps several hundred input variables and may take several hours of computer time to generate a single output observation. Investigation of techniques for efficiently selecting input values has led to the development of Latin hypercube sampling by McKay, Conover and Beckman (1979). Procedures for looking at the effect of different distributional assumptions on input variables have been examined in Iman and Conover (1980).

While much effort has been expended toward development of new statistical techniques for computer modeling, relatively little attention has been given to the problem of incorporating the dependences that may exist among the input variables. Typically the model input variables are assumed to be independent (Iman, Helton, and Campbell (1978)). A study presently underway at Sandia Laboratories is examining mechanisms by which radionuclides might escape a waste depository in bedded salt (Campbell and Cranwell (1980)). The assumption of independence among input variables may not be appropriate for the models used in this study. For example, significant correlations are expected to exist between hydraulic properties in the vicinity of the disposal site and the time for circulating groundwater to contact radioactive waste.

One approach to incorporating dependences is to consider linear combinations of the independent input variables to achieve a desired correlation structure. In the case of normal random variables and random sampling, this approach is well known to produce a multivariate normal input vector. However, if the samples are obtained using Latin hypercube sampling, then this approach will destroy the integrity of the Latin hypercube sample. That is, the values obtained from this linear combination will no longer map back into each of the original Latin hypercube sample intervals, which collectively span the range of each input variable. In addition, the linear combinations of nonnormal random variables will adversely affect both the random sample and the Latin hypercube sample, as the marginal distributions may no longer resemble the original marginal distributions desired on the input variables.

Another approach to incorporating dependences has been developed by Johnson and Ramberg (1979). By viewing the marginal distributions as transformations of normal distributions, a correlation structure can be imposed as follows. An original normal independently distributed input vector is first transformed to a correlated multivariate normal vector as described above. The appropriate transformation is then used to obtain the desired marginal distributions. However, the means, variances, and correlations of the transformed variables are difficult to control. Johnson and Ramberg show how to control these moments in the multivariate case for lognormal and inverse hyperbolic sine distributions, but the mathematics is intractable for the multivariate logit-normal distribution.

In this paper, we present a method based on rank correlations which incorporates the desired rank dependence among the input variables. The method has the following desirable properties.

1) It is distribution free. That is, it may be used with equal facility on all types of input distribution functions.

2) It is simple. No unusual mathematical techniques are required to implement the technique.

3) It can be applied to any sampling scheme for which correlated input could logically be considered, while preserving the intent of the sampling scheme. That is, the same numbers originally selected as input values are retained; only their pairing is affected to achieve the desired rank correlation. This means that in Latin hypercube sampling the integrity of the intervals is maintained. If some lattice structure is used for selection of values, that same structure is retained.

4) The marginal distributions remain intact.

Our approach is based on the premise that rank correlation is a meaningful way to define dependences among input variables. That is, a correlation coefficient computed on raw data may lose meaning and interpretation with nonnormal data or in the presence of outliers. On the other hand, rank correlation coefficients can be quite meaningful in most modeling situations, even when the data are normal.

In Section 2, we explain the proposed technique for including dependences among the input variables, and provide an example of the technique. Section 3 presents the results of a simulation study. An application is discussed in Section 4. The final section contains a discussion and summary. Algorithms useful for implementing the procedure explained in this paper are given in the Appendix.

2. THE METHOD

Suppose that a random row vector X has a correlation matrix I. That is, the elements of X are uncorrelated. Let C be the desired correlation matrix of some transformation of X. Because C is positive definite and symmetric, C may be written as $C = PP'$ where P is a lower triangular matrix (Scheuer and Stoller (1962)). Then the transformed vector XP' has the desired correlation matrix C. This is the theoretical basis for our method.

Let the number of input variables be denoted by K, and let N be the sample size. Let R be an NxK matrix whose columns represent K independent permutations of the integers from 1 to N. Each row of R, say R_i, has K independent components, where each component assumes one of the values from 1 to N with equal probability. Then the row vector R_i has population correlation matrix I. Multiplication by P', $R_i P'$, results in the desired population correlation matrix C. Multiplication of the entire matrix R by P', $RP' = R^*$, gives a matrix R^* whose rows have the same multivariate distribution as $R_i P'$. Any particular realization r^* of R^* will have a sample correlation that estimates C. That is, if the sample correlation matrix associated with R is exactly equal to I, then the sample correlation matrix of R^* would be C. Therefore, to avoid the problem associated with R not necessarily having a sample correlation matrix equal to I, a matrix S is found such that $STS' = C$ where T is the sample correlation matrix associated with R. Consider only realizations of R which have distinct (nonidentical) columns, so that T is positive definite and symmetric. The Cholesky factorization may be used to find the lower triangular matrix Q such that $T = QQ'$. This along with the fact that $C = PP'$ allows the equation involving S to be rewritten as $SQQ'S' = PP'$ which implies $SQ = P$ or $S = PQ^{-1}$. Note that S is also lower triangular. The matrix $R^* = RS'$ has a correlation matrix exactly equal to C.

For the rank correlation matrix of the input values to be approximately equal to C, the values in each column of the NxK input matrix are rearranged so that they will have the <u>same ordering</u> as the corresponding column of R^*. A numerical example will now be given to illustrate the method.

Suppose the rank correlation matrix C is desired for 6 input variables. For a sample size of 15, Algorithm C in

$$C = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & .75 & -.70 \\ 0 & 0 & 0 & .75 & 1 & -.95 \\ 0 & 0 & 0 & -.70 & -.95 & 1 \end{bmatrix}$$

the Appendix is used to obtain a 15 x 6 matrix R. Each column

$$R = \begin{bmatrix} 15 & 15 & 1 & 1 & 11 & 6 \\ 3 & 5 & 13 & 3 & 7 & 12 \\ 5 & 12 & 5 & 14 & 15 & 5 \\ 13 & 8 & 4 & 10 & 8 & 1 \\ 14 & 6 & 11 & 12 & 9 & 14 \\ 9 & 1 & 3 & 4 & 6 & 9 \\ 2 & 4 & 7 & 9 & 1 & 7 \\ 8 & 3 & 9 & 6 & 4 & 13 \\ 10 & 7 & 12 & 13 & 12 & 15 \\ 6 & 9 & 6 & 2 & 14 & 3 \\ 1 & 13 & 14 & 15 & 5 & 2 \\ 7 & 2 & 15 & 7 & 2 & 4 \\ 11 & 11 & 2 & 11 & 3 & 8 \\ 12 & 10 & 10 & 8 & 13 & 10 \\ 4 & 14 & 8 & 5 & 10 & 11 \end{bmatrix}$$

of R represents a random permutation of the integers from 1 to 15. The rank correlation matrix of R is given by T.

$$T = \begin{bmatrix} 1.0000 & .0607 & -.4036 & -.0821 & .2536 & .1750 \\ .0607 & 1.0000 & -.2857 & .1321 & .5071 & -.2643 \\ -.4036 & -.2857 & 1.0000 & .2714 & -.1679 & .2429 \\ -.0821 & .1321 & .2714 & 1.0000 & -.0464 & -.0393 \\ .2536 & .5071 & -.1679 & -.0464 & 1.0000 & .0571 \\ .1750 & -.2643 & .2429 & -.0393 & .0571 & 1.0000 \end{bmatrix}$$

The lower triangular matrices P and Q such that $PP' = C$ and $QQ' = T$, are obtained from Algorithm A in the Appendix.

$$P = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & .75 & .6614 & 0 \\ 0 & 0 & 0 & -.70 & -.6425 & .3117 \end{bmatrix}$$

$$Q = \begin{bmatrix} 1.0000 & 0 & 0 & 0 & 0 & 0 \\ .0607 & .9982 & 0 & 0 & 0 & 0 \\ -.4036 & -.2617 & .8767 & 0 & 0 & 0 \\ -.0821 & .1374 & .3128 & .9362 & 0 & 0 \\ .2536 & .4927 & .0723 & -.1238 & .8200 & 0 \\ .1750 & -.2754 & .2754 & -.0782 & .1450 & .8891 \end{bmatrix}$$

The inverse of Q can be found by use of Algorithm B in the Appendix. The matrix S equals PQ^{-1},

$$S = \begin{bmatrix} 1.0000 & 0 & 0 & 0 & 0 & 0 \\ -.0608 & 1.0018 & 0 & 0 & 0 & 0 \\ .4422 & .2990 & 1.1406 & 0 & 0 & 0 \\ -.0511 & -.2469 & -.3811 & 1.0681 & 0 & 0 \\ -.2495 & -.6254 & -.3904 & .9077 & .8066 & 0 \\ .1459 & .6954 & .2558 & -.8302 & -.8455 & .3505 \end{bmatrix}$$

and finally, the matrix R^* equals RS'.

$$
R^* = \begin{bmatrix}
15 & 14.12 & 12.26 & -3.78 & -3.73 & 4.85 \\
3 & 4.83 & 17.65 & -3.14 & -.58 & 3.04 \\
5 & 11.72 & 11.50 & 9.83 & 14.10 & -12.20 \\
13 & 7.22 & 12.70 & 6.52 & 5.72 & -6.23 \\
14 & 5.16 & 20.53 & 6.43 & 6.61 & -3.64 \\
9 & .45 & 7.70 & 2.42 & 4.43 & -2.46 \\
2 & 3.89 & 10.06 & 5.86 & 3.24 & -1.00 \\
8 & 2.52 & 14.70 & 1.83 & 1.29 & 1.75 \\
10 & 6.40 & 20.20 & 7.07 & 9.92 & -6.28 \\
6 & 8.65 & 12.19 & -2.68 & 3.64 & -3.78 \\
1 & 12.96 & 20.30 & 7.43 & 3.80 & -3.21 \\
7 & 1.58 & 20.80 & .91 & -.89 & .15 \\
11 & 10.35 & 10.43 & 7.71 & 2.00 & .90 \\
12 & 9.29 & 19.70 & 1.65 & 4.60 & -2.87 \\
4 & 13.78 & 15.08 & -1.37 & -.27 & 3.61
\end{bmatrix}
$$

It only remains to generate the NxK matrix of input vectors, according to any desired method or distribution, as if the K input random variables were independent of each other. Then the values of the variable in each column are arranged so they have the same order (rank) as the corresponding column in R^*. Thus the sample rank correlation of the input vectors will be the same as the sample rank correlation of R^*, given by L for this example. Also, the identity of the original marginal distributions on the input variables has been maintained, as the procedure explained in this section merely provides a means for pairing the variables and does not change the numbers themselves.

$$L = \begin{bmatrix} 1.0000 & .0607 & .0464 & -.0250 & .1643 & -.0536 \\ .0607 & 1.0000 & -.0071 & .0643 & .0000 & .0393 \\ .0464 & -.0071 & 1.0000 & -.1000 & -.0143 & -.0536 \\ -.0250 & .0643 & -.1000 & 1.0000 & .7036 & -.6286 \\ .1643 & .0000 & -.0143 & .7036 & 1.0000 & -.9071 \\ -.0536 & .0393 & -.0536 & -.6286 & -.9071 & 1.0000 \end{bmatrix}$$

3. SIMULATION RESULTS

The rank correlation matrix L in Section 2 for the matrix R^* does not turn out to be exactly equal to C. The brief simulation study reported in this section examines the sampling behavior of the sample rank correlation matrix L for sample sizes N = 15, 25, 50, 100, where the desired correlation matrix is C as given in Section 2. The simulation results in Table 1 show that the bias, if any, is small. The observed mean rank correlations for 100 repetitions of R are close to the desired values in almost every case, i.e., within one or two standard deviations ($s_{\overline{X}} = s/\sqrt{100}$). The estimates improve, that is, the bias and the standard deviation get smaller, as N gets larger, which one might expect.

Table 1. Means and Standard Deviations of Rank Correlations for 100 Simulation Runs Recorded by Matrix Position and Sample Size.

i,j	Desired Correlation	N = 15		N = 25		N = 50		N = 100	
		$\bar{x}$	s	$\bar{x}$	s	$\bar{x}$	s	$\bar{x}$	s
1,2	0.0	.0056	.0686	-.0015	.0427	.0033	.0215	-.0011	.0124
1,3	0.0	.0041	.0622	.0094	.0378	.0002	.0202	-.0004	.0103
1,4	0.0	-.0003	.0702	.0047	.0456	-.0015	.0219	.0011	.0128
1,5	0.0	-.0027	.0739	.0111	.0454	.0014	.0306	.0008	.0178
1,6	0.0	-.0042	.0730	-.0032	.0447	.0002	.0270	.0014	.0185
2,3	0.0	-.0055	.0611	.0024	.0413	-.0014	.0291	-.0005	.0114
2,4	0.0	-.0110	.0610	-.0109	.0466	.0029	.0223	.0015	.0096
2,5	0.0	-.0071	.0738	-.0068	.0466	.0017	.0272	.0021	.0152
2,6	0.0	.0089	.0817	.0008	.0510	.0007	.0286	.0001	.0182
3,4	0.0	-.0006	.0866	-.0032	.0537	-.0003	.0205	.0004	.0116
3,5	0.0	-.0096	.0887	-.0022	.0462	.0050	.0314	.0009	.0189
3,6	0.0	-.0131	.0860	.0018	.0519	-.0032	.0300	-.0002	.0211
4,5	0.75	.7242	.0617	.7291	.0354	.7412	.0201	.7430	.0091
4,6	-0.70	-.6768	.0612	-.6766	.0358	-.6892	.0211	-.6917	.0100
5,6	-0.95	-.9225	.0411	-.9337	.0178	-.9421	.0110	-.9455	.0054

4. AN APPLICATION

Thus far in this paper, we have restricted our attention to a 6 x 6 correlation matrix as an easy and convenient means of demonstrating the method and summarizing the simulation results. This section presents an application of the method to a model used to estimate the risk associated with geologic disposal of radioactive waste. Input to this model includes time to groundwater contact with radioactive waste which is correlated with other input variables such as hydraulic, thermal, and mechanical properties of several rock types near the waste depository. Thus it is necessary to define a target correlation structure between properties of the rock units near the depository and the time to groundwater contact with radioactive waste. In this example, 15 variables are defined including the ones just mentioned. Thus the desired correlation matrix is a 15 x 15 symmetric matrix which must be positive definite. The nonzero target correlations are indicated in parentheses in Table 2, along with the actual rank correlation structure generated using the method of the previous sections, with N = 100.

Examination of the entries in Table 2 shows excellent agreement with the target correlation matrix even though no attempt was made to improve on the entries by considering other matrices resulting from a new 100 x 15 matrix of ranks R. That is, the user of this method is free to generate as many rank correlation matrices as desired before beginning the

Table 2. Actual rank correlations generated from a sample of size N = 100 for the input variables used in a model used to estimate the risk associated with geologic disposal of radioactive waste. Numbers in parenthesis represent the nonzero target correlations.

Variable Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14
2	-.0151													
3	-.0048	.0173												
4	.0014	-.0077	-.0118											
5	.2845 (.3000)	-.2864 (-.3000)	.0240	-.0052										
6	-.0066	.0090	.0026	-.0031	-.0099									
7	.0002	.0053	.0044	.0024	-.0003	-.0181								
8	-.0041	.0085	-.0024	.0176	.0183	.0160	.0034							
9	-.0015	.0017	-.0067	.0003	-.0076	.0091	-.0003	.0178						
10	-.0033	.0090	-.0094	.0111	.0016	-.0154	-.0010	-.0073	-.0151					
11	-.0135	.7027 (.7000)	.0186	.0072	-.0045	.0019	-.0073	.0357	-.0167	.0142				
12	.4424 (.4500)	.4843 (.5000)	.0127	-.0047	-.0218	-.0116	.0046	.0069	-.0101	.0125	-.0131			
13	-.3573 (-.3500)	.0239	-.0149	.0102	-.0107	-.0143	-.0073	.0225	.0174	-.0105	-.0006	.0010		
14	.0074	-.3331 (-.3500)	.0044	-.0037	-.0054	-.0162	.0125	-.0041	.0015	-.0072	.0015	.0127	-.0310	
15	-.0202	.0003	-.0046	-.0160	-.0234	.0110	-.0144	-.0237	-.0097	.0198	-.0072	-.0099	.0001	.0027

Variable Number

actual computer model runs, but for this example, we considered only one such matrix. It is worth noting that the largest difference between the sample correlations and the target correlations is 0.0357, out of 105 pairs of variables.

5. SUMMARY AND DISCUSSION

A method for introducing rank correlations among observations on independent random variables is given in this paper. This method, unlike methods based on linear combinations of random variables, preserves the exact marginal distributions, may be used with any distributions, is simple to use, and may be applied to any sampling scheme for which correlated variables could logically be considered. Simulation studies and the application in a computer model with many variables indicate that the expected value of the rank correlation matrix obtained using this procedure is very close to the desired form. It is worth noting that even if the desired correlation matrix is I, this method can be relied on to produce a sample rank correlation matrix which more closely resembles orthogonal input than one would have using a strictly random input. That is, the variance associated with sample rank correlations in random sampling tends to decrease at the rate n, whereas the simulation results indicate that the variance using this method tends to decrease at a rate close to n^2.

It may be noted that the sample correlations in Section 2 for correlated random variables, matrix L, appear to be in the tails of their respective sampling distributions as estimated in Table 1. However, we should point out that we used the first and only complete example that we generated, and nothing prevents the prospective user of this method from generating several matrices of ranks, computing L for each one, and choosing that matrix that provides the most preferred rank correlations. This approach would permit a pairing of values of input variables that would yield rank correlations as close to the desired structure as the user thinks is necessary.

In any type of computer modeling involving random sampling of the input variables, whether it is simple random sampling, stratified sampling, or Latin hypercube sampling, the validity of the model output depends to a great extent on how closely the sampled joint distribution of the input variables agrees with the true joint distribution. That is, if a correlation structure exists among the input variables, but the actual sampling takes place as if the input variables were independent, the theoretical properties of the statistics formed from the output may no longer be valid. Estimators intended to be unbiased or consistent may not be. The procedure presented in this paper can be expected to bring the joint distribution of the input variables closer than would be attained under the assumption of independence. A user's manual and computer listing for a Latin hypercube sampling program which contains the technique presented in this report is available (Iman, Davenport, and Zeigler (1980)).

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APPENDIX

Algorithm A.

To factor a given K x K correlation matrix $C = (c_{ij})$ into $C = PP'$, where $P = (p_{ij})$ is a lower triangular matrix, the Cholesky factorization scheme (Scheuer and Stoller (1962)) may be used. The elements of P are determined recursively, column by column as follows. The first column of values is given by $p_{i1} = c_{i1}$, $1 \leq i \leq K$. For each succeeding column the diagonal term is

$$p_{jj} = \left(1 - \sum_{k=1}^{j-1} p_{jk}^2\right)^{1/2}$$, and the remaining terms are

$$p_{ij} = \left(c_{ij} - \sum_{k=1}^{j-1} p_{ik} \; p_{jk}\right) / p_{jj} \qquad 1 < j < i \leq K \; .$$

Of course $p_{ij} = 0$ for all $i < j \leq K$.

Algorithm B.

To find the inverse of the lower triangular matrix P given in Algorithm A proceed as follows. Let $A = P^{-1}$. The diagonal elements of A are given by $a_{jj} = 1/p_{jj}$, $1 \leq j \leq K$. The remaining terms of A are

$$a_{ij} = - \sum_{k=j+1}^{i} a_{ik} \; p_{kj} / p_{jj} \qquad \begin{array}{l} j = K-1, K-2, \ldots, 1 \\ j < i < K \end{array}$$

and $a_{ij} = 0$ for all $i < j \le K$. Note that A is also a lower trangular matrix and its computation first requires finding the diagonal elements and then moving from right to left away from the diagonal element to complete each succeeding row.

Algorithm C

```
C      THIS SUBROUTINE WILL PROVIDE A RANDOM PERMUTATION OF
C      THE INTEGERS 1,2,...,N AND IS BASED ON ALGORITHM 235
C      IN COMMUN. ASSOC. COMPUTING MACH. BY R. DURSTENFELD
C      (1964).
C
C      ON THE VERY FIRST CALL TO THIS SUBROUTINE THE VECTOR
C      ID WILL CONTAIN THE INTEGERS 1 TO N ORDERED FROM
C      SMALLEST TO LARGEST.  ADDITIONAL CALLS TO THIS
C      SUBROUTINE WILL USE THE ARRANGEMENT OF INTEGERS
C      CREATED ON THE PREVIOUS CALL.  UDGEN IS A USER
C      SUPPLIED U(0,1) RANDOM NUMBER GENERATOR.

       SUBROUTINE MIX(ID,N)
       DIMENSION ID(1)
       DO 1 I=2,N
       J=N+2-I
       K=J*UDGEN(0.) + 1
       L=ID(J)
       ID(J)=ID(K)
    1  ID(K)=L
       RETURN
       END
```

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