

ON USING SINGULAR CORRELATION MATRICES FOR MULTIVARIATE NORMAL DISTRIBUTION

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Abstract: This work presents a new approach to the management of singular correlation matrices in the multivariate normal distribution setting. The non-invertibility of singular correlation matrices makes them difficult to analyze statistically, necessitating the use of specialist methods to accurately evaluate multivariate normal probability. With support for arbitrary single correlation matrices, the suggested approach provides a fast and accurate solution for such cases. The method provides academics and practitioners dealing with complicated data structures with a flexible tool that takes into consideration. The study also expands the use of this technique to the simultaneous creation of confidence intervals. Its applicability for large sample sizes is especially significant, since it addresses a major difficulty in statistical inference. This methodology not only improves the validity of probability evaluations when singular correlation matrices are present, but it also advances the statistical toolbox that can be used for multivariate normal distribution analysis in practical contexts by strengthening the construction of simultaneous confidence intervals

Keywords: multivariate normal, singular distribution, numerical integration, statistical computation

1. INTRODUCTION

Let X_1, \dots, X_m ($m \geq 2$) be the standardized m -variate normal random variates with a correlation matrix $\{\rho_{jk}^{(m)}\}$.

Consider the probability

$$\Pr \left[\bigcap_{j=1}^m (X_j \leq b_j); \{\rho_{jk}^{(m)} = \alpha_{jk}\} \right] \quad (1)$$

where $b_1, \dots, b_m \in \mathbb{R}$ and $\{\rho_{jk}^{(m)} = \alpha_{jk}\}$ denotes the correlation matrix $\rho_{jk}^{(m)}$ with entry α_{jk} in the j^{th} row and k -th column for $j \neq k$ and entry 1 for $j = k$, where $1 \leq j, k \leq m$. The methods for evaluating the probability in equation (1) with various non-singular correlation structures have been extensively studied by [1–8]. For example, in order to evaluate m -variate normal probability with a non-singular negative product structure $\left(\{\rho_{jk}^{(1)} = -\alpha_j \alpha_k\} \text{ where } 1 < m \text{ and } \sum_{j=1}^m \frac{\alpha_j^2}{1+\alpha_j^2} = 1 \right)$, [4] proved that for any $2 \leq i < m$

$$\Pr \left[\bigcap_{j=1}^m (X_j \leq b_j); \{\rho_{jk}^{(m)} = \alpha_j \alpha_k\} \right] = \int_{-\infty}^{\infty} \prod_{j=1}^1 \left[\Phi \left(\frac{b_j - i\alpha_j z}{\sqrt{1+\alpha_j^2}} \right) \right] \phi(z) dz \quad (2)$$

where ϕ is the standard normal density function and extended to complex domain and defined by

$$\phi(x + iy) = e^{\frac{x}{2}} \int_{-\infty}^x e^{-isy} \phi(s) ds \quad (3)$$

where $i^2 = -1$.

As $1-m$ has a single correlation structure, [9] demonstrated that the conclusion in equation (2) is invalid and developed a novel theory to evaluate one-sided multivariate normal probabilities with such unique correlation structure, after changing (2) for $1-m$ to assess the two-sided probability in the form, the result cannot be extended.

$$\Pr \left[\bigcap_{j=1}^m (|X_j| \leq b_j); \{\rho_{jk}^{(m)} = -\alpha_j \alpha_k\} \right] \quad (4)$$

where $b_j > 0$ for $j = 1, \dots, m$.

A method for assessing equation (3) for $m=3$ was developed by [10], with the additional constraint that, for $m \geq 4$, $\alpha_1 = \alpha_2 = \dots = \alpha_m = -1/(m-1)$. For each $m \geq 4$, [11] offered an alternative method to assess the upper and lower limits for (3).

This work presents an innovative method for assessing (3) with any kind of arbitrary single correlation structures. A comparative study between the novel methodology and the current method is carried out using numerical and simulation research. The new method is then used, provided that the sample size is high enough, to assess the critical values for the simultaneous creation of all pairwise confidence intervals and simultaneous confidence intervals for multinomial proportions.

2. SINGULAR MULTIVARIATE NORMAL INTEGRAL EVALUATION

■ Negative Product Correlation Structure

Let X_1, \dots, X_m be the standardized m -variate normal variates with a singular negative product correlation structure, i. e. $\rho_{jk}^{\{m\}} = -\alpha_j \alpha_k$ with $\sum_{j=1}^m \frac{\alpha_j^2}{1+\alpha_j^2} = 1$. Denote the events $A_j = \{X_j: |X_j| \leq b_j\}$ for $j = 1, \dots, m$ and $J_r^m = \{(j_1, \dots, j_r): 1 \leq j_1 < j_2 < \dots < j_r \leq m\}$ be a set in on r -dimensional space with all the $j; j_i (1 < i < m)$ being integers. [11] derived the following inequalities:

$$\sum_{r=1}^{m-2} (-1)^{r+1} \sum_{J_r^m} P_r \left[\left(\bigcap_{l=1}^r A_{j_l} \right) \cap A_m \right] - \Pr[A_m] \leq \Pr \left[\bigcap_{j=1}^m A_j \right] \leq 1 - \sum_{r=1}^{m-2} (-1)^{r+1} \sum_{J_r^m} P_r \left[\bigcap_{l=1}^r A_{j_l} \right] \quad (5)$$

when m is an odd integer, and

$$\sum_{r=1}^{m-2} (-1)^{r+1} \sum_{J_r^m} P_r \left[\bigcap_{l=1}^r A_{j_l} \right] - 1 \leq \Pr \left[\bigcap_{j=1}^m A_j \right] \leq \Pr[A_m] - \sum_{r=1}^{m-2} (-1)^{r+1} \sum_{J_r^m} P_r \left[\left(\bigcap_{l=1}^r A_{j_l} \right) \cap A_m \right] \quad (6)$$

In the event when m is even. Observe that the multivariate normal probabilities with non-singular negative product correlation structures are used to represent the upper and lower bounds for the unique multivariate normal probability. Therefore, after extending the solution in equation (2) as follows, the boundaries may be numerically evaluated:

$$\Pr \left[\bigcap_{j=1}^l A_{j_i} \left\{ \rho_{jk}^{\{m\}} = -\alpha_j \alpha_k \right\} \right] = \int_{-\infty}^{\infty} \prod_{j=1}^l \left[\Phi \left(\frac{b_j - i\alpha_j z}{\sqrt{1+\alpha_j^2}} \right) - \Phi \left(\frac{-b_j - i\alpha_j z}{\sqrt{1+\alpha_j^2}} \right) \right] \phi(z) dz \quad (7)$$

when $2 \leq l < m$ and $\Pr[A_m] = 2\Phi(b_j) - 1$ when $l = 1$.

Kwong's inequalities can be utilized recursively to express all probabilities in terms of nonsingular multivariate normal probabilities, which can then be computed using any available method. This allows for the evaluation of both upper and lower bounds for an m -variate normal distribution with any arbitrary singular correlation matrix of rank k ($k < m$). But as m -climbs, the calculation time also increases quickly, as does the discrepancy between the precise value and the boundaries. For any unique multivariate normal probability, Kwong's inequalities are consequently neither a precise or efficient method when $m-k > 1$. In the next part, a novel method is developed.

■ General Correlation Structure

The definition of the multivariate normal distribution, as it is commonly understood, is given when the variance-covariance matrix Σ is positive definite. Described as:

$$F(a, b, \Sigma) = \Pr \left[\bigcap_{j=1}^m (a_j \leq X_j \leq b_j); \Sigma \right] = \frac{(2\pi)^{-\frac{m}{2}}}{\sqrt{|\Sigma|}} \int_{a_1}^{b_1} \dots \int_{a_m}^{b_m} e^{-\frac{1}{2} x' \Sigma^{-1} x} dx_m \dots dx_1 \quad (8)$$

A key phase in the advancement of the numerical techniques expounded by [7] involved transforming to F via $x = Cy$, whereby C represents the Cholesky factor of Σ ($\Sigma = CC^{ij}$).

$$F(a, b, \Sigma) = (2\pi)^{-\frac{m}{2}} \int_{a \leq Cy \leq b} e^{-\frac{1}{2}y'y} dy \quad (9)$$

The findings tends to extend this method to situations in which Σ is positive semi-definite and demonstrate that a comparable interpretation of F may be applied in these scenarios as well. Let D be a $m \times m$ diagonal matrix with nonnegative diagonal elements d_1, d_2, \dots, d_m . and let $\Sigma = UDU'$ be a singular value decomposition for Σ . In the event where k is the rank of Σ and $k < m$, then $d_{k+1} = d_{k+2} = \dots = d_m = 0$.

Now define $\Sigma(\epsilon) = \Sigma + \epsilon I$ for $\epsilon > 0$ Then

$$\Sigma(\epsilon) = UDU' + \epsilon I = U(D + \epsilon I)U' = UD(\epsilon)U',$$

where $D(\epsilon) = D + \epsilon I$, so $\Sigma(\epsilon)$ is positive definite, and $F(a, b, \Sigma)$ is properly defined and let $V(\epsilon) = UD(\epsilon)^{\frac{1}{2}}$, so $\Sigma(\epsilon) = V(\epsilon)V'(\epsilon)$, and let $x = V(\epsilon)v$.

Then,

$$F(a, b, \Sigma) = (2\pi)^{-\frac{m}{2}} \int_{a \leq V(\epsilon)v \leq b} e^{-\frac{1}{2}v'vdv}. \quad (10)$$

Taking the limit as ϵ approaches zero, we have

$$F(a, b, \Sigma) = (2\pi)^{-\frac{m}{2}} \int_{a \leq Vv \leq b} e^{-\frac{1}{2}v'vdv}. \quad (11)$$

where $V = V(0)$. V can be written as $V = \hat{U}D^{\frac{1}{2}}$, where U is an $m \times m$ matrix with its first k columns as the first k columns of U and remaining $m - k$ columns as columns of zeros, because $d_{k+1} = d_{k+2} = \dots = d_m = 0$. For a final step, we determine an $m \times m$ orthogonal matrix Q so that $C = VQ'$ is lower triangular. The Q required for this step is an $m \times m$ identity matrix except for its principal $k \times k$ submatrix which is the $k \times k$ orthogonal matrix required to make the principal $k \times k$ sub matrix of V lower triangular (see Golub and Van Loan, 1996, for a description of how such a Q can be determined). Then, if $v = Q'y$, $F(a, b, \Sigma) = (2\pi)^{-\frac{m}{2}} \int_{a \leq Cy \leq b} e^{-\frac{1}{2}y'y} dy$, where C is lower triangular and $c_{ij} = 0$ if $j > k$. The integration region defined by $a \leq Cy \leq b$ places no constraint on the variables $y_{k+1}, y_{k+2}, \dots, y_m$, and all possible values between $-\infty$ and ∞ for these variables are consistent with the definition of the integration region, so the innermost $m - k$ integrals are all equal to one.

Therefore

$$F(a, b, \Sigma) = (2\pi)^{-\frac{k}{2}} \int_{a \leq Cy \leq b} e^{-\frac{1}{2}y'y} dy \quad (12)$$

where C is now the $m \times k$ matrix obtained by removing the original $m - k$ zero columns from the original C and $y = (y_1, y_2, \dots, y_k)'$. This matrix C can be computed directly using the generalized Cholesky decomposition algorithm described by [12].

Next, in accordance with [7] methodology, rewrite each of the inequalities $a \leq Cy \leq b$ using the lower triangular structure of C , and explicitly state the integration limits for F to yield F in the following form:

$$F(a, b, \Sigma) = (2\pi)^{-\frac{k}{2}} \int_{a'_1}^{b'_1} e^{-\frac{y_1^2}{2}} \int_{a'_2(y_1)}^{b'_2(y_1)} e^{-\frac{y_2^2}{2}} \dots \int_{a'_k(y_1, \dots, y_{k-1})}^{b'_k(y_1, \dots, y_{k-1})} e^{-\frac{y_k^2}{2}} dy \quad (13)$$

where $a'_k(y_1, \dots, y_{k-1}) = \frac{a_i - \sum_{j=1}^{i-1} c_{ij}y_j}{c_{ik}}$ and $b'_k(y_1, \dots, y_{k-1}) = \frac{b_i - \sum_{j=1}^{i-1} c_{ij}y_j}{c_{ik}}$, for $i = 1, 2, \dots, k$. But this definition of F is not complete if $k < m$, because we must take into account the $m - k$ additional constraints $a_i \leq \sum_{j=1}^i c_{ij}y_j \leq b_i$ for $i = k + 1, k + 2, \dots, m$, that the k integration variables must satisfy. There are various cases to consider. In order to introduce the general cases, the findings consider the case where $c_{ik} \neq 0$ for all $i > k$. In this case we only need to place additional constraints on y_k and modify the definitions of a'_k and b'_k . We first rewrite the last $m - k + 1$ constraint in the form $a_i - \sum_{j=1}^{k-1} c_{ij}y_j \leq c_{ik}y_k \leq b_i - \sum_{j=1}^{k-1} c_{ij}y_j$, for $i = k, k + 1, \dots, m$.

Then we divide these constraints into two groups, the first group consisting of the constraints where $c_{i,k} > 0$ and the second group consisting of the constraints where $c_{i,k} < 0$. For both groups,

we divide by $c_{i,k}$, to produce explicit constraints on y_k , but for the second group we must change the order of the inequalities. The revised limits for y_k can now be written as

$$\check{a}'_k(y_1, \dots, y_{k-1}) = \max \left(\max_{c_{i,k} > 0} \left(\frac{a_i - \sum_{j=1}^{k-1} c_{i,j} y_j}{c_{i,k}} \right), \max_{c_{i,k} < 0} \left(\frac{b_i - \sum_{j=1}^{k-1} c_{i,j} y_j}{c_{i,k}} \right) \right) \quad (14)$$

$$\check{b}'_k(y_1, \dots, y_{k-1}) = \max \left(\check{a}'_k(y_1, \dots, y_{k-1}), \min \left(\min_{c_{i,k} > 0} \left(\frac{b_i - \sum_{j=1}^{k-1} c_{i,j} y_j}{c_{i,k}} \right), \min_{c_{i,k} < 0} \left(\frac{a_i - \sum_{j=1}^{k-1} c_{i,j} y_j}{c_{i,k}} \right) \right) \right)$$

In the cases where $c_{i,k} = 0$ for some i 's, with $i > k$, the associated constraints for these i 's do not affect y_k , so the constraints for some of other variables need to be adjusted. For these general cases, we first reorder all of the constraints into groups of sizes l_1, l_2, \dots, l_k , with $l_1 + l_2 + \dots + l_k = m$, so that if we denote the reordered constraints by $a \leq \bar{C}y \leq b$ then the first l_1 rows of \bar{C} have the form $(*, 0, \dots, 0)$, the next l_2 rows of \bar{C} have the form $(?, *, 0, \dots, 0)$, and so on with the last l_k rows of \bar{C} in the form $(?, \dots, ?, *)$, where $*$ denotes a nonzero and $?$ denotes zero or nonzero. Then, for each $i, i = 1, \dots, k$ the set of l_i constraints are rewritten and merged to produce a single constraint on y_i ; using the procedure that we described for y_k . When this process is complete, the integral for F can be written as

$$F(a, b, \Sigma) = (2\pi)^{-\frac{k}{2}} \int_{\check{a}'_1}^{\check{b}'_1} e^{-\frac{y_1^2}{2}} \int_{\check{a}'_2(y_1)}^{\check{b}'_2(y_1)} e^{-\frac{y_2^2}{2}} \dots \int_{\check{a}'_k(y_1, \dots, y_{k-1})}^{\check{b}'_k(y_1, \dots, y_{k-1})} e^{-\frac{y_k^2}{2}} dy \quad (15)$$

In order to put F into a form that is easy to use with standard numerical integration methods, two more transformations are required. First, let $y_i = \Phi^{-1}(z_i)$, for $i = 1, 2, \dots, k$ so that $\phi(y_i)dy_i = dz_i$. Then

$$F(a, b, \Sigma) = (2\pi)^{-\frac{k}{2}} \int_{d_1}^{c_1} \int_{d_2(z_1)}^{c_2(z_1)} \dots \int_{d_k(z_1, \dots, z_{k-1})}^{c_k(z_1, \dots, z_{k-1})} dz$$

with

$$d_i(z_1, \dots, z_{i-1}) = \bar{\Phi}(a'_i(\Phi^{-1}(z_1), \dots, \Phi^{-1}(z_{i-1}))),$$

and

$$c_i(z_1, \dots, z_{i-1}) = \bar{\Phi}(b'_i(\Phi^{-1}(z_1), \dots, \Phi^{-1}(z_{i-1}))),$$

Finally, let $z_i = d_i + (e_i - d_i)u_i$, for $i = 1, \dots, k$, so $dz_i = (e_i - d_i)du_i$. Then

$$F(a, b, \Sigma) = (e_1 - d_1) \int_0^1 (e_2(u_1) - d_2(u_1)) \dots \int_0^1 (e_k(u_1, \dots, u_{k-1}) - d_k(u_1, \dots, u_{k-1})) \int_0^1 du$$

The innermost integral is one, so the numerical problem involves the estimation of a $(k-1)$ dimensional integral.

3. NUMERICAL AND SIMULATION STUDIES

Assume that Z_j for $j = 1, \dots, m$ are independently and normally distributed with mean 0 and variance $(1 + \alpha_j^2)$. Let $\bar{Z} = \sum_{j=1}^m Z_j \alpha_j^2 / (1 + \alpha_j^2)$. [9] showed that the standardized multivariate normal random variables with singular correlation structure given in equation (3) can be generated by the transformation $X_j = a_j(Z_j - \bar{Z})$ for $j = 1, \dots, m$, where $\sum_{j=1}^m \alpha_j^2 / (1 + \alpha_j^2) = 1$. Therefore, for any given b_j and a_j for $j = 1, \dots, m$, we generate all the Z_j and transform each of them to X_j based on equation (4). Then, we observe whether absolute value of each X_j is less than its corresponding b_j for $j = 1, \dots, m$, respectively.

The process is repeated N times, and the nominal probabilities from the simulation and a standard error are calculated. Those simulated probabilities are compared with two bounds obtained numerically according to Section 2.1, and with the numerical evaluation of the F integrals described in Section 2.2. Randomized lattice rules were used for the numerical integration of F , and the absolute accuracy requested was 0.001 [13]. For this method, the amount of work required was measured as the number N of integrand values (values) required to estimate F with error less than 0.001. The error estimates used for the randomized lattice rules were three times the standard

errors for these randomized rules. In order to compare these values with values from the simulation method, we used the same for the simulation method, and report an error estimate for the simulation that is three times the standard error for the simulation method.

It is obvious that the differences among the two bounds are negligible in all the considered cases. However, the computational time of evaluating the bounds increases rapidly as m increases. It is impractical to compute the bounds for $m > 12$. The computational time of new approach described in Section 2.2 also increases with m , but the estimate values of all the cases considered in this study were obtained in a short period of computational time. The error estimates for the simulation method, using the same number of function values, were in all cases significantly larger than the error estimates for the new method. The new method can also be applied to the multivariate normal distributions with any arbitrary singular correlation structures. Therefore, we conclude that the proposed approach provides an efficient and accurate way to estimate the Fintegrals with any singular correlation matrices.

Table 1: Bounds and Estimated Values for MVN Probabilities

b_i 's			f Values	f Values
	Upper	Lower	Simulated	F Estimate
$\alpha_i^2/(1 + \alpha_i^2)$'s	Bound	Bound	Error Est.	Error Est.
(2.3, 2.2, 2.1, 2.0)			4224	4224
	.887369	.887310	.888968	.887541
(.2, .1, .4, .3)			.014504	.000374
(.5, 2.4, 1.0, 2.0, 1.6)			496	496
	.232658	.232373	.286290	.232567
(.1, .2, .2, .2, .3)			.060951	.000642
(2.2, 2.4, 2.5, 2.0, 2.1)			6992	6992
	.880775	.880773	.879720	.878440
(.3, .1, .05, .5, .05)			.011671	.000682
(2.4, .5, 1.2, .4, 1.9, 2.0)			496	496
	.089252	.089103	.066532	.089192
(.1, .1, .2, .2, .2, .2)			.033603	.000479
(1.6, 1.7, 1.8, 1.4, 2.1, 2.5, 1.6)			6692	6692
	.554366	.554366	.560212	.554429
(.1, .1, .2, .2, .2, .1, .1)			.017809	.000979
(2.0, 2.1, 1.9, 1.8, 2.0, 2.1, 2.2, 2.3)			6692	6692
	.714231	.714231	.698227	.713891
(.1, .1, .1, .1, .1, .15, .05, .2, 2)			.016470	.000985
(.4, 2.2, 2.5, 3.1, .9, 1.8, .8, 2.3, 2.9)			496	496
	.102861	.102861	.098790	.102832
(.01, .02, .07, .1, .15, .05, .3, .2, .1)			.040234	.000269
(2.8, 2.9, 2.8, 2.7, 2.4, 3.3, 3.4, 2.5, 2.6, 2.7)			1248	1248
	.935023	.935023	.927885	.934968
(.1, .05, .05, .04, .06, .1, .15, .15, .1, .2)			.021976	.000658
(3.0, 2.8, 2.4, 2.5, 1.9, 2.2, 2.1, 2.0, 2.4, 2.5, .9, 1.8)			6992	6992
	.475903	.475903	.496281	.475583
(.02, .08, .04, .06, .1, .1, .16, .14, .15, .1, .05)			.017939	.000827
(2.5, 2.7, 3.4, .9, 2.4, 1.7, 1.8, 2.3, 2.4, 2.6, .9, .8)			496	496
	.185877	.185877	.181452	.185936
(.01, .03, .06, .05, .05, .1, .15, .05, .1, .14, .16, .1)			.051966	.000689

4. CONCLUSION

Investigating the use of singular correlation matrices in the context of the multivariate normal distribution has shown an innovative method to handling the complexities involved in singular correlation matrices. This work is important because it advances statistical methods, especially in situations when singularity presents difficulties for traditional approaches.

A critical gap in statistical modeling is filled by the suggested method, as variable dependencies frequently result in singular correlation matrices. Historically, multivariate studies have faced

difficulties with singular matrices due to their non-invertibility. By utilizing singular correlation matrices to their full potential rather than viewing them as obstacles, the approach offers a more holistic viewpoint.

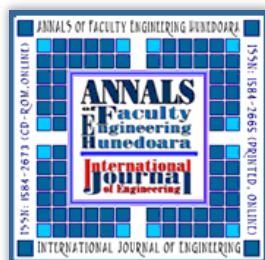
The effective use of the proposed method in the context of calculating simultaneous pairwise confidence intervals for multinomial proportions is one noteworthy application. This application becomes more significant with suitably large sample sizes. In these types of situations, singularities frequently impede the traditional techniques for calculating confidence intervals, producing undefinable or erroneous outcomes. The method, on the other hand, shows persistence in overcoming these difficulties, opening the door for more solid and trustworthy statistical conclusions.

The methodology's effectiveness is especially noticeable when multinomial percentage estimate is involved, as category dependencies can make standard studies more difficult. By using a novel method, the results not only get over the drawbacks of singular correlation matrices but also improve the accuracy of confidence interval estimations all at once and comprehensively.

With the growing complexity of real-world datasets in statistical studies, the suggested technique offers a useful resource for both practitioners and scholars. Its flexibility and efficiency when dealing with singular correlation matrices present a viable path for improving statistical modeling methods and enhancing the precision of conclusions in the areas of multinomial proportion estimation and multivariate normal distribution.

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