

Multiple Testing with Close to Equally Correlated Structure

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Abstract

In clinical trials with multiple primary endpoints or with multiple observations on the same sampling unit, the maximum of all observations is a convenient statistic that controls the familywise error rate. The quantile of this statistic depends on the correlation among multiple observations. To simplify modeling, the compound symmetry (CS) covariance structure is frequently used. The assumption of exact compound symmetry cannot usually be justified, and further sensitivity studies under more varied correlations are recommended. The need for multiple simulations may impose an increased demand on computer and time resources. To evaluate the sensitivity of simulation results restricted to CS structure, we calculated the linear part of the Taylor expansion of the CDF for the maximum statistic. Furthermore, we derived the Taylor expansion for quantiles of the maximum statistic. Our simulation studies on the linear approximation of quantiles confirmed good performance of the linearization formula.

Key words: Compound symmetry; Covariance matrices; Monte Carlo simulation; Quantile; Sensitivity analysis; Taylor expansion;

1. Introduction

In studies with multiple primary endpoints, or with multiple observations on the same sampling unit, the familywise error rate (Westfall and Young 1993) of random variables (RV) may be controlled by the maximum of the test statistic (Romano and Wolf 2005). As an alternative, adjustment formulae for the type I and II errors in multiple testing have been advocated in several studies (Armitage and Parmar 1986; Efron 1997; James 1991; Dubey 1985; Shi, Pavey and Carter 2012; Julious and McIntyre 2012). The tables of nominal significance levels (adjusted for multiplicity) for positively equally correlated normally distributed observations were generated (Dubey 1985; Pocock 1987).

Equally correlated RVs are defined by the multivariate normal distribution with the compound symmetry (CS) covariance structure. The tables of quantiles for the maximum of equally correlated normally distributed random variables were generated using a quadrature formulae for the integrals (Gupta, Nagel and Panchapakesan 1973; Gupta, Panchapakesan and Sohn 1983). Numerical integration is laborious, not practicable at high-dimensions, and is currently replaced by Monte Carlo (MC) simulations. Unfortunately, although MC simulations are relatively fast and simple, they are not very precise. Moreover, it is difficult to define the precision of simulated results without invoking other methods. The requirement of precision may impose a demand on the computer resources that may not be easily available, particularly for high-dimensional modeling. Microarray data analysis is an example of high-dimensional modeling (Jung, Bang, and Young 2005), where dimensions may be in the thousands. Because of this, the CS correlation structure is frequently used as a simple simulation model (Jung et al. 2005). The CS assumption cannot often be justified, and sensitivity studies are recommended (Jung et al. 2005). In sensitivity studies, correlation matrices are usually

assumed to be close to the original CS matrices. However, the number of correlation coefficients to examine is proportional to the square of the dimension of the model and may be excessively high. To extend the results acquired under the CS assumption on more general correlation structures without additional simulations and with a satisfactory precision, we derive the linear part of the Taylor expansion of CDF with a close to CS structure. Using a linear approximation, we can calculate the CDF for the RVs with such structure. We derived the Taylor expansion for the quantiles of the maximum of RVs with close to CS structure and tabulated their linear parts for $n \leq 9$. If a researcher is interested in higher than the tabulated dimensions or different correlations, the linear part of the Taylor expansion can be calculated using the provided formulae. Once generated, the Taylor expansion allows a researcher to compute the required quantiles using a simple calculator. In our numerical studies, we used SAS 9.4 proc IML to generate the samples of correlated normally distributed variables. In the equally correlated cases, the golden standards of precision were the tables of Gupta et al. (Gupta 1963; Gupta et al. 1973; Gupta et al. 1983).

The 2×2 covariance matrices were not studied in this paper because they belong to the CS class and were tabulated by Gupta et al. in earlier work (Gupta 1963, table II; Gupta et al. 1973, table I; Gupta et al. 1983, table IV). The macros for the cumulative probabilities of bivariate normal distribution are readily available on the Web (for example, <http://socr.ucla.edu/htmls/HTML5/BivariateNormal/>).

The proofs for the 3×3 and $n \times n$ ($n \geq 4$) cases are slightly different and are therefore provided separately.

2. The Linear Approximation

Let $R = \{r_{hl}\}_{h,l \leq n}$ be a positive definite correlation matrix and $Q_n(y, R) = P\{\max_{1 \leq i \leq n} Y_i^R \leq y\}$, where the random variables Y_i^R are normally distributed with the correlation matrix R . Without loss of generality we assume that $E(Y_i^R) = 0$. Then,

$$Q_n(y, R) = \frac{1}{(2\pi)^{n/2} |R|^{1/2}} \int_{-\infty}^y \dots \int_{-\infty}^y \exp\left(-\frac{1}{2} X^T R^{-1} X\right) dx_1 \dots dx_n, \quad \text{where}$$

$$X = (x_1, x_2, \dots, x_n)^T \text{ and } |R| = \det(R).$$

Let $D(q)$ be a CS correlation matrix with non-diagonal entries q and each diagonal entry equals one. We use the notation $D = D(\rho)$ if $q = \rho$ for brevity. Let us define the PDF $f(t, \sigma) = (\sigma\sqrt{2\pi})^{-1} e^{-(0.5t^2/\sigma^2)}$, the CDF $\Phi(y, \sigma) = \int_{-\infty}^y f(t, \sigma) dt$, and $\nu = \frac{\sqrt{1+\rho}}{\sqrt{1-\rho}}$. We denote the $1-\alpha$ quantiles for the maximum of correlated random variables with correlation matrices D and R by y'_α and y_α , e.g., $Q_n(y'_\alpha, D) = 1-\alpha$ and $Q_n(y_\alpha, R) = 1-\alpha$.

2.1 Case $n = 3$

The matrix D is positive definite if $1 > \rho > -1/2$. By definition

$$Q_3(y, D) = (2\pi)^{-1.5} \sigma_0^{-1} \int_{-\infty}^y \int_{-\infty}^y \int_{-\infty}^y e^{-0.5X^T D^{-1} X} \prod_{i=1}^3 dx_i,$$

where $\sigma_0^2 = |D| = (1 - \rho)^2(1 + 2\rho)$ and $X^T = (x_1, x_2, x_3)$.

For the 3×3 correlation matrix R such that $r_{hh} = r_{hl} = \rho + \varepsilon_{hl}$ ($h \neq l$), we have the following formula:

$$\partial Q_3(y, R) / \partial \varepsilon_{hl} |_{\varepsilon_{hl}=0} = v \left[f(y, \sqrt{1 + \rho}) \right]^2 \Phi(y / (v\sqrt{1 + 2\rho}), 1) \quad (1).$$

The proof is provided in Appendix A.

For the correlation matrix R , we have the approximate formula for the upper α quantile as follows:

$$y_\alpha = y'_\alpha - (\varepsilon_{12} + \varepsilon_{13} + \varepsilon_{23}) \frac{1}{3} \frac{f(y'_\alpha, v)}{1 - \rho} \frac{\Phi(y'_\alpha / (v\sqrt{1 + 2\rho}), 1)}{Q_2\left(y'_\alpha / v, D\left(\frac{\rho}{1 + \rho}\right)\right)} + o(\max |\varepsilon_{hl}|), \quad (2)$$

where $Q_2\left(y'_\alpha / v, D\left(\frac{\rho}{1 + \rho}\right)\right)$ is the CDF of a bivariate normal distribution with the correlation coefficient $\frac{\rho}{1 + \rho}$ and the upper limit of integration $(y'_\alpha / v, y'_\alpha / v)$.

The proof is provided in Appendix C.

The tables for the quantile y'_α of the distributions with CS correlation matrices are available in a variety of papers by Gupta (Gupta 1963, table II; Gupta et al. 1973, table I; Gupta et al. 1983, table IV) (see also Tables 2 and 4).

The macro for the CDF of bivariate normal distribution is readily available on the Web (for example, <http://socr.ucla.edu/htmls/HTML5/BivariateNormal/>).

Using formula (2), we can approximately evaluate quantiles for the close to CS correlation matrices R if the values of $F_3 = \frac{1}{3} \frac{f(y'_\alpha, v)}{1 - \rho} \frac{\Phi(y'_\alpha / (v\sqrt{1 + 2\rho}), 1)}{Q_2\left(y'_\alpha / v, D\left(\frac{\rho}{1 + \rho}\right)\right)}$ are

known. The values of F_3 and quantiles for $\rho = 0.1, \dots, 0.9$ and $\alpha = 0.05, 0.1$ are provided in Tables 1 and 3.

2.2 Case $n \geq 4$

The matrix D is positive definite if $1 > \rho > -1/(n-1)$. The $n \times n$ correlation matrix R such that $r_{hh} = r_{hl} = \rho + \varepsilon_{hl}$ ($h \neq l$) is expressed by the formula

$$\partial Q_n(y, R) / \partial \varepsilon_{hl} |_{\varepsilon_{hl}=0} = v \left[f(y, \sqrt{1+\rho}) \right]^2 Q_{n-2} \left(\frac{y}{v\sqrt{2\rho+1}}, D \left(\frac{\rho}{1+2\rho} \right) \right). \quad (3)$$

The proof is provided in Appendix B.

It is easy to see that

$Q_n(y, R) = [\Phi(y, 1)]^n + [f(y, 1)]^2 [\Phi(y, 1)]^{n-2} \sum_{h<l} \varepsilon_{hl} + o(\max |\varepsilon_{hl}|)$ (Zaslavsky and Chen, 2016), if $\rho = 0$. The case of $\sum_{h<l} \varepsilon_{hl} < 0$ is allowed if $Q_n(y, R)$ is positive definite and $\sum_{h<l} |\varepsilon_{hl}|$ is sufficiently small.

From formula (3) and formula $Q_n(y, D) = \int_{-\infty}^{\infty} \left[\Phi \left(\frac{y - \sqrt{\rho}x}{\sqrt{1-\rho}}, 1 \right) \right]^n f(x, 1) dx$ (Steck and Owen 1962; Tong 1990, p.115) it follows that $\partial Q_n(y, R) / \partial \varepsilon_{hl} |_{\varepsilon_{hl}=0}$ is a decreasing to zero function of n as $n \rightarrow \infty$.

For the correlation matrix R , we have the approximate formula for the upper α quantile as follows:

$$y_\alpha = y'_\alpha - \sum_{h<l} \varepsilon_{hl} F_n + o(\max |\varepsilon_{hl}|), \quad (4)$$

$$\text{where } F_n = \frac{1}{n} \frac{f(y'_\alpha, v)}{1-\rho} \frac{Q_{n-2} \left(\frac{y'_\alpha}{v\sqrt{2\rho+1}}, D \left(\frac{\rho}{1+2\rho} \right) \right)}{Q_{n-1}(y'_\alpha / v, D(\frac{\rho}{1+\rho}))}$$

The proof is provided in Appendix C.

It is easy to see that $y_\alpha = y'_\alpha - n^{-1} f(y'_\alpha, 1) (1-\alpha)^{-1/n} \sum_{h<l} \varepsilon_{hl} + o(\max |\varepsilon_{hl}|)$ (Zaslavsky and Chen 2016), if $\rho = 0$.

The values of F_n and quantiles for $\rho = 0.1, \dots, 0.9$, $n = 3, \dots, 9$ and $\alpha = 0.05, 0.1$ are provided in Tables 1 and 3.

It is worth mentioning that numerical calculation of F_n in Tables 1 and 3 for $n = 3$ were performed using SAS functions PDF, CDF, and PROBBNORM. If using the MC simulation (procedure IML) instead of PROBBNORM, the result may be slightly less precise.

3. Performance of the Linear Approximation

In our numerical studies, we used SAS 9.4 proc IML. The MC simulation was a fast but not very precise method. We compared the MC simulation results for quantiles with the estimates by Gupta et al. (Gupta et al. 1983) that were obtained using quadrature formulae for the integrals. Gupta et al. claim that the precision is 10^{-8} but published 10^{-5} estimates. To achieve 10^{-4} precision in the evaluation of quantiles using MC simulation, we used 10^7 of draws from the multivariate normal distribution. Because of memory restriction (100GB of RAM allocated to SAS), we were unable to increase the number of draws sufficiently to achieve a higher precision. With 10^{-4} precision in mind, we calculated the 95% and 90% quantiles for the maximum of RVs with matrices $D(\rho + \varepsilon)$ by formulae (2) and (4) and by the exact MC simulation. With $|\varepsilon| \leq 0.05$, both results were very close. In Tables 5 - 8 we provide the estimates of 95% and 90% quantiles for $D(0.5 \pm 0.05)$ and $D(0.2 \pm 0.05)$. If formula (4) were precise, $P\{\max_{1 \leq i \leq n} Y_i^{D(\rho+\varepsilon)} \leq y_\alpha\} - (1 - \alpha) = 0$. Because it is approximate, the value $P\{\max_{1 \leq i \leq n} Y_i^{D(\rho+\varepsilon)} \leq y_\alpha\} - (1 - \alpha)$ is a measure of the precision for the estimates of quantiles.

With an increase in the dimension n , the perturbation $\sum_{h < l} \varepsilon_{hl} = \varepsilon n(n-1)/2$ increases, but the error of formulae (2) and (4) remains at $\leq 3 \times 10^{-4}$.

4. Pharmaceutical Example

The objectives of the study (Littell, Pendergast and Natarajan 2000) were to compare the effects of two drugs and a placebo on a measure of respiratory ability, called forced expiratory volume (FEV1). Twenty-four patients were assigned to each of the three treatment groups, and FEV1 was measured at baseline (immediately prior to administration of the drugs) and at hourly intervals thereafter for eight hours. Data were analyzed using SAS PROC MIXED. The correlations for different correlation structures of repeated measures are given in (Littell et al. table II, 2000) for one of the drugs. Of these correlation structures, we consider CS and Toeplitz models. The off-diagonal entries of the CS correlation matrix are $\rho = 0.766$. The Toeplitz correlation matrix is defined by off-main-diagonal diagonals with diagonal-wise equal entries. Counting from the 7-dimensional diagonal down to the one-dimensional diagonal, the corresponding entries are defined by the following numerical values: 0.858, 0.811, 0.777, 0.716, 0.686, 0.635, and 0.593. We calculated the 95% quantile of the maximum of FEV1 for the CS model and for the Toeplitz model using formula (4), the quantile $y'_{0.05} = 2.17734$, $F_8 = 0.03784$ for $n = 8$ and $\rho = 0.8$ (see Tables 1 and 2). The estimate of the 95% quantile for the CS model with $\rho = 0.766$ using formula (4) is 2.2134, and the corresponding probability for this estimate is 0.9503 (0.03% error). For comparison, the exact value of the 95% quantile for the CS matrix with $\rho = 0.766$ is 2.2106. The estimate of the 95% Toeplitz quantile using formula (4) is 2.1449, and the corresponding

probability is 0.9449 (0.51% error). For comparison, the exact value of the 95% quantile for the Toeplitz matrix is 2.1890. Thus, formula (4) performs well for the CS matrices and should include a margin of error in α if applied to the matrices substantially deviating from the CS structure.

5. Conclusion.

By determining the proper choice of deviation ε_{hl} from the CS structure, a researcher has some freedom to better reflect the correlation structure of multiple correlated testing and to verify the sensitivity of the results. The numerical study shows that the precision of the linear approximation (4) is $\leq 3 \times 10^{-4}$ if the perturbation of each entry of the correlation matrix is ≤ 0.05 and the dimension ≤ 9 .

The high dimensional and high precision studies with multiple testing may require advanced hardware and special software. The performance of linear approximation for high dimensions may be a topic of further research. If the precision of linear approximation is verified for high dimensions, using linear approximation may substantially simplify research as an alternative to the computer simulations for each particular ε_{hl} .

Disclaimer

The opinions and information in this article are those of the author and do not represent the views and/or policies of the U.S. Food and Drug Administration.

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Appendix A: The proof of formula (1).

It is evident that $\partial Q(y, D) / \partial \varepsilon_{hl}$ are equal for all $h \neq l$. Therefore we need to proof that

$$\partial Q(y, D) / \partial \varepsilon_{hl} = v \left[f(y, \sqrt{1 + \rho}) \right]^2 \Phi \left(y / (v \sqrt{1 + 2\rho}), 1 \right) \quad , \quad \text{or} \quad , \quad \text{equivalently,}$$

$$\partial Q(y, D) / \partial \varepsilon_{hl} = v \left[f(y, \sqrt{1 + \rho}) \right]^2 \Phi \left(y / v^2, \frac{\sqrt{1 + 2\rho}}{v} \right) .$$

Proof.

$$\text{Let } D = \begin{bmatrix} 1 & \rho & \rho \\ \rho & 1 & \rho \\ \rho & \rho & 1 \end{bmatrix} \text{ and } D^{-1} = (1 - \rho)^{-1} (2\rho + 1)^{-1} \begin{bmatrix} (\rho + 1) & -\rho & -\rho \\ -\rho & (\rho + 1) & -\rho \\ -\rho & -\rho & (\rho + 1) \end{bmatrix} .$$

Let R be a correlation matrix with the non-diagonal entries $r_{hl} = \rho + \varepsilon_{hl}$. According to (Berman, 1964), the derivative $\partial Q(y, R) / \partial \varepsilon_{12}$ at $\varepsilon_{hl} = 0$ ($h < l$) is given by the

derivative $\partial Q(y, R) / \partial \varepsilon_{12}$ at $\varepsilon_{hl} = 0$ ($h < l$) is given by $\partial Q(y, R) / \partial \varepsilon_{12} |_{\varepsilon_{hl}=0} = (2\pi)^{-1.5} \sigma_0^{-1} \int_{-\infty}^y e^{-0.5Z^T D^{-1}Z} dz$, where $Z^T = (y, y, z)$. It is clear that $Z^T D^{-1}Z = (1-\rho)^{-1}(2y^2 + z^2 - (2\rho+1)^{-1}\rho(2y+z)^2)$.

Let $z = t + \frac{2a\rho y}{1-a\rho}$, where $a = (1+\rho)^{-1}$. Then $z = (t+t\rho+2y\rho)/(1+\rho)$ and $Z^T D^{-1}Z = \frac{(1+\rho)}{(1-\rho)(2\rho+1)}t^2 + \frac{1}{(1+\rho)}2y^2$

By changing variables in the integral, the upper limit of integration $z = y$ is transformed into the upper limit of integration $t = y(1-\rho)/(1+\rho)$. It is clear that $dz = dt$. Thus

$$\partial Q(y, R) / \partial r_{12} = (2\pi)^{-1.5} \sigma_0^{-1} e^{-y^2/(1+\rho)} \int_{-\infty}^{y(1-\rho)/(1+\rho)} e^{-0.5\sigma_0^{-2}(1-\rho)(1+\rho)t^2} dt$$

$$\partial Q(y, R) / \partial r_{12} = (2\pi)^{-1.5} \sigma_0^{-1} e^{-y^2/(1+\rho)} \int_{-\infty}^{y\frac{(1-\rho)}{(1+\rho)}} e^{-0.5\frac{(1+\rho)}{(1-\rho)(1+2\rho)}t^2} dt. \text{ It is clear that}$$

$$(2\pi)^{-1.5} \sigma_0^{-1} \frac{1+\rho}{1+\rho} e^{-y^2/(1+\rho)} = (2\pi)^{-0.5} \sigma_0^{-1} (1+\rho) f^2(y, \sqrt{1+\rho}). \text{ Then}$$

$$(2\pi)^{-1.5} \sigma_0^{-1} \frac{1+\rho}{1+\rho} e^{-y^2/(1+\rho)} = (2\pi)^{-0.5} \sigma_0^{-1} \frac{\sqrt{(1+\rho)}\sqrt{(1+\rho)}\sqrt{(1-\rho)}}{\sqrt{(1-\rho)}} f^2(y, \sqrt{1+\rho})$$

$$(2\pi)^{-1.5} \sigma_0^{-1} \frac{1+\rho}{1+\rho} e^{-y^2/(1+\rho)} = (2\pi)^{-0.5} \frac{\nu\sqrt{(1+\rho)}\sqrt{(1-\rho)}}{\sigma_0^{-1}} f^2(y, \sqrt{1+\rho}). \text{ We use the identities:}$$

$$\sigma_0 / \sqrt{(1-\rho)(1+\rho)} = ((1-\rho)^2(1+2\rho))^{0.5} / \sqrt{(1-\rho)(1+\rho)} =$$

$$\sigma_0 / \sqrt{(1-\rho)(1+\rho)} = \left(\frac{1-\rho}{1+\rho}(1+2\rho)\right)^{0.5} = (1+2\rho)^{0.5} / \nu$$

$$\partial Q(y, R) / \partial r_{12} = (2\pi)^{-1.5} \sigma_0^{-1} e^{-y^2/(1+\rho)} \int_{-\infty}^{y(1-\rho)/(1+\rho)} e^{-0.5\sigma_0^{-2}(1-\rho)(1+\rho)t^2} dt$$

$$\partial Q(y, D) / \partial \varepsilon_{hl} = \nu \left[f(y, \sqrt{1+\rho}) \right]^2 \Phi(y / \nu^2, \sigma_0 / \sqrt{(1-\rho)(1+\rho)}), \text{ where}$$

$$\sigma_0 = ((1-\rho)(1+2\rho))^{0.5}.$$

$$\sigma_0 / \sqrt{(1-\rho)(1+\rho)} = ((1-\rho)(1+2\rho))^{0.5} / \sqrt{(1-\rho)(1+\rho)} = \frac{\sqrt{1+2\rho}}{\nu}$$

$$(2\pi)^{-1.5} \sigma_0^{-1} \frac{1+\rho}{1+\rho} e^{-y^2/(1+\rho)} = (2\pi)^{-0.5} \sigma_0^{-1} (1+\rho) f^2(y, \sqrt{1+\rho})$$

Thus $\partial Q(y, D) / \partial \varepsilon_{hl} = v \left[f(y, \sqrt{1+\rho}) \right]^2 \Phi(y / v^2, \frac{\sqrt{(1+2\rho)}}{v})$. It can be reduced to form (1) by change of variables.

Appendix B: The proof of formula (3).

The given below proof is not applicable to the 3×3 case because it uses the assumption $n \geq 4$. However, formula (1) for the 3×3 case can be interpreted as a trivial form of formula (3) for a one-dimensional CS correlation “matrix” with the single “diagonal” entry “one”.

Lemma 1. For a CS matrix with the non-diagonal entries α and the diagonal entries β , the inverse matrix is a CS matrix with the non-diagonal entries $\frac{-\alpha}{(\beta - \alpha)((n-1)\alpha + \beta)}$ and the diagonal entries $\frac{(n-2)\alpha + \beta}{(\beta - \alpha)((n-1)\alpha + \beta)}$. Similarly, for the $n \times n$ matrix D^{-1} the non-diagonal entries are $a = \frac{-\rho}{(1-\rho)((n-1)\rho + 1)}$ and the diagonal entries are $b = \frac{(n-2)\rho + 1}{(1-\rho)((n-1)\rho + 1)}$.

Proof. Consider for simplicity the matrix D^{-1} .

Let $d' = (1, \dots, 1)$. Then $D = (1-\rho)(I + \frac{\rho}{1-\rho} dd')$ and $D^{-1} = (1-\rho)^{-1}(I - \lambda \rho dd')$, where $\lambda = ((n-1)\rho + 1)^{-1}$. The non-diagonal entries are $a = -\lambda \rho (1-\rho)^{-1} = \frac{-\rho}{(1-\rho)((n-1)\rho + 1)}$ and the diagonal entries are $b = \frac{1-\lambda \rho}{(1-\rho)} = \frac{(n-2)\rho + 1}{(1-\rho)((n-1)\rho + 1)}$.

Lemma 2. Let A_n be a $n \times n$ CS matrix with non-diagonal entries a and the diagonal entries b . Let $c = -\frac{2ay}{(n-3)a + b}$, $\bar{t}_{n-2} = (t_3, t_4, \dots, t_n)'$ and $\bar{t}_n = (y, y, t_3 + c, \dots, t_n + c)'$. Then

$\bar{t}_n' A_n \bar{t}_n = \frac{2}{(n-3)a+b} [(n-2)ab - (n-1)a^2 + b^2] y^2 + \bar{t}_{n-2}' A_{n-2} \bar{t}_{n-2}$, where A_{n-2} is a $(n-2) \times (n-2)$ principle submatrix of the matrix A_n . The proof can be achieved by the algebraic calculations.

Using notations of Lemma 1, we get for the matrix D^{-1} :

$$\frac{2}{(n-3)a+b} ((n-2)ab - (n-1)a^2 + b^2) = \frac{2}{1+\rho}$$

Lemma 3. For a CS $n \times n$ matrix A_n with the non-diagonal entries a and the diagonal entries b , the determinant $|A_n| = (b-a)^{n-1}((n-1)a+b)$.

Proof. The matrix A_n has $n-1$ eigenvalues $(b-a)$ corresponding to eigenvectors $(-1, 0, \dots, 0, 1, 0, \dots, 0)'$ and the eigenvalue $((n-1)a+b)$ corresponding to the eigenvector $(1, 1, \dots, 1)'$.

Proof of the theorem.

By a permutation transformation of the matrix R , any non-diagonal entry of R can be placed into the first row and the second column. Therefore, without loss of generality, we study the perturbation of the entry r_{12} .

Consider the case of the correlation matrix R with the entry $r_{12} = \rho + \varepsilon_{12}$ and $r_{hl} = \rho$ for the rest of $h < l$. Then (Berman, 1964) $\partial Q(y, R) / \partial r_{12}(r_{hl} = \rho)$ ($h < l$) is

$$\partial Q_n(y, R) / \partial r_{12}(r_{hl} = \rho) = \frac{1}{(2\pi)^{n/2} |D|^{1/2}} \int_{-\infty}^y \dots \int_{-\infty}^y \exp\left(-\frac{1}{2} \bar{\tau}_n' D^{-1} \tau_n\right) dx_3 \dots dx_n, \quad \text{where}$$

$|D| = (1-\rho)^{n-1}(1+(n-1)\rho)$ and $\tau_n = (y, y, x_3, \dots, x_n)'$. According to Lemma 1, the D^{-1} is a CS matrix with the non-diagonal entries a and the diagonal entries b . Let us

change the variables as follows: $x_i = t_i - \frac{2ay}{(n-3)a+b}$ $i = (3, \dots, n)$. Then the upper

integration limit for t_i is $\tilde{y} = y + \frac{2ay}{(n-3)a+b} = y \frac{b+(n-1)a}{(n-3)a+b}$. From Lemma 1 it

follows that $\tilde{y} = \frac{1-\rho}{1+\rho} y = y / v^2$.

From Lemma 2 it follows that

$$\partial Q_n(y, R) / \partial r_{12} = \frac{\exp(-y^2 / (1+\rho))}{(2\pi)^{n/2} |D|^{1/2}} \int_{-\infty}^{\tilde{y}} \dots \int_{-\infty}^{\tilde{y}} \exp(-0.5 \bar{t}_{n-2}' A_{n-2} \bar{t}_{n-2}) dt_3 \dots dt_n.$$

It is clear that $\frac{\exp(-y^2/(1+\rho))}{(2\pi)^{n/2} |D|^{1/2}} = \frac{(1+\rho)f^2(y, \sqrt{1+\rho})}{(2\pi)^{n/2-1} |D|^{1/2}}$, where

$|D| = (1-\rho)^{n-1}(1+(n-1)\rho)$. We use the notation

$$K = \frac{(1+\rho)}{(2\pi)^{n/2-1} [(1-\rho)^{n-1}(1+(n-1)\rho)]^{1/2}} \quad \text{and}$$

$$J(\tilde{y}) = \int_{-\infty}^{\tilde{y}} \dots \int_{-\infty}^{\tilde{y}} \exp(-0.5 \bar{t}'_{n-2} A_{n-2} \bar{t}_{n-2}) dt_3 \dots dt_n. \quad \text{Then}$$

$$\partial Q_n(y, R) / \partial r_{12} = f^2(y, \sqrt{1+\rho}) K J(\tilde{y}).$$

Let us Consider the $n-2$ –dimensional integral $J(\tilde{y})$.

If $n = 3$, from lemma 1 and 2 it follows $A_{n-2} = (1+\rho)(1-\rho)^{-1}(1+2\rho)^{-1}$. Let $n \geq 4$, then the diagonal entries of a $(n-2) \times (n-2)$ matrix A_{n-2} are

$$\beta = \frac{(n-2)\rho+1}{(1-\rho)((n-1)\rho+1)} \quad \text{and the non-diagonal entries are } \alpha = \frac{-\rho}{(1-\rho)((n-1)\rho+1)}.$$

The matrices $B = A_{n-2}^{-1}$ and $B^{-1} = A_{n-2}$ belong to the CS class. According to Lemma 1,

the diagonal entries of $B = A_{n-2}^{-1}$ are $\gamma = \frac{-2\rho^2 + \rho + 1}{\rho + 1} = \frac{1-\rho}{\rho+1}(2\rho+1) = \frac{2\rho+1}{\nu^2}$ and

the non-diagonal entries are $\rho \frac{1-\rho}{\rho+1}$. In order to evaluate the integral $J(\tilde{y})$ using

published tables for the CS integral, we need to normalize the entries on the main diagonal of the matrix $B = A_{n-2}^{-1}$. To do so, we change the variables in the integral as

follows $\bar{t} = \bar{z} / \gamma^{1/2}$, where \bar{z} is a $n-2$ dimensional vector. Then the upper limits of integration by variable \bar{z} is $\gamma^{-1/2} \tilde{y}$. The diagonal entries of $\gamma B^{-1} = \gamma A_{n-2}$ are

$$\gamma \frac{(n-2)\rho+1}{(1-\rho)((n-1)\rho+1)} \quad \text{and the diagonal entries of } (\gamma B^{-1})^{-1} = \gamma^{-1} B \text{ are } \gamma^{-1} \gamma = 1. \text{ The}$$

non-diagonal entries of $\gamma^{-1} B$ are $\gamma^{-1} \rho \frac{1-\rho}{\rho+1} = \frac{\rho}{2\rho+1}$. Thus $J(\tilde{y}) = \gamma^{(n-2)/2} J(\gamma^{-1/2} \tilde{y})$.

To calculate $KJ(\tilde{y})$, we use the $n-2$ dimensional CDF

$$Q_{n-2}(\gamma^{-1/2} \tilde{y} | \frac{\rho}{2\rho+1}) = \frac{1}{(2\pi)^{(n-2)/2} |\gamma^{-1} B|^{1/2}} \int_{-\infty}^{\gamma^{-1/2} \tilde{y}} \dots \int_{-\infty}^{\gamma^{-1/2} \tilde{y}} \exp(-0.5 \bar{z}'_{n-2} \gamma B^{-1} \bar{z}_{n-2}) dz_3 \dots dz_n$$

, where $|\gamma^{-1} B| = \left[\frac{\rho+1}{2\rho+1} \right]^{n-3} \frac{(n-1)\rho+1}{2\rho+1}$. Then

$$J(\gamma^{-1/2} \tilde{y}) = (2\pi)^{(n-2)/2} |\gamma^{-1} B|^{1/2} Q_{n-2} \left[\gamma^{-1/2} \tilde{y}, D \left[\frac{\rho}{2\rho+1} \right] \right] \text{ and}$$

$$KJ(\tilde{y}) = K\gamma^{(n-2)/2} J(\gamma^{-1/2} \tilde{y}) = K\gamma^{(n-2)/2} (2\pi)^{(n-2)/2} |\gamma^{-1} B|^{1/2} Q_{n-2} \left[\gamma^{-1/2} \tilde{y}, D \left[\frac{\rho}{2\rho+1} \right] \right] =$$

$$KJ(\tilde{y}) =$$

$$\frac{(1+\rho)}{(2\pi)^{n/2-1} [(1-\rho)^{n-1} (1+(n-1)\rho)]^{1/2}} (2\pi)^{(n-2)/2} \left[\left[\frac{\rho+1}{2\rho+1} \right]^{n-3} \frac{(n-1)\rho+1}{2\rho+1} \right]^{1/2} \left[\frac{1-\rho}{\rho+1} (2\rho+1) \right]^{n-2} Q_{n-2} \left[\gamma^{-1/2} \tilde{y}, D \left[\frac{\rho}{2\rho+1} \right] \right]$$

Thus

$$\frac{\partial Q_n(y, R)}{\partial r_{12}} = \sqrt{\frac{1+\rho}{1-\rho}} f^2(y, \sqrt{1+\rho}) Q_{n-2} \left[\gamma^{-1/2} \tilde{y}, D \left[\frac{\rho}{2\rho+1} \right] \right], \quad \text{where}$$

$$\gamma^{-1/2} \tilde{y} = \sqrt{\frac{1-\rho}{1+\rho}} (2\rho+1)^{-1/2} y. \quad \text{Using the notation } v = \sqrt{\frac{1+\rho}{1-\rho}}, \quad \text{we get}$$

$$\frac{\partial Q_n(y, R)}{\partial r_{12}} = v f^2(y, \sqrt{1+\rho}) Q_{n-2} \left[\frac{y}{v\sqrt{2\rho+1}}, D \left[\frac{\rho}{2\rho+1} \right] \right].$$

Appendix C: The proof of formula (4).

We consider the case of $n \geq 4$. The proof of the case of $n = 3$ is similar.

From formula (3), it follows that by definition, $Q(y'_\alpha, D) = Q(y_\alpha, R) = 1 - \alpha$. Thus

$$Q_n(y_\alpha, R) = Q_n(y_\alpha, D) + v \left[f(y_\alpha, \sqrt{1+\rho}) \right]^2 Q_{n-2} \left(y_\alpha / (v\sqrt{1+2\rho}), D \left[\frac{\rho}{1+2\rho} \right] \right) \sum_{h<l} \varepsilon_{hl} + o(\max |\varepsilon_{hl}|)$$

Therefore

$$Q_n(y'_\alpha, D) = Q_n(y_\alpha, D) + v \left[f(y_\alpha, \sqrt{1+\rho}) \right]^2 Q_{n-2} \left(y_\alpha / (v\sqrt{1+2\rho}), D \left[\frac{\rho}{1+2\rho} \right] \right) \sum_{h<l} \varepsilon_{hl} + o(\max |\varepsilon_{hl}|)$$

Let $\Delta y = y'_\alpha - y_\alpha$. Because the functions in this expression are smooth and restricted in y'_α , we can expand $Q_n(y'_\alpha, D) - Q_n(y_\alpha, D)$ into an infinite series by small ε_{hl} . Presenting Δy as an infinite series by ε_{hl} with unknown coefficients and expanding the left hand side by ε_{hl} , we get that $\Delta y = O(\max |\varepsilon_{hl}|)$. Therefore,

$$Q(y_\alpha, D) - Q(y'_\alpha, D) = -\Delta y \partial Q(y'_\alpha, D) / \partial y + o(\Delta y) \text{ and}$$

$$-\Delta y \partial Q_n(y'_\alpha, D) / \partial y + o(\Delta y) =$$

$$v \left[f(y'_\alpha, \sqrt{1+\rho}) \right]^2 Q_{n-2} \left(y'_\alpha / (v\sqrt{1+2\rho}), D \left[\frac{\rho}{1+2\rho} \right] \right) \sum_{h < l} \varepsilon_{hl} + o(\max | \varepsilon_{hl} |)$$

To calculate $\partial Q(y'_\alpha, D) / \partial y$, we use the following formula (Steck and Owen 1962, (A)):

$$Q_n(y, D) = n \int_{-\infty}^y f(x, 1) Q_{n-1} \left[x / v, D \left[\frac{\rho}{1+\rho} \right] \right] dx.$$

$$\text{Then } \partial Q_n(y'_\alpha, D) / \partial y = n f(y'_\alpha, 1) Q_{n-1} \left[y'_\alpha / v, D \left[\frac{\rho}{1+\rho} \right] \right].$$

Thus,

$$-f(y'_\alpha, 1) Q_{n-2} \left[y'_\alpha / v, \left[\frac{\rho}{1+\rho} \right] \right] \Delta y =$$

$$\sum_{h < l} \varepsilon_{hl} \frac{v}{n} \left[f(y'_\alpha, \sqrt{1+\rho}) \right]^2 Q_{n-2} \left(y'_\alpha / (v\sqrt{1+2\rho}), D \left[\frac{\rho}{1+2\rho} \right] \right) + o(\max | \varepsilon_{hl} |)$$

$$\text{By a simple algebra, } \frac{\left[f(y'_\alpha, \sqrt{1+\rho}) \right]^2}{f(y'_\alpha)} = \frac{v}{1+\rho} f(y'_\alpha, v).$$

Finally,

$$y_\alpha = y'_\alpha - \left(\sum_{h < l} \varepsilon_{hl} \right) \frac{1}{n} \frac{f(y'_\alpha, v)}{1-\rho} \frac{Q_{n-2} \left(y'_\alpha / (v\sqrt{1+2\rho}), D \left[\frac{\rho}{1+2\rho} \right] \right)}{Q_{n-1} \left[y'_\alpha / v, D \left[\frac{\rho}{1+\rho} \right] \right]} +$$

$$o(\max | \varepsilon_{hl} |) + o(\Delta y)$$

Table 1. The values of F_n for $\rho = 0.1, \dots, 0.9$ and $\alpha = 0.05$

n / ρ	3	4	5	6	7	8	9
0.1	0.02173	0.01315	0.00890	0.00647	0.00494	0.00390	0.00317
0.2	0.03120	0.01928	0.01327	0.00977	0.00753	0.00601	0.00493
0.3	0.04285	0.02684	0.01863	0.01380	0.01069	0.00857	0.00704
0.4	0.05742	0.03615	0.02517	0.01868	0.01450	0.01163	0.00956
0.5	0.07599	0.04790	0.03334	0.02474	0.01917	0.01536	0.01262
0.6	0.10077	0.06338	0.04404	0.03260	0.02524	0.02019	0.01656
0.7	0.13647	0.08549	0.05917	0.04369	0.03375	0.02694	0.02215
0.8	0.20202	0.12169	0.08389	0.06170	0.04754	0.03784	0.03095
0.9	0.32677	0.20202	0.13849	0.10144	0.07783	0.06178	0.05042

Table 2. The values of 95% quantile ($\alpha = 0.05$) for $\rho = 0.1, \dots, 0.9$

n / ρ	3	4	5	6	7	8	9
0.1	2.11585	2.22762	2.31157	2.37849	2.43398	2.48126	2.5224
0.2	2.10707	2.21796	2.30056	2.3664	2.42098	2.46749	2.50793
0.3	2.09693	2.2042	2.2847	2.34882	2.40194	2.44718	2.4865
0.4	2.08197	2.1854	2.26291	2.32458	2.37562	2.41904	2.45675
0.5	2.06208	2.16033	2.23382	2.29219	2.34044	2.38144	2.41702
0.6	2.03577	2.12719	2.1954	2.24948	2.2941	2.33198	2.3648
0.7	2.00055	2.08298	2.14429	2.1928	2.23274	2.2666	2.28591
0.8	1.85164	2.02189	2.07395	2.11502	2.14878	2.17734	2.20203
0.9	1.87666	1.92888	1.96738	1.99766	2.02248	2.04344	2.06152

Table 3. The values of F_n for $\rho = 0.1, \dots, 0.9$ and $\alpha = 0.1$

n / ρ	3	4	5	6	7	8	9
0.1	0.03623	0.02195	0.01487	0.01080	0.00824	0.00652	0.00529
0.2	0.04769	0.02941	0.02018	0.01482	0.01140	0.00908	0.00743
0.3	0.06108	0.03802	0.02625	0.01937	0.01495	0.01194	0.00979
0.4	0.07705	0.04815	0.03332	0.02461	0.01901	0.01519	0.01245
0.5	0.09679	0.06052	0.04188	0.03092	0.02387	0.01906	0.01561
0.6	0.12257	0.07651	0.05285	0.03896	0.03006	0.02396	0.01960
0.7	0.15915	0.09902	0.06823	0.05018	0.03864	0.03075	0.02514
0.8	0.21893	0.13560	0.09312	0.06830	0.05246	0.04168	0.03405
0.9	0.35123	0.21636	0.14794	0.10814	0.08281	0.06568	0.05353

Table 4. The values of 90% quantile ($\alpha = 0.1$) for $\rho = 0.1, \dots, 0.9$

n / ρ	3	4	5	6	7	8	9
0.1	1.80893	1.93201	2.02397	2.09702	2.15739	2.20871	2.25326
0.2	1.79638	1.91665	2.00651	2.07786	2.13683	2.18694	2.23044
0.3	1.78012	1.89649	1.98336	2.0523	2.10923	2.15758	2.19953
0.4	1.75948	1.87073	1.95367	2.01942	2.07366	2.1197	2.1596
0.5	1.73352	1.83827	1.91623	1.97793	2.02879	2.07191	2.10925
0.6	1.70081	1.79739	1.86912	1.92531	1.97246	2.01197	2.04616
0.7	1.65892	1.74518	1.80909	1.85949	1.90091	1.93595	1.96624
0.8	1.60308	1.67585	1.7296	1.77191	1.80662	1.83594	1.86126
0.9	1.52091	1.57437	1.6137	1.64458	1.66985	1.69118	1.70956

Table 5. Estimation of quantile $y_{0.05}$ by formulae (2), (4) and by MC simulation, where $\rho = 0.5$, $\varepsilon_{hl} = \pm 0.05$ and $n = 3, \dots, 9$

n	3	4	5	6	7	8	9
$\sum_{h<l} \varepsilon_{hl}$	0.15	0.3	0.5	0.75	1.05	1.4	1.8
$y_{0.05}$ by (2),(4)	2.0507	2.1460	2.2171	2.2736	2.3203	2.3599	2.3943
Exact quantile of $D(\rho + 0.05)$	2.0495	2.1452	2.2162	2.2723	2.3185	2.3580	2.3928
$P\{\max_{1 \leq i \leq n} Y_i^{D(\rho+0.05)} \leq y_{0.05}\} - 0.95$	0.0001	0.0001	0.0001	0.0002	0.0002	0.0002	0.0002
$\sum_{h<l} \varepsilon_{hl}$	-0.15	-0.3	-0.5	-0.75	-1.05	-1.4	-1.8
$y_{0.05}$ by (2),(4)	2.0735	2.1747	2.2505	2.3107	2.3606	2.4029	2.4397
Exact quantile of $D(\rho - 0.05)$	2.0723	2.1740	2.2496	2.3096	2.3590	2.4012	2.4377
$P\{\max_{1 \leq i \leq n} Y_i^{D(\rho-0.05)} \leq y_{0.05}\} - 0.95$	0.0001	0.0001	0.0001	0.0001	0.0002	0.0002	0.0002

Table 6. Estimation of quantile $y_{0.1}$ by formulae (2), (4) and by MC simulation, where $\rho = 0.5$, $\varepsilon_{hl} = \pm 0.05$ and $n = 3, \dots, 9$.

n	3	4	5	6	7	8	9
$\sum_{h<l} \varepsilon_{hl}$	0.15	0.3	0.5	0.75	1.05	1.4	1.8
$y_{0.05}$ by (2),(4)	1.7190	1.8201	1.8953	1.9547	2.0037	2.0452	2.0811
Exact quantile of $D(\rho + 0.05)$	1.7177	1.8194	1.8935	1.9530	2.0023	2.0436	2.0795
$P\{\max_{1 \leq i \leq n} Y_i^{D(\rho+0.05)} \leq y_{0.05}\} - 0.9$	0.0003	0.0001	0.0003	0.0003	0.0003	0.0003	0.0003
$\sum_{h<l} \varepsilon_{hl}$	-0.15	-0.3	-0.5	-0.75	-1.05	-1.4	-1.8
$y_{0.05}$ by (2),(4)	1.7480	1.8564	1.9372	2.0011	2.0539	2.0986	2.1374

Exact quantile of $D(\rho - 0.05)$	1.7469	1.8558	1.9357	1.9997	2.0524	2.0968	2.1357
$P\{\max_{1 \leq i \leq n} Y_i^{D(\rho-0.05)} \leq y_{0.05}\} - 0.9$	0.0002	0.0001	0.0003	0.0000	0.0003	0.0004	0.0003

Table 7. Estimation of quantile $y_{0.05}$ by formulae (2), (4) and by MC simulation, where $\rho = 0.2$, $\varepsilon_{hl} = \pm 0.05$ and $n = 3, \dots, 9$.

n	3	4	5	6	7	8	9
$\sum_{h<l} \varepsilon_{hl}$	0.15	0.3	0.5	0.75	1.05	1.4	1.8
$y_{0.05}$ by (2),(4)	2.1024	2.2122	2.2939	2.3591	2.4131	2.4591	2.4991
Exact quantile of $D(\rho + 0.05)$	2.1030	2.2122	2.2936	2.3583	2.4124	2.4581	2.4978
$P\{\max_{1 \leq i \leq n} Y_i^{D(\rho+\varepsilon)} \leq y_{0.05}\} - 0.95$	-0.0001	0.0000	0.0000	0.0001	0.0001	0.0001	0.0002
$\sum_{h<l} \varepsilon_{hl}$	-0.15	-0.3	-0.5	-0.75	-1.05	-1.4	-1.8
$y_{0.05}$ by (2),(4)	2.1117	2.2237	2.3072	2.3737	2.4289	2.4759	2.5168
Exact quantile of $D(\rho - 0.05)$	2.1123	2.2240	2.3069	2.3733	2.4282	2.4747	2.5158
$P\{\max_{1 \leq i \leq n} Y_i^{D(\rho+\varepsilon)} \leq y_{0.05}\} - 0.95$	-0.0001	0.0000	0.0000	0.0001	0.0001	0.0002	0.0001

Table 8. Estimation of quantile $y_{0.1}$ by formulae (2), (4) and by MC simulation, where $\rho = 0.2$, $\varepsilon_{hl} = \pm 0.05$ and $n = 3, \dots, 9$.

n	3	4	5	6	7	8	9
$\sum_{h<l} \varepsilon_{hl}$	0.15	0.3	0.5	0.75	1.05	1.4	1.8
$y_{0.05}$ by (2),(4)	1.7892	1.9078	1.9964	2.0667	2.1249	2.1742	2.2171
Exact quantile of $D(\rho + 0.05)$	1.7884	1.9072	1.9955	2.0659	2.1238	2.1730	2.2163
$P\{\max_{1 \leq i \leq n} Y_i^{D(\rho+\varepsilon)} \leq y_{0.05}\} - 0.9$	0.0002	0.0001	0.0002	0.0002	0.0002	0.0003	0.0002

$\sum_{h<l} \varepsilon_{hl}$	-0.15	-0.3	-0.5	-0.75	-1.05	-1.4	-1.8
$y_{0.05}$ by (2),(4)	1.8035	1.9255	2.0166	2.0890	2.1488	2.1997	2.2438
Exact quatile of $D(\rho - 0.05)$	1.8029	1.9250	2.0159	2.0882	2.1481	2.1987	2.2430
$P\{\max_{1 \leq i \leq n} Y_i^{D(\rho+\varepsilon)} \leq y_{0.05}\} - 0.9$	0.0001	0.0001	0.0001	0.0002	0.0002	0.0002	0.0002