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On the asymptotic distribution of likelihood ratio test when parameters lie on the boundary

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Abstract The paper discusses statistical inference dealing with the asymptotic theory of likelihood ratio tests when some parameters may lie on boundary of the parameter space. We derive a closed form solution for the case when one parameter of interest and one nuisance parameter lie on the boundary. The asymptotic distribution is *not* always a mixture of several chi-square distributions. For the cases when one parameter of interest and two nuisance parameters or two parameters of interest and one nuisance parameter are on the boundary, we provide an explicit solution which can be easily computed by simulation. These results can be used in many applications, e.g. testing for random effects in genetics. Contrary to the claim of some authors in the applied literature that use of chi-square distribution with degrees of freedom as in case of interior parameters will be too conservative when some parameters are on the boundary, we show that when nuisance parameters are on the boundary, that approach may often be anti-conservative.

Keywords Likelihood ratio test · Nuisance parameters on the boundary · One-sided tests · Parameters of interest on the boundary · Quadratic forms

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1 Introduction

The asymptotic distribution of the LRT in non-standard situations, in particular when parameters of interest and/or nuisance parameters are on the boundary of a parameter space, is important in many applications, e.g., in variance components testing in many natural science applications. In the field of genetics and biology, there is indeed a considerable amount of interest in statistical issues when some parameters may lie on the boundaries: in almost 1,000 references to Self and Liang (1987) pioneering paper on parameters on the boundary, about half come from genetics and biology fields.

It is well known that, under some very general conditions, the usual asymptotic theory of estimation based on the maximum likelihood estimates (MLEs) and the usual asymptotic theory of tests based on the likelihood ratio tests (LRTs) are valid, and provide useful tools for meaningful statistical inference in large samples. Typically, we conclude the asymptotic normality of the MLE $\hat{\boldsymbol{\theta}} = (\hat{\theta}_1, \cdots, \hat{\theta}_p)$ of $\boldsymbol{\theta}$ and the asymptotic chi-square distribution of $-2ln(LRT)$ with a suitable df under a null hypothesis. However, it should be noted that the validity of such results is based on a *crucial* assumption that the unknown parameter vector $\boldsymbol{\theta}$ is an *interior* point of Ω, the underlying parameter space of $\boldsymbol{\theta}$. In many applications, it can often hold that some parameters may lie on the boundaries, thus making the standard asymptotic results on MLEs and LRTs unjustified and incorrect. Fortunately, this has been recognized long time ago, and some corrective measures can be taken.

Based on Chernoff (1954), Feder (1968), Moran (1971), Chant (1974) and Self and Liang (1987), the following general result under fairly standard regularity conditions on the joint density of $\mathbf{X} = (X_1, \ldots, X_N)$ and nature of $\boldsymbol{\theta}$ can be stated. The conditions which are typical Cramer-type and require, among others, twice differentiability of the underlying joint pdf and finiteness of the Fisher information matrix, are satisfied in many applications.

Let $\hat{\boldsymbol{\theta}}_N$ denote the MLE of $\boldsymbol{\theta}$ when the likelihood function $L(\boldsymbol{\theta}|\mathbf{X})$ is maximized with respect to (wrt) $\boldsymbol{\theta} \in \Omega$. Assume that $\Omega = \Omega_1 \times \cdots \Omega_p$, and Ω_i is taken to be one of two possible forms: open intervals $\Omega_i = (\theta_{i0}, \infty)$ and half-closed intervals $\Omega_i = [\theta_{i0}, \infty)$ for some real θ_{i0}. Thus, some parameters belong to interior sets while others to boundary sets. The maximization of the likelihood wrt $\boldsymbol{\theta}$ would then mean unrestricted maximization in a product of open intervals and *half-closed* intervals, depending on which parameters can assume their boundary values. We will call these *natural* restrictions on $\boldsymbol{\theta}$ and reserve the use of the term *restricted* maximization to the situation when the components of $\boldsymbol{\theta}$ are restricted by a null hypothesis of the form $H_0 : \boldsymbol{\theta} \in \Omega_0$.

To make matters simple and easy to understand, let us consider the following two testing problems about one parameter, say θ_1, of $\boldsymbol{\theta}$.

Problem 1 Test the null hypothesis $H_0 : \theta_1 = \theta_{10} + \delta$ versus $H_1 : \theta_1 \neq \theta_{10} + \delta$ where $\delta > 0$ and naturally θ_1 is an interior point of Ω_1.

Problem 2 Test the null hypothesis $H_0 : \theta_1 = \theta_{10}$ versus $H_1 : \theta_1 > \theta_{10}$ where θ_{10} is the boundary point of $\Omega_1 = [\theta_{10}, \infty)$.

The following proposition is adapted from Self and Liang (1987) although its various versions appear in the other references cited above.

Proposition 1.1 (Self and Liang 1987)

(a) *Consider the problem of testing the null hypothesis $H_0 : \theta_1 = \theta_{10} + \delta$ versus $H_1 : \theta_1 \neq \theta_{10} + \delta$, for some $\delta > 0$ when $\Omega_1 = (\theta_{10}, \infty)$, and suppose we compute the LRT by maximizing $L(\boldsymbol{\theta}|\mathbf{X})$ wrt $\boldsymbol{\theta} \in \Omega$ and also under H_0. Write $\Omega_0 = \{\boldsymbol{\theta} : \theta_1 = \theta_{10} + \delta, \theta_2, \cdots, \theta_p$ unspecified$\}$ Then the null distribution of the profile log likelihood based LRT using $\mathbf{X}$, namely, the null distribution of*

$$-2\ln\left[\frac{\max_{\boldsymbol{\theta}\in\Omega_0} L(\boldsymbol{\theta}|\mathbf{X})}{\max_{\boldsymbol{\theta}\in\Omega} L(\boldsymbol{\theta}|\mathbf{X})}\right] \tag{1.1}$$

is asymptotically equivalent to the distribution of the profile log likelihood based LRT using $\mathbf{Z}$ under $N[\boldsymbol{\theta}, \Sigma]$, namely, the distribution of

$$\min_{\boldsymbol{\theta}\in\Omega_0^*} Q(\boldsymbol{\theta}|\mathbf{Z}) - \min_{\boldsymbol{\theta}\in\Omega^*} Q(\boldsymbol{\theta}|\mathbf{Z}) \tag{1.2}$$

when $\boldsymbol{\theta} = \mathbf{0}$. Here Ω^* is a translation of Ω by Ω_0 so that it includes the point 0 in the parameter space of $\mathbf{Z}$.

(b) *Consider the problem of testing the null hypothesis $H_0 : \theta_1 = \theta_{10}$ versus $H_1 : \theta_1 > \theta_{10}$, and suppose we compute the LRT by maximizing $L(\boldsymbol{\theta}|\mathbf{X})$ wrt $\boldsymbol{\theta} \in \Omega$ and also under H_0. Write $\Omega_0 = \{\boldsymbol{\theta} : \theta_1 = \theta_{10}, \theta_2, \ldots, \theta_p$ unspecified$\}$. Then the null distribution of the profile log likelihood based LRT using $\mathbf{X}$, namely, the null distribution of*

$$-2\ln\left[\frac{\max_{\boldsymbol{\theta}\in\Omega_0} L(\boldsymbol{\theta}|\mathbf{X})}{\max_{\boldsymbol{\theta}\in\Omega} L(\boldsymbol{\theta}|\mathbf{X})}\right] \tag{1.3}$$

is asymptotically equivalent to the distribution of the profile log likelihood based LRT using $\mathbf{Z}$ under $N[\boldsymbol{\theta}, \Sigma]$, namely, the distribution of

$$\min_{\boldsymbol{\theta}\in\Omega_0^*} Q(\boldsymbol{\theta}|\mathbf{Z}) - \min_{\boldsymbol{\theta}\in\Omega^*} Q(\boldsymbol{\theta}|\mathbf{Z}) \tag{1.4}$$

when $\boldsymbol{\theta} = \mathbf{0}$.

Remark 1.1 In the above, $Q(\boldsymbol{\theta}|\mathbf{Z}) = (\mathbf{Z} - \boldsymbol{\theta})'[\Sigma]^{-1}(\mathbf{Z} - \boldsymbol{\theta})$ is the exponent of the normal likelihood of $\mathbf{Z}$ with mean $\boldsymbol{\theta}$ and dispersion Σ. In (*a*), the minimum under $\boldsymbol{\theta} \in \Omega_0^*$ is computed when $\theta_1 = \delta$ and $\theta_2, \cdots, \theta_p$ are unspecified in $(-\infty, \infty)$, and minimum under $\boldsymbol{\theta} \in \Omega^*$ is computed when all the parameters $\boldsymbol{\theta}$ are unspecified in $(-\infty, \infty)$. In (*b*), the minimum under $\boldsymbol{\theta} \in \Omega_0^*$ is computed when $\theta_1 = 0$ and $\theta_2, \cdots, \theta_p$ are unspecified in $(-\infty, \infty)$, and minimum under $\boldsymbol{\theta} \in \Omega^*$ is computed when $\theta_1 \geq 0$ and all the other parameters $\boldsymbol{\theta}$ are unspecified in $(-\infty, \infty)$. This is the simplest result of its kind for one parameter of interest on the boundary and no nuisance parameter being on the boundary.

Remark 1.2 A point about Σ is in order here. Usually, this is taken as the inverse of the Fisher Information matrix evaluated at the MLEs of $\boldsymbol{\theta}$ (Self and Liang 1987).

Self and Liang (1987) discussed at length the computation of the LRT based on $\mathbf{Z}$ and its null distribution under various forms of the null hypothesis: parameters of interest on the boundary or beyond the boundary as well as the nuisance parameters on the boundary or beyond the boundary. In general, as expected, it follows that the null distribution of the LRT based on $\mathbf{Z}$ is central chi-square when the null parameter space Ω_0^* consists only of interior points. However, this distribution is far from being chi-square (quite often a mixture of chi-squares) when Ω_0^* contains some boundary points of $\boldsymbol{\theta}$ as in Problem 2 above. Unfortunately, the derivation of the distribution of the LRT based on $\mathbf{Z}$ in Self and Liang (1987) is quite complicated in many useful cases, and is well beyond the reach of common users.

The main object of this paper is to explicitly derive the asymptotic distribution of the LRT based on $\mathbf{Z}$ for a parameter of interest lying on the boundary in the presence of one or two nuisance parameters also lying on the boundary. Our results also cover the case of two parameters of interest and one nuisance parameter all lying on the boundary. This is achieved by essentially spelling out the geometric-based methods of Self and Liang (1987) with clarity and detailed explanations using algebraic approach. It is expected that from the application point of view, these cases would serve quite well.

The organization of the rest of the paper is as follows. Section 2.1 considers one parameter of interest and one nuisance parameter lying on the boundaries. Section 2.2 considers one parameter of interest and two nuisance parameters lying on the boundaries as well as two parameters of interest and one nuisance parameter lying on the boundaries. Some details of these cases appear in Appendix A and B. Unlike in Self and Liang (1987), our solution in Section 2.1 corresponding to one nuisance parameter being on the boundary is explicit in some situations, and percentage points of the LRT can be readily computed. Again, unlike in Self and Liang (1987), our explicit solution in Section 2.2, although quite involved, can be readily used to simulate the percentage points of the LRT. We have demonstrated this in a few cases in Section 3. Applications of our results are discussed in Section 4.

2 Main results

Assume $\mathbf{X} \sim f(\mathbf{x}|\boldsymbol{\theta})$ where $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_p)$ and $\theta_i \in \Omega_i = (\theta_{i0}, \infty)$ or $[\theta_{i0}, \infty)$, depending on whether θ_i is an interior point or a boundary point. Here, typically, $\mathbf{X}$ is a collection of either *iid* or just independent random variables and $f(.|.)$ stands for their joint *pdf* or the likelihood function.

From Self and Liang (1987), it follows that the asymptotic distribution of the LRT for $H_0 : \theta_1 = \theta_{10}$ versus $H_1 : \theta_1 > \theta_{10}$ based on $\mathbf{X}$ is the same as the *exact* distribution of the LRT for $H_0 : \theta_1 = 0$ versus $H_1 : \theta_1 > 0$ based on

$\mathbf{Z} \sim N[\boldsymbol{\theta}, \Sigma]$ under $\boldsymbol{\theta} = \mathbf{0}$ where Σ is known and $\boldsymbol{\theta} = (\theta_1, \theta_2, \cdots, \theta_p)$ with $\theta_2 \geq 0$ and $\theta_3, \ldots, \theta_p$ being *unrestricted* in case of one nuisance parameter on the boundary (Case 8 of Self and Liang 1987), and $\theta_2 \geq 0, \theta_3 \geq 0$ and $\theta_4, \ldots, \theta_p$ being *unrestricted* in case of two nuisance parameters on the boundary. Obviously, a $(1-\alpha)$ level lower confidence bound of θ_1 is obtained as the minimum of all *accepted* values of θ_{10} when the above null hypothesis H_0 is carried out at level α. Case of two parameters of interest and one nuisance parameter on the boundaries is very similar to the latter case.

Based on standard normal theory, it follows that the distribution of the LRT for H_0 versus H_1 based on $\mathbf{Z}$ is nothing but the distribution of the difference $\Delta(\mathbf{Z})$ of two quadratic forms in $\mathbf{Z}$: $Q_0(\mathbf{Z}) - Q_1(\mathbf{Z})$. These quadratic forms in $\mathbf{Z}$ which are essentially *restricted* and *unrestricted* minimums of the basic normal quadratic form $Q(\boldsymbol{\theta}|\mathbf{Z}) = (\mathbf{Z} - \boldsymbol{\theta})'[\Sigma]^{-1}(\mathbf{Z} - \boldsymbol{\theta})$ are computed below. We now consider the two cases separately.

2.1 One nuisance parameter on the boundary

Assume that $\theta_2 \in \Omega_2 = [\theta_{20}, \infty), \theta_i \in \Omega_i = (\theta_{i0}, \infty), i = 3, \ldots, p$.

Theorem 2.1 *The asymptotic null distribution of the LRT for $\rho \geq 0$ is a mixture of χ_0^2, χ_1^2, χ_2^2 with mixing coefficients $1/2 - q$, $1/2$, q, where $q = \sin^{-1}(\rho)/2\pi$ and ρ is correlation between Z_1 and Z_2. Such a mixture representation does not hold for $\rho < 0$.*

Proof The proof of the theorem is rather long, and will be given in several steps.

The quadratic $Q_1(\mathbf{Z})$, which is the unrestricted minimum of $Q(\boldsymbol{\theta}|\mathbf{Z})$, is obtained by minimizing $Q(\boldsymbol{\theta}|\mathbf{Z})$ *wrt* $\boldsymbol{\theta}$, subject to the *natural* restrictions: $\theta_1 \geq 0, \theta_2 \geq 0$. From the computations in Sinha et al. (2007), $Q_1(\mathbf{Z})$ is easily obtained as

$$\begin{aligned}
\min\nolimits_{\theta_1 \geq 0, \theta_2 \geq 0} Q(\boldsymbol{\theta}|\mathbf{Z}) &= 0, && \textit{if } Z_1 > 0, Z_2 > 0 \\
&= \left(Z_1 - Z_{1.2}, Z_2\right)'\left[\Sigma_{2\times 2}\right]^{-1} \\
&\quad \left(Z_1 - Z_{1.2}, Z_2\right), && \textit{if } Z_{1.2} > 0, Z_2 < 0 \\
&= \left(Z_1, Z_2 - Z_{2.1}\right)'\left[\Sigma_{2\times 2}\right]^{-1} \\
&\quad \left(Z_1, Z_2 - Z_{2.1}\right), && \textit{if } Z_{2.1} > 0, Z_1 < 0 \\
&= \left(Z_1, Z_2\right)'\left[\Sigma_{2\times 2}\right]^{-1} \\
&\quad \left(Z_1, Z_2\right), && \textit{if } Z_{1.2} < 0, Z_{2.1} < 0,
\end{aligned} \tag{2.1}$$

where Z_1 and Z_2 are the components of $\mathbf{Z}$ and $\Sigma_{2\times 2}$ represents the 2×2 variance-covariance matrix of (Z_1, Z_2).

Since $Z_{1.2} = Z_1 - \rho\sigma_1 Z_2/\sigma_2$ and $Z_{2.1} = Z_2 - \rho\sigma_2 Z_1/\sigma_1$, we get $Z_1 - Z_{1.2} = \rho\sigma_1 Z_2/\sigma_2$ and $Z_2 - Z_{2.1} = \rho\sigma_2 Z_1/\sigma_1$. Hence

$$\begin{aligned}
\min_{\theta_1\geq 0,\theta_2\geq 0} Q(\boldsymbol{\theta}|\mathbf{Z}) &= 0, && \textit{if } Z_1 > 0,\ Z_2 > 0\\
&= Z_2^2/\sigma_2^2, && \textit{if } Z_{1.2} > 0,\ Z_2 < 0\\
&= Z_1^2/\sigma_1^2, && \textit{if } Z_{2.1} > 0,\ Z_1 < 0\\
&= \big(Z_1, Z_2\big)'\big[\Sigma_{2\times 2}\big]^{-1}\big(Z_1, Z_2\big), && \textit{if } Z_{1.2} < 0,\ Z_{2.1} < 0,
\end{aligned} \tag{2.2}$$

To compute the quadratic $Q_0(\mathbf{Z})$, the restricted minimum of $Q(\boldsymbol{\theta}|\mathbf{Z})$ under the null hypothesis $H_0 : \theta_1 = 0$, we compute the minimum value of the quadratic form $Q(\boldsymbol{\theta}|\mathbf{Z})$, minimizing *wrt* the remaining parameters under the constraint that $\theta_2 \geq 0$. Naturally what is really needed here is the minimum value of $Q(\theta_2|Z_1, Z_2, \theta_1 = 0)$ when $\theta_2 \geq 0$ where

$$Q\big(\theta_2|Z_1, Z_2, \theta_1 = 0\big) = Z_1^2/\sigma_1^2 + \big(Z_{2.1} - \theta_2\big)^2\big/\sigma_{2.1}^2 \tag{2.3}$$

with $Z_{2.1} = Z_2 - \rho\sigma_2 Z_1/\sigma_1$ and $\sigma_{2.1}^2 = \sigma_2^2(1-\rho^2)$. Obviously,

$$\begin{aligned}
\min_{\theta_2\geq 0} Q\big(\theta_2|Z_1, Z_2, \theta_1 = 0\big) &= Z_1^2\big/\sigma_1^2 && \textit{if } Z_{2.1} > 0\\
&= Z_1^2\big/\sigma_1^2 + Z_{2.1}^2\big/\sigma_{2.1}^2 && \textit{if } Z_{2.1} < 0.
\end{aligned} \tag{2.4}$$

Noting that

$$\begin{aligned}
-2\ln LRT(\mathbf{Z}) &= \min_{\theta_2\geq 0} Q\big(\theta_2|Z_1, Z_2, \theta_1 = 0\big)\\
&\quad - \min_{\theta_1,\theta_2\geq 0} Q\big(\theta_1, \theta_2|Z_1, Z_2\big),
\end{aligned} \tag{2.5}$$

we now combine Eqs. 2.2 and 2.4 to derive the expression for $-2\ln LRT(\mathbf{Z})$ and hence its null distribution under $\theta_1 = 0$.

Towards this end, let us write $U = Z_1/\sigma_1$ and $V = Z_2/\sigma_2$ so that $(U, V) \sim N[0, 0, 1, 1, \rho]$ under H_0, and we consider two separate cases depending on the sign of ρ.

Let $\rho \geq 0$. We have clearly displayed in Fig. 1 the various scenarios in the sample space of Z_1 and Z_2 corresponding to Eqs. 2.2 and 2.4. This figure and the equations readily enable us to compute

$$\begin{aligned}
-2\ln LRT(\mathbf{Z}) &= U^2, && \textit{if } V - \rho U > 0, U > 0\\
&= \frac{U^2 + V^2 - 2\rho UV}{1-\rho^2}, && \textit{if } V - \rho U < 0, U > 0, V > 0\\
&= \frac{(U-\rho V)^2}{1-\rho^2}, && \textit{if } V - \rho U < 0, V < 0, U - \rho V > 0\\
&= 0, && \textit{if } V - \rho U < 0, U - \rho V < 0\\
&= 0, && \textit{if } V - \rho U > 0, U < 0
\end{aligned} \tag{2.6}$$

Obviously, the exact null distribution of $-2\ln LRT(\mathbf{Z})$ is quite involved. It needs to be derived by first computing the conditional null distributions of each

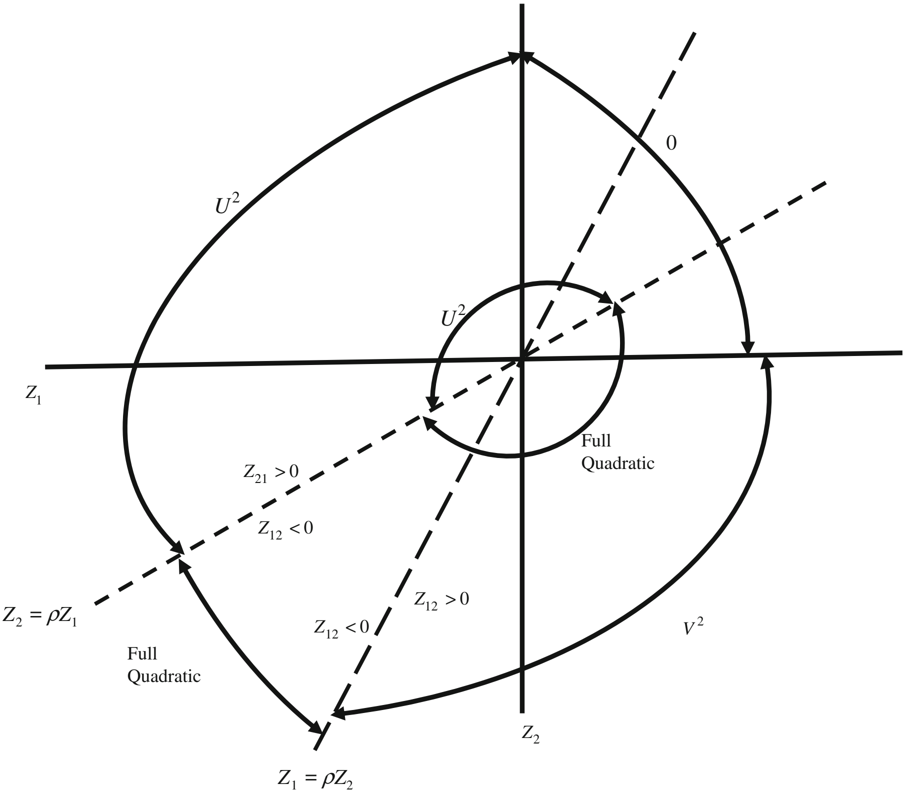

Fig. 1 $\rho \geq 0$. Inner circle corresponds to restricted minimum and outer circle to unrestricted minimum (Eqs. 2.2 and 2.4)

part of $-2\ln LRT(\mathbf{Z})$, given the conditioning event, and then multiplying by the probabilities of these conditioning events.

We first compute the component probabilities of the five *regions* in Eq. 2.6.

1. $Pr[regionI] = Pr[V - \rho U > 0, U > 0] = 1/4$ (by independence).
2. $Pr[regionII] = Pr[V - \rho U < 0, U > 0, V > 0] = Pr[V < \rho U, U > 0] - Pr[V < \rho U, U > 0, V < 0] = \frac{1}{4} - Pr[U > 0, V < 0] = \frac{1}{4} - Pr[-U < 0, V < 0] = \frac{1}{4} - \frac{cos^{-1}(\rho)}{2\pi}$. This probability is 0 when $\rho = 0$.
3. $Pr[regionIII] = Pr[V - \rho U < 0, V < 0, U - \rho V > 0] = Pr[V < 0, U - \rho V > 0] = \frac{1}{4}$ (by independence).
4. $Pr[regionIV] = \frac{\cos^{-1}(\rho)}{2\pi}$, as $(V - \rho U, U - \rho V) \sim N[0, 0, 1 - \rho^2, 1 - \rho^2, -\rho(1 - \rho^2)]$, resulting in $P[V - \rho U < 0, U - \rho V < 0] = \cos^{-1}(\rho)/2\pi$. This probability is $\frac{1}{4}$ when $\rho = 0$.
5. $Pr[regionV] = Pr[V - \rho U > 0, U < 0] = \frac{1}{4}$ (by independence).

The total probability of all five regions is 1, as expected. We now derive the cumulative distribution function (CDF) of $-2lnLRT(\mathbf{Z}) = W(say)$ based on Eq. 2.6. By definition, for $w \geq 0$,

$$\begin{aligned}
Pr\big[W \leq w\big] &= Pr\big[U^2 \leq w, V - \rho U > 0, U > 0\big] \\
&\quad + Pr\left[\frac{U^2 + V^2 - 2\rho UV}{1-\rho^2} \leq w, V - \rho U < 0, U > 0, V > 0\right] \\
&\quad + Pr\left[\frac{(U - \rho V)^2}{1-\rho^2} \leq w, V - \rho U < 0, V < 0, U - \rho V > 0\right] \\
&\quad + Pr\big[V - \rho U < 0, U - \rho V < 0\big] \\
&\quad + Pr\big[V - \rho U > 0, U < 0\big] \qquad (2.7)
\end{aligned}$$

As explained earlier, the first term, fourth term and fifth term are easily obtained. Using the fact that the events $[V - \rho U < 0, V < 0, U - \rho V > 0]$ and $[V < 0, U - \rho V > 0]$ are equivalent and the independence of V and $U - \rho V$, the third term can be computed as

$$Pr\left[\frac{(U - \rho V)^2}{1-\rho^2} \leq w, V < 0, U - \rho V > 0\right] = \frac{1}{4} Pr\big[\chi_1^2 \leq w\big] \qquad (2.8)$$

It remains to compute the most crucial second term. Obviously, this term is 0 when $\rho = 0$. Writing $X = (V - \rho U)/\sqrt{1-\rho^2}$ and $Y = U$ so that $(X, Y) \sim iid \sim N(0, 1)$, the second term for $\rho > 0$ is evaluated as

$$\begin{aligned}
&Pr\big[X^2 + Y^2 \leq w, Y > 0, X < 0, \rho Y + X\sqrt{1-\rho^2} > 0\big] \\
&= \int_0^{\rho\sqrt{w}} \left[\int_{\frac{x\sqrt{1-\rho^2}}{\rho}}^{\sqrt{w-x^2}} \phi(y)dy\right] \phi(x)dx \qquad (2.9)
\end{aligned}$$

where $\phi(.)$ is the standard normal pdf. Combining the above terms, we get the following.

1. For $\rho = 0$,

$$Pr[W \leq w] = \frac{1}{2}\big(1 + Pr\big[\chi_1^2 \leq w\big]\big) \qquad (2.10)$$

2. For $\rho > 0$,

$$\begin{aligned}
Pr[W \leq w] &= \frac{\cos^{-1}\rho}{2\pi} + \frac{1}{4} + \frac{1}{2} Pr\big[\chi_1^2 \leq w\big] \\
&\quad + \int_0^{\rho\sqrt{w}} \left[\int_{\frac{x\sqrt{1-\rho^2}}{\rho}}^{\sqrt{w-x^2}} \phi(y)dy\right] \phi(x)dx \qquad (2.11)
\end{aligned}$$

The derivative of the last term of the *CDF* in Eq. 2.11.

$$\frac{d}{dw}\left[\int_0^{\rho\sqrt{w}}\left[\int_{\frac{x\sqrt{1-\rho^2}}{\rho}}^{\sqrt{w-x^2}}\phi(y)dy\right]\phi(x)dx\right]=\left[\frac{\sin^{-1}\rho}{2\pi}\right]\frac{e^{-w/2}}{2}. \tag{2.12}$$

The *pdf* $g(w)$ of W at $w>0$ is then simplified as

$$\begin{aligned} g(w) &= \frac{1}{2}f(\chi_1^2) \qquad \textit{if} \;\; \rho=0 \\ &= \frac{1}{2}f\big(\chi_1^2\big)+\frac{\sin^{-1}\rho}{2\pi}f\big(\chi_2^2\big) \qquad \textit{if} \;\; \rho>0 \end{aligned} \tag{2.13}$$

Noting that $\sin^{-1}\rho+\cos^{-1}\rho=\frac{\pi}{2}$, the final expression of the *CDF* $G(w)$ of W can be expressed as

$$\begin{aligned} G(w) &= \frac{1}{2}-\frac{\sin^{-1}\rho}{2\pi}+\frac{1}{2}Pr\big[\chi_1^2\le w\big] \\ &\quad +\frac{\sin^{-1}\rho}{2\pi}Pr\big[\chi_2^2\le w\big] \end{aligned} \tag{2.14}$$

□

Remark 2.1 Theorem 2.1 provides a closed form and explicit solution for Case 8 of Self and Liang (1987). This also spells out the situation, namely, $\rho\ge 0$, under which a mixture of chisquare representation holds. The explicit analysis for $\rho<0$ shows that such a chisquare representation does not hold (see Kopylev and Sinha 2010 for details).

2.2 Two nuisance parameters on the boundary

Assume that $\theta_i\in\Omega_i=[\theta_{i0},\infty)$, $i=2,3$, $\theta_i\in\Omega_i=(\theta_{i0},\infty)$, $i=4,\ldots,p$.

To compute $Q_1(\mathbf{Z})$ and $Q_0(\mathbf{Z})$ in this case which essentially involves minimization *wrt three* parameters, we write $Q(\mathbf{Z})$ under H_0 as $Q_0(\mathbf{Z}|H_0)=Q_0(Z_1,Z_2,Z_3|\theta_1=0,\theta_2\ge 0,\theta_3\ge 0)+Q(Z_4,\ldots,Z_p|\theta_4,\cdots,\theta_p)$, and further decompose the first term as

$$\begin{aligned} &Q_0\big(Z_1,Z_2,Z_3|\theta_1=0,\theta_2\ge 0,\theta_3\ge 0\big) \\ &\quad =\frac{Z_1^2}{\sigma_1^2}+\big(Z_2-\theta_2-\rho_{12}\sigma_2 Z_1/\sigma_1,\,Z_3-\theta_3-\rho_{13}\sigma_3 Z_1/\sigma_1\big)'\mathbf{A}^{-1} \\ &\qquad \times\big(Z_2-\theta_2-\rho_{12}\sigma_2 Z_1/\sigma_1,\,Z_3-\theta_3-\rho_{13}\sigma_3 Z_1/\sigma_1\big) \end{aligned} \tag{2.15}$$

where

$$\mathbf{A}=\begin{pmatrix}\sigma_2^2(1-\rho_{12}^2) & \sigma_2\sigma_3(\rho_{23}-\rho_{12}\rho_{13}) \\ \sigma_2\sigma_3(\rho_{23}-\rho_{12}\rho_{13}) & \sigma_3^2(1-\rho_{13}^2)\end{pmatrix}. \tag{2.16}$$

Write $Y_2 = Z_{2.1} = Z_2 - \rho_{12}\sigma_2 Z_1/\sigma_1$ and $Y_3 = Z_{3.1} = Z_3 - \rho_{13}\sigma_3 Z_1/\sigma_1$, and

$$Y_{2.3} = Y_2 - \frac{\sigma_2\left(\rho_{23} - \rho_{12}\rho_{13}\right)}{\sigma_3\left(1 - \rho_{13}^2\right)} Y_3$$

$$Y_{3.2} = Y_3 - \frac{\sigma_3\left(\rho_{23} - \rho_{12}\rho_{13}\right)}{\sigma_2\left(1 - \rho_{12}^2\right)} Y_2. \tag{2.17}$$

It then follows from Eqs. 39 and 40 of Sinha et al. (2007) that the $\min_{\theta_1=0,\theta_2\geq 0,\theta_3\geq 0} Q_0(\boldsymbol{\theta}|\mathbf{Z})$ will consist of four terms depending on the signs of the four *residual* random variables: Y_2, Y_3, $Y_{2.3}$, $Y_{3.2}$. To be specific, we write

$$U_1 = Z_1/\sigma_1, \quad U_2 = \frac{Y_2}{\sigma_2\sqrt{1 - \rho_{12}^2}}, \quad U_3 = \frac{Y_3}{\sigma_3\sqrt{1 - \rho_{13}^2}} \tag{2.18}$$

so that $U_1 \sim N[0, 1]$ is independent of (U_2, U_3), and

$$\left(U_2, U_3\right) \sim N_2\left[0, 0, 1, 1, c_{23}\right], c_{23} = \frac{\rho_{23} - \rho_{12}\rho_{13}}{\sqrt{\left(1 - \rho_{12}^2\right)\left(1 - \rho_{13}^2\right)}}. \tag{2.19}$$

Note that the expressions of the *restricted* MLEs of θ_2 and θ_3 under H_0 quoted below are from the Eq. 39 of Sinha et al. (2007)

$$\begin{aligned}
\left(\hat{\theta}_2, \hat{\theta}_3\right)'_{\text{null}} &= (Y_2, Y_3)', && \textit{if} \quad Y_2 > 0, Y_3 \geq 0 \\
&= (Y_{2.3}, 0)', && \textit{if} \quad Y_{2.3} \leq 0, Y_3 \leq 0 \\
&= (0, Y_{3.2})', && \textit{if} \quad Y_2 \leq 0, Y_{3.2} > 0 \\
&= (0, 0)', && \textit{if} \quad Y_{2.3} < 0, Y_{3.2} < 0.
\end{aligned} \tag{2.20}$$

Using Eq. 2.20, upon direct simplification, the minimum value of $Q_0(\mathbf{Z})$ under H_0 is (quoted from the Eq. 40 of Sinha et al. 2007)

$$\begin{aligned}
\min_{\theta_1=0,\theta_2\geq 0,\theta_3\geq 0} Q_0(\boldsymbol{\theta}|\mathbf{Z}) &= U_1^2, && \textit{if} \quad U_2 > 0, U_3 > 0 \\
&= U_1^2 + U_2^2, && \textit{if} \quad U_2 < 0, U_{3.2} > 0 \\
&= U_1^2 + U_3^2, && \textit{if} \quad U_3 < 0, U_{2.3} > 0 \\
&= \text{full quadratic}, && \textit{if} \quad U_{2.3} < 0, U_{3.2} < 0
\end{aligned} \tag{2.21}$$

where

$$U_{2.3} = U_2 - c_{23}U_3, \quad U_{3.2} = U_3 - c_{23}U_2 \tag{2.22}$$

and the term *full quadratic* refers to the quadratic term $Q_0(\mathbf{Z})$ under $\theta_1 = \theta_2 = \theta_3 = 0$. Obviously, U_2 is independent of $U_{3.2}$ and U_3 is independent of $U_{2.3}$.

Returning to the computation of $Q_1(\mathbf{Z})$, the *unrestricted* minimum of $Q(\mathbf{Z}|\boldsymbol{\theta})$ under the natural constraints: $\theta_1 \geq 0, \theta_2 \geq 0, \theta_3 \geq 0$, we recall from the

Eq. 44 of Sinha et al. (2007) the following MLEs of the above three crucial parameters:

$$\begin{aligned}
\left(\hat{\theta}_1, \hat{\theta}_2, \hat{\theta}_3\right)' = \left(Z_1, Z_2, Z_3\right)', &\quad \textit{if} \quad Z_1 \geq 0, Z_2 \geq 0, Z_3 \geq 0 \\
= (0, Z_{2.1}, Z_{3.1})', &\quad \textit{if} \quad Z_1 < 0, Z_{2.1} > 0, Z_{3.1} \geq 0 \\
= (Z_{1.2}, 0, Z_{3.2})', &\quad \textit{if} \quad Z_2 < 0, Z_{1.2} > 0, Z_{3.2} \geq 0 \\
= (Z_{1.3}, Z_{2.3}, 0)', &\quad \textit{if} \quad Z_3 < 0, Z_{1.3} \geq 0, Z_{2.3} \geq 0 \\
= (0, 0, Z_{3.12})', &\quad \textit{if} \quad Z_{1.2} \leq 0, Z_{2.1} \leq 0, Z_{3.12} > 0 \\
= (0, Z_{2.13}, 0)', &\quad \textit{if} \quad Z_{1.3} < 0, Z_{3.1} < 0, Z_{2.13} > 0 \\
= (Z_{1.23}, 0, 0)', &\quad \textit{if} \quad Z_{2.3} < 0, Z_{3.2} < 0, Z_{1.23} > 0 \\
= (0, 0, 0)', &\quad \textit{if} \quad Z_{1.23} \leq 0, Z_{2.13} \leq 0, Z_{3.12} \leq 0. \quad (2.23)
\end{aligned}$$

where $Z_{..}$ are the *usual* residual terms, defined in the Appendix B. Naturally we need to plug in these estimates of the MLEs in $Q(Z_1, Z_2, Z_3|\theta_1, \theta_2, \theta_3)$ and simplify to get an expression of the unrestricted minimum, i.e., $Q_1(\mathbf{Z})$. Towards this end, we express all the relevant terms appearing above in terms of U_1, U_2, U_3 and proceed in a systematic manner, taking one region at a time. We also provide the *minimum* value of the quadratic in each case.

Theorem 2.2 *The expression for the likelihood ratio test statistic which is the difference $Q_0(\mathbf{Z}) - Q_1(\mathbf{Z})$ is obtained by using Eq. 2.23 and all the results under Cases* I–VIII *in the Appendix A.*

Remark 2.2 For the case of two parameters of interest and one nuisance parameter lying on the boundaries, the unrestricted minimum $Q_1(\mathbf{Z})$ is exactly the same as above, and is given in Cases I–VIII. The restricted minimum is given by

$$\begin{aligned}
Q_0\left(Z_1, Z_2, Z_3|\theta_1 = 0, \theta_2 = 0, \theta_3 \geq 0\right) &= \frac{Z_1^2}{\sigma_1^2} + \frac{Z_2^2}{\sigma_2^2}, \quad \textit{if } Z_{3.12} > 0 \\
&= \frac{Z_1^2}{\sigma_1^2} + \frac{Z_2^2}{\sigma_2^2} + \frac{Z_{3.12}^2}{\sigma_{3.12}^2}, \quad \textit{if } Z_{3.12} < 0.
\end{aligned} \tag{2.24}$$

In terms of U, using Eq. B.9

$$Q_0(\mathbf{Z}) = U_1^2 + \left(1-\rho_{12}^2\right)\left(U_2 + \frac{\rho_{12}}{\sqrt{1-\rho_{12}^2}}U_1\right)^2, \qquad if \quad U_{3.2} > 0$$

$$= U_1^2 + \left(1-\rho_{12}^2\right)\left(U_2 + \frac{\rho_{12}}{\sqrt{1-\rho_{12}^2}}U_1\right)^2 + U_{3.2}^2, \quad if \quad U_{3.2} < 0 \quad (2.25)$$

where $U_{3.2}$ is defined in Eq. 2.22.

3 Simulations

To verify the accuracy of the analytically derived distribution of $Q_0(\mathbf{Z}) - Q_1(\mathbf{Z})$ in Section 2, it was simulated and verified against the actual distribution of the above difference based on numerical optimization, as described below. All computations were performed in R (R Development Core Team 2006).

1. Simulation of the analytically derived distribution. The analytically derived expression for the asymptotic distribution of the LRT was simulated by first generating 1E6 realizations of the normal vector U with mean 0 and correlation structure described in Eqs. 2.6 and 2.19 and then expressing restricted and unrestricted minimums Q_0 and Q_1 and their difference in terms of vector U. The upper percentiles of the simulated distribution of the difference $Q_0 - Q_1$ are summarized in Tables 1 and 2 for selected combinations of correlation coefficients.

Table 1 Upper percentiles of the asymptotic distribution of the LRT (for $\rho \geq 0$) calculated by simulation, numerical optimization and closed form distribution

ρ_1, ρ_2, ρ_3	Method	Closed form	Percentiles 0.90	0.95	0.975	0.99
$0, 0, \rho$;	sim	$1/2 * \chi_0^2 +$	1.646	2.715	3.849	5.435
ρ-any ≥ 0	theor	$1/2 * \chi_1^2$	1.656	2.713	3.860	5.417
	optim		1.650	2.695	3.866	5.517
.2,0,0	sim	Eq. 2.14	1.835	2.945	4.140	5.771
	theor	$\rho = 0.2$	1.838	2.956	4.140	5.740
	optim		1.849	2.935	4.120	5.648
.9,0,0	sim	Eq. 2.14	2.640	**3.889**	**5.159**	**6.899**
	theor	$\rho = 0.9$	2.643	3.884	5.183	6.903
	optim		2.613	3.846	5.140	6.892
χ_1^2			2.706	3.841	5.024	6.635

The last row shows corresponding percentiles of the chi-square with one-degree of freedom—the asymptotic distribution of the LRT when complications due to boundary parameters are ignored. In column Method, *sim* stands for simulation of the analytical distribution and *optim* stands for the numerical optimization as described above, and *theor* stands for the closed form percentiles. Percentiles exceeding corresponding percentiles of χ_1^2, i.e. situations when use of χ_1^2 is anti-conservative, are in bold

Table 2 Upper percentiles of the asymptotic distribution of the LRT (for $\rho \geq 0$) calculated by simulation, numerical optimization when closed form distribution is not available

ρ_1, ρ_2, ρ_3	Method	Percentiles			
		0.90	0.95	0.975	0.99
.8, .8, .6	sim	**3.339**	**4.690**	**6.076**	**7.933**
	optim	3.362	4.703	6.076	7.913
.2, .8, −.2	sim	**3.074**	**4.409**	**5.771**	**7.569**
	optim	3.103	4.415	5.759	7.498
.2, .8, .3	sim	2.559	3.808	**5.079**	**6.802**
	optim	2.561	3.810	5.117	6.874
.2, .8, .6	sim	2.249	3.413	4.644	6.270
	optim	2.237	3.410	4.635	6.274
.5, .5, −.2	sim	**2.981**	**4.317**	**5.653**	**7.476**
	optim	2.960	4.290	5.657	7.511
.5, .5, .3	sim	2.627	**3.910**	**5.228**	**6.983**
	optim	2.643	3.982	5.274	6.977
.5, .5, .6	sim	2.502	3.729	5.002	**6.768**
	optim	2.463	3.713	5.042	6.690
.2, .2, −.8	sim	2.502	3.756	**5.047**	**6.802**
	optim	2.506	3.763	5.011	6.809
.2, .2, .9	sim	1.894	3.021	4.211	5.863
	optim	1.888	2.988	4.207	5.839
0, .8, −.5	sim	**3.105**	**4.440**	**5.768**	**7.575**
	optim	3.085	4.405	5.767	7.635
0, .8, .5	sim	1.979	3.060	4.201	5.762
	optim	1.974	3.072	4.216	5.842
−.5, −.5, .6	sim	0.842	1.607	2.460	3.659
	optim	0.850	1.620	2.477	3.657
−.8, .8, .8	sim	0.377	0.848	1.390	2.188
	optim	0.378	0.845	1.396	2.192
χ^2_1		2.706	3.841	5.024	6.635

See legend of Table 1 for details

2. Numerical optimization. The distribution of the LRT was calculated by numerically optimizing numerator and denominator of the LRT based on **Z** of the single tri-variate normal variable with corresponding constraints on nuisance parameters. The constrained numerical optimization was performed using R function *optim()*. The procedure was repeated 1E5 times and upper percentiles of the resulting distribution are summarized in Tables 1 and 2.

Tables 1 and 2 demonstrate that the upper percentiles of the analytically derived distribution are very close to the closed form solution, when a closed form solution is available, and also to the numerical optimization of the restricted and unrestricted quadratic forms, for the selected correlation structures. The full distribution of the LRT was similarly very close (not shown).

4 Discussion

In some applications, it is not uncommon to ignore the possibility of the nuisance parameters on the boundary and claim that using usual chi-square with one degree of freedom will result in too conservative a test (e.g., Visscher

2006 and Meyer 2008 in the field of genetics, Stoel et al. 2006 in the field of psychology). Morris et al. (2009) also recommend stopping enforcing constraints on the nuisance parameters. Our results demonstrate that when one or more nuisance parameters are on the boundary, using chi square with one degree of freedom may result in anti-conservative tests for a wide range of correlation structures (Tables 1 and 2).

When, however, applied literature pays serious attention to nuisance parameters on the boundary, Case 8 of Self and Liang (1987), which is our Theorem 2.1, is often cited, but sheer complexity of the asymptotic distribution for Case 8 in Self and Liang (1987) makes its use in applied science a *daunting* task. Thus, while acknowledging that the use of chi-square approximation is likely to be inaccurate, most authors still use this result in absence of a better alternative! We believe that the closed form solution, derived in Section 2.1 and verified by simulations in Section 3, would render an easy application of the correct asymptotic distribution for a very important case when one of the nuisance parameters, in addition to a single parameter of interest, are on the boundaries, and correlation is non-negative.

We should also mention another situation of interest in applications, namely, Case 7 of Self and Liang (1987), when two parameters of interest, but no nuisance parameters, are on the boundary (e.g., Dominicus et al. 2006). Unfortunately, this example in Self and Liang (1987) has probabilities of the mixture components inverted, most likely a misprint. The mixing probability for χ^2_0 should be p, not $1 - p$, where $p = a\cos(\rho)/2\pi$. A lucky erroneous inversion of the sign of ρ in Dominicus et al. (2006) calculations allows them to make the correct recommendation for their applied case.

We conclude this paper with the hope that the use of correct asymptotic distributions for one and two nuisance parameters on the boundary would lead to a considerable improvement of the one-side testing.

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Appendix A

In the following, matrix $\mathbf{R}$ is defined as

$$\mathbf{R} = \begin{pmatrix} 1 & \rho_{12} & \rho_{13} \\ \rho_{12} & 1 & \rho_{23} \\ \rho_{13} & \rho_{23} & 1 \end{pmatrix}.$$

Case I $MLE = (Z_1, Z_2, Z_3)$ over Region $R_I : Z_1 \geq 0, Z_2 \geq 0, Z_3 \geq 0.$

Obviously, the minimum value of the quadratic here is $Q_I = 0$ and the region R_I can be reexpressed in terms of U_1, U_2, U_3 as:

$$R_I : U_1 > 0, U_2 + \frac{U_1\rho_{12}}{\sqrt{1-\rho_{12}^2}} > 0, U_3 + \frac{U_1\rho_{13}}{\sqrt{1-\rho_{13}^2}} > 0. \tag{A.1}$$

Case II $MLE = (0, Z_{2.1}, Z_{3.1})$ over Region $R_{II} : Z_1 < 0, Z_{2.1} \geq 0, Z_{3.1} \geq 0.$

Obviously, the minimum value of the quadratic here is Q_{II} given by the following expression

$$\begin{aligned} Q_{II} &= (Z_1, Z_2 - Z_{2.1}, Z_3 - Z_{3.1})'[\Sigma]^{-1}\big(Z_1, Z_2 - Z_{2.1}, Z_3 - Z_{3.1}\big) \\ &= U_1^2\big(1, \rho_{12}, \rho_{13}\big)'\mathbf{R}^{-1}\big(1, \rho_{12}, \rho_{13}\big) \end{aligned} \tag{A.2}$$

and the region R_{II} can be reexpressed in terms of U_1, U_2, U_3 as:

$$R_{II} : U_1 < 0, U_2 > 0, U_3 > 0. \tag{A.3}$$

Case III $MLE = (Z_{1.2}, 0, Z_{3.2})$ over region $R_{III} : Z_2 < 0, Z_{1.2} \geq 0, Z_{3.2} \geq 0.$

Obviously, the minimum value of the quadratic here is Q_{III} given by the following expression

$$\begin{aligned} Q_{III} &= \big(Z_1 - Z_{1.2}, Z_2, Z_3 - Z_{3.2}\big)'[\Sigma]^{-1}\big(Z_1 - Z_{1.2}, Z_2, Z_3 - Z_{3.2}\big) \\ &= \left(Z_1\rho_{12}^2 + \rho_{12}\sigma_1\frac{Y_2}{\sigma_2}, Y_2 + \rho_{12}\sigma_2\frac{Z_1}{\sigma_1}, \rho_{12}\rho_{23}\frac{Z_1}{\sigma_1}\right)'[\Sigma]^{-1} \\ &\quad\times\left(Z_1\rho_{12}^2 + \rho_{12}\sigma_1\frac{Y_2}{\sigma_2}, Y_2 + \rho_{12}\sigma_2\frac{Z_1}{\sigma_1}, \rho_{12}\rho_{23}\frac{Z_1}{\sigma_1}\right) \\ &= \left[\rho_{12}\frac{Z_1}{\sigma_1} + \frac{Y_2}{\sigma_2}\right]^2\big(\rho_{12}, 1, \rho_{23}\big)'\mathbf{R}^{-1}\big(\rho_{12}, 1, \rho_{23}\big) \\ &= \left[U_2 + \frac{\rho_{12}U_1}{\sqrt{1-\rho_{12}^2}}\right]^2\big(1-\rho_{12}^2\big)\big(\rho_{12}, 1, \rho_{23}\big)'\mathbf{R}^{-1}\big(\rho_{12}, 1, \rho_{23}\big) \end{aligned} \tag{A.4}$$

and the region R_{III} can be reexpressed in terms of U_1, U_2, U_3 as

$$\begin{aligned}
R_{III} \ : \ & Z_2 < 0, \quad Z_{1.2} > 0, \quad Z_{3.2} > 0 \\
& \sim Y_2 + \rho_{12}\sigma_2 \frac{Z_1}{\sigma_1} < 0,\ Z_1 - \frac{\rho_{12}}{1-\rho_{12}^2}\frac{\sigma_1}{\sigma_2} Y_2 > 0, \\
& \quad \left(\rho_{13} - \rho_{12}\rho_{23}\right)\frac{Z_1}{\sigma_1} - \rho_{23}\frac{Y_2}{\sigma_2} + \frac{Y_3}{\sigma_3} > 0 \\
& \sim \rho_{12}\frac{Z_1}{\sigma_1} + \frac{Y_2}{\sigma_2} < 0,\ \frac{Z_1}{\sigma_1} - \frac{\rho_{12}}{1-\rho_{12}^2} \times \frac{Y_2}{\sigma_2} > 0, \\
& \quad \left(\rho_{13} - \rho_{12}\rho_{23}\right)\frac{Z_1}{\sigma_1} > \rho_{23}\frac{Y_2}{\sigma_2} - \frac{Y_3}{\sigma_3} > 0 \\
& \sim U_2 + \frac{\rho_{12}}{\sqrt{1-\rho_{12}^2}} U_1 < 0,\ U_1 > \frac{\rho_{12}}{\sqrt{1-\rho_{12}^2}} U_2, \\
& \quad c_{13} U_1 > \frac{\rho_{23}}{\sqrt{1-\rho_{13}^2}} U_2 - \frac{U_3}{\sqrt{1-\rho_{12}^2}},
\end{aligned} \tag{A.5}$$

where $c_{13} = \frac{\rho_{13}-\rho_{12}\rho_{23}}{\sqrt{(1-\rho_{12}^2)(1-\rho_{13}^2)}}$.

Case IV $MLE = (Z_{1.3}, Z_{2.3}, 0)$ over region $R_{VI} : Z_3 < 0,\ Z_{1.3} \geq 0,\ Z_{2.3} \geq 0.$

Similarly to the previous case

$$\begin{aligned}
Q_{IV} &= \left(Z_1 - Z_{1.3}, Z_2 - Z_{2.3}, Z_3\right)'[\Sigma]^{-1}\left(Z_1 - Z_{1.3}, Z_3 - Z_{2.3}, Z_3\right) \\
&= \left(Z_1\rho_{13}^2 + \rho_{13}\sigma_1\frac{Y_3}{\sigma_3}, \rho_{13}\rho_{23}\sigma_2\frac{Z_1}{\sigma_1} + \rho_{23}\sigma_2\frac{Y_3}{\sigma_3}, Y_3 + \rho_{13}\sigma_3\frac{Z_1}{\sigma_1}\right)' \\
&\quad \times [\Sigma]^{-1}\left(Z_1\rho_{13}^2 + \rho_{13}\sigma_1\frac{Y_3}{\sigma_3}, \rho_{13}\rho_{23}\sigma_2\frac{Z_1}{\sigma_1} + \rho_{23}\sigma_2\frac{Y_3}{\sigma_3}, Y_3 + \rho_{13}\sigma_3\frac{Z_1}{\sigma_1}\right) \\
&= \left(\frac{Z_1}{\sigma_1}\rho_{13}^2 + \rho_{13}\frac{Y_3}{\sigma_3}, \rho_{13}\rho_{23}\frac{Z_1}{\sigma_1} + \rho_{23}\frac{Y_3}{\sigma_3}, \frac{Y_3}{\sigma_3} + \rho_{13}\frac{Z_1}{\sigma_1}\right)' \mathbf{R^{-1}} \\
&\quad \times \left(\frac{Z_1}{\sigma_1}\rho_{13}^2 + \rho_{13}\frac{Y_3}{\sigma_3}, \rho_{13}\rho_{23}\frac{Z_1}{\sigma_1} + \rho_{23}\frac{Y_3}{\sigma_3}, \frac{Y_3}{\sigma_3} + \rho_{13}\frac{Z_1}{\sigma_1}\right) \\
&= \left[U_3 + \frac{\rho_{13}U_1}{\sqrt{1-\rho_{13}^2}}\right]^2 \left(1-\rho_{13}^2\right)\left(\rho_{13}, \rho_{23}, 1\right)'\mathbf{R}^{-1}(\rho_{13}, \rho_{23}, 1)
\end{aligned} \tag{A.6}$$

$$
\begin{aligned}
R_{IV} &: Z_3 < 0, \quad Z_{1.3} > 0, \quad Z_{2.3} > 0 \\
&\sim Y_3 + \rho_{13}\sigma_3 \frac{Z_1}{\sigma_1} < 0,\, Z_1\left(1-\rho_{13}^2\right) - \rho_{13}\sigma_1 \frac{Y_3}{\sigma_3} > 0, \\
&\quad \rho_{23}\frac{Y_3}{\sigma_3} + \frac{Y_2}{\sigma_2} > 0 \\
&\sim \rho_{13}\frac{Z_1}{\sigma_1} + \frac{Y_3}{\sigma_3} < 0,\, \frac{Z_1}{\sigma_1} - \frac{\rho_{13}}{1-\rho_{13}^2} \times \frac{Y_3}{\sigma_3}, \\
&\quad \left(\rho_{12} - \rho_{13}\rho_{23}\right)\frac{Z_1}{\sigma_1} > \rho_{23}\frac{Y_3}{\sigma_3} - \frac{Y_2}{\sigma_2} > 0 \\
&\sim U_3 + \frac{\rho_{13}}{\sqrt{1-\rho_{13}^2}} U_1 < 0,\, U_1 > \frac{\rho_{13}}{\sqrt{1-\rho_{13}^2}} U_3, \\
&\quad c_{12}U_1 > \frac{\rho_{23}}{\sqrt{1-\rho_{12}^2}} U_3 - \frac{U_2}{\sqrt{1-\rho_{13}^2}},
\end{aligned}
\tag{A.7}
$$

where $c_{12} = \frac{\rho_{12}-\rho_{13}\rho_{23}}{\sqrt{(1-\rho_{12}^2)(1-\rho_{13}^2)}}$.

Case V $MLE = (0, 0, Z_{3.12})$ over Region $R_V : Z_{1.2} < 0,\, Z_{2.1} < 0,\, Z_{3.12} > 0$.

$$
\begin{aligned}
Q_V &= \left(Z_1, Z_2, Z_3 - Z_{3.12}\right)'[\Sigma]^{-1}\left(Z_1, Z_2, Z_3 - Z_{3.12}\right) \\
&= \left(Z_1, Y_2 + \rho_{12}\sigma_2\frac{Z_1}{\sigma_1}, \rho_{13}\sigma_3\frac{Z_1}{\sigma_1} + \sigma_3\frac{Y_2(\rho_{23}-\rho_{12}\rho_{13})}{\sigma_2(1-\rho_{12}^2)}\right)' \Sigma^{-1} \\
&\quad \times \left(Z_1, Y_2 + \rho_{12}\sigma_2\frac{Z_1}{\sigma_1}, \rho_{13}\sigma_3\frac{Z_1}{\sigma_1} + \sigma_3\frac{Y_2\left(\rho_{23}-\rho_{12}\rho_{13}\right)}{\sigma_2\left(1-\rho_{12}^2\right)}\right) \\
&= \left[\frac{Z_1}{\sigma_1}\left(1, \rho_{12}, \rho_{13}\right) + \frac{Y_2}{\sigma_2}\left(0, 1, \frac{\rho_{23}-\rho_{12}\rho_{13}}{1-\rho_{12}^2}\right)\right]' \mathbf{R}^{-1} \\
&\quad \times \left[\frac{Z_1}{\sigma_1}\left(1, \rho_{12}, \rho_{13}\right) + \frac{Y_2}{\sigma_2}\left(0, 1, \frac{\rho_{23}-\rho_{12}\rho_{13}}{1-\rho_{12}^2}\right)\right] \\
&= \left[U_1\left(1, \rho_{12}, \rho_{13}\right) + U_2\left(0, \sqrt{1-\rho_{12}^2}, \frac{\rho_{23}-\rho_{12}\rho_{13}}{\sqrt{1-\rho_{12}^2}}\right)\right]' \mathbf{R}^{-1} \\
&\quad \times \left[U_1(1, \rho_{12}, \rho_{13}) + U_2\left(0, \sqrt{1-\rho_{12}^2}, \frac{\rho_{23}-\rho_{12}\rho_{13}}{\sqrt{1-\rho_{12}^2}}\right)\right]
\end{aligned}
\tag{A.8}
$$

$$
\begin{aligned}
R_V \;:\; & Z_{1.2} < 0,\, Z_{2.1} < 0,\, Z_{3.12} > 0 \\
& \sim \frac{Z_1}{\sigma_1} < \frac{Y_2}{\sigma_2}\frac{\rho_{12}}{1-\rho_{12}^2},\, Y_2 < 0,\, \frac{Y_3}{\sigma_3} > \frac{Y_2}{\sigma_2}\frac{\left(\rho_{23}-\rho_{12}\rho_{13}\right)}{1-\rho_{12}^2} \\
& \sim U_1 < \frac{\rho_{12}}{\sqrt{1-\rho_{12}^2}} U_2,\, U_2 < 0,\, U_{3.2} > 0
\end{aligned}
\tag{A.9}
$$

Case VI $MLE = (0, Z_{2.13}, 0)$ over the region $R_{VI} : Z_{1.3} < 0,\, Z_{3.1} < 0,\, Z_{2.13} > 0$.

$$
\begin{aligned}
Q_{VI}(\mathbf{Z}|\hat{\boldsymbol{\theta}}) &= \left(Z_1, Z_2 - Z_{2.13}, Z_3\right)' \Sigma^{-1} \left(Z_1, Z_2 - Z_{2.13}, Z_3\right) \\
&= \left(Z_1, \rho_{12}\sigma_2 \frac{Z_1}{\sigma_1} + \sigma_2 \left[\frac{\rho_{23}-\rho_{12}\rho_{13}}{1-\rho_{13}^2}\right]\frac{Y_3}{\sigma_3}, Y_3 + \rho_{13}\sigma_3 \frac{Z_1}{\sigma_1}\right)' \Sigma^{-1} \\
&\quad \times \left(Z_1, \rho_{12}\sigma_2 \frac{Z_1}{\sigma_1} + \sigma_2 \left[\frac{\rho_{23}-\rho_{12}\rho_{13}}{1-\rho_{13}^2}\right]\frac{Y_3}{\sigma_3}, Y_3 + \rho_{13}\sigma_3 \frac{Z_1}{\sigma_1}\right) \\
&= \left(\frac{Z_1}{\sigma_1}, \rho_{12}\frac{Z_1}{\sigma_1} + \left[\frac{\rho_{23}-\rho_{12}\rho_{13}}{1-\rho_{13}^2}\right]\frac{Y_3}{\sigma_3}, \frac{Y_3}{\sigma_3} + \rho_{13}\frac{Z_1}{\sigma_1}\right)' \mathbf{R}^{-1} \\
&\quad \times \left(\frac{Z_1}{\sigma_1}, \rho_{12}\frac{Z_1}{\sigma_1} + \left[\frac{\rho_{23}-\rho_{12}\rho_{13}}{1-\rho_{13}^2}\right]\frac{Y_3}{\sigma_3}, \frac{Y_3}{\sigma_3} + \rho_{13}\frac{Z_1}{\sigma_1}\right) \\
&= \left[\frac{Z_1}{\sigma_1}\left(1, \rho_{12}, \rho_{13}\right) + \frac{Y_3}{\sigma_3}\left(0, \frac{\rho_{23}-\rho_{12}\rho_{13}}{1-\rho_{13}^2}, 1\right)\right]' \mathbf{R}^{-1} \\
&\quad \times \left[\frac{Z_1}{\sigma_1}(1, \rho_{12}, \rho_{13}) + \frac{Y_3}{\sigma_3}\left(0, \frac{\rho_{23}-\rho_{12}\rho_{13}}{1-\rho_{13}^2}, 1\right)\right] \\
&= \left[U_1\left(1, \rho_{12}, \rho_{13}\right) + U_3\left(0, \frac{\rho_{23}-\rho_{12}\rho_{13}}{\sqrt{1-\rho_{13}^2}}, \sqrt{1-\rho_{13}^2}\right)\right]' \mathbf{R}^{-1} \\
&\quad \times \left[U_1(1, \rho_{12}, \rho_{13}) + U_3\left(0, \frac{\rho_{23}-\rho_{12}\rho_{13}}{\sqrt{1-\rho_{13}^2}}, \sqrt{1-\rho_{13}^2}\right)\right]
\end{aligned}
\tag{A.10}
$$

$$
R_{VI} : U_1 < \frac{\rho_{13}}{\sqrt{1-\rho_{13}^2}} U_3,\, U_3 < 0,\, U_{2.3} > 0. \tag{A.11}
$$

Case VII $MLE = (Z_{1.23}, 0, 0)$ over the region $R_{VII}: Z_{2.3} < 0,\ Z_{3.2} < 0,\ Z_{1.23} > 0.$

To compute the quadratic $Q_{VII}(\mathbf{Z}|\hat{\boldsymbol{\theta}})$, note from Eq. B.6 that

$$\frac{Z_1 - Z_{1.23}}{\sigma_1} = \frac{Z_1}{\sigma_1}\frac{\rho_{12}^2 + \rho_{13}^2 - 2\rho_{12}\rho_{13}\rho_{23}}{1-\rho_{23}^2} + \frac{Y_2}{\sigma_2}\frac{\rho_{12} - \rho_{13}\rho_{23}}{1-\rho_{23}^2} + \frac{Y_3}{\sigma_3}\frac{\rho_{13} - \rho_{12}\rho_{23}}{1-\rho_{23}^2} \tag{A.12}$$

This yields

$$\begin{aligned}
&\left[\frac{Z_1 - Z_{1.23}}{\sigma_1}, \frac{Z_2}{\sigma_2}, \frac{Z_3}{\sigma_3}\right] \\
&= \left[\frac{Z_1}{\sigma_1}\frac{\rho_{12}^2 + \rho_{13}^2 - 2\rho_{12}\rho_{13}\rho_{23}}{1-\rho_{23}^2} + \frac{Y_2}{\sigma_2}\frac{\rho_{12} - \rho_{13}\rho_{23}}{1-\rho_{23}^2}\right. \\
&\qquad \left. + \frac{Y_3}{\sigma_3}\frac{\rho_{13} - \rho_{12}\rho_{23}}{1-\rho_{23}^2}, \frac{Y_2}{\sigma_2} + \rho_{12}\frac{Z_1}{\sigma_1}, \frac{Y_3}{\sigma_3} + \rho_{13}\frac{Z_1}{\sigma_1}\right] \\
&= \left[\frac{Z_1}{\sigma_1}\left(\frac{\rho_{12}^2 + \rho_{13}^2 - 2\rho_{12}\rho_{13}\rho_{23}}{1-\rho_{23}^2}, \rho_{12}, \rho_{13}\right)\right. \\
&\qquad \left. + \frac{Y_2}{\sigma_2}\left(\frac{\rho_{12} - \rho_{13}\rho_{23}}{1-\rho_{23}^2}, 1, 0\right) + \frac{Y_3}{\sigma_3}\left(\frac{\rho_{13} - \rho_{12}\rho_{23}}{1-\rho_{23}^2}, 0, 1\right)\right] \\
&= \left[U_1\left(\frac{\rho_{12}^2 + \rho_{13}^2 - 2\rho_{12}\rho_{13}\rho_{23}}{1-\rho_{23}^2}, \rho_{12}, \rho_{13}\right)\right. \\
&\qquad \left. + U_2\sqrt{1-\rho_{12}^2}\left(\frac{\rho_{12} - \rho_{13}\rho_{23}}{1-\rho_{23}^2}, 1, 0\right) + U_3\sqrt{1-\rho_{13}^2}\left(\frac{\rho_{13} - \rho_{12}\rho_{23}}{1-\rho_{23}^2}, 0, 1\right)\right] \\
&= \mathbf{V}(say).
\end{aligned} \tag{A.13}$$

Hence $Q_{VII}(\mathbf{Z}|\hat{\boldsymbol{\theta}}) = \mathbf{V}'\mathbf{R}^{-1}\mathbf{V}$.

From Eq. B.3, note that

$$\begin{aligned}
Z_{2.3} < 0 &\sim \frac{Z_1}{\sigma_1}(\rho_{12} - \rho_{13}\rho_{23}) + \frac{Y_2}{\sigma_2} - \rho_{23}\frac{Y_3}{\sigma_3} < 0 \\
&\sim U_1(\rho_{12} - \rho_{13}\rho_{23}) + U_2\sqrt{1-\rho_{12}^2} - U_3\rho_{23}\sqrt{1-\rho_{13}^2} < 0.
\end{aligned} \tag{A.14}$$

Similarly, from Eq. B.4, we get

$$Z_{3.2} < 0 \sim \frac{Z_1}{\sigma_1}(\rho_{13} - \rho_{12}\rho_{23}) - \rho_{23}\frac{Y_2}{\sigma_2} + \frac{Y_3}{\sigma_3} < 0$$
$$\sim U_1(\rho_{13} - \rho_{12}\rho_{23}) - U_2\rho_{23}\sqrt{1-\rho_{12}^2} + U_3\sqrt{1-\rho_{13}^2} < 0. \tag{A.15}$$

Finally, from Eq. B.6, we get

$$Z_{1.23} > 0 \sim \frac{Z_1}{\sigma_1}\left(1 - \rho_{12}^2 - \rho_{13}^2 - \rho_{23}^2 + 2\rho_{12}\rho_{13}\rho_{23}\right)$$
$$> \frac{Y_2}{\sigma_2}(\rho_{12} - \rho_{13}\rho_{23}) + \frac{Y_3}{\sigma_3}(\rho_{13} - \rho_{12}\rho_{23})$$
$$\sim U_1\frac{\left(1 - \rho_{12}^2 - \rho_{13}^2 - \rho_{23}^2 + 2\rho_{12}\rho_{13}\rho_{23}\right)}{\sqrt{\left(1-\rho_{12}^2\right)\left(1-\rho_{13}^2\right)}}$$
$$> U_2\frac{\rho_{12} - \rho_{13}\rho_{23}}{\sqrt{1-\rho_{13}^2}} + U_3\frac{\rho_{13} - \rho_{12}\rho_{23}}{\sqrt{1-\rho_{12}^2}}. \tag{A.16}$$

Case VIII $MLE = (0, 0, 0)$ over the region $R_{VIII} : Z_{1.23} < 0, Z_{2.13} < 0, Z_{3.12} < 0.$

$$Q_{VIII}(\mathbf{Z}|\hat{\boldsymbol{\theta}}) = \text{full quadratic} = U_1^2 + \frac{U_2^2 + U_3^2 - 2c_{23}U_2U_3}{1 - c_{23}^2}. \tag{A.17}$$

To describe R_{VIII}, from Eq. B.6

$$Z_{1.23} < 0 \sim \frac{U_1\left(1 - \rho_{12}^2 - \rho_{13}^2 - \rho_{23}^2 + 2\rho_{12}\rho_{13}\rho_{23}\right)}{\sqrt{1-\rho_{12}^2}\sqrt{1-\rho_{13}^2}}$$
$$< \frac{U_2(\rho_{12} - \rho_{13}\rho_{23})}{\sqrt{1-\rho_{12}^2}} + \frac{U_3(\rho_{13} - \rho_{12}\rho_{23})}{\sqrt{1-\rho_{13}^2}}. \tag{A.18}$$

Also, it is easy to verify that $Z_{2.13} = U_{2.3}$ and $Z_{3.12} = U_{3.2}$. Hence R_{VIII} can be expressed as

$$R_{VIII} : U_{2.3} < 0, U_{3.2} < 0,$$
$$\frac{U_1\left(1 - \rho_{12}^2 - \rho_{13}^2 - \rho_{23}^2 + 2\rho_{12}\rho_{13}\rho_{23}\right)}{\sqrt{1-\rho_{12}^2}\sqrt{1-\rho_{13}^2}}$$
$$< \frac{U_2(\rho_{12} - \rho_{13}\rho_{23})}{\sqrt{1-\rho_{12}^2}} + \frac{U_3(\rho_{13} - \rho_{12}\rho_{23})}{\sqrt{1-\rho_{13}^2}}. \tag{A.19}$$

Appendix B

Here we express some standard residuals which are used in Appendix A in terms of Z_1, Y_2 and Y_3.

- $Z_{1.2}$

$$Z_{1.2} = Z_1 - \sigma_1\rho_{12}\frac{Z_2}{\sigma_2} = Z_1 - \sigma_1\rho_{12}\left[\frac{Y_2}{\sigma_2} + \rho_{12}\frac{Z_1}{\sigma_1}\right]$$
$$= Z_1\left(1-\rho_{12}^2\right) - \sigma_1\rho_{12}\frac{Y_2}{\sigma_2}. \tag{B.1}$$

- $Z_{1.3}$ By symmetry with $Z_{1.2}$, we readily get

$$Z_{1.3} = Z_1\left(1-\rho_{13}^2\right) - \sigma_1\rho_{13}\frac{Y_3}{\sigma_3}. \tag{B.2}$$

- $Z_{2.3}$

$$Z_{2.3} = Z_2 - \sigma_2\rho_{23}\frac{Z_3}{\sigma_3} = \left[Y_2 + \sigma_2\rho_{12}\frac{Z_1}{\sigma_1}\right] - \sigma_2\rho_{23}\left[\rho_{13}\frac{Z_1}{\sigma_1} + \frac{Y_3}{\sigma_3}\right]$$
$$= \sigma_2(\rho_{12} - \rho_{13}\rho_{23})\frac{Z_1}{\sigma_1} + Y_2 - \sigma_2\rho_{23}\frac{Y_3}{\sigma_3}. \tag{B.3}$$

- $Z_{3.2}$ By symmetry with $Z_{2.3}$, we readily get

$$Z_{3.2} = \sigma_3(\rho_{13} - \rho_{12}\rho_{23})\frac{Z_1}{\sigma_1} - \sigma_3\rho_{23}\frac{Y_2}{\sigma_2} + Y_3. \tag{B.4}$$

- $Z_{1.23}$ This term which is the residual of Z_1, given Z_2 and Z_3, is defined as $Z_1 - E(Z_1|Z_2, Z_3)$. Recalling that $Z \sim N[\mathbf{0}, \Sigma]$ and writing $\mathbf{B}_{2\times 2} =$ dispersion matrix of (Z_2, Z_3), we get

$$E(Z_1|Z_2, Z_3) = (\sigma_{12}, \sigma_{13})\mathbf{B}^{-1}(Z_2, Z_3)'$$
$$= \frac{(\sigma_{12}\sigma_{33} - \sigma_{13}\sigma_{23}, -\sigma_{12}\sigma_{23} + \sigma_{13}\sigma_{22})(Z_2, Z_3)'}{\sigma_{22}\sigma_{33} - \sigma_{23}^2}$$
$$= \frac{(\sigma_{12}\sigma_{33} - \sigma_{13}\sigma_{23})Z_2 + (-\sigma_{12}\sigma_{23} + \sigma_{13}\sigma_{22})Z_3}{\sigma_{22}\sigma_{33} - \sigma_{23}^2}$$
$$= \sigma_1\frac{\rho_{12} - \rho_{13}\rho_{23}}{1-\rho_{23}^2}\frac{Z_2}{\sigma_2} + \sigma_1\frac{\rho_{13} - \rho_{12}\rho_{23}}{1-\rho_{23}^2}. \tag{B.5}$$

Now replacing Z_2 by $Y_2 + \sigma_2\rho_{12}\frac{Z_1}{\sigma_1}$ and Z_3 by $Y_3 + \sigma_3\rho_{13}\frac{Z_1}{\sigma_1}$ and simplifying, we get

$$Z_{1.23} = Z_1\frac{1 - \rho_{12}^2 - \rho_{13}^2 - \rho_{23}^2 + 2\rho_{12}\rho_{13}\rho_{23}}{1-\rho_{23}^2} \tag{B.6}$$
$$- \sigma_1\frac{\rho_{12} - \rho_{13}\rho_{23}}{1-\rho_{23}^2}\frac{Y_2}{\sigma_2} - \sigma_1\frac{\rho_{13} - \rho_{12}\rho_{23}}{1-\rho_{23}^2}\frac{Y_3}{\sigma_3}.$$

- $Z_{2.13}$ This term which is the residual of Z_2, given Z_1 and Z_3, is defined as $Z_2 - E(Z_2|Z_1, Z_3)$. Using symmetry with $E(Z_1|Z_2, Z_3)$, we readily get

$$E(Z_2|Z_1, Z_3) = \sigma_2 \frac{\rho_{12} - \rho_{13}\rho_{23}}{1-\rho_{13}^2}\frac{Z_1}{\sigma_1} + \sigma_2 \frac{\rho_{23} - \rho_{12}\rho_{13}}{1-\rho_{13}^2}\frac{Z_3}{\sigma_3} \tag{B.7}$$

Now replacing Z_2 by $Y_2 + \sigma_2\rho_{12}\frac{Z_1}{\sigma_1}$ and Z_3 by $Y_3 + \sigma_3\rho_{13}\frac{Z_1}{\sigma_1}$ and noting that the coefficient of Z_1 is 0, we get

$$Z_{2.13} = Y_2 - \sigma_2 \times \frac{\rho_{23} - \rho_{12}\rho_{13}}{1-\rho_{13}^2} \times \frac{Y_3}{\sigma_3}. \tag{B.8}$$

- $Z_{3.12}$ By symmetry with $Z_{2.13}$, we readily get

$$Z_{3.12} = Y_3 - \sigma_3 \times \frac{\rho_{23} - \rho_{12}\rho_{13}}{1-\rho_{12}^2} \times \frac{Y_2}{\sigma_2}. \tag{B.9}$$

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