Statistical Analysis of Diffusion Tensors in Diffusion-weighted Magnetic
Resonance Image Data (Technical Details) *

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Abstract

In this technical report, we give detailed information about how to establish asymptotic theory for one-step weighted least-squares estimates of tensors, estimated eigenvalues and eigenvectors, and pseudo-likelihood ratio statistics. We establish the strong convergence rate and asymptotic normality for the one-step weighted least-squares estimates of tensors. We derive the first-order and second-order expansions of the eigenvalues and eigenvectors of the estimated diffusion tensors. We also derive the asymptotic distributions of pseudo-likelihood ratio statistics under the null hypotheses to classify tensor morphologies.

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1 Assumptions

The following assumptions are needed to facilitate the technical details, although they are not the weakest possible conditions.

(C1) The errors $\eta_i$ are independent and $\sup_i E\eta_i^2 < \infty$.

(C2) $\lambda_{\min}(A_n) \to \infty$.

(C3) $\theta_*$ is an interior point of $\Theta$ and $\sup_i b_i < \infty$;

(C4) $\lim_{C \to \infty} \sup_i E[\eta_i^2 1\{|\eta_i| > C\}] = 0$ and $\inf_i E[\eta_i^2] > 0$, where $1(\cdot)$ denotes the indicator function.

(C5) $\max_{1 \leq i \leq n} z_i^T (A_n)^{-1} z_i \to 0$ as $n \to \infty$.

(C6) $\sup_i E[\eta_i^3] < \infty$.

(C7) $\sum_{i=1}^n z_i z_i^T$ is always positive definite for $n \geq 7$, and the distribution of $(\log S_1, \ldots, \log S_n)$ is absolutely continuous with respect to $n$–dimensional Lebesgue measure.

(C8) The three eigenvalues of $\hat{D}$ are distinct with probability one.

(C9) $\sqrt{n}\text{vecs}(\hat{D} - D)$ converges to a multivariate normal distribution with mean $0$ and covariance matrix $\Sigma_D$.

(C10) $Q_n$ converges to a matrix $Q$, which satisfies $0 < \lambda_{\min}(Q) \leq \lambda_{\max}(Q) < \infty$, where $Q_n = G_{n,s}^{1/2} B_{n,s}^{-1} G_{n,s}^{1/2}$ and $\lambda_{\max}(Q)$ denotes the maximum eigenvalue of $Q$.

Comments. Conditions (C1)-(C2) are sufficient and necessary conditions for $\hat{\theta}_{LS}$ to be strongly consistency (Lai, Robbins, and Wei 1979; Chen, Hu, and Ying 1999). Condition (C3) is a natural condition for diffusion tensor imaging, because diffusion tensor is associated with the covariance matrix of a diffusion process and $b_i$, the $b$ factor, usually range from 0 to 3,000 s/mm$^2$ (Kingsley 2006 a, b, c). Conditions (C4)-(C6) are standard conditions to establish the asymptotic normality of $\hat{\theta}_{LS}$ for a linear heteroskedastic model (Eicker 1963; White 1980). Condition (C7) is similar to the condition used for sample covariance matrix in Okamoto (1973). Conditions (C1)-(C7) are sufficient conditions for Conditions (C8) and (C9). Condition (C10) is required to ensure the asymptotic distributions of $PLRT(i)$.  

1
2 Proof of Theorem 1

Lemma 1. Assume that

(D1) \( \sum_{i=1}^{n} z_{n,i} z_{n,i}^T = I_7 \), where \( z_{n,i} \) is a \( 7 \times 1 \) vector;

(D2) \( |f_{n,i}(\theta)| \leq C_1 ||\theta|| \) and \( |f_{n,i}(\theta_1) - f_{n,i}(\theta_2)| \leq C_2 ||\theta_1 - \theta_2|| \) for all \( i = 1, \cdots, n \), where \( C_1 \) and \( C_2 \) are constants;

(D3) \( \{\epsilon_i : i = 1, \cdots, n\} \) is a sequence of independent random variables satisfying \( E\epsilon_i = 0 \) and \( \sup_i E|\epsilon_i| < \infty \);

(D4) \( \lim_{n \to \infty} \sup_i z_{n,i}^T z_{n,i} = 0 \) and \( \sup_i E\epsilon_i^2 < \infty \).

We have the following results.

(i) If assumptions (D1)-(D3) are true, then \( \sup_i ||\theta|| \leq M e^T_k W_n(\theta) e_l \rightarrow 0 \) in probability for all \( k, l = 1, \cdots, 7 \), where \( W_n(\theta) = \sum_{i=1}^{n} (z_{n,i} z_{n,i}^T f_{n,i}(a_n \theta) \epsilon_i, \lim_{n \to \infty} a_n = 0 \) and \( e_k \) is a \( 7 \times 1 \) vector with the \( k \)-th component as one and zero otherwise;

(ii) If assumptions (D1)-(D4) are true, then \( \sup_i ||\theta|| \leq M e^T_k W_n'(\theta) e_l \rightarrow 0 \) in probability for all \( k, l = 1, \cdots, 7 \), where \( W_n'(\theta) = \sum_{i=1}^{n} (z_{n,i} z_{n,i}^T f_{n,i}(\theta) \epsilon_i). \)

Proof of Lemma 1: The proof consists of two steps as follows:

Step 1: \( W_n(\theta) \) (or \( W_n'(\theta) \)) converges to zero in probability for each \( ||\theta|| \leq M \);

Step 2: \( \{W_n(\theta) : n \geq 1\} \) (or \( \{W_n'(\theta) : n \geq 1\} \)) is stochastically equicontinuous on \( ||\theta|| \leq M \).

We prove Steps 1 and 2 for \( W_n(\theta) \) as follows. For Step 1, let \( B_n = \sum_{i=1}^{n} |(e_k^T z_{n,i} z_{n,i}^T e_l)| |\epsilon_i| \).

We have

\[
EB_n \leq (\sup_i E|\epsilon_i|) \sum_{i=1}^{n} |e_k^T z_{n,i} z_{n,i}^T e_l| \leq 7(\sup_i E|\epsilon_i|)
\]

and \( \sup_{n \geq 1} EB_n < \infty \), which yields \( B_n = O_p(1) \). Thus,

\[
|(e_k^T W_n(\theta) e_l| \leq a_n C_1 MB_n = a_n O_p(1) = o_p(1)
\]

holds for any \( ||\theta|| \leq M \). For Step 2, because \( |W_n(\theta) - W_n(\theta')| \leq C_2 a_n ||\theta - \theta'||B_n \) and \( B_n = O_p(1) \), Lemma 1 (a) of Andrews (1992) yields the statement in Step 2.

We prove Steps 1 and 2 for \( W_n'(\theta) \) as follows. To check Step 1, we apply the weak law of large numbers (Theorem 1 in Chow and Teicher 1988; p.338). We check the following three
conditions stated as follows:

\[(i) \sum_{i=1}^{n} P\{|X_{n,i}| \geq \epsilon\} \rightarrow 0 \quad \text{for} \quad \epsilon > 0; \]

\[(ii) \sum_{i=1}^{n} \text{Var}(X_{n,i}^2 \mathbb{1}\{|X_{n,i}| < 1\}) \rightarrow 0; \quad (iii) \sum_{i=1}^{n} E(X_{n,i} \mathbb{1}\{|X_{n,i}| < 1\}) \rightarrow 0; \]

where \(X_{n,i} = (e_k^T z_{n,i} z_{n,i}^T e_l) f_{n,i}(\theta) \epsilon_i\). Using the Mapkob and Cauchy-Schwartz inequality, we can prove condition (i) by noting that

\[\sum_{i=1}^{n} P\{|X_{n,i}| \geq \epsilon\} \leq \epsilon - 2 \sum_{i=1}^{n} E|X_{n,i}|^2 \leq \epsilon - 2 C_1 M \sum_{i=1}^{n} (z_{n,i}^T z_{n,i})^2 E|\epsilon_i|^2 \leq C \sup_i z_{n,i}^T z_{n,i},\]

where \(C\) and \(C_1\) are constants. Condition (ii) can be proved by noting that

\[\sum_{i=1}^{n} \text{Var}(X_{n,i}^2 \mathbb{1}\{|X_{n,i}| < 1\}) \leq \sum_{i=1}^{n} E|X_{n,i}|^2 \leq C \sup_i z_{n,i}^T z_{n,i}.\]

To check condition (iii), we note that \(\sum_{i=1}^{n} E(X_{n,i} \mathbb{1}\{|X_{n,i}| < 1\})\) can be bounded by

\[\sum_{i=1}^{n} E(X_{n,i} \mathbb{1}\{|X_{n,i}| \geq 1\}) \leq \sum_{i=1}^{n} z_{n,i}^T z_{n,i} E[|\epsilon_i| \mathbb{1}\{(\max_j z_{n,j}^T z_{n,j})|\epsilon_i| \geq 1\}] \leq \sum_{i=1}^{n} z_{n,i}^T z_{n,i} \sqrt{E|\epsilon_i|^2} \sqrt{P\{(\max_j z_{n,j}^T z_{n,j})|\epsilon_i| \geq 1\}} \leq (\max_j z_{n,j}^T z_{n,j}) C,\]

because \(E(X_{n,i}) = 0\). To check Step 2, we can show that \(\{W_n'(\theta) : n \geq 1\}\) is stochastically equicontinuous on \(||\theta|| \leq M\) by following the same reasoning for \(W_n(\theta)\). This completes the proof of Lemma 1.

**Proof of Theorem 1**: To prove Theorem 1 (a), we consider two different cases for \(\hat{\theta}^{(0)}\) in \(\Theta_s,\delta'\): a fixed \(\hat{\theta}^{(0)}\) and a random \(\hat{\theta}^{(0)}\).

We prove Theorem 1 (a) for the fixed \(\hat{\theta}^{(0)} \in \Theta_s,\delta'\) as follows. It follows from condition (C3) that

\[0 < m = \inf_{i \geq 1, \theta \in \Theta_s,\delta'} \exp(2z_i^T \theta) \leq \sup_{i \geq 1, \theta \in \Theta_s,\delta'} \exp(2z_i^T \theta) = M < \infty,\]

where \(\Theta_s,\delta' = \{\theta : ||\theta - \theta_s|| \leq \delta'\}\) for any \(\delta' > 0\). Thus, for all \(\theta \in \Theta_s,\delta'\), we have \(mA_n \leq B_n(\theta) \leq MA_n\) and

\[m\lambda_{\min}(A_n) \leq \lambda_{\min}(B_n(\theta)) \leq M\lambda_{\min}(A_n).\]
By using (C1) and (C2), we can use equation (1) and Theorem 1 of Lai et al. (1979) to infer, for any $\delta > 0$ and $\theta \in \Theta_{\star, \delta'}$, we have

$$\left( \sum_{i=1}^{n} \exp(2z_i^T \theta) z_i z_i^T \right)^{-1} \sum_{i=1}^{n} \exp(2z_i^T \theta) z_i \eta_i = o \left( \left\{ \log \lambda_{\min}(A_n) \right\}^{1+\delta} / \lambda_{\min}(A_n) \right)^{1/2}$$

almost surely. See also Theorem 1 of Chen et al. (1999).

For the random $\hat{\theta}(0)$, such as $\hat{\theta}_{LS}$, we prove Theorem 1 (a) by showing that

$$\sup_{\theta \in \Theta_{\star, \delta'}} \left\| B_n(\theta) \right\|^{-1} \sum_{i=1}^{n} \exp(2z_i^T \theta) z_i \eta_i = o \left( \left\{ \log \lambda_{\min}(A_n) \right\}^{1+\delta} / \lambda_{\min}(A_n) \right)^{1/2}$$

holds almost surely. It follows from equation (1) that it is sufficient to show that

$$\sup_{\theta \in \Theta_{\star, \delta'}} \left\| A_n^{-1} \sum_{i=1}^{n} \exp(2z_i^T \theta) z_i \eta_i \right\| = o \left( \left\{ \log \lambda_{\min}(A_n) \right\}^{1+\delta} / \lambda_{\min}(A_n) \right)^{1/2}$$

a.s. (2)

To prove (2), we mainly generalize the methods used in Lai et al. (1979), who proved strong consistency of $\hat{\theta}_{LS}$. Note that an extra term $\exp(2z_i^T \theta)$ appears with each $\epsilon_i$. The proof consists of three steps. We first show that

$$\sum_{i=1}^{\infty} c_i \exp(2z_i^T \theta) \eta_i$$

converges a.s. for all sequences $\{c_i\}$ such that $\sum_{i=1}^{n} c_i^2 < \infty$. (3)

Second, we apply the same techniques used in Lai et al. (1979) to prove a general version of Theorem 2 in Lai et al. (1979), in which we replace $\epsilon_i$ by $\exp(2z_i^T \theta) \eta_i$ for all $i$. Finally, we apply a Chung-style uniform law of large numbers in Zaman (1989) to prove (2).

To avoid replicating the proof in Lai et al. (1979), we only show (3) as follows. Let $S_n(\theta) = \sum_{i=1}^{n} c_i \exp(2z_i^T \theta) \eta_i$, $\| \cdot \|$ is the common $L_2$ norm, $\| \cdot \|_0$ is the supremum norm:

$$\| f \|_0 = \sup_{\theta \in \Theta_{\star, \delta'}} | f(\theta) |$$

and $\| \cdot \|_L$ is the Lipschitz norm given by

$$\| f \|_L = \sup_{\theta \in \Theta_{\star, \delta'}} | f(\theta) | + \sup_{\theta, \theta' \in \Theta_{\star, \delta'}, \theta \neq \theta'} | f(\theta) - f(\theta') | \| \theta - \theta' \|^{-1}.$$

We first show that the series of random function $S_n(\theta)$ converges uniformly in quadratic mean. Under assumption (C1), we use the type 2 inequality (Araujo and Gine 1980; Zaman 1989) to conclude that for any $m, n$,

$$E \| S_n(\theta) - S_m(\theta) \|_0^2 \leq C \sum_{i=m}^{n} E \| c_i \exp(2z_i^T \theta) \eta_i \|_L^2 \leq CM^2 \sup_i (E \eta_i^2) \sum_{i=m}^{n} c_i^2,$$

where $C$ is a constant. Thus, the series $\{ S_n(\theta) : n \geq 1 \}$ is Cauchy in quadratic mean and is convergent in quadratic mean. We can apply the Ito-Nisio lemma (Ito and Nisio 1968)
to conclude that $S_n(\theta)$ converges uniformly to a limit function $s(\theta) \in \{ f(\theta) \mid f : \Theta_{\alpha, \beta'} \to (-\infty, +\infty) \text{ and } ||f||_0 < \infty \}$ almost surely. This completes the proof of (3).

To prove Theorem 1 (b), we first prove that

$$[G_n(\hat{\theta}(k))]^{-1/2}B_n(\hat{\theta}(k)) (\hat{\theta}(k) - \theta_*) = [G_n(\theta_*)]^{-1/2} \sum_{i=1}^{n} \omega_{i,s} z_{i} \eta_{i} [1 + o_p(1)],$$

and then we apply the Lindeberg-Feller Theorem to prove that $[G_n(\theta_*)]^{-1/2} \sum_{i=1}^{n} \omega_{i,s} z_{i} \eta_{i}$ converges to $N(0, \sigma^2 I_T)$, where $\omega_{i,s} = \exp(z^T \theta_*)$.

Because $[G_n(\hat{\theta}(k))]^{-1/2}B_n(\hat{\theta}(k)) (\hat{\theta}(k) - \theta_*)$ can be written as

$$[G_n(\hat{\theta}(k))]^{-1/2}B_n(\hat{\theta}(k)) [B_n(\hat{\theta}(k-1))]^{-1} \sum_{i=1}^{n} \omega_{i}^{(k-1)} z_{i} \eta_{i},$$

we can prove (4) by using the following steps:

$$||[G_n(\hat{\theta}(k))]^{-1}G_n(\theta_*) - I_T|| + ||B_n(\hat{\theta}(k)) [B_n(\hat{\theta}(k-1))]^{-1} - I_T|| \to 0 \text{ a.s.,}$$

(5)

$$[G_n(\theta_*)]^{-1/2} \sum_{i=1}^{n} \omega_{i}^{(k-1)} z_{i} \eta_{i} = [G_n(\theta_*)]^{-1/2} \sum_{i=1}^{n} \omega_{i,s} z_{i} \eta_{i} [1 + o_p(1)].$$

(6)

It follows from Theorem 1 (a) and conditions (C2) and (C3) that (5) is true. Furthermore, by using (C3) and Theorem 1 (a), we have that $\sup_i |\omega_{i}^{(k-1)} - \omega_{i,s}|$ converges to zero almost surely. Thus, (6) is proved, and so is (4). It follows from conditions (C1)-(C5) and the Lindeberg-Feller Theorem that $[G_n(\theta_*)]^{-1/2} \sum_{i=1}^{n} \omega_{i,s} z_{i} \eta_{i}$ converges to $N(0, I_T)$ in distribution.

To prove Theorem 1 (c), let $T_n(\theta) = [G_n(\theta_*)]^{-1/2} F_n(\theta) [G_n(\theta_*)]^{-1/2} - I_T$. We note that $T_n(\hat{\theta}(k))$ can be rewritten as

$$[G_n(\theta_*)]^{-1/2} \sum_{i=1}^{n} z_{i} z_{i}^T \exp(4z_{i}^T \theta_*) E\eta_{i}^2 [\exp(4z_{i}^T \Delta^{(k)}) e_i(\hat{\theta}^{(k)})^2 / E\eta_{i}^2 - 1] [G_n(\theta_*)]^{-1/2},$$

where $\Delta^{(k)} = \hat{\theta}^{(k)} - \theta_*$. Now $e_i(\hat{\theta}^{(k)})^2 = \eta_{i}^2 - 2z_{i}^T \Delta^{(k)} \eta_{i} + (z_{i}^T \Delta^{(k)})^2$, $T_n(\hat{\theta}(k))$ can be written as the sum of term (I), term (II), and term (III), where

$$\text{term (I)} = \sum_{i=1}^{n} z_{n,i} z_{n,i}^T \exp(4z_{i}^T \Delta^{(k)}) [\eta_{i}^2 - E\eta_{i}^2] / E\eta_{i}^2,$$

$$\text{term (II)} = \sum_{i=1}^{n} z_{n,i} z_{n,i}^T \exp(4z_{i}^T \Delta^{(k)}) [-2z_{i}^T \Delta^{(k)} \eta_{i}] / E\eta_{i}^2.$$
\[
\text{term (III)} = \sum_{i=1}^{n} z_{n,i} z_{n,i}^T \{ \exp(4z_i^T \Delta^{(k)}) (z_i^T \Delta^{(k)})^2 / E\eta_i^2 + \exp(4z_i^T \Delta^{(k)}) - 1 \},
\]
and \( z_{n,i} = [G_n(\theta_\ast)]^{-1/2} z_i \exp(2z_i^T \theta_\ast) \sqrt{E\eta_i^2} \). Because
\[
\sup_i | \exp(4z_i^T \Delta^{(k)}) (z_i^T \Delta^{(k)})^2 / E\eta_i^2 + \exp(4z_i^T \Delta^{(k)}) - 1 | \leq C_3 |\Delta^{(k)}|,
\]
term (III) converges to zero almost surely. Applying Lemma 1 leads to the result that every element of terms (I) and (II) converges to zero in probability.

3 Proof of Theorem 2

Proof of Theorem 2: We prove Theorem 2 (a) for \( \hat{\theta}_{LS} \) as follows. The estimated eigenvalues \( \{m_1, m_2, m_3\} \) are the roots of
\[
g(m) = |\hat{D} - mI_3| = m^3 - m^2 I_1(\hat{D}) + mI_2(\hat{D}) - I_3(\hat{D}) = 0,
\]
where \( I_1(\hat{D}) = \text{trace}[\hat{D}] \), \( I_3(\hat{D}) = |\hat{D}| \), and
\[
I_2(\hat{D}) = \hat{D}_{11} \hat{D}_{22} + \hat{D}_{11} \hat{D}_{33} + \hat{D}_{22} \hat{D}_{33} - (\hat{D}_{12}^2 + \hat{D}_{13}^2 + \hat{D}_{23}^2).
\]
Let \( d(\hat{D}) \) be the discriminant of the polynomial \( g(m) \). We know (Okamoto, 1973) that

the eigenvalues of \( \hat{D} \) are distinct if and only if \( d(\hat{D}) \neq 0 \).

Thus, it suffices to prove that \( d(\hat{D}) \neq 0 \) holds with probability one. Because \( \hat{\theta}_{LS} \) is a linear combination of \( \log S_i \) and \( d(\hat{D}) \) is a polynomial in the elements of \( \hat{D} \), \( d(\hat{D}) \) is a polynomial in the elements of \( \{\log S_1, \cdots, \log S_n\} \), denoted as \( f(\log S_1, \cdots, \log S_n) \). Using the lemma in Okamoto (1973), we only need to show that \( f(\log S_1, \cdots, \log S_n) \) is not identically zero. If we set \( \log S_i = z_i^T \theta_{0*} \), in which \( \theta_{0*} \) corresponds to a diffusion tensor with three distinct eigenvalues, then \( f(z_1^T \theta_{0*}, \cdots, z_n^T \theta_{0*}) \) is not equal to zero. This proves Theorem 2 (a).

We prove Theorem 2 (b) in two steps. In Step 1, we consider any fixed \( \hat{\theta}^{(0)} \in \Theta_{s, \delta} \). Thus,
\[
\hat{\theta}^{(1)} = \sum_{i=1}^{n} z_i z_i^T \exp(2z_i^T \hat{\theta}^{(0)})^{-1} \sum_{i=1}^{n} \exp(2z_i^T \hat{\theta}^{(0)}) z_i \log S_i
\]
is a polynomial function of \{\log S_1, \cdots, \log S_n\}. Similar to the argument for Theorem 2 (a), we can use the lemma in Okamoto (1973) to complete the proof of Theorem 2 (b).

In Step 2, we consider any random \( \hat{\theta}^{(0)} \in \Theta_{*,\delta'} \). Note that \( \hat{\theta}^{(1)} = [B_n(\hat{\theta}_{LS})]^{-1} \sum_{i=1}^n \exp(2z_i^T \hat{\theta}_{LS})z_i \log S_i \). Let \( \hat{D}^{(1)} \) be the diffusion tensor of \( \hat{\theta}^{(1)} \) and let \( d(\hat{D}^{(1)}) \) be the discriminant of the polynomial \( g(m) = |mI_3 - \hat{D}^{(1)}| = 0 \). Thus, by using Fubini’s Theorem, we have \( P(\{d(\hat{D}^{(1)}) = 0\} | \hat{\theta}_{LS} \in \Theta_{*,\delta'}) \) can be written as

\[
\int P(\{d(\hat{D}^{(1)}) = 0\} | \hat{\theta}_{LS} = \theta, \hat{\theta}_{LS} \in \Theta_{*,\delta'}) P(\hat{\theta}_{LS} = \theta | \hat{\theta}_{LS} \in \Theta_{*,\delta'}) d\theta,
\]

where \( \{d(\hat{D}^{(1)}) = 0\} \) denotes the event \( d(\hat{D}^{(1)}) = 0 \), \( p(\hat{\theta}_{LS} = \theta | \hat{\theta}_{LS} \in \Theta_{*,\delta'}) \) is the conditional density function of \( \hat{\theta}_{LS} \) given \( \hat{\theta}_{LS} \in \Theta_{*,\delta'} \), and \( P(\{d(\hat{D}^{(1)}) = 0\} | \hat{\theta}_{LS} = \theta, \hat{\theta}_{LS} \in \Theta_{*,\delta'}) \) is the conditional probability of \( \{d(\hat{D}^{(1)}) = 0\} \) given \( \hat{\theta}_{LS} = \theta \) and \( \hat{\theta}_{LS} \in \Theta_{*,\delta'} \). We note that \( \hat{\theta}_{LS} \) is a linear combination of \( \{\log S_i : i = 1, \cdots, n\} \) and \( \hat{\theta}^{(1)} \) given \( \hat{\theta}_{LS} = \theta \) is a linear function of \( \{\log S_i : i = 1, \cdots, n\} \). It follows from Okamoto’s (1973) lemma that \( P(\{d(\hat{D}^{(1)}) = 0\} | \hat{\theta}_{LS} = \theta, \hat{\theta}_{LS} \in \Theta_{*,\delta'}) = 0 \) holds for almost every \( \theta \in \Theta_{*,\delta'} \). Thus, \( P(\{d(\hat{D}^{(1)}) = 0\} | \hat{\theta}_{LS} \in \Theta_{*,\delta'}) = 0 \).

4 Proof of Theorem 3

**Proof of Theorem 3.** For an isotropic tensor, we have \( \Lambda = \lambda I_3 \), \( \Gamma = I_3 \), and \( C_n^T = E \). Recall that \( T_n = \lambda I_3 + n^{-1/2}U_n \), we have

\[
T_n = C_n^TMC_n = C_n^T(\lambda I_3 + n^{-1/2}H_n)C_n = \lambda I_3 + n^{-1/2}C_n^TH_nC_n,
\]

where \( H_n = \sqrt{n}(M - \lambda I_3) \). Thus, \( U_n = C_n^TH_nC_n \), and \( C_n \) and \( H_n \) are uniquely defined as continuous functions of \( U_n \) with the proper ordering except on a set of probability 0. Using a theorem due to Rubin (Anderson, 2003; Theorem 13.5.3), we can infer that the limiting distribution of \( H_n \) and \( C_n \) is determined by \( C_n^THC = U \) and the distribution of \( U \), in which \( H = \text{diag}(h_1, h_2, h_3) \) and \( C = (c_{ij}) \) satisfy \( h_1 > h_2 > h_3, c_{ii} > 0 \) for \( i = 1, 2, 3 \), and \( C_n^TC = I_{3x3} \). Note that the density of the distribution of \( U \) is proportional to \( |\Sigma_U|^{-1/2} \exp\{-\frac{1}{2} \text{vecs}(U)^T\Sigma_U^{-1} \text{vecs}(U)\} \). Using a result due to Hsu, P.L. (Deemer and Olkin,
1951), we can obtain that the Jacobian of the transformation from $U$ to $H$ and $C$ is proportional to $(h_1 - h_2)(h_2 - h_3)(h_1 - h_3)$. Thus, combining the above two results, we can obtain the joint density of $H$ and $C$ as given in Theorem 3.

Because $h_1 \geq h_2 \geq h_3$ are three eigenvalues of $U$, $-h_3 \geq -h_2 \geq -h_1$ are the corresponding eigenvalues of $-U$. Moreover, since $U$ and $-U$ follow the same distribution, $h_2$ and $-h_2$ follow the same distribution. Thus, $E(h_2) = E(-h_2)$, which yields that $E(h_2) = 0$. Similarly, we can show that $E(h_1 + h_2 + h_3) = 0$. We can use the explicit form of $p(h, C)$ to infer that $E(h_1 - h_2) > 0$ and $E(h_2 - h_3) > 0$. Finally, we get $E(h_1) > E(h_2) = 0 > E(h_3)$.

5 Proof of Theorem 4

Proof of Theorem 4. We have $T_n = \Lambda + n^{-1/2}U_n = C_n^TMC_n = C_n^T(\Lambda + n^{-1/2}H_n)C_n$. Using a matrix representation, we get

$$
\begin{pmatrix}
\lambda_1 I_2 & 0 \\
0^T & \lambda_3 \\
\end{pmatrix} + n^{-1/2}
\begin{pmatrix}
U_{n,11} & U_{n,12} \\
U_{n,21} & U_{n,22} \\
\end{pmatrix}
= \begin{pmatrix}
C_{n,11}^T & n^{-1/2}F_{n,21}^T \\
C_{n,12}^T & C_{n,22} \\
\end{pmatrix} 
\begin{pmatrix}
\lambda_1 C_{n,11}^T C_{n,11} & 0 \\
0^T & \lambda_3 C_{n,22}^2 \\
\end{pmatrix} + n^{-1/2} \times
\begin{pmatrix}
C_{n,11}^T H_{n,1} C_{n,11} & \lambda_1 C_{n,11}^T F_{n,12} + \lambda_3 F_{n,21}^T C_{n,22} \\
\lambda_1 F_{n,12}^T C_{n,11} + \lambda_3 C_{n,22} F_{n,21} & C_{n,22}^2 h_{n,3} \\
\end{pmatrix} + n^{-1}M_n,
$$

where $F_{n,12} = \sqrt{n}C_{n,12}$, $F_{n,21} = \sqrt{n}C_{n,21}$, and $M_n$ is given by

$$
\begin{pmatrix}
M_{n,11} & M_{n,12} \\
M_{n,21} & M_{n,22} \\
\end{pmatrix} = \begin{pmatrix}
(\lambda_3 + n^{-1/2}h_{n,3}) F_{n,21}^T F_{n,21} & C_{n,11}^T H_{n,1} F_{n,12} + h_{n,3} C_{n,22} F_{n,21}^T \\
F_{n,12}^T H_{n,1} C_{n,11} + h_{n,3} C_{n,22} F_{n,21} & \lambda_1 F_{n,12}^T F_{n,12} + n^{-1/2} F_{n,12}^T H_{n,1} F_{n,12} \\
\end{pmatrix}.
$$
Because $C_n^T C_n = C_n C_n^T = I_3$, we know that

$$
\begin{pmatrix}
I_2 & 0 \\
0^T & 1
\end{pmatrix}
= 
\begin{pmatrix}
C_{n,11}^T C_{n,11} & 0 \\
0^T & C_{n,22}^2
\end{pmatrix}
+ n^{-1/2} \times
$$

$$
\begin{pmatrix}
0 & C_{n,11}^T \mathbf{F}_{n,12} + \mathbf{F}_{n,21}^T C_{n,22} \\
\mathbf{F}_{n,12}^T C_{n,11} + C_{n,22} \mathbf{F}_{n,21} & 0
\end{pmatrix}
+ n^{-1} \begin{pmatrix}
\mathbf{F}_{n,21}^T \mathbf{F}_{n,21} & 0 \\
0^T & \mathbf{F}_{n,12}^T \mathbf{F}_{n,12}
\end{pmatrix}.
$$

This gives

$$
C_{n,11}^T C_{n,11} = I_2 - n^{-1} \mathbf{F}_{n,21}^T \mathbf{F}_{n,21}, \quad C_{n,11} C_{n,11}^T = I_2 - n^{-1} \mathbf{F}_{n,12}^T \mathbf{F}_{n,12},
$$

$$
C_{n,11}^T \mathbf{F}_{n,12} + \mathbf{F}_{n,21}^T C_{n,22} = 0, \quad \text{and} \quad C_{n,22}^2 = 1 - n^{-1} \mathbf{F}_{n,12}^T \mathbf{F}_{n,12}.
$$

Combining the above results, we get

$$
\mathbf{U}_{n,11} = C_{n,11}^T \mathbf{H}_{n,1} C_{n,11} + n^{-1/2} (\mathbf{M}_{n,11} - \lambda_1 \mathbf{F}_{n,21}^T \mathbf{F}_{n,21}),
$$

$$
\mathbf{U}_{n,12} = (\lambda_1 - \lambda_3) C_{n,11}^T \mathbf{F}_{n,12} + n^{-1/2} \mathbf{M}_{n,12},
$$

and $\mathbf{U}_{n,22} = C_{n,22}^2 h_{n,3} + n^{-1/2} (\mathbf{M}_{n,22} - \lambda_3 \mathbf{F}_{n,12}^T \mathbf{F}_{n,12})$. Furthermore, by following the same reasoning in Theorem 13.5.1 of Anderson (2003) and Anderson (1963), it follows that

$$
\begin{align*}
C_{n,11}^T \mathbf{H}_{n,1} C_{n,11} &= \mathbf{U}_{n,11} + n^{-1/2} (\lambda_1 - \lambda_3) \mathbf{F}_{n,21}^T \mathbf{F}_{n,21} + o_p(n^{-1/2}), \\
h_{n,3} &= \mathbf{U}_{n,22} - (\lambda_1 - \lambda_3) n^{-1/2} \mathbf{F}_{n,12}^T \mathbf{F}_{n,12} + o_p(n^{-1/2}), \\
C_{n,22}^2 &= 1 - n^{-1} \mathbf{F}_{n,12}^T \mathbf{F}_{n,12} + o_p(n^{-1}), \\
C_{n,11}^T \mathbf{F}_{n,12} &= - \mathbf{F}_{n,21}^T C_{n,22} = - \mathbf{F}_{n,21}^T + o_p(n^{-1/2}), \quad \text{and} \\
C_{n,11}^T \mathbf{F}_{n,12} &= o_p(1) = (\mathbf{U}_{n,12} - n^{-1/2} \mathbf{M}_{n,12})/(\lambda_1 - \lambda_3) + o_p(n^{-1/2}).
\end{align*}
$$

The above results lead to Theorem 4 (a), (b), and (c). By using the transformation given by $\hat{h}_1 = -h_2$ and $\hat{h}_2 = -h_1$, we can prove that $E(h_1 + h_2) = 0$ and $E(h_1) > 0 > E(h_2)$.

By using $C_n^T = \Gamma^T \mathbf{E}$, we obtain $\mathbf{E} = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3) = \Gamma C_n^T$, which leads to

$$
(\mathbf{e}_1, \mathbf{e}_2) = (\mathbf{v}_1, \mathbf{v}_2) C_{n,11}^T + n^{-1/2} \mathbf{v}_3 \mathbf{U}_{n,12}^T C_{n,11}^T / (\lambda_1 - \lambda_3) + o_p(n^{-1/2}).
$$
Furthermore, by using (8), we have

\[ \sqrt{n}(e_3 - v_3) = (v_1, v_2)F_{n,21}^T - 0.5v_3n^{-1/2}F_{n,12}^TF_{n,12} + o_p(n^{-1/2}) \]

\[ = -(v_1, v_2)[I_2 - n^{-1/2}(C_{n,11}C_{n,11} - U_{n,22}I_2)(\lambda_1 - \lambda_3)^{-1}]U_{n,12}(\lambda_1 - \lambda_3)^{-1} \]

\[ - 0.5v_3n^{-1/2}U_{n,21}C_{n,11}C_{n,11}U_{n,12}/(\lambda_1 - \lambda_3)^2 + o_p(n^{-1/2}). \]

Using (9) and the results in Theorem 4 (a), (b), and (c), the proof of Theorem 4 (d) immediately follows.

Proof of Corollaries 1 and 2. The technical arguments are similar to the proof of Theorem 4 and thus the details are omitted for brevity.

6 Proof of Theorem 5

Proof of Theorem 5: The key idea in deriving the asymptotic distributions of PLRT(i) is as follows. After some algebraic and probabilistic manipulations, we get

\[ \ell_n(\theta|\hat{\theta}_{LS}) - \ell_n(\theta_*) = \hat{\theta}^{(1)}B_n(\hat{\theta}_{LS})\hat{\theta}^{(1)} - (\theta - \hat{\theta}^{(1)})^TB_n(\hat{\theta}_{LS})(\theta - \hat{\theta}^{(1)}) \]

(10)

\[ = Z_n^TQ_nZ_n - [K_n(\theta - \theta_*) - Z_n]^TQ_n[K_n(\theta - \theta_*) - Z_n] + o_p(1), \]

where \( K_n = G_{n,s}^{-1/2}B_{n,s}, Q_n = G_{n,s}^{1/2}B_{n,s}^{-1}G_{n,s}^{1/2}, \) and \( Z_n = C_{n,s}^{-1/2}\sum_{i=1}^n z_i\eta_i\omega_{i,s}, \) in which \( G_{n,s} = G_n(\theta_*) \), \( B_{n,s} = B_n(\theta_*) \), and \( \omega_{i,s} = \exp(2z_i^T\theta_*) \). Thus, we establish a quadratic expansion of \( \ell_n(\theta|\hat{\theta}_{LS}) \) in \( \theta \) about \( \theta_* \). Finally, we apply the asymptotic results in Andrews (2001) and Zhu and Zhang (2006) to deriving the limiting distributions of PLRT(i).

It follows from Theorem 1 of Andrews (2001) that

\[ \max_{\theta \in \Theta(i)} \ell_n(\theta|\hat{\theta}_{LS}) = \ell_n(\theta_*) + Z_n^TQ_nZ_n - \max_{\omega \in \Omega(i)} [\omega - Z_n]^TQ_n[\omega - Z_n] + o_p(1), \]

(11)

in which \( \{K_n(\theta - \theta_*)/b_n : n \geq 1\} \) locally approximates a cone \( \Omega(j) \), where \( K_n = |G_n(\theta_*)|^{-1/2}B_n(\theta_*) \), \( b_n \to \infty \), and \( b_n \leq C\lambda_{\min}(K_n) \leq C\sqrt{\lambda_{\min}(A_n)}. \) The parameter spaces \( \Theta(i) \) can be, respec-
tively, written as

\[ \Theta(1) = \{ (\log S_0, \lambda) : \log S_0 \in R, \ D = \lambda I_3 \geq 0 \}, \]

\[ \Theta(2) = \{ (\log S_0, a, b, c, d) : \log S_0 \in R, \ D = a^2 I_3 - a^2 \sin^2(b)vv^T \}, \quad \text{and} \quad (12) \]

\[ \Theta(3) = \{ (\log S_0, a, b, c, d) : \log S_0 \in R, \ D = a^2 \sin^2(b)I_3 + a^2[1 - \sin^2(b)]vv^T \}, \]

in which \( v = (\cos(d), \cos(c) \sin(d), \sin(c) \sin(d))^T \). Therefore, we have

\[
PLRT(j) = \max_{\omega \in \Omega(j)} [\omega - Z_n]^T Q_n [\omega - Z_n] + o_p(1).
\]

To derive the asymptotic distribution of \( PLRT(j) \), we only need to study the geometric structure of \( \Omega(j) \) for \( j = 1, 2, 3 \).

For \( \theta \in \Theta(1) \), \( \theta = G_1 \xi \), where

\[
\xi = \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix} \quad \text{and} \quad G_1^T = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 \end{pmatrix}.
\]

Thus, the isotropic hypotheses can be written as \( H_0^{(1)} : \theta = G_1 \xi, \xi \in R^2 \) versus \( H_1^{(1)} : \theta \in \Theta \).

Because \( D \) has the form \( \lambda I_3 \) with \( \lambda > 0 \) under \( H_0^{(1)} \), we can get \( \Omega(1) = \{ \omega : \omega = G_1 \xi, \xi \in R^2 \} \).

Finally, we obtain that \( PLRT(1) \) converges to \( X(1) = Z^T [Q - QG_1^T (G_1 Q G_1^T)^{-1} G_1 Q] Z \) in distribution.

For \( \theta \in \Theta(2) \), we consider two different cases of \( D = \lambda_1 I_3 - (\lambda_1 - \lambda_3) v_3 v_3^T : \lambda_1 - \lambda_3 > 0 \) and \( \lambda_1 = \lambda_3 \). If \( \lambda_1 > \lambda_3 \), we define

\[
\xi^T = (\xi_1, \xi_2, \xi_3, \xi_4, \xi_5) = (S_0, \lambda_1, \sqrt{\lambda_1 - \lambda_3} v_3^T)
\]

and \( \xi^* \) is the true value under the null hypothesis \( H_0^{(2)} \). Thus, \( \theta \) can be written as a function of \( \xi \) as follow:

\[
\theta(\xi) = (\xi_1, \xi_2 - \xi_3^2, -\xi_3 \xi_4, -\xi_3 \xi_5, \xi_2 - \xi_4^2, -\xi_4 \xi_5, \xi_2 - \xi_5^2)^T.
\]

Differentiating \( \theta \) with respect to \( \xi \), we can prove that the rank of \( \partial \theta(\xi)/\partial \xi \) evaluating at \( \xi^* \) is 5, because \( \xi_{3,*}^2 + \xi_{4,*}^2 + \xi_{5,*}^2 = \lambda_1 - \lambda_3 > 0 \). Let \( G_2 = \partial \theta(\xi^*)/\partial \xi \), we get that \( \Omega(2) = \{ \omega : \).
$\omega = G_2^T \xi, \xi \in R^5$ and $PLRT(2)$ converges to $X(2) = Z^T [Q - QG_2^T (G_2QG_2^T)^{-1} G_2Q] Z$ in distribution.

Thus, we introduce a new parametrization $\omega$ can be written as $Hence, $\theta$ can be written as

$$\theta(\xi|e) = (\xi_1,\xi_2 - \xi_3 e_1, -\xi_3 e_1 e_2, -\xi_3 e_1 e_3, \xi_2 - \xi_3 e_2 e_3, \xi_2 - \xi_3 e_3)$$

Let $\Theta(2|e) = \{\theta : \theta = \theta(\xi|e)\}$. Differentiating $\theta(\xi|e)$ with respect to $\xi$ for any given $e$, it follows that the rank of $G_3(e)$ is 3 and $\Theta(2|e)$ can be approximated by $\Omega(2|e) = \{\omega : \omega = G_3(e)^T \xi, \xi \in [0,\infty]\}$. Finally, we have

$$PLRT(2) = \max_{ee^T e=1, \omega \in \Omega(2|e)} [Z_n - \omega]^T Q_n [Z_n - \omega] + o_p(1)$$

Similar to $PLRT(2)$, we can establish the asymptotic distribution of $PLRT(3)$.

7 Approximating $X(i)$

Because similar procedure can be developed for $X(2)$ and $X(3)$, we only give a procedure for approximating $X(1)$ as follows. First, $X(1)$ can be written as $Z^T \Sigma(1) Z$ and $\Sigma(1) = Q - QG_1^T (G_1QG_1^T)^{-1} G_1Q$, in which $Q$ is the limit of $Q_n$, $G_1$ is a matrix defined in the proof of Theorem 5, and $Z$ is a multivariate Gaussian random vector that has mean $\theta$ and covariance matrix $I_7$. Second, we can construct a consistent estimate of $\Sigma(1)$, $\hat{\Sigma}(1) = \hat{Q} - \hat{Q}G_1^T (G_1\hat{Q}G_1^T)^{-1} G_1\hat{Q}$, where $\hat{Q} = F_n(\hat{\theta}(1))^{1/2} B_n(\hat{\theta}(1))^{-1} F_n(\hat{\theta}(1))^{1/2}$. Third, we can approximate $X(1)$ by a scaled $\chi^2$ distribution $c_1 \chi^2(\nu_1)$, where $\nu_1$ is the degree of freedom (Chou et al. 1991). Fourth, we use the moment matching technique to match the mean and variance of $c_1 \chi^2(\nu_1)$ with those of $X(1)$ in order to estimate $c_1$ and $\nu_1$. Finally, we have $c_1 = \sum_{i=1}^{6} \gamma_i^2 / \sum_{i=1}^{6} \gamma_i$ and $\nu_1 = (\sum_{i=1}^{6} \gamma_i)^2 / \sum_{i=1}^{6} \gamma_i^2$, where $\gamma_i$ are eigenvalues of $\hat{\Sigma}(1)$. 

12
REFERENCES


