

# On Second-Order Error Terms In Fully Exponential Laplace Approximations.

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## Abstract

Posterior means can be expressed as the ratio of integrals, which is called *fully exponential form*. To approximate the posterior means analytically, Laplace's method might be useful. In this article, we present explicit error terms of order  $n^{-1}$ , and of order  $n^{-2}$  in the Laplace approximations with asymptotic modes. Moreover, we give second-order error terms in fully exponential Laplace approximations to posterior means with asymptotic modes, which are proposed by Miyata (2004).

## 1. Introduction

Laplace's method for the asymptotic evaluation of integrals (Laplace, 1847) is a simple and useful technique. This method has been applied frequently in statistical theory by many authors (Mosteller and Wallace 1964; Lindley 1980; Tierney and Kadane 1986).  $\Theta = \Theta_1 \times \cdots \times \Theta_d \subseteq \mathbb{R}^d$  is an open parameter space of  $\boldsymbol{\theta} \equiv (\theta_1, \dots, \theta_d)^T$ , where  $T$  denotes the transpose of a matrix. Suppose that  $(\Omega, \mathcal{A})$  is a measurable space,  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  is a family of probability distributions on  $(\Omega, \mathcal{A})$ , and  $\{\mathbf{X}_i : i = 1, 2, \dots\}$  is a stochastic process on  $(\Omega, \mathcal{A})$  with  $\mathbf{X}_i$ 's taking values in  $(\mathcal{X}, \mathcal{B})$  where  $\mathcal{X}$  is a subset of  $\mathbb{R}$ , and  $\mathcal{B}$  is the class of Borel subsets of  $\mathcal{X}$ . We will assume that for all  $n$ , the distributions of  $\tilde{\mathbf{X}} = (\mathbf{X}_1, \dots, \mathbf{X}_n)$  are dominated by a  $\sigma$ -finite measure, and we will denote a density of  $\tilde{\mathbf{X}}$  under  $P_\theta$  by  $p_n(\mathbf{x}|\boldsymbol{\theta})$ . Note that  $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n, \dots)$  is the observed sequence and  $p_n(\mathbf{x}|\boldsymbol{\theta})$  depends on the first  $n$  observation  $\tilde{\mathbf{x}} = (\mathbf{x}_1, \dots, \mathbf{x}_n)$ . Let  $\theta_0$  be a true parameter, and let "a.e.  $P_{\theta_0}$ " be abbreviated to "a.e." or omitted. Let  $g^+(\boldsymbol{\theta})$  be a smooth and strictly positive function. The purpose of this article is to give first-order and second-order error terms in the fully exponential Laplace approximation to the posterior mean

$$E[g^+(\boldsymbol{\Theta})] = \frac{\int_{\Theta} g^+(\boldsymbol{\theta}) p_n(\mathbf{x}|\boldsymbol{\theta}) \pi(\boldsymbol{\theta}) d\boldsymbol{\theta}}{\int_{\Theta} p_n(\mathbf{x}|\boldsymbol{\theta}) \pi(\boldsymbol{\theta}) d\boldsymbol{\theta}}, \quad (1.1)$$

where  $\Theta$  is an open subset of  $\mathbb{R}^d$ ,  $p_n(\mathbf{x}|\boldsymbol{\theta})$  is the likelihood, and  $\pi$  is a prior. Although  $\Theta$  also denotes a random vector with a posterior distribution, we can see from the context which  $\Theta$  indicates. For convenience, the integrals in (1.1) are reexpressed as

$$E[g^+(\boldsymbol{\Theta})] = \frac{\int_{\Theta} \exp\{-nh_n^*(\boldsymbol{\theta})\} d\boldsymbol{\theta}}{\int_{\Theta} \exp\{-nh_n(\boldsymbol{\theta})\} d\boldsymbol{\theta}}, \quad (1.2)$$

where  $h_n^*(\boldsymbol{\theta}) = -n^{-1} \log[g^+(\boldsymbol{\theta}) p_n(\mathbf{x}|\boldsymbol{\theta}) \pi(\boldsymbol{\theta})]$  and  $h_n(\boldsymbol{\theta}) = -n^{-1} \log[p_n(\mathbf{x}|\boldsymbol{\theta}) \pi(\boldsymbol{\theta})]$ .

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Section 2 sketches out the concept of asymptotic modes, and describes the Laplace approximations with asymptotic modes. In particular, the first-order and second-order errors are given in an explicit form. In Section 3, we give the explicit error terms of order  $n^{-2}$  in a fully exponential Laplace approximation to a posterior mean of  $g^+$ .

## 2. Asymptotic modes and Laplace's approximations

This section introduces the Laplace method for an integral of the form  $\int_{\Theta} e^{-nh_n(\boldsymbol{\theta})} d\boldsymbol{\theta}$  with an asymptotic mode of  $-h_n(\boldsymbol{\theta})$ . For convenience of exposition, we write

$$\frac{\partial^s}{\partial\theta_{i_1}\cdots\partial\theta_{i_s}}h_n(\boldsymbol{\theta}) \equiv h_{i_1\dots i_s}(\boldsymbol{\theta}), \quad \sum_{i_1\dots i_s} \equiv \sum_{i_1=1}^d \cdots \sum_{i_s=1}^d,$$

and the first and second derivatives are represented by

$$D^1h_n(\boldsymbol{\theta}) \equiv \frac{\partial}{\partial\boldsymbol{\theta}}h_n(\boldsymbol{\theta}) = \left(\frac{\partial}{\partial\theta_1}h_n(\boldsymbol{\theta}), \dots, \frac{\partial}{\partial\theta_d}h_n(\boldsymbol{\theta})\right)^T$$

$$D^2h_n(\boldsymbol{\theta}) \equiv \frac{\partial^2}{\partial\boldsymbol{\theta}\partial\boldsymbol{\theta}^T}h_n(\boldsymbol{\theta}) = \begin{pmatrix} \frac{\partial^2}{\partial\theta_1\partial\theta_1}h_n(\boldsymbol{\theta}) & \cdots & \frac{\partial^2}{\partial\theta_1\partial\theta_d}h_n(\boldsymbol{\theta}) \\ \vdots & \ddots & \vdots \\ \frac{\partial^2}{\partial\theta_d\partial\theta_1}h_n(\boldsymbol{\theta}) & \cdots & \frac{\partial^2}{\partial\theta_d\partial\theta_d}h_n(\boldsymbol{\theta}) \end{pmatrix}.$$

We say that  $\hat{\boldsymbol{\theta}}$  is an asymptotic mode of  $-h_n$  if  $\hat{\boldsymbol{\theta}}$  converges to the exact mode of  $-h_n(\boldsymbol{\theta})$  as the sample size  $n$  tends to infinity. The exact mode of  $-h_n(\boldsymbol{\theta})$  is denoted by  $\hat{\boldsymbol{\theta}}_{EX}$ . Note that since  $\hat{\boldsymbol{\theta}}_{EX}$  satisfies  $D^1h_n(\hat{\boldsymbol{\theta}}_{EX}) = 0$ , it is also taken as an asymptotic mode for  $-h_n$ . Additionally, the following asymptotic modes are defined.

**Definition 1**  $\hat{\boldsymbol{\theta}}$  is an asymptotic mode of order  $n^{-1}$  for  $-h_n$  if  $\|\hat{\boldsymbol{\theta}} - \hat{\boldsymbol{\theta}}_{EX}\| \rightarrow 0$  a.e., and  $D^1h_n(\hat{\boldsymbol{\theta}}) = O(n^{-1})$  a.e.

**Remark 1.** Let  $h_n(\boldsymbol{\theta}) = -n^{-1}\log[p_n(\mathbf{x}|\boldsymbol{\theta})\pi(\boldsymbol{\theta})]$ . The maximum likelihood estimator  $\hat{\boldsymbol{\theta}}_{ML}$  for  $p_n(\mathbf{x}|\boldsymbol{\theta})$  is an asymptotic mode of order  $n^{-1}$  for  $-h_n$  because  $D^1h_n(\hat{\boldsymbol{\theta}}_{ML}) = -n^{-1}\pi(\hat{\boldsymbol{\theta}}_{ML}) = O(n^{-1})$ , and  $\hat{\boldsymbol{\theta}}_{ML}$  converges to the exact mode of  $-h_n(\boldsymbol{\theta})$ , as  $n$  tends to infinity under suitable conditions. For the convergence of  $\hat{\boldsymbol{\theta}}_{ML}$ , see Heyde and Johnstone (1979).

**Definition 2**  $\hat{\boldsymbol{\theta}}$  is an asymptotic mode of order  $n^{-2}$  for  $-h_n$  if  $\|\hat{\boldsymbol{\theta}} - \hat{\boldsymbol{\theta}}_{EX}\| \rightarrow 0$  a.e., and  $D^1h_n(\hat{\boldsymbol{\theta}}) = O(n^{-2})$  a.e.

**Remark 2.** Let  $\hat{\boldsymbol{\theta}}_{ML}$  be the maximum likelihood estimator for  $p(\mathbf{x}|\boldsymbol{\theta})$ , and let  $h_n(\boldsymbol{\theta}) = -n^{-1}\log[p(\mathbf{x}|\boldsymbol{\theta})\pi(\boldsymbol{\theta})]$ . Then, it follows from the same argument as in the proof of Theorem 3 of Miyata (2004) that  $\hat{\boldsymbol{\theta}}_{ML}^* \equiv \hat{\boldsymbol{\theta}}_{ML} - [D^2h_n(\hat{\boldsymbol{\theta}}_{ML})]^{-1}D^1h_n(\hat{\boldsymbol{\theta}}_{ML})$  satisfies  $D^1h_n(\hat{\boldsymbol{\theta}}_{ML}^*) = O(n^{-2})$ .

Subsequently, we introduce the regularity conditions (A1), (A2), (A3), (A4) and (A5) for which the asymptotic expansions for  $\int_{\Theta} e^{-nh_n(\boldsymbol{\theta})} d\boldsymbol{\theta}$  will be valid. Let  $\|\mathbf{a}\| \equiv (\mathbf{a}^T\mathbf{a})^{1/2}$  for any vector

$\mathbf{a}$ ,  $|\cdot|$  denote the determinant of a matrix. We use  $B_\delta(\hat{\boldsymbol{\theta}})$  to denote the open ball of radius  $\delta$  centered at  $\hat{\boldsymbol{\theta}}$ , namely  $B_\delta(\hat{\boldsymbol{\theta}}) = \{\boldsymbol{\theta} \in \Theta : \|\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}\| < \delta\}$ . Let  $\{\hat{\boldsymbol{\theta}}\} \equiv \{\hat{\boldsymbol{\theta}} : n = 1, 2, \dots\}$  be the sequence of asymptotic modes.

We list the following assumptions for  $(\{h_n(\boldsymbol{\theta})\}, \{\hat{\boldsymbol{\theta}}\})$ :

(A1)  $\{h_n(\boldsymbol{\theta}) : n = 1, 2, \dots\}$  is a sequence of eight times continuously differentiable real functions on  $\Theta$ .

There exists positive numbers  $\epsilon$ ,  $M$ ,  $\zeta$  and an integer  $n_0$  such that for the asymptotic mode  $\hat{\boldsymbol{\theta}}$ ,  $n \geq n_0$  implies

(A2) the integral  $\int_{\Theta} e^{-nh_n(\boldsymbol{\theta})} d\boldsymbol{\theta}$  is finite;

(A3) for all  $\boldsymbol{\theta} \in B_\epsilon(\hat{\boldsymbol{\theta}})$  and all  $1 \leq j_1, \dots, j_m \leq d$  with  $m = 1, \dots, 8$ ,

$\|h_n(\boldsymbol{\theta})\| < M$  and  $\|\partial^m h_n(\boldsymbol{\theta}) / \partial \theta_{j_1} \cdots \partial \theta_{j_m}\| < M$ ;

(A4)  $D^2 h_n(\hat{\boldsymbol{\theta}})$  is positive definite and  $|D^2 h_n(\hat{\boldsymbol{\theta}})| > \zeta$ ;

(A5) for all  $\delta$  for which  $0 < \delta < \epsilon$ ,  $B_\delta(\hat{\boldsymbol{\theta}}) \subseteq \Theta$  and

$$|nD^2 h_n(\hat{\boldsymbol{\theta}})|^{1/2} C_n(\hat{\boldsymbol{\theta}})^{-1} \int_{\Theta - B_\delta(\hat{\boldsymbol{\theta}})} \exp\{-n[h_n(\boldsymbol{\theta}) - h_n(\hat{\boldsymbol{\theta}})]\} d\boldsymbol{\theta} = O(n^{-3}),$$

where  $C_n(\hat{\boldsymbol{\theta}}) = \exp\left(\frac{n}{2} D^1 h(\hat{\boldsymbol{\theta}})^T [D^2 h(\hat{\boldsymbol{\theta}})]^{-1} D^1 h(\hat{\boldsymbol{\theta}})\right)$ . The pair  $(\{h_n\}, \{\hat{\boldsymbol{\theta}}\})$  will be said to satisfy the *analytical assumptions for the asymptotic-mode Laplace method* if (A1), (A2), (A3), (A4) and (A5) are satisfied for the asymptotic mode  $\hat{\boldsymbol{\theta}}$ .

Our conditions (A1)–(A5) are analogous to those of Kass, Tierney and Kadane (1990) except  $\hat{\boldsymbol{\theta}}$  is an asymptotic mode. If  $\hat{\boldsymbol{\theta}}$  is an asymptotic mode of order  $n^{-1}$ ,  $\int_{\Theta - B_\delta(\hat{\boldsymbol{\theta}})} \exp\{-n[h_n(\boldsymbol{\theta}) - h_n(\hat{\boldsymbol{\theta}})]\} d\boldsymbol{\theta} = O(n^{-3-d/2})$  holds under (A5). Hence (A5) means that the probability outside a neighborhood of the  $\hat{\boldsymbol{\theta}}$  converges to zero as the sample size  $n$  tends to infinity. Let  $h_{j_1 \dots j_m}$  denote the  $m$ th partial derivative  $\partial^m h_n(\boldsymbol{\theta}) / \partial \theta_{j_1} \cdots \partial \theta_{j_m}$  with respect to  $\boldsymbol{\theta}$  evaluated at  $\hat{\boldsymbol{\theta}}$ , for example,  $h_{112}$  means  $\partial^3 h_n(\hat{\boldsymbol{\theta}}) / \partial \hat{\theta}_1^2 \partial \hat{\theta}_2$ . Let  $h^{ij}$  be the components of  $[D^2 h(\hat{\boldsymbol{\theta}})]^{-1}$  and  $\mathbf{b} = (b_i) \equiv -[D^2 h_n(\hat{\boldsymbol{\theta}})]^{-1} D^1 h_n(\hat{\boldsymbol{\theta}})$ . We define the sixth, eighth, tenth, and twelfth central moments of a multivariate normal distribution having covariance matrix  $[nD^2 h(\hat{\boldsymbol{\theta}})]^{-1}$  as  $\mu_{ijkrs}$ ,  $\mu_{ijkrstu}$ ,  $\mu_{ijkrstuvw}$ , and  $\mu_{ijkrstuvwxy}$ , respectively.

**Theorem 3.** Suppose that  $\hat{\boldsymbol{\alpha}}$  is an asymptotic mode of order  $n^{-1}$  for  $-h_n$  and the pair  $(\{h_n(\boldsymbol{\alpha})\}, \{\hat{\boldsymbol{\alpha}}\})$  satisfies *analytical assumptions for the asymptotic-mode Laplace method*. Then it follows that for large  $n$ ,

$$\int_{\Theta} e^{-nh_n(\boldsymbol{\theta})} d\boldsymbol{\theta} = (2\pi)^{d/2} |\Sigma|^{1/2} e^{-nh_n(\hat{\boldsymbol{\alpha}})} C_n(\hat{\boldsymbol{\alpha}}) \left(1 + \frac{\lambda_{1n}}{n} + \frac{\lambda_{2n}}{n^2} + O(n^{-3})\right), \quad (2.1)$$

where  $C_n(\hat{\boldsymbol{\alpha}}) = \exp\left(\frac{n}{2} D^1 h_n(\hat{\boldsymbol{\alpha}})^T [D^2 h_n(\hat{\boldsymbol{\alpha}})]^{-1} D^1 h_n(\hat{\boldsymbol{\alpha}})\right)$ ,

$$\begin{aligned}
\lambda_{1n} &= -\frac{1}{2} \sum_{ijk} h_{ijk}(\hat{\boldsymbol{\alpha}})(nb_i)h^{jk} - \frac{1}{8} \sum_{ijkq} h_{ijkq}(\hat{\boldsymbol{\alpha}})h^{ij}h^{kq} \\
&\quad + \frac{1}{72} \sum_{ijkqrs} h_{ijk}(\hat{\boldsymbol{\alpha}})h_{qrs}(\hat{\boldsymbol{\alpha}})\mu_{ijkqrs}n^3, \\
\lambda_{2n} &= -\frac{n^3}{6} \sum h_{ijk}b_ib_jb_k - \frac{n^2}{4} \sum h_{ijkq}h^{ij}b_kb_q + \frac{n^4}{12} \sum h_{ijk}h_{qrs}b_ib_j\mu_{kqrs} \\
&\quad + \frac{n^4}{8} \sum h_{ijk}h_{qrs}b_ib_q\mu_{jkrs} - \frac{n^3}{24} \sum h_{ijkqr}b_i\mu_{jkqr} \\
&\quad - \frac{n^3}{720} \sum h_{ijkqrs}\mu_{ijkqrs} + \frac{n^4}{48} \sum h_{ijk}h_{qrst}b_i\mu_{jkqrst} \\
&\quad + \frac{n^4}{36} \sum h_{ijk}h_{qrst}b_q\mu_{ijkrst} + \frac{n^4}{1152} \sum h_{ijkq}h_{rstu}\mu_{ijkqrst} \\
&\quad + \frac{n^4}{720} \sum h_{ijk}h_{qrst}\mu_{ijkqrst} - \frac{n^5}{144} \sum h_{ijk}h_{qrs}h_{tuv}b_i\mu_{jkqrstuv} \\
&\quad - \frac{n^5}{1728} \sum h_{ijk}h_{qrs}h_{tuv}\mu_{ijkqrstuvw} \\
&\quad + \frac{n^6}{31104} \sum h_{ijk}h_{qrs}h_{tuv}h_{wxy}\mu_{ijkqrstuvwxy},
\end{aligned} \tag{2.2}$$

$\Sigma \equiv [nD^2h(\hat{\boldsymbol{\alpha}})]^{-1} = (n^{-1}h^{ij})$ , and  $\mu_{ijkqrs}$  are the sixth central moments of a multivariate Normal distribution having covariance matrix  $\Sigma$ .

Note that  $\lambda_{1n}$  and  $\lambda_{2n}$  are of order  $O(1)$ . The proof is given in Appendix C.

**Theorem 4.** Suppose that  $\hat{\boldsymbol{\theta}}$  is an asymptotic mode of order  $n^{-2}$  for  $-h_n$  and the pair  $(\{h_n(\boldsymbol{\theta})\}, \{\hat{\boldsymbol{\theta}}\})$  satisfies *analytical assumptions for the asymptotic-mode Laplace method*. Then it follows that for large  $n$ ,

$$\int_{\Theta} e^{-nh_n(\boldsymbol{\theta})} d\boldsymbol{\theta} = (2\pi)^{d/2} |\Sigma|^{1/2} e^{-nh_n(\hat{\boldsymbol{\theta}})} C_n(\hat{\boldsymbol{\theta}}) \left( 1 + \frac{a_{1n}}{n} + \frac{a_{2n}}{n^2} + O(n^{-3}) \right), \tag{2.3}$$

where  $C_n(\hat{\boldsymbol{\theta}}) = \exp\left(\frac{n}{2} D^1 h_n(\hat{\boldsymbol{\theta}})^T [D^2 h_n(\hat{\boldsymbol{\theta}})]^{-1} D^1 h_n(\hat{\boldsymbol{\theta}})\right)$ ,

$$\begin{aligned}
a_{1n} &= -\frac{1}{8} \sum_{ijkq} h_{ijkq}h^{ij}h^{kq} + \frac{n^3}{72} \sum_{ijkqrs} h_{ijk}h_{qrs}\mu_{ijkqrs}, \\
a_{2n} &= -\frac{1}{2} \sum_{ijk} h_{ijk}(n^2b_i)h^{jk} - \frac{n^3}{720} \sum_{ijkqrs} h_{ijkqrs}\mu_{ijkqrs} \\
&\quad + \frac{n^4}{1152} \sum h_{ijkq}h_{rstu}\mu_{ijkqrst} + \frac{n^4}{720} \sum h_{ijk}h_{qrst}\mu_{ijkqrst} \\
&\quad - \frac{n^5}{1728} \sum h_{ijk}h_{qrs}h_{tuv}\mu_{ijkqrstuvw} \\
&\quad + \frac{n^6}{31104} \sum h_{ijk}h_{qrs}h_{tuv}h_{wxy}\mu_{ijkqrstuvwxy},
\end{aligned}$$

and  $\Sigma \equiv [nD^2h(\hat{\boldsymbol{\theta}})]^{-1} = (n^{-1}h^{ij})$ .

$a_{1n}$ , and  $a_{2n}$  are of order  $O(1)$ , and the proof is given in Appendix C.

**Remark 5.**  $O(n^{-3})$  includes  $h_i, \dots, h_{ijkqrst}, h^{ij}, b_i$ ,

$$\begin{aligned} & \frac{-n}{8!} \int_{B_\delta(\hat{\theta})} \exp\left(-\frac{1}{2}(\boldsymbol{\theta} - \mathbf{y})^T \Sigma^{-1}(\boldsymbol{\theta} - \mathbf{y})\right) h_{ijkqrstu}(\gamma_1) z_i z_j z_k z_q z_r z_s z_t z_u d\boldsymbol{\theta}, \\ & \int_{\boldsymbol{\theta} - B_\delta(\hat{\theta})} \exp\{-n[h_n(\boldsymbol{\theta}) - h_n(\hat{\theta})]\} d\boldsymbol{\theta} \\ & \text{and } \int_{B_\delta(\hat{\theta})} n(\boldsymbol{\theta}|\hat{\theta} + \mathbf{b}, [nD^2 h_n(\hat{\theta})]^{-1}) R_{5n}(k_n(\boldsymbol{\theta}, \hat{\theta})) d\boldsymbol{\theta}, \end{aligned}$$

where  $\gamma_1$  is a point between  $\boldsymbol{\theta}$  and  $\hat{\theta}$ ,

$$k_n(\boldsymbol{\theta}, \hat{\theta}) = -n \left( \frac{1}{6} \sum_{ijk} h_{ijk} z_i z_j z_k + \dots + \frac{1}{7!} \sum_{ijkqrst} h_{ijkqrst} z_i \dots z_t + \frac{1}{8!} \sum_{ijkqrstu} h_{ijkqrstu}(\gamma_2) z_i \dots z_u \right)$$

$\gamma_2$  is a point between  $\boldsymbol{\theta}$  and  $\hat{\theta}$

$$R_{5n}(k_n(\boldsymbol{\theta}, \hat{\theta})) = \frac{k_n(\boldsymbol{\theta}, \hat{\theta})^5}{4!} \int_0^1 (1 - \lambda)^4 \exp\{\lambda k_n(\boldsymbol{\theta}, \hat{\theta})\} d\lambda.$$

### 3. Main results

This section mainly gives the explicit error terms of order  $n^{-2}$  in the fully exponential Laplace approximations to posterior means. Let  $\mathbf{b}^* = (b_i^*) \equiv -[D^2 h_n^*(\hat{\theta})]^{-1} D^1 h_n^*(\hat{\theta})$

**Theorem 6.** Let  $\hat{\theta}$  be an asymptotic mode of order  $n^{-2}$  for  $-h_n(\boldsymbol{\theta})$ , and  $\hat{\theta}_N$  is a single Newton step from  $\hat{\theta}$  toward the maximum of  $-h_n^*(\boldsymbol{\theta})$ , i.e.,  $\hat{\theta}_N \equiv \hat{\theta} - [D^2 h_n^*(\hat{\theta})]^{-1} D^1 h_n^*(\hat{\theta})$ . If pairs  $(\{h_n(\boldsymbol{\theta})\}, \{\hat{\theta}\})$  and  $(\{h_n^*(\boldsymbol{\theta})\}, \{\hat{\theta}_N\})$  satisfy *analytical assumptions for the asymptotic-mode Laplace method*, Then

$$E[g(\boldsymbol{\theta})] = \left( \frac{|D^2 h_n(\hat{\theta})|}{|D^2 h_n^*(\hat{\theta}_N)|} \right)^{1/2} \frac{C_n^*(\hat{\theta}_N)}{C_n(\hat{\theta})} \frac{\exp[-nh^*(\hat{\theta}_N)]}{\exp[-nh(\hat{\theta})]} \left( 1 + \frac{c_n}{n^2} + O(n^{-3}) \right), \quad (3.1)$$

where  $C_n^*(\hat{\theta}_N) = \exp\{(n/2)D^1 h_n^*(\hat{\theta}_N)^T [D^2 h_n^*(\hat{\theta}_N)]^{-1} D^1 h_n^*(\hat{\theta}_N)\}$  and

$$\begin{aligned} c_n = & -\frac{n^2}{2} \sum h_{ijk} b_i^* h^{jk} + \frac{n^2}{2} \sum h_{ijk} b_i h^{jk} + \frac{1}{4} \sum h_{ijkq} h_{l\alpha\beta} h^{ij} h^{k\alpha} h^{\beta q} h^{lm} G_m \\ & - \frac{1}{4} \sum h_{ijkq} h^{ij} h^{k\alpha} h^{\beta q} G_{\alpha\beta} - \frac{1}{8} \sum h_{ijkql} h^{ij} h^{kq} h^{lm} G_m + \frac{1}{8} \sum h^{ij} h^{kq} G_{ijkq} \\ & + \frac{1}{36} \sum h_{\alpha ijk} h_{qrs} h^{\alpha\beta} [n^3 \mu_{ijkqrs}] G_\beta - \frac{1}{36} \sum h_{qrs} [n^3 \mu_{ijkqrs}] G_{ijk} \\ & - \frac{1}{8} \sum_{ijkqrs\alpha\beta lm} h_{ijk} h_{qrs} h_{l\alpha\beta} h^{jk} h^{rs} h^{i\alpha} h^{\beta q} h^{lm} G_m + \frac{1}{8} \sum_{ijkqrs\alpha\beta} h_{ijk} h_{qrs} h^{jk} h^{rs} h^{i\alpha} h^{\beta q} G_{\alpha\beta} \\ & - \frac{1}{4} \sum_{ijkqrs\alpha\beta lm} h_{ijk} h_{qrs} h_{l\alpha\beta} h^{jr} h^{ks} h^{i\alpha} h^{\beta q} h^{lm} G_m + \frac{1}{4} \sum_{ijkqrs\alpha\beta} h_{ijk} h_{qrs} h^{jr} h^{ks} h^{i\alpha} h^{\beta q} G_{\alpha\beta} \\ & - \frac{1}{4} \sum_{ijkqrs\alpha\beta lm} h_{ijk} h_{qrs} h_{l\alpha\beta} h^{kq} h^{rs} h^{i\alpha} h^{\beta j} h^{lm} G_m + \frac{1}{4} \sum_{ijkqrs\alpha\beta} h_{ijk} h_{qrs} h^{kq} h^{rs} h^{i\alpha} h^{\beta j} G_{\alpha\beta}. \end{aligned}$$

Note that  $c_n$  is of order  $O(1)$ . The first term in the right side of  $c_n$  is reexpressed as

$$-\frac{n^2}{2} \sum h_{ijk} b_i^* h^{jk} = \frac{1}{4} \sum_{ijklm\alpha\beta} h_{ijk} h_{l\alpha\beta} h^{il} h^{jk} h^{\alpha r} h^{\beta m} G_r G_m + O(n^{-1}). \quad (3.2)$$

If  $\hat{\boldsymbol{\theta}}$  is replaced with the exact mode  $\hat{\boldsymbol{\theta}}_{EX}$  of  $-h_n(\boldsymbol{\theta})$  in (3.1), then it follows that

$$E[g(\boldsymbol{\Theta})] = \left( \frac{|D^2 h_n(\hat{\boldsymbol{\theta}}_{EX})|}{|D^2 h_n^*(\hat{\boldsymbol{\theta}}_N)|} \right)^{1/2} C_n^*(\hat{\boldsymbol{\theta}}_N) \frac{\exp[-nh^*(\hat{\boldsymbol{\theta}}_N)]}{\exp[-nh(\hat{\boldsymbol{\theta}}_{EX})]} \left( 1 + \frac{\dot{c}_n}{n^2} + O(n^{-3}) \right), \quad (3.3)$$

where  $\dot{c}_n$  is  $c_n$  with the term  $(n^2/2) \sum h_{ijk} b_i h^{jk}$  being 0. Furthermore, the approximation with  $\hat{\boldsymbol{\theta}}_N$  with the exact mode of  $-h_n^*$  is equivalent to the Tierney–Kadane approximation. As a generalized form, the following result holds.

**Theorem 7.** Suppose that  $\hat{\boldsymbol{\theta}}$  and  $\tilde{\boldsymbol{\theta}}$  are asymptotic modes of order  $n^{-2}$  for  $-h_n(\boldsymbol{\theta})$  and  $-h_n^*(\boldsymbol{\theta})$  respectively. Then

$$E[g(\boldsymbol{\Theta})] = \left( \frac{|D^2 h_n(\hat{\boldsymbol{\theta}})|}{|D^2 h_n^*(\tilde{\boldsymbol{\theta}})|} \right)^{1/2} \frac{C_n^*(\tilde{\boldsymbol{\theta}}) \exp[-nh^*(\tilde{\boldsymbol{\theta}})]}{C_n(\hat{\boldsymbol{\theta}}) \exp[-nh(\hat{\boldsymbol{\theta}})]} \left( 1 + O(n^{-2}) \right). \quad (3.4)$$

## Appendix A: Lemmas concerning matrices

This section prepares some lemmas concerning matrices to prove the main results.

**Lemma 8.** Suppose that  $\mathbf{a}$  is a  $1 \times d$  matrix,  $\mathbf{M}$  is a  $d \times d$  symmetric matrix. Then,

$$\mathbf{a}^T(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}) + (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})^T \mathbf{M}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}) = (\boldsymbol{\theta} - \mathbf{y})^T \mathbf{M}(\boldsymbol{\theta} - \mathbf{y}) - \frac{1}{4} \mathbf{a}^T \mathbf{M}^{-1} \mathbf{a},$$

where  $\mathbf{y} = \hat{\boldsymbol{\theta}} - (1/2)\mathbf{M}^{-1}\mathbf{a}$ .

*Proof.*

$$\begin{aligned} & (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}} + \frac{1}{2}\mathbf{M}^{-1}\mathbf{a})^T \mathbf{M}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}} + \frac{1}{2}\mathbf{M}^{-1}\mathbf{a}) - \frac{1}{4} \mathbf{a}^T \mathbf{M}^{-1} \mathbf{a} \\ &= (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})^T \mathbf{M}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}) + \frac{1}{2} \mathbf{a}^T \mathbf{M}^{-1} \mathbf{M}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}) + (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})^T \mathbf{M} \frac{1}{2} \mathbf{M}^{-1} \mathbf{a} + \frac{1}{2} \mathbf{a}^T \mathbf{M}^{-1} \mathbf{M} \frac{1}{2} \mathbf{M}^{-1} \mathbf{a} \\ &\quad - \frac{1}{4} \mathbf{a}^T \mathbf{M}^{-1} \mathbf{a} \\ &= \mathbf{a}^T(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}) + (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})^T \mathbf{M}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}). \end{aligned}$$

**Lemma 9.** Let  $\mathbf{I}_d$  be a  $d \times d$  unit matrix. For any  $d \times d$  matrix  $\mathbf{A}$  and any scalar  $x$ ,

$$|\mathbf{A} + x\mathbf{I}_d| = \sum_{r=0}^d x^r \sum_{\{i_1, \dots, i_r\}} |\mathbf{A}^{\{i_1, \dots, i_r\}}|, \quad (\text{A.1})$$

where  $|\cdot|$  denotes the determinant of a matrix,  $\{i_1, \dots, i_r\}$  is an  $r$ -dimensional subset of the first  $d$  positive integers  $1, \dots, d$  (and the second summation is over all  $\binom{d}{r}$  such subsets), and  $\mathbf{A}^{\{i_1, \dots, i_r\}}$  is the  $(d-r) \times (d-r)$  principal submatrix of  $\mathbf{A}$  obtained by striking out the  $i_1, \dots, i_r$ th rows and columns. (For  $r = d$ , the sum  $\sum_{\{i_1, \dots, i_r\}} |\mathbf{A}^{\{i_1, \dots, i_r\}}|$  is to be interpreted as 1.) Note that the expression (A.1) is a polynomial in  $x$ , the coefficient of  $x^0$  (i.e., the constant term of the polynomial) equals  $|\mathbf{A}|$ , and the coefficient of  $x^{d-1}$  equals  $\text{tr}(\mathbf{A})$ .

*Proof.* See Harville (1997; corollary 13.7.4, p.197).

**Lemma 10.** For  $d \times d$  nonsingular matrices  $\mathbf{A}$  and  $\mathbf{B}$ ,

$$\frac{d}{dt} \left( \frac{|\mathbf{A} - (t/n)\mathbf{B}|}{|\mathbf{A}|} \right) \Big|_{t=0} = -\frac{1}{n} \text{tr}(\mathbf{B}\mathbf{A}^{-1}).$$

*Proof.* Using Lemma 8 and the relation between an inverse matrix and the cofactors, we have

$$\begin{aligned} & \frac{d}{dt} \left( \frac{|\mathbf{A} - (t/n)\mathbf{B}|}{|\mathbf{A}|} \right) \Big|_{t=0} \\ &= \frac{d}{dt} \left( |\mathbf{B}\mathbf{A}^{-1}| \left| \mathbf{A}\mathbf{B}^{-1} - \frac{t}{n} \mathbf{I}_d \right| \right) \Big|_{t=0} \\ &= \frac{d}{dt} \left( |\mathbf{B}\mathbf{A}^{-1}| \left[ |\mathbf{A}\mathbf{B}^{-1}| - \frac{t}{n} \sum_{\{i_1\}} |(\mathbf{A}\mathbf{B}^{-1})^{\{i_1\}}| + \frac{t^2}{n^2} \xi + \dots + \frac{(-t)^d}{n^d} \right] \right) \Big|_{t=0} \\ &= -\frac{1}{n} \frac{1}{|\mathbf{A}\mathbf{B}^{-1}|} \sum_{\{i_1\}} |(\mathbf{A}\mathbf{B}^{-1})^{\{i_1\}}| \\ &= -\frac{1}{n} \text{tr}(\mathbf{A}\mathbf{B}^{-1})^{-1} \\ &= -\frac{1}{n} \text{tr}(\mathbf{B}\mathbf{A}^{-1}), \end{aligned}$$

where  $\xi = \sum_{\{i_1, i_2\}} |(\mathbf{A}\mathbf{B}^{-1})^{\{i_1, i_2\}}|$  and  $\{i_1\}$  and  $\{i_1, i_2\}$  are the same notations as in Lemma 8. Hence this lemma is proved.

**Lemma 11.** For  $d \times d$  nonsingular matrices  $\mathbf{A}$  and  $\mathbf{B}$  and any scalar  $x$ , it follows that

$$(\mathbf{A} + x\mathbf{B})^{-1} - \mathbf{A}^{-1} = O(x). \quad (\text{A.2})$$

*Proof.* Multiplying  $(\mathbf{A} + x\mathbf{B})^{-1}(\mathbf{A} + x\mathbf{B}) = \mathbf{I}_d$  by  $\mathbf{A}^{-1}$  from the right side yields

$$(\mathbf{A} + x\mathbf{B})^{-1} - \mathbf{A}^{-1} = -x(\mathbf{A} + x\mathbf{B})^{-1}\mathbf{B}\mathbf{A}^{-1}. \quad (\text{A.3})$$

Hence the lemma is proved.

**Lemma 12.** For  $d \times d$  nonsingular matrices  $\mathbf{A}$  and  $\mathbf{B}$ ,

$$\frac{d}{dt} (\mathbf{A} - \frac{t}{n}\mathbf{B})^{-1} \Big|_{t=0} = \frac{1}{n} \mathbf{A}^{-1} \mathbf{B} \mathbf{A}^{-1}.$$

*Proof:* Using (A.3),

$$\frac{(\mathbf{A} - (t/n)\mathbf{B})^{-1} - \mathbf{A}^{-1}}{t} = \frac{1}{n} (\mathbf{A} - \frac{t}{n}\mathbf{B})^{-1} \mathbf{B} \mathbf{A}^{-1}. \quad (\text{A.4})$$

Hence, letting  $t \rightarrow 0$  yields the lemma.

## Appendix B: Some lemmas

This section presents some lemmas required in the evaluation of the asymptotic errors in Sections 2 and 3.

**Lemma 13.** Let  $n$  denote a sample size, and let  $z_i \equiv \Theta_i - \hat{\theta}_i$ . Suppose that  $\Theta = (\Theta_1, \dots, \Theta_d)^T$  is according to  $N_d(\hat{\theta} + \mathbf{b}, \Sigma)$ , where  $\hat{\theta} = (\hat{\theta}_1, \dots, \hat{\theta}_d)^T$ ,  $\mathbf{b} = (b_1, \dots, b_d)^T = O(n^{-1})$ , and  $\Sigma = (\mu_{ij})$  is the covariance matrix with  $\mu_{ij} = O(n^{-1})$ . Then we have the following results.

$$(a) \ E[(\Theta_i - \hat{\theta}_i)(\Theta_j - \hat{\theta}_j)(\Theta_k - \hat{\theta}_k)] = \underbrace{b_i \mu_{jk} + b_j \mu_{ik} + b_k \mu_{ij}}_{O(n^{-2})} + \underbrace{b_i b_j b_k}_{O(n^{-3})}$$

$$(b) \ E[(\Theta_i - \hat{\theta}_i)(\Theta_j - \hat{\theta}_j)(\Theta_k - \hat{\theta}_k)(\Theta_q - \hat{\theta}_q)] = \underbrace{\mu_{ij} \mu_{kq} + \mu_{ik} \mu_{jq} + \mu_{iq} \mu_{kj}}_{O(n^{-2})} + \sum_{[m_1, m_2]_4} \underbrace{b_{m_1} b_{m_2} \mu_{m_3 m_4}}_{O(n^{-3})} + b_i b_j b_k b_q,$$

where  $[m_1, m_2]_4$  indicates ways of a pair chosen among four alphabets  $i, j, k$ , and  $q$ . Hence the summation  $\sum_{[m_1, m_2]_4}$  is over  $\binom{4}{2}$ .

$$(c) \ E[z_i z_j z_k z_q z_r] = \sum_{[m_1]_5} \underbrace{b_{m_1} \mu_{m_2 m_3 m_4 m_5}}_{O(n^{-3})} + \sum_{[l_1, l_2, l_3]_5} \underbrace{b_{l_1} b_{l_2} b_{l_3} \mu_{l_4 l_5}}_{O(n^{-4})} + b_i b_j b_k b_q b_r,$$

where  $[m_1]_5$  indicates ways of one chosen among five alphabets  $i, j, k, q$ , and  $r$ , and  $[l_1, l_2, l_3]_5$  indicates ways of a triple chosen among  $i, j, k, q$ , and  $r$ . The notations  $[l_1, l_2, l_3, l_4]_6$ ,  $[m_1, m_2]_6$ , etc below are also defined similarly.

$$(d) \ E[z_i z_j z_k z_q z_r z_s] = \underbrace{\mu_{ijkqrs}}_{O(n^{-3})} + \sum_{[m_1, m_2]_6} \underbrace{b_{m_1} b_{m_2} \mu_{m_3 m_4 m_5 m_6}}_{O(n^{-4})} + \sum_{[l_1, l_2, l_3, l_4]_6} \underbrace{b_{l_1} b_{l_2} b_{l_3} b_{l_4} \mu_{l_5 l_6}}_{O(n^{-5})} + b_i b_j b_k b_q b_r b_s$$

$$(e) \ E[z_i z_j z_k z_q z_r z_s z_t] = \sum_{[m_1]_7} \underbrace{b_{m_1} \mu_{m_2 m_3 m_4 m_5 m_6 m_7}}_{O(n^{-4})} + \sum_{[l_1, l_2, l_3]_7} b_{l_1} b_{l_2} b_{l_3} \mu_{l_4 l_5 l_6 l_7} + \sum_{[n_1, n_2, n_3, n_4, n_5]_7} b_{n_1} b_{n_2} b_{n_3} b_{n_4} b_{n_5} \mu_{n_6 n_7} + b_i b_j b_k b_q b_r b_s b_t$$

$$(f) \ E[\underbrace{z_i z_j z_k z_q z_r z_s z_t z_u}_8] = \underbrace{\mu_{ijkqrstu}}_{O(n^{-4})} + O(n^{-5})$$

$$(g) \ E[\underbrace{z_i z_j z_k z_q z_r z_s z_t z_u z_v}_9] = \sum_{[m_1]_9} \underbrace{b_{m_1} \mu_{m_2 m_3 m_4 m_5 m_6 m_7 m_8 m_9}}_{O(n^{-5})} + O(n^{-6})$$

$$(h) \ E[\underbrace{z_i z_j z_k z_q z_r z_s z_t z_u z_v z_w}_{10}] = \underbrace{\mu_{ijkqrstuvw}}_{O(n^{-5})} + O(n^{-6})$$

$$(i) \ E[\underbrace{z_i z_j z_k z_q z_r z_s z_t z_u z_v z_w z_x z_y}_{12}] = \underbrace{\mu_{ijkqrstuvwxy}}_{O(n^{-6})} + O(n^{-7})$$



*Proof of (a).* Putting  $u_i \equiv \Theta_i - (\hat{\theta}_i + b_i)$ ,  $E[u_i] = 0$ , and  $E[u_i u_j] = \mu_{ij}$ . By using the binomial theorem and the result in which odd moments of  $u_i$  are 0, we have

$$\begin{aligned}
& E[(\Theta_i - \hat{\theta}_i)(\Theta_j - \hat{\theta}_j)(\Theta_k - \hat{\theta}_k)] \\
&= E\left[(\Theta_i - (\hat{\theta}_i + b_i) + b_i)(\Theta_j - (\hat{\theta}_j + b_j) + b_j)(\Theta_k - (\hat{\theta}_k + b_k) + b_k)\right] \\
&= E[(u_i + b_i)(u_j + b_j)(u_k + b_k)] \\
&= E[u_i u_j u_k] + b_i E[u_j u_k] + b_j E[u_i u_k] + b_k E[u_i u_j] \\
&\quad + b_i b_j E[u_k] + b_j b_k E[u_i] + b_i b_k E[u_j] + b_i b_j b_k \\
&= b_i \mu_{jk} + b_j \mu_{ik} + b_k \mu_{ij} + b_i b_j b_k.
\end{aligned}$$

*Proof of (b).*

$$\begin{aligned}
& E[(\Theta_i - \hat{\theta}_i)(\Theta_j - \hat{\theta}_j)(\Theta_k - \hat{\theta}_k)(\Theta_q - \hat{\theta}_q)] \\
&= E\left[(\Theta_i - (\hat{\theta}_i + b_i) + b_i)(\Theta_j - (\hat{\theta}_j + b_j) + b_j)(\Theta_k - (\hat{\theta}_k + b_k) + b_k)(\Theta_q - (\hat{\theta}_q + b_q) + b_q)\right] \\
&= E[(u_i + b_i)(u_j + b_j)(u_k + b_k)(u_q + b_q)] \\
&= E[u_i u_j u_k u_q] + \sum_{[m_1]_4} b_{m_1} \underbrace{E[u_{m_2} u_{m_3} u_{m_4}]}_0 + \sum_{[m_1, m_2]_4} b_{m_1} b_{m_2} E[u_{m_3} u_{m_4}] \\
&\quad + \sum_{[m_1, m_2, m_3]_4} b_{m_1} b_{m_2} b_{m_3} \underbrace{E[u_{m_4}]}_0 + b_i b_j b_k b_q \\
&= \mu_{ijkl} + \sum_{[m_1, m_2]_4} b_{m_1} b_{m_2} E[u_{m_3} u_{m_4}] + b_i b_j b_k b_q.
\end{aligned}$$

*Proof of (c).*

$$\begin{aligned}
& E[z_i z_j z_k z_q z_r] \\
&= E[(\Theta_i - (\hat{\theta}_i + b_i) + b_i)(\Theta_j - (\hat{\theta}_j + b_j) + b_j) \cdots (\Theta_r - (\hat{\theta}_r + b_r) + b_r)] \\
&= E[(u_i + b_i)(u_j + b_j)(u_k + b_k)(u_q + b_q)(u_r + b_r)] \\
&= \underbrace{\mu_{ijklr}}_0 + \sum_{[m_1]_5} b_{m_1} E[u_{m_2} u_{m_3} u_{m_4} u_{m_5}] + \sum_{[m_1, m_2]_5} b_{m_1} b_{m_2} \underbrace{E[u_{m_3} u_{m_4} u_{m_5}]}_0 \\
&\quad + \sum_{[m_1, m_2, m_3]_5} b_{m_1} b_{m_2} b_{m_3} E[u_{m_4} u_{m_5}] + \sum_{[m_1, m_2, m_3, m_4]_5} b_{m_1} b_{m_2} b_{m_3} b_{m_4} E[u_{m_5}] + b_i b_j b_k b_q b_r \\
&= \sum_{[m_1]_5} b_{m_1} \mu_{m_2 m_3 m_4 m_5} + \sum_{[m_1, m_2, m_3]_5} b_{m_1} b_{m_2} b_{m_3} \mu_{m_4 m_5} + b_i b_j b_k b_q b_r.
\end{aligned}$$

Proof of (d).

$$\begin{aligned}
& E[z_i z_j z_k z_q z_r z_s] \\
&= E[(u_i + b_i)(u_j + b_j)(u_k + b_k)(u_q + b_q)(u_r + b_r)(u_s + b_s)] \\
&= \mu_{ijkqrs} + \sum_{[m_1]_6} b_{m_1} \underbrace{E[u_{m_2} u_{m_3} u_{m_4} u_{m_5} u_{m_6}]}_0 \\
&\quad + \sum_{[m_1, m_2]_6} b_{m_1} b_{m_2} E[u_{m_3} u_{m_4} u_{m_5} u_{m_6}] + \sum_{[m_1, m_2, m_3]_6} b_{m_1} b_{m_2} b_{m_3} E[u_{m_4} u_{m_5} u_{m_6}] \\
&\quad + \sum_{[m_1, m_2, m_3, m_4]_6} b_{m_1} b_{m_2} b_{m_3} b_{m_4} E[u_{m_5} u_{m_6}] + \sum_{[m_1, m_2, m_3, m_4, m_5]_6} b_{m_1} b_{m_2} b_{m_3} b_{m_4} b_{m_5} E[u_{m_6}] \\
&\quad\quad\quad + b_i b_j b_k b_q b_r b_s.
\end{aligned}$$

Similarly, (e)–(h) can be proved.

Let  $G(\boldsymbol{\theta}) \equiv \log g^+(\boldsymbol{\theta})$  and let  $G_{j_1 \dots j_m}$  denote the  $m$ th partial derivatives  $\partial^m G(\boldsymbol{\theta}) / \partial \theta_{j_1} \dots \theta_{j_m}$  evaluated at  $\boldsymbol{\theta} = \hat{\boldsymbol{\theta}}$ . For example,  $G_{213} = \partial^3 G(\hat{\boldsymbol{\theta}}) / \partial \hat{\theta}_2 \partial \hat{\theta}_1 \partial \hat{\theta}_3$ . For simplicity, we let  $h_n^* = h^*$  and  $h_n = h$ .

**Lemma 14.** Let  $\hat{\boldsymbol{\theta}}$  be an asymptotic mode of order  $n^{-2}$  for  $-h(\boldsymbol{\theta})$ , and let  $h^*(\boldsymbol{\theta}) \equiv h(\boldsymbol{\theta}) - (1/n)G(\boldsymbol{\theta})$ . Suppose that  $h^*(\boldsymbol{\theta})$  and  $h(\boldsymbol{\theta})$  are five times continuously differentiable sequences on  $\Theta$ ,  $G(\boldsymbol{\theta})$  is four times continuously differentiable, and  $[D^2 h(\hat{\boldsymbol{\theta}})]^{-1}$  exists. Then the following results hold:

$$\begin{aligned}
\text{(a)} \quad & h^*(\hat{\boldsymbol{\theta}}_N) - h(\hat{\boldsymbol{\theta}}) = -\frac{1}{n}G(\hat{\boldsymbol{\theta}}) + \underbrace{\frac{1}{n}D^1 h(\hat{\boldsymbol{\theta}})^T [D^2 h(\hat{\boldsymbol{\theta}})]^{-1} D^1 G(\hat{\boldsymbol{\theta}})}_{O(n^{-3})} + O(n^{-2}) \\
\text{(b)} \quad & D^1 h^*(\hat{\boldsymbol{\theta}}_N) - D^1 h(\hat{\boldsymbol{\theta}}) = O(n^{-2}) \\
\text{(c)} \quad & h_{ij}^*(\hat{\boldsymbol{\theta}}_N) - h_{ij}(\hat{\boldsymbol{\theta}}) = \frac{1}{n}D^1 h_{ij}(\hat{\boldsymbol{\theta}})^T [D^2 h(\hat{\boldsymbol{\theta}})]^{-1} D^1 G(\hat{\boldsymbol{\theta}}) - \frac{1}{n}G_{ij}(\hat{\boldsymbol{\theta}}) + O(n^{-2}) \\
& \quad = \frac{1}{n} \sum_{\alpha, \beta} h_{\alpha ij} h^{\alpha \beta} G_\beta - \frac{1}{n}G_{ij} + O(n^{-2}) \\
\text{(d)} \quad & h_{ijk}^*(\hat{\boldsymbol{\theta}}_N) - h_{ijk}(\hat{\boldsymbol{\theta}}) = \frac{1}{n}D^1 h_{ijk}(\hat{\boldsymbol{\theta}})^T [D^2 h(\hat{\boldsymbol{\theta}})]^{-1} D^1 G(\hat{\boldsymbol{\theta}}) - \frac{1}{n}G_{ijk}(\hat{\boldsymbol{\theta}}) + O(n^{-2}) \\
& \quad = \frac{1}{n} \sum_{\alpha \beta} h_{\alpha ijk} h^{\alpha \beta} G_\beta - \frac{1}{n}G_{ijk} + O(n^{-2}) \\
\text{(e)} \quad & h_{ijkq}^*(\hat{\boldsymbol{\theta}}_N) - h_{ijkq}(\hat{\boldsymbol{\theta}}) = \frac{1}{n}D^1 h_{ijkq}(\hat{\boldsymbol{\theta}})^T [D^2 h(\hat{\boldsymbol{\theta}})]^{-1} D^1 G(\hat{\boldsymbol{\theta}}) - \frac{1}{n}G_{ijkq}(\hat{\boldsymbol{\theta}}) + O(n^{-2}) \\
& \quad = \frac{1}{n} \sum_{\alpha \beta} h_{\alpha ijkq} h^{\alpha \beta} G_\beta - \frac{1}{n}G_{ijkq} + O(n^{-2}) \\
\text{(f)} \quad & h^{ij}(\hat{\boldsymbol{\theta}}_N) - h^{ij}(\hat{\boldsymbol{\theta}}) = \frac{1}{n}D^1 h^{ij}(\hat{\boldsymbol{\theta}})^T [D^2 h(\hat{\boldsymbol{\theta}})]^{-1} D^1 G(\hat{\boldsymbol{\theta}}) + O(n^{-2}) \\
& \quad = -\frac{1}{n} \sum_{\alpha \beta l m} h^{i\alpha} h_{l\alpha \beta} h^{\beta j} h^{lm} G_m + O(n^{-2})
\end{aligned}$$

$$(g) \ h^{*ij}(\hat{\boldsymbol{\theta}}_N) - h^{ij}(\hat{\boldsymbol{\theta}}) = -\frac{1}{n} \sum_{\alpha,\beta,l,m} h^{i\alpha} h_{l\alpha\beta} h^{\beta j} h^{lm} G_m + \frac{1}{n} \sum_{\alpha,\beta} h^{i\alpha} G_{\alpha\beta} h^{\beta j} + O(n^{-2})$$

*Proof of (a).* From  $Dh^*(\hat{\boldsymbol{\theta}}) = Dh(\hat{\boldsymbol{\theta}}) - (1/n)DG(\hat{\boldsymbol{\theta}}) = -(1/n)DG(\hat{\boldsymbol{\theta}}) + O(n^{-2})$

$$\hat{\boldsymbol{\theta}}_N - \hat{\boldsymbol{\theta}} = -[D^2h^*(\hat{\boldsymbol{\theta}})]^{-1}D^1h^*(\hat{\boldsymbol{\theta}}) \quad (\text{B.1})$$

$$= \frac{1}{n}[D^2h(\hat{\boldsymbol{\theta}})]^{-1}D^1G(\hat{\boldsymbol{\theta}}) + O(n^{-2}) \quad (\text{B.2})$$

It follows from the result (B.2) that

$$\begin{aligned} h^*(\hat{\boldsymbol{\theta}}_N) - h(\hat{\boldsymbol{\theta}}) &= h(\hat{\boldsymbol{\theta}}_N) - h(\hat{\boldsymbol{\theta}}) - \frac{1}{n}G(\hat{\boldsymbol{\theta}}_N) \\ &= D^1h(\hat{\boldsymbol{\theta}})^T(\hat{\boldsymbol{\theta}}_N - \hat{\boldsymbol{\theta}}) - \frac{1}{n}G(\hat{\boldsymbol{\theta}}_N) + O(n^{-2}) \\ &= D^1h(\hat{\boldsymbol{\theta}})^T \left\{ \frac{1}{n}[D^2h(\hat{\boldsymbol{\theta}})]^{-1}D^1G(\hat{\boldsymbol{\theta}}) \right\} - \frac{1}{n}G(\hat{\boldsymbol{\theta}}) + O(n^{-2}) \\ &= \frac{1}{n}D^1h(\hat{\boldsymbol{\theta}})^T[D^2h(\hat{\boldsymbol{\theta}})]^{-1}D^1G(\hat{\boldsymbol{\theta}}) - \frac{1}{n}G(\hat{\boldsymbol{\theta}}) + O(n^{-2}). \end{aligned}$$

*Proof of (b).* Because  $\hat{\boldsymbol{\theta}}_N$  is an asymptotic mode of order  $n^{-2}$  for  $-h^*$ , this is immediate from Miyata (2004, p.1047).

*Proof of (c).* Because  $D^2h^*(\hat{\boldsymbol{\theta}}_N) = D^2h(\hat{\boldsymbol{\theta}}_N) - (1/n)D^2G(\hat{\boldsymbol{\theta}}_N)$ , arguing as in the proof of (a) of Lemma 13, we have

$$\begin{aligned} h_{ij}^*(\hat{\boldsymbol{\theta}}_N) - h_{ij}(\hat{\boldsymbol{\theta}}) &= h_{ij}(\hat{\boldsymbol{\theta}}_N) - h_{ij}(\hat{\boldsymbol{\theta}}) - \frac{1}{n}G_{ij}(\hat{\boldsymbol{\theta}}_N) \\ &= D^1h_{ij}(\hat{\boldsymbol{\theta}})^T(\hat{\boldsymbol{\theta}}_N - \hat{\boldsymbol{\theta}}) - \frac{1}{n}G_{ij}(\hat{\boldsymbol{\theta}}_N) + O(n^{-2}) \\ &= D^1h_{ij}(\hat{\boldsymbol{\theta}})^T \left\{ \frac{1}{n}[D^2h(\hat{\boldsymbol{\theta}})]^{-1}D^1G(\hat{\boldsymbol{\theta}}) \right\} - \frac{1}{n}G_{ij}(\hat{\boldsymbol{\theta}}) + O(n^{-2}) \\ &= \frac{1}{n}D^1h_{ij}(\hat{\boldsymbol{\theta}})^T[D^2h(\hat{\boldsymbol{\theta}})]^{-1}D^1G(\hat{\boldsymbol{\theta}}) - \frac{1}{n}G_{ij}(\hat{\boldsymbol{\theta}}) + O(n^{-2}) \\ &= \frac{1}{n} \sum_{\alpha,\beta} h_{\alpha ij} h^{\alpha\beta} G_{\beta}(\hat{\boldsymbol{\theta}}) - \frac{1}{n}G_{ij}(\hat{\boldsymbol{\theta}}) + O(n^{-2}). \end{aligned}$$

*Proof of (d).* Arguing as in the proof of (a) of Lemma 13,

$$\begin{aligned} h_{ijk}^*(\hat{\boldsymbol{\theta}}_N) - h_{ijk}(\hat{\boldsymbol{\theta}}) &= h_{ijk}(\hat{\boldsymbol{\theta}}_N) - h_{ijk}(\hat{\boldsymbol{\theta}}) - \frac{1}{n}G_{ijk}(\hat{\boldsymbol{\theta}}_N) \\ &= D^1h_{ijk}(\hat{\boldsymbol{\theta}})^T(\hat{\boldsymbol{\theta}}_N - \hat{\boldsymbol{\theta}}) - \frac{1}{n}G_{ijk}(\hat{\boldsymbol{\theta}}_N) + O(n^{-2}) \\ &= D^1h_{ijk}(\hat{\boldsymbol{\theta}})^T \left\{ \frac{1}{n}[D^2h(\hat{\boldsymbol{\theta}})]^{-1}D^1G(\hat{\boldsymbol{\theta}}) \right\} - \frac{1}{n}G_{ijk}(\hat{\boldsymbol{\theta}}) + O(n^{-2}) \\ &= \frac{1}{n}D^1h_{ijk}(\hat{\boldsymbol{\theta}})^T[D^2h(\hat{\boldsymbol{\theta}})]^{-1}D^1G(\hat{\boldsymbol{\theta}}) - \frac{1}{n}G_{ijk}(\hat{\boldsymbol{\theta}}) + O(n^{-2}) \\ &= \frac{1}{n} \sum_{\alpha,\beta} h_{\alpha ijk} h^{\alpha\beta} G_{\beta}(\hat{\boldsymbol{\theta}}) - \frac{1}{n}G_{ijk}(\hat{\boldsymbol{\theta}}) + O(n^{-2}). \end{aligned}$$

*Proof of (e).* This is the same as that of (d) essentially.

*Proof of (f).* It follows from (B.2) that

$$\begin{aligned} h^{ij}(\hat{\boldsymbol{\theta}}_N) - h^{ij}(\hat{\boldsymbol{\theta}}) &= D^1 h^{ij}(\hat{\boldsymbol{\theta}})^T (\hat{\boldsymbol{\theta}}_N - \hat{\boldsymbol{\theta}}) + O(n^{-2}) \\ &= \frac{1}{n} D^1 h^{ij}(\hat{\boldsymbol{\theta}})^T [D^2 h(\hat{\boldsymbol{\theta}})]^{-1} D^1 G(\hat{\boldsymbol{\theta}}) + O(n^{-2}) \end{aligned} \quad (\text{B.3})$$

By using the matrix algebra (D.A. Harville p.308),

$$\frac{\partial}{\partial \hat{\theta}_k} [D^2 h(\hat{\boldsymbol{\theta}})]^{-1} = -[D^2 h(\hat{\boldsymbol{\theta}})]^{-1} \frac{\partial}{\partial \hat{\theta}_k} D^2 h(\hat{\boldsymbol{\theta}}) [D^2 h(\hat{\boldsymbol{\theta}})]^{-1}.$$

Hence,

$$\frac{\partial}{\partial \hat{\theta}_k} h^{ij}(\hat{\boldsymbol{\theta}}) = - \sum_{\alpha, \beta} h^{i\alpha} h_{k\alpha\beta} h^{\beta j}.$$

Therefore,

$$D^1 h^{ij}(\hat{\boldsymbol{\theta}}) = - \sum_{\alpha, \beta} h^{i\alpha} h^{\beta j} D^1 h_{\alpha\beta}(\hat{\boldsymbol{\theta}}).$$

Thus

$$\begin{aligned} h^{ij}(\hat{\boldsymbol{\theta}}_N) - h^{ij}(\hat{\boldsymbol{\theta}}) &= \frac{1}{n} \left( - \sum_{\alpha\beta} h^{i\alpha} h^{\beta j} D^1 h_{\alpha\beta}(\hat{\boldsymbol{\theta}})^T \right) [D^2 h(\hat{\boldsymbol{\theta}})]^{-1} D^1 G(\hat{\boldsymbol{\theta}}) + O(n^{-2}) \\ &= -\frac{1}{n} \sum_{\alpha\beta kl} h^{i\alpha} h_{k\alpha\beta} h^{\beta j} h^{kl} G_l + O(n^{-2}). \end{aligned}$$

*Proof of (g).* It follows from (A.3) that

$$\begin{aligned} [D^2 h^*(\hat{\boldsymbol{\theta}}_N)]^{-1} - [D^2 h(\hat{\boldsymbol{\theta}})]^{-1} &= [D^2 h(\hat{\boldsymbol{\theta}}_N) - \frac{1}{n} D^2 G(\hat{\boldsymbol{\theta}}_N)]^{-1} - [D^2 h(\hat{\boldsymbol{\theta}})]^{-1} \\ &= [D^2 h(\hat{\boldsymbol{\theta}}_N)]^{-1} - [D^2 h(\hat{\boldsymbol{\theta}})]^{-1} + \frac{1}{n} [D^2 h^*(\hat{\boldsymbol{\theta}}_N)]^{-1} D^2 G(\hat{\boldsymbol{\theta}}_N) [D^2 h(\hat{\boldsymbol{\theta}}_N)]^{-1} \\ &= [D^2 h(\hat{\boldsymbol{\theta}}_N)]^{-1} - [D^2 h(\hat{\boldsymbol{\theta}})]^{-1} + \frac{1}{n} [D^2 h(\hat{\boldsymbol{\theta}})]^{-1} D^2 G(\hat{\boldsymbol{\theta}}) [D^2 h(\hat{\boldsymbol{\theta}})]^{-1} + O(n^{-2}). \end{aligned}$$

Using (f) of this lemma, we have

$$\begin{aligned} h^{*ij}(\hat{\boldsymbol{\theta}}_N) - h^{ij}(\hat{\boldsymbol{\theta}}) &= h^{ij}(\hat{\boldsymbol{\theta}}_N) - h^{ij}(\hat{\boldsymbol{\theta}}) + \frac{1}{n} \begin{pmatrix} h^{1j} & & \\ & \dots & \\ h^{dj} & & \end{pmatrix} D^2 G(\hat{\boldsymbol{\theta}}) \begin{pmatrix} h^{1j} \\ \vdots \\ h^{dj} \end{pmatrix} + O(n^{-2}) \\ &= -\frac{1}{n} \sum_{\alpha\beta lm} h^{i\alpha} h_{l\alpha\beta} h^{\beta j} h^{lm} G_m + \frac{1}{n} \sum_{\alpha\beta} h^{i\alpha} G_{\alpha\beta} h^{\beta j} + O(n^{-2}). \end{aligned}$$

The following expansions are used to derive the fully exponential Laplace approximations in Section 3.

**Lemma 15.** Suppose that  $\hat{\boldsymbol{\theta}}$  is an asymptotic mode of order  $n^{-2}$  for  $-h(\hat{\boldsymbol{\theta}})$ . Let  $\mu_{ijkqrs}^*$  be sixth central moments of a multivariate Normal distribution with mean  $\mathbf{0}$  and covariance  $\Sigma^* = [nD^2h^*(\hat{\boldsymbol{\theta}}_N)]^{-1}$ . Let

$$\Delta^{k_5k_6} = \sum_{\alpha\beta lm} h^{k_5\alpha} h_{l\alpha\beta} h^{\beta k_6} h^{lm} G_m - \sum_{\alpha\beta} h^{k_5\alpha} h^{\beta k_6} G_{\alpha\beta}.$$

Then the following results hold.

$$(a) \quad n^3(\mu_{ijkqrs}^* - \mu_{ijkqrs}) = -\frac{1}{n} \sum_{\langle k_1, k_2, \dots, k_6 \rangle} h^{k_1k_2} h^{k_3k_4} \Delta^{k_5k_6} + O(n^{-2}),$$

where  $\mathcal{A}$ ,  $\mathcal{A}$ , and  $\mathcal{B}$  are three rooms in which two rooms are the same, and the other is different from them, and  $\langle k_1, k_2, \dots, k_6 \rangle$  denotes ways to arrange elements  $i, j, k, q, r$  and  $s$  into the three rooms  $\mathcal{A}$ ,  $\mathcal{A}$ , and  $\mathcal{B}$  by two alphabets. Hence the summation  $\sum_{\langle k_1, k_2, \dots, k_6 \rangle}$  is over  $\binom{6}{2} \cdot \binom{4}{2} / 2 = 45$  terms.

(b)

$$\begin{aligned} & \sum_{ijkqrs} h_{ijk} h_{qrs} n^3 (\mu_{ijkqrs}^* - \mu_{ijkqrs}) \\ &= -\frac{9}{n} \sum_{ijkqrs\alpha\beta lm} h_{ijk} h_{qrs} h_{l\alpha\beta} h^{jk} h^{rs} h^{i\alpha} h^{\beta q} h^{lm} G_m + \frac{9}{n} \sum_{ijkqrs\alpha\beta} h_{ijk} h_{qrs} h^{jk} h^{rs} h^{i\alpha} h^{\beta q} G_{\alpha\beta} \\ & - \frac{18}{n} \sum_{ijkqrs\alpha\beta lm} h_{ijk} h_{qrs} h_{l\alpha\beta} h^{jr} h^{ks} h^{i\alpha} h^{\beta q} h^{lm} G_m + \frac{18}{n} \sum_{ijkqrs\alpha\beta} h_{ijk} h_{qrs} h^{jr} h^{ks} h^{i\alpha} h^{\beta q} G_{\alpha\beta} \\ & - \frac{18}{n} \sum_{ijkqrs\alpha\beta lm} h_{ijk} h_{qrs} h_{l\alpha\beta} h^{kq} h^{rs} h^{i\alpha} h^{\beta j} h^{lm} G_m + \frac{18}{n} \sum_{ijkqrs\alpha\beta} h_{ijk} h_{qrs} h^{kq} h^{rs} h^{i\alpha} h^{\beta j} G_{\alpha\beta} \\ & + O(n^{-2}). \end{aligned}$$

$$(c) \quad n^3 \sum_{ijkqrs} \{h_{ijk}^*(\hat{\boldsymbol{\theta}}_N) - h_{ijk}(\hat{\boldsymbol{\theta}})\} h_{qrs} \mu_{ijkqrs}^* \\ = \frac{1}{n} \sum_{ijkqrs\alpha\beta} h_{\alpha ijk} h_{qrs} h^{\alpha\beta} (n^3 \mu_{ijkqrs}) G_\beta - \sum_{ijkqrs} h_{qrs} (n^3 \mu_{ijkqrs}) G_{ijk} + O(n^{-2}).$$

$$(d) \quad h_l^*(\hat{\boldsymbol{\theta}}_N) = \frac{1}{2n^2} \sum_{r\alpha\beta} h_{l\alpha\beta} h^{\alpha r} h^{\beta m} G_r G_m + O(n^{-3}).$$

*Proof of (a).* It is well known that sixth central moments of the Normal distribution are decomposed with elements of the covariance matrix i.e.,

$$\mu_{ijkqrs}^* = \frac{1}{n^3} \left( \underbrace{h^{*ij} h^{*kq} h^{*rs} + h^{*ij} h^{*kr} h^{*qs} + \dots + h^{*is} h^{*jr} h^{*kq}}_{15 \text{ terms}} \right), \quad (B.4)$$

where  $h^{*ij}$  are  $(i, j)$ -elements of  $[D^2h^*(\hat{\boldsymbol{\theta}}_N)]^{-1}$ . For example, see Kass et al. (1990, p.477).

From (g) of Lemma 13,  $h^{*ij}(\hat{\boldsymbol{\theta}}_N) = h^{ij}(\hat{\boldsymbol{\theta}}) - \frac{\Delta^{ij}}{n} + O(n^{-2})$ .

Then we have

$$\begin{aligned}
& h^{*ij}(\hat{\theta}_N)h^{*kq}(\hat{\theta}_N)h^{*rs}(\hat{\theta}_N) \\
&= h^{ij}(\hat{\theta})h^{kq}(\hat{\theta})h^{rs}(\hat{\theta}) \\
&- \frac{1}{n}h^{ij}(\hat{\theta})h^{kq}(\hat{\theta})\left(\sum_{\alpha\beta lm} h^{r\alpha}h_{l\alpha\beta}h^{\beta s}h^{lm}G_m - \sum_{\alpha\beta} h^{r\alpha}h^{\beta s}G_{\alpha\beta}\right) \\
&- \frac{1}{n}h^{ij}(\hat{\theta})h^{rs}(\hat{\theta})\left(\sum_{\alpha\beta lm} h^{k\alpha}h_{l\alpha\beta}h^{\beta q}h^{lm}G_m - \sum_{\alpha\beta} h^{k\alpha}h^{\beta q}G_{\alpha\beta}\right) \\
&- \frac{1}{n}h^{kq}(\hat{\theta})h^{rs}(\hat{\theta})\left(\sum_{\alpha\beta lm} h^{i\alpha}h_{l\alpha\beta}h^{\beta j}h^{lm}G_m - \sum_{\alpha\beta} h^{i\alpha}h^{\beta j}G_{\alpha\beta}\right) + O(n^{-2}) \\
&= h^{ij}(\hat{\theta})h^{kq}(\hat{\theta})h^{rs}(\hat{\theta}) - \frac{1}{n}h^{ij}(\hat{\theta})h^{kq}(\hat{\theta})\Delta^{rs} - \frac{1}{n}h^{ij}(\hat{\theta})h^{rs}(\hat{\theta})\Delta^{kq} \\
&\quad - \frac{1}{n}h^{kq}(\hat{\theta})h^{rs}(\hat{\theta})\Delta^{ij} + O(n^{-2}), \tag{B.5}
\end{aligned}$$

where

$$\Delta^{ij} = \sum_{\alpha,\beta,l,m} h^{i\alpha}h_{l\alpha\beta}h^{\beta j}h^{lm}G_m - \sum_{\alpha,\beta} h^{i\alpha}h^{\beta j}G_{\alpha\beta}. \tag{B.6}$$

Substitution of (B.5) into the decomposition (B.4) leads to the equation (a).

*Proof of (b).* From Lemma 14 (a), we have

$$\begin{aligned}
& \sum_{ijkqrs} h_{ijk}h_{qrs}n^3(\mu_{ijkqrs}^* - \mu_{ijkqrs}) \\
&= -\frac{1}{n}\sum_{ijkqrs} h_{ijk}h_{qrs}\left(\underbrace{h^{ij}h^{kq}\Delta^{rs} + h^{ij}\Delta^{kq}h^{rs} + \Delta^{ij}h^{kq}h^{rs} + \dots + h^{is}h^{jr}\Delta^{kq}}_{45\text{terms}}\right) + O(n^{-2}) \\
&= -\frac{1}{n}\sum_{ijkqrs} h_{ijk}h_{qrs}\sum_{\langle k_1k_2\dots k_6 \rangle} h^{k_1k_2}h^{k_3k_4}\Delta^{k_5k_6} + O(n^{-2}). \tag{B.7}
\end{aligned}$$

Equation (B.7) are divided into three kinds of terms,  $\sum h_{ijk}h_{qrs}\Delta^{iq}h^{jk}h^{rs}$ ,  $\sum h_{ijk}h_{qrs}\Delta^{iq}h^{jr}h^{ks}$ , and  $\sum h_{ijk}h_{qrs}\Delta^{ij}h^{kq}h^{rs}$  as described below. Note that  $\sum h_{ijk}h_{qrs}h^{ij}h^{kq}\Delta^{rs}$  and  $\sum h_{ijk}h_{qrs}\Delta^{ij}h^{kq}h^{rs}$  are the same if the suffixes  $i$  and  $j$  are exchanged for  $r$  and  $s$ . The second summation in (B.7) is

$$\begin{aligned}
& \sum_{\langle k_1 k_2 \dots k_6 \rangle} h^{k_1 k_2} h^{k_3 k_4} \Delta^{k_5 k_6} \\
&= h^{ij} h^{kq} \Delta^{rs} + h^{ij} h^{kr} \Delta^{qs} + h^{ij} h^{ks} \Delta^{qr} + h^{ik} h^{jq} \Delta^{rs} + h^{ik} h^{jr} \Delta^{qs} + h^{ik} h^{js} \Delta^{qr} \\
&+ h^{iq} h^{jk} \Delta^{rs} + h^{iq} h^{jr} \Delta^{ks} + h^{iq} h^{js} \Delta^{kr} + h^{ir} h^{jk} \Delta^{qs} + h^{ir} h^{jq} \Delta^{ks} + h^{ir} h^{js} \Delta^{kq} \\
&+ h^{is} h^{jk} \Delta^{qr} + h^{is} h^{jq} \Delta^{kr} + h^{is} h^{jr} \Delta^{kq} + \underbrace{h^{ij} \Delta^{kq} h^{rs} + h^{ij} \Delta^{kr} h^{qs} + h^{ij} \Delta^{ks} h^{qr}} \\
&+ \underbrace{h^{ik} \Delta^{jq} h^{rs} + h^{ik} \Delta^{jr} h^{qs} + h^{ik} \Delta^{js} h^{qr}} + h^{iq} \Delta^{jk} h^{rs} + h^{iq} \Delta^{jr} h^{ks} + h^{iq} \Delta^{js} h^{kr} \\
&+ h^{ir} \Delta^{jk} h^{qs} + h^{ir} \Delta^{jq} h^{ks} + h^{ir} \Delta^{js} h^{kq} + h^{is} \Delta^{jk} h^{qr} + h^{is} \Delta^{jq} h^{kr} + h^{is} \Delta^{jr} h^{kq} \\
&+ \Delta^{ij} h^{kq} h^{rs} + \Delta^{ij} h^{kr} h^{qs} + \Delta^{ij} h^{ks} h^{qr} + \Delta^{ik} h^{jq} h^{rs} + \Delta^{ik} h^{jr} h^{qs} + \Delta^{ik} h^{js} h^{qr} \\
&+ \underbrace{\Delta^{iq} h^{jk} h^{rs}} + \underbrace{\Delta^{iq} h^{jr} h^{ks} + \Delta^{iq} h^{js} h^{kr}} + \underbrace{\Delta^{ir} h^{jk} h^{qs}} + \underbrace{\Delta^{ir} h^{jq} h^{ks} + \Delta^{ir} h^{js} h^{kq}} \\
&+ \underbrace{\Delta^{is} h^{jk} h^{qr}} + \underbrace{\Delta^{is} h^{jq} h^{kr} + \Delta^{is} h^{jr} h^{kq}}.
\end{aligned}$$

Then we classify the foregoing equation into three type listed below.

① (The underline) In the suffixes  $k_5$  and  $k_6$  of  $\Delta^{k_5 k_6}$ , one is from  $i, j$  and  $k$ , and another is from  $q, r$  and  $s$ . Additionally, in  $k_3$  and  $k_4$  of  $h^{k_3 k_4}$ , one is from  $i, j$  and  $k$ , and another is from  $q, r$  and  $s$ . (全部で18通り)

② (The underbrace) In the suffixes  $k_5$  and  $k_6$  of  $\Delta^{k_5 k_6}$ , one is from  $i, j$  and  $k$ , and another is from  $q, r$  and  $s$ . Additionally, the suffixes  $k_3$  and  $k_4$  have two alphabets in either  $(i, j, k)$  or  $(q, r, s)$ . (全部で9通り)

③ The suffixes  $k_5$  and  $k_6$  of  $\Delta^{k_5 k_6}$  have two alphabets in either  $(i, j, k)$  or  $(q, r, s)$ . (全部で18通り)

Consequently,

$$\begin{aligned}
& \sum_{ijkqrs} h_{ijk} h_{qrs} n^3 (\mu_{ijkqrs}^* - \mu_{ijkqrs}) \\
&= -\frac{9}{n} \sum h_{ijk} h_{qrs} \Delta^{iq} h^{jk} h^{rs} - \frac{18}{n} \sum h_{ijk} h_{qrs} \Delta^{iq} h^{jr} h^{ks} \\
&\quad - \frac{18}{n} \sum h_{ijk} h_{qrs} \Delta^{ij} h^{kq} h^{rs} + O(n^{-2}) \\
&= -\frac{9}{n} \sum h_{ijk} h_{qrs} h^{jk} h^{rs} \left( \sum_{\alpha, \beta, l, m} h^{i\alpha} h_{l\alpha\beta} h^{\beta q} h^{lm} G_m - \sum_{\alpha, \beta} h^{i\alpha} G_{\alpha\beta} h^{\beta q} \right) \\
&\quad - \frac{18}{n} \sum_{ijkqrs} h_{ijk} h_{qrs} h^{jr} h^{ks} \left( \sum_{\alpha, \beta, l, m} h^{i\alpha} h_{l\alpha\beta} h^{\beta q} h^{lm} G_m - \sum_{\alpha, \beta} h^{i\alpha} G_{\alpha\beta} h^{\beta q} \right) \\
&\quad - \frac{18}{n} \sum_{ijkqrs} h_{ijk} h_{qrs} h^{kq} h^{rs} \left( \sum_{\alpha, \beta, l, m} h^{i\alpha} h_{l\alpha\beta} h^{\beta j} h^{lm} G_m - \sum_{\alpha, \beta} h^{i\alpha} G_{\alpha\beta} h^{\beta j} \right) + O(n^{-2}).
\end{aligned}$$

Thus the foregoing equation becomes

$$\begin{aligned}
& -\frac{9}{n} \sum_{ijkqrs\alpha\beta lm} h_{ijk} h_{qrs} h_{l\alpha\beta} h^{jk} h^{rs} h^{i\alpha} h^{\beta q} h^{lm} G_m + \frac{9}{n} \sum_{ijkqrs\alpha\beta} h_{ijk} h_{qrs} h^{jk} h^{rs} h^{i\alpha} h^{\beta q} G_{\alpha\beta} \\
& -\frac{18}{n} \sum_{ijkqrs\alpha\beta lm} h_{ijk} h_{qrs} h_{l\alpha\beta} h^{jr} h^{ks} h^{i\alpha} h^{\beta q} h^{lm} G_m + \frac{18}{n} \sum_{ijkqrs\alpha\beta} h_{ijk} h_{qrs} h^{jr} h^{ks} h^{i\alpha} h^{\beta q} G_{\alpha\beta} \\
& -\frac{18}{n} \sum_{ijkqrs\alpha\beta lm} h_{ijk} h_{qrs} h_{l\alpha\beta} h^{kq} h^{rs} h^{i\alpha} h^{\beta j} h^{lm} G_m + \frac{18}{n} \sum_{ijkqrs\alpha\beta} h_{ijk} h_{qrs} h^{kq} h^{rs} h^{i\alpha} h^{\beta j} G_{\alpha\beta} \\
& + O(n^{-2}).
\end{aligned}$$

*Proof of (c).* It follows from Lemma 13 (d) that

$$\begin{aligned}
& n^3 \sum_{ijkqrs} (h_{ijk}^*(\hat{\theta}_N) - h_{ijk}(\hat{\theta})) h_{qrs} \mu_{ijkqrs}^* \\
& = n^3 \sum_{ijkqrs} \left( \frac{1}{n} \sum_{\alpha,\beta} h_{\alpha ijk} h^{\alpha\beta} G_\beta - \frac{1}{n} G_{ijk} + O(n^{-2}) \right) h_{qrs} \left( \mu_{ijkqrs} + O(n^{-4}) \right) \\
& = \frac{1}{n} \sum_{ijkqrs\alpha\beta} h_{\alpha ijk} h_{qrs} h^{\alpha\beta} (n^3 \mu_{ijkqrs}) G_\beta - \sum_{ijkqrs} h_{qrs} (n^3 \mu_{ijkqrs}) G_{ijk} + O(n^{-2})
\end{aligned}$$

Hence, (c) is proved.

*Proof of (d)* Expanding the first derivatives  $h_l^*(\hat{\theta}_N)$  around  $\hat{\theta}$ , and using (B.1) and (B.2) yields

$$\begin{aligned}
h_l^*(\hat{\theta}_N) &= h_l^*(\hat{\theta}) + D^1 h_l^*(\hat{\theta})^T (\hat{\theta}_N - \hat{\theta}) + \frac{1}{2} (\hat{\theta}_N - \hat{\theta})^T D^2 h_l^*(\hat{\theta}) (\hat{\theta}_N - \hat{\theta}) + O(n^{-3}) \\
&= h_l^*(\hat{\theta}) + D^1 h_l^*(\hat{\theta})^T \left( -[D^2 h^*(\hat{\theta})]^{-1} D^1 h^*(\hat{\theta}) \right) \\
&\quad + \frac{1}{2} \left( \frac{1}{n} [D^2 h(\hat{\theta})]^{-1} D^1 G(\hat{\theta}) \right)^T D^2 h_l^*(\hat{\theta}) \left( \frac{1}{n} [D^2 h(\hat{\theta})]^{-1} D^1 G(\hat{\theta}) \right) + O(n^{-3}).
\end{aligned}$$

It follows from definition of an inverse matrix that

$$D^1 h_l^*(\hat{\theta})^T [D^2 h^*(\hat{\theta})]^{-1} = (0, \dots, 0, \underset{l}{1}, 0, \dots, 0).$$

Thus we have

$$\begin{aligned}
h_l^*(\hat{\theta}_N) &= h_l^*(\hat{\theta}) - h_l^*(\hat{\theta}) + \frac{1}{2n^2} D^1 G(\hat{\theta})^T [D^2 h(\hat{\theta})]^{-1} D^2 h_l(\hat{\theta}) [D^2 h(\hat{\theta})]^{-1} D^1 G(\hat{\theta}) + O(n^{-3}) \\
&= \frac{1}{2n^2} D^1 G(\hat{\theta})^T [D^2 h(\hat{\theta})]^{-1} D^2 h_l(\hat{\theta}) [D^2 h(\hat{\theta})]^{-1} D^1 G(\hat{\theta}) + O(n^{-3}) \\
&= \frac{1}{2n^2} \left( \sum_r h^{1r} G_r \cdots \sum_r h^{dr} G_r \right) D^2 h_l(\hat{\theta}) \begin{pmatrix} \sum_q h^{1q} G_q \\ \vdots \\ \sum_q h^{dq} G_q \end{pmatrix} + O(n^{-3}) \\
&= \frac{1}{2n^2} \sum_{l\alpha\beta qr} h_{l\alpha\beta} h^{\alpha r} h^{\beta q} G_r G_q + O(n^{-3}).
\end{aligned}$$

Hence, the lemma is proved.



## Appendix C: Proofs of the main results

This section proves the main results. The notations are the same as in Sections 2 and 3.

*Proof of Theorem 1.*

$$\int_{\boldsymbol{\theta}} e^{-nh(\boldsymbol{\theta})} d\boldsymbol{\theta} = \int_{B_\delta(\boldsymbol{\theta})} e^{-nh(\boldsymbol{\theta})} d\boldsymbol{\theta} + \int_{\boldsymbol{\theta}-B_\delta(\boldsymbol{\theta})} e^{-nh(\boldsymbol{\theta})} d\boldsymbol{\theta}.$$

First, we evaluate the first term in the r.h.s.

By expanding  $h(\boldsymbol{\theta})$  about  $\hat{\boldsymbol{\theta}}$ ,

$$\begin{aligned} h(\boldsymbol{\theta}) &= h(\hat{\boldsymbol{\theta}}) + \sum_i h_i(\hat{\boldsymbol{\theta}}) z_i + \frac{1}{2} \sum_{ij} h_{ij}(\hat{\boldsymbol{\theta}}) z_i z_j + \frac{1}{6} \sum_{ijk} h_{ijk}(\hat{\boldsymbol{\theta}}) z_i z_j z_k \\ &\quad + \frac{1}{24} \sum_{ijkq} h_{ijkq}(\hat{\boldsymbol{\theta}}) z_i z_j z_k z_q + \frac{1}{120} \sum h_{ijkqr}(\hat{\boldsymbol{\theta}}) z_i z_j z_k z_q z_r \\ &\quad + \frac{1}{720} \sum h_{ijkqrs}(\hat{\boldsymbol{\theta}}) z_i z_j z_k z_q z_r z_s + R_{1n}, \end{aligned}$$

where  $R_{1n} \equiv (1/7!) \sum h_{ijkqrst} z_i z_j z_k z_q z_r z_s z_t + r_{1n}$ , and  $r_{1n}$  is bounded over  $B_\epsilon(\hat{\boldsymbol{\theta}})$  by a polynomial in  $z_i z_j z_k z_q z_r z_s z_t z_u$ . By using Lemma 7, we have

$$\begin{aligned} &\sum_i h_i(\hat{\boldsymbol{\theta}}) z_i + \frac{1}{2} \sum_{ij} h_{ij}(\hat{\boldsymbol{\theta}}) z_i z_j \\ &= D^1 h(\hat{\boldsymbol{\theta}})^T (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}) + \frac{1}{2} (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})^T D^2 h(\hat{\boldsymbol{\theta}}) (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}) \\ &= \frac{1}{2} (\boldsymbol{\theta} - \mathbf{y})^T D^2 h(\hat{\boldsymbol{\theta}}) (\boldsymbol{\theta} - \mathbf{y}) - \frac{1}{4} D^1 h(\hat{\boldsymbol{\theta}})^T \left[ \frac{1}{2} D^2 h(\hat{\boldsymbol{\theta}}) \right]^{-1} D^1 h(\hat{\boldsymbol{\theta}}), \end{aligned}$$

where  $\mathbf{y} = \hat{\boldsymbol{\theta}} - [D^2 h(\hat{\boldsymbol{\theta}})]^{-1} D^1 h(\hat{\boldsymbol{\theta}})$ .

Using the expansion  $e^x = 1 + x + (1/2)x^2 + (1/6)x^3 + (1/24)x^4 + (1/120)e^{\tau_1} x^5$ , where  $\tau_1$  is a point between 0 and  $x$ , it follows that

$$\begin{aligned} &\exp \left\{ -n \left[ \frac{1}{6} \sum_{ijk} h_{ijk}(\hat{\boldsymbol{\theta}}) z_i z_j z_k + \cdots + \frac{1}{720} \sum h_{ijkqrs}(\hat{\boldsymbol{\theta}}) z_i z_j z_k z_q z_r z_s + R_{1n} \right] \right\} \\ &= \left\{ 1 - n \left( \frac{1}{6} \sum h_{ijk} z_i z_j z_k + \frac{1}{24} \sum h_{ijkq} z_i z_j z_k z_q + \frac{1}{120} \sum h_{ijkqr} z_i z_j z_k z_q z_r \right. \right. \\ &\quad \left. \left. + \frac{1}{720} \sum h_{ijkqrs} z_i z_j z_k z_q z_r z_s + R_{1n} \right) \right. \\ &\quad + \frac{n^2}{2} \left( \frac{1}{36} \left[ \sum_{ijk} h_{ijk} z_i z_j z_k \right]^2 + 2 \cdot \frac{1}{6} \cdot \frac{1}{24} \left[ \sum_{ijk} h_{ijk} z_i z_j z_k \right] \left[ \sum_{qrst} h_{qrst} z_q z_r z_s z_t \right] \right. \\ &\quad \left. + \left( \frac{1}{24} \right)^2 \left[ \sum h_{ijkq} z_i z_j z_k z_q \right]^2 + 2 \cdot \frac{1}{6} \cdot \frac{1}{120} \left[ \sum h_{ijk} z_i z_j z_k \right] \left[ \sum_{qrstu} h_{qrstu} z_q z_r z_s z_t z_u \right] + R_{2n} \right) \\ &\quad - \frac{n^3}{6} \left( \left( \frac{1}{6} \right)^3 \left[ \sum_{ijk} h_{ijk} z_i z_j z_k \right]^3 + \binom{3}{2} \cdot \left( \frac{1}{6} \right)^2 \cdot \frac{1}{24} \left[ \sum_{ijk} h_{ijk} z_i z_j z_k \right]^2 \left[ \sum_{qrst} h_{qrst} z_q z_r z_s z_t \right] + R_{3n} \right) \\ &\quad \left. + \frac{n^4}{24} \left( \left( \frac{1}{6} \right)^4 \left[ \sum_{ijk} h_{ijk} z_i z_j z_k \right]^4 + R_{4n} \right) + R_{5n} \right\} \\ &= J_n(\boldsymbol{\theta}, \hat{\boldsymbol{\theta}}) + R_n, \end{aligned} \tag{C.1}$$

where  $R_{2n}$ ,  $R_{3n}$ , and  $R_{4n}$  are the rests of terms squared, cubed, and to the fourth power in the bracket,  $R_{5n}$  is a term with polynomials of degree greater than or equal to 15, and  $R_n$  is the sum of all terms involving  $R_{1n}$ ,  $R_{2n}$ ,  $R_{3n}$ ,  $R_{4n}$ , and  $R_{5n}$ .

In (C.1),  $J_n(\boldsymbol{\theta}, \hat{\boldsymbol{\theta}})$  is

$$\begin{aligned}
J_n(\boldsymbol{\theta}, \hat{\boldsymbol{\theta}}) &= 1 - \frac{n}{6} \sum h_{ijk} z_i z_j z_k - \frac{n}{24} \sum h_{ijkq} z_i z_j z_k z_q \\
&+ \frac{n^2}{72} \sum h_{ijk} h_{qrs} z_i z_j z_k z_q z_r z_s \\
&- \frac{n}{120} \sum h_{ijkqr} z_i z_j z_k z_q z_r - \frac{n}{720} \sum h_{ijkqrs} z_i z_j z_k z_q z_r z_s \\
&+ \frac{n^2}{144} \sum h_{ijk} h_{qrst} z_i z_j z_k z_q z_r z_s z_t + \frac{n^2}{1152} \sum h_{ijkq} h_{rstu} z_i z_j z_k z_q z_r z_s z_t z_u \\
&+ \frac{n^2}{720} \sum h_{ijk} h_{qrst} z_i z_j z_k z_q z_r z_s z_t z_u \\
&- \frac{n^3}{1296} \sum h_{ijk} h_{qrs} h_{tuv} z_i z_j z_k z_q z_r z_s z_t z_u z_v \\
&- \frac{n^3}{1728} \sum h_{ijk} h_{qrs} h_{tuv} z_i z_j z_k z_q z_r z_s z_t z_u z_v z_w \\
&+ \frac{n^4}{31104} \sum h_{ijk} h_{qrs} h_{tuv} h_{wxy} z_i z_j z_k z_q z_r z_s z_t z_u z_v z_w z_x z_y.
\end{aligned}$$

From (C.1), we have

$$\begin{aligned}
&\int_{B_\delta(\hat{\boldsymbol{\theta}})} e^{-nh(\boldsymbol{\theta})} d\boldsymbol{\theta} \\
&= e^{-nh(\hat{\boldsymbol{\theta}})} \cdot \exp \left\{ \frac{n}{4} D^1 h(\hat{\boldsymbol{\theta}})^T \left[ \frac{1}{2} D^2 h(\hat{\boldsymbol{\theta}}) \right]^{-1} D^1 h(\hat{\boldsymbol{\theta}}) \right\} \\
&\times \int_{B_\delta(\hat{\boldsymbol{\theta}})} \exp \left( -\frac{1}{2} (\boldsymbol{\theta} - \mathbf{y})^T \left( \frac{1}{n} D^2 h(\hat{\boldsymbol{\theta}})^{-1} \right)^{-1} (\boldsymbol{\theta} - \mathbf{y}) \right) \\
&\times \exp \left\{ -n \left( \frac{1}{6} \sum_{ijk} h_{ijk}(\hat{\boldsymbol{\theta}}) z_i z_j z_k + \cdots + \frac{1}{720} \sum h_{ijkqrs} z_i z_j z_k z_q z_r z_s + R_{1n} \right) \right\} d\boldsymbol{\theta}. \\
&= e^{-nh(\hat{\boldsymbol{\theta}})} C_n(\hat{\boldsymbol{\theta}}) \int_{B_\delta(\hat{\boldsymbol{\theta}})} \exp \left( -\frac{1}{2} (\boldsymbol{\theta} - \mathbf{y})^T \Sigma^{-1} (\boldsymbol{\theta} - \mathbf{y}) \right) J_n(\boldsymbol{\theta}, \hat{\boldsymbol{\theta}}) d\boldsymbol{\theta}, \tag{C.2}
\end{aligned}$$

$$+ e^{-nh(\hat{\boldsymbol{\theta}})} C_n(\hat{\boldsymbol{\theta}}) \int_{B_\delta(\hat{\boldsymbol{\theta}})} \exp \left( -\frac{1}{2} (\boldsymbol{\theta} - \mathbf{y})^T \Sigma^{-1} (\boldsymbol{\theta} - \mathbf{y}) \right) R_n d\boldsymbol{\theta} \tag{C.3}$$

where  $\Sigma = [nD^2 h(\hat{\boldsymbol{\theta}})]^{-1}$ . Second, we evaluate (C.3). The terms composing  $R_n$  may be represented explicitly using the mean value form of the remainders in terms of higher derivatives of  $h$  evaluated at points between  $\hat{\boldsymbol{\theta}}$  and  $\boldsymbol{\theta}$ , for example, one such term is

$(-n/8!) \sum h_{ijkqrstu}(\gamma_1) z_i z_j z_k z_q z_r z_s z_t z_u$ , where  $\gamma_1$  is a point between  $\boldsymbol{\theta}$  and  $\hat{\boldsymbol{\theta}}$ . It is one piece of the error term appearing as  $R_n$ . Because it follows from condition (A3) that  $\|h_{ijkqrstu}(\gamma_1)\| < M$

on  $B_\delta(\hat{\boldsymbol{\theta}})$ , we have

$$\begin{aligned}
& \left\| \frac{-n}{8!} \int_{B_\delta(\hat{\boldsymbol{\theta}})} \exp\left(-\frac{1}{2}(\boldsymbol{\theta} - \mathbf{y})^T \Sigma^{-1}(\boldsymbol{\theta} - \mathbf{y})\right) h_{ijklrstu}(\gamma_1) z_i z_j z_k z_q z_r z_s z_t z_u d\boldsymbol{\theta} \right\| \\
& \leq \frac{nM}{8!} \int_{B_\delta(\hat{\boldsymbol{\theta}})} \exp\left(-\frac{1}{2}(\boldsymbol{\theta} - \mathbf{y})^T \Sigma^{-1}(\boldsymbol{\theta} - \mathbf{y})\right) \|z_i z_j z_k z_q z_r z_s z_t z_u\| d\boldsymbol{\theta} \\
& = |\Sigma|^{1/2} \times O(n^{-3}).
\end{aligned} \tag{C.4}$$

The other terms are similar. Thus (C.3) becomes  $(2\pi)^{d/2} e^{-nh(\hat{\boldsymbol{\theta}})} |\Sigma|^{1/2} C_n(\hat{\boldsymbol{\theta}}) \times O(n^{-3})$ .

Third, we evaluate (C.2). Since there exists a symmetric matrix  $\mathbf{A}^{1/2}$  such that  $\mathbf{A}^{1/2} \mathbf{A}^{1/2} = D^2 h(\hat{\boldsymbol{\theta}})$ , putting  $n^{1/2} \mathbf{A}^{1/2}(\boldsymbol{\theta} - \mathbf{y}) = \mathbf{u}$ , we have

$$\begin{aligned}
\Theta - B_\delta(\hat{\boldsymbol{\theta}}) &= \{\boldsymbol{\theta} : (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})^T (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}) > \delta^2\} \\
&= \{\boldsymbol{\theta} : (\mathbf{u} - n^{1/2} \mathbf{A}^{1/2} \mathbf{b})^T [D^2 h(\hat{\boldsymbol{\theta}})]^{-1} (\mathbf{u} - n^{1/2} \mathbf{A}^{1/2} \mathbf{b}) > n\delta^2\} \\
&\subseteq \{\boldsymbol{\theta} : \frac{1}{\lambda_1} (\mathbf{u} - n^{1/2} \mathbf{A}^{1/2} \mathbf{b})^T (\mathbf{u} - n^{1/2} \mathbf{A}^{1/2} \mathbf{b}) > n\delta^2\} \\
&\subseteq \{\boldsymbol{\theta} : 2\mathbf{u}^T \mathbf{u} + 2n\mathbf{b}^T \mathbf{A}^{1/2} \mathbf{A}^{1/2} \mathbf{b} > n\lambda_1 \delta^2\} \\
&= \{\boldsymbol{\theta} : \mathbf{u}^T \mathbf{u} > nc_2\} \\
&= \{\boldsymbol{\theta} : (\boldsymbol{\theta} - \mathbf{y})^T \Sigma^{-1}(\boldsymbol{\theta} - \mathbf{y}) > nc_2\},
\end{aligned}$$

where  $\lambda_1$  is the smallest eigenvalue of  $D^2 h(\hat{\boldsymbol{\theta}})$ ,  $\mathbf{b} = (b_i) \equiv -[D^2 h(\hat{\boldsymbol{\theta}})]^{-1} D^1 h(\hat{\boldsymbol{\theta}})$  and  $c_2 = (1/2)\{\lambda_1 \delta^2 - 2D^1 h(\hat{\boldsymbol{\theta}})^T [D^2 h(\hat{\boldsymbol{\theta}})]^{-1} D^1 h(\hat{\boldsymbol{\theta}})\}$ . Note that  $c_2 > 0$  for large  $n$  because  $\lambda_1$  is strictly positive from the assumption (A4). Hence, once again putting  $n^{1/2} \mathbf{A}^{1/2}(\boldsymbol{\theta} - \mathbf{y}) = \mathbf{u} = (u_i)$ , we have

$$\begin{aligned}
& \int_{\Theta - B_\delta(\hat{\boldsymbol{\theta}})} \exp\left(-\frac{1}{2}(\boldsymbol{\theta} - \mathbf{y})^T \Sigma^{-1}(\boldsymbol{\theta} - \mathbf{y})\right) J_n(\boldsymbol{\theta}, \hat{\boldsymbol{\theta}}) d\boldsymbol{\theta} \\
& \leq \left( \int_{(\boldsymbol{\theta} - \mathbf{y})^T \Sigma^{-1}(\boldsymbol{\theta} - \mathbf{y}) > nc_2} \exp\left(-\frac{1}{2}(\boldsymbol{\theta} - \mathbf{y})^T \Sigma^{-1}(\boldsymbol{\theta} - \mathbf{y})\right) J_n(\boldsymbol{\theta}, \hat{\boldsymbol{\theta}}) d\boldsymbol{\theta} \right)^{1/2} \\
& = |\Sigma|^{1/2} \left( \int_{\mathbf{u}^T \mathbf{u} > nc_2} \exp\left(-\frac{1}{2}\mathbf{u}^T \mathbf{u}\right) Po(\mathbf{u}) d\mathbf{u} \right)^{1/2},
\end{aligned}$$

where  $Po(\mathbf{u})$  denotes a term with multivariate polynomials in  $u_1, \dots, u_d$  of finite degree. Consequently,

$$\int_{\Theta - B_\delta(\hat{\boldsymbol{\theta}})} \exp\left(-\frac{1}{2}(\boldsymbol{\theta} - \mathbf{y})^T \Sigma^{-1}(\boldsymbol{\theta} - \mathbf{y})\right) J_n(\boldsymbol{\theta}, \hat{\boldsymbol{\theta}}) d\boldsymbol{\theta}.$$

becomes the term of exponentially decreasing error by the same argument as in Kass et al. (1990, pp.478-479). This allows the replacement of the domain in (C.2) by the whole Euclidean space. Therefore, (C.2) is replaced with

$$e^{-nh(\hat{\boldsymbol{\theta}})} C_n(\hat{\boldsymbol{\theta}}) \int_{\mathbb{R}^d} \exp\left(-\frac{1}{2}(\boldsymbol{\theta} - \mathbf{y})^T \Sigma^{-1}(\boldsymbol{\theta} - \mathbf{y})\right) J_n(\boldsymbol{\theta}, \hat{\boldsymbol{\theta}}) d\boldsymbol{\theta}.$$

Since  $\Sigma = (h^{ij}/n)$ , it follows from Lemma 12 (a) that

$$nE^N[(\Theta_i - \hat{\theta}_i)(\Theta_j - \hat{\theta}_j)(\Theta_k - \hat{\theta}_k)] = b_i h^{jk} + b_j h^{ik} + b_k h^{ij} + nb_i b_j b_k.$$

Then, using  $D^1h(\hat{\boldsymbol{\theta}}) = O(n^{-1})$ , we have

$$E^N \left[ -\frac{n}{6} \sum_{ijk} h_{ijk}(\hat{\boldsymbol{\theta}}) z_i z_j z_k \right] = -\frac{1}{2n} \sum_{ijk} h_{ijk}(\hat{\boldsymbol{\theta}}) (nb_i) h^{jk} - \frac{n}{6} \sum_{ijk} h_{ijk} b_i b_j b_k. \quad (\text{C.5})$$

Moreover,

$$\begin{aligned} E^N \left[ -\frac{n}{24} \sum_{ijkq} h_{ijkq} z_i z_j z_k z_q \right] &= -\frac{n}{24} \sum_{ijkq} h_{ijkq} E[z_i z_j z_k z_q] \\ &= -\frac{n}{24} \sum_{ijkq} h_{ijkq} \left( \frac{h^{ij}}{n} \cdot \frac{h^{kq}}{n} + \frac{h^{ik}}{n} \cdot \frac{h^{jq}}{n} + \frac{h^{iq}}{n} \cdot \frac{h^{kj}}{n} + \sum_{[m_1, m_2]_4} b_{m_1} b_{m_2} \frac{h^{m_3 m_4}}{n} + b_i b_j b_k b_q \right) \\ &= -\frac{1}{8n} \sum_{ijkq} h_{ijkq} h^{ij} h^{kq} - \frac{n}{24} \cdot \frac{1}{n} \cdot \binom{4}{2} \sum_{ijkq} h_{ijkq} h^{ij} b_k b_q - \frac{n}{24} \sum_{ijkq} h_{ijkq} b_i b_j b_k b_q \\ &= -\frac{1}{8n} \sum_{ijkq} h_{ijkq} h^{ij} h^{kq} - \frac{1}{4} \sum_{ijkq} h_{ijkq} h^{ij} b_k b_q + O(n^{-3}) \end{aligned} \quad (\text{C.6})$$

Similarly, applying (iii)–(xi) of Appendix E to the other expanded terms in  $J_n(\boldsymbol{\theta}, \hat{\boldsymbol{\theta}})$ , and then combining (C.5) and (C.6) yields

$$\int_{B_\delta(\hat{\boldsymbol{\theta}})} e^{-nh(\boldsymbol{\theta})} d\boldsymbol{\theta} = (2\pi)^{d/2} |\Sigma|^{1/2} e^{-nh(\hat{\boldsymbol{\theta}})} C_n(\hat{\boldsymbol{\theta}}) \left( 1 + \frac{\lambda_{1n}}{n} + \frac{\lambda_{2n}}{n^2} + O(n^{-3}) \right), \quad (\text{C.7})$$

where  $C_n(\hat{\boldsymbol{\theta}}) = \exp\{(n/2)D^1h(\hat{\boldsymbol{\theta}})^T[D^2h(\hat{\boldsymbol{\theta}})]^{-1}D^1h(\hat{\boldsymbol{\theta}})\}$ ,

$$\lambda_{1n} = -\frac{1}{2} \sum_{ijk} h_{ijk}(\hat{\boldsymbol{\theta}}) (nb_i) h^{jk} - \frac{1}{8} \sum_{ijkq} h_{ijkq}(\hat{\boldsymbol{\theta}}) h^{ij} h^{kq} + \frac{1}{72} \sum_{ijkqrs} h_{ijk}(\hat{\boldsymbol{\theta}}) h_{qrs}(\hat{\boldsymbol{\theta}}) \mu_{ijkqrs} n^3,$$

and  $\mu_{ijkqrs}$  are the sixth central moments of a multivariate Normal distribution having covariance matrix  $[nD^2h(\hat{\boldsymbol{\theta}})]^{-1}$ .

On the other hand, it follows from assumption (A.5) of Section 2 that

$$\int_{\boldsymbol{\theta} - B_\delta(\hat{\boldsymbol{\theta}})} e^{-nh(\boldsymbol{\theta})} d\boldsymbol{\theta} = (2\pi)^{d/2} |\Sigma|^{1/2} e^{-nh(\hat{\boldsymbol{\theta}})} C_n(\hat{\boldsymbol{\theta}}) \times O(n^{-3}). \quad (\text{C.8})$$

Therefore, combining (C.7) and (C.8) yields the result.

**Lemma 16.** Suppose that  $\hat{\boldsymbol{\theta}}$  is an asymptotic mode of order  $n^{-2}$  for  $-h$ . Then it follows that  $D^1h^*(\hat{\boldsymbol{\theta}}_N) = O(n^{-2})$ .

*Proof.* Expanding  $\partial h^*(\hat{\boldsymbol{\theta}}_N)/\partial \theta_i$  around  $\hat{\boldsymbol{\theta}}$  yields, for  $i = 1, \dots, d$ ,

$$\frac{\partial}{\partial \theta_i} h^*(\hat{\boldsymbol{\theta}}_N) = \frac{\partial}{\partial \theta_i} h^*(\hat{\boldsymbol{\theta}}) + (D^1 \frac{\partial}{\partial \theta_i} h^*(\hat{\boldsymbol{\theta}}))^T (\hat{\boldsymbol{\theta}}_N - \hat{\boldsymbol{\theta}}) + (\hat{\boldsymbol{\theta}}_N - \hat{\boldsymbol{\theta}})^T \left[ D^2 \frac{\partial}{\partial \theta_i} h^*(\xi_i) \right] (\hat{\boldsymbol{\theta}}_N - \hat{\boldsymbol{\theta}}), \quad (\text{C.9})$$

where  $\xi_i$  is an interior point on the line from  $\hat{\boldsymbol{\theta}}$  to  $\hat{\boldsymbol{\theta}}_N$ .

Writing (C.9) in a matrix form gives

$$D^1h^*(\hat{\boldsymbol{\theta}}_N) = D^1h^*(\hat{\boldsymbol{\theta}}) + D^2h^*(\hat{\boldsymbol{\theta}})^T (\hat{\boldsymbol{\theta}}_N - \hat{\boldsymbol{\theta}}) + R^*(\xi), \quad (\text{C.10})$$

where  $R^*(\xi) = ((\hat{\theta}_N - \hat{\theta})^T [D^2 \partial h^*(\xi_1) / \partial \theta_1] (\hat{\theta}_N - \hat{\theta}), \dots, (\hat{\theta}_N - \hat{\theta}) [D^2 \partial h^*(\xi_d) / \partial \theta_d] (\hat{\theta}_N - \hat{\theta}))^T$ . Substituting  $\hat{\theta}_N - \hat{\theta} = -[D^2 h^*(\hat{\theta})]^{-1} D^1 h^*(\hat{\theta})$  into (C.10), we have

$$D^1 h^*(\hat{\theta}_N) = D^1 h^*(\hat{\theta}) - D^2 h^*(\hat{\theta}) [D^2 h^*(\hat{\theta})]^{-1} D^1 h^*(\hat{\theta}) + O(n^{-2}) = O(n^{-2}).$$

*Proof of Theorem 5.*

$$\begin{aligned} & \frac{\int e^{-nh^*(\theta)} d\theta}{\int e^{-nh(\theta)} d\theta} \\ &= \left( \frac{|D^2 h(\hat{\theta})|}{|D^2 h^*(\hat{\theta}_N)|} \right)^{1/2} \frac{C_n^*(\hat{\theta}_N) \exp[-nh^*(\hat{\theta}_N)]}{C_n(\hat{\theta}) \exp[-nh(\hat{\theta})]} \frac{1 + \frac{a_{1n}^*}{n} + \frac{a_{2n}^*}{n^2} + O(n^{-3})}{1 + \frac{a_{1n}}{n} + \frac{a_{2n}}{n^2} + O(n^{-3})} \\ &= \left( \frac{|D^2 h(\hat{\theta})|}{|D^2 h^*(\hat{\theta}_N)|} \right)^{1/2} \frac{C_n^*(\hat{\theta}_N) \exp[-nh^*(\hat{\theta}_N)]}{C_n(\hat{\theta}) \exp[-nh(\hat{\theta})]} \\ & \quad \times \left( 1 + \frac{a_{1n}^* - a_{1n}}{n} + \frac{a_{2n}^* - a_{2n} - a_{1n}(a_{1n}^* - a_{1n})}{n^2} + O(n^{-3}) \right) \end{aligned}$$

First, we shall evaluate  $a_{1n}^* - a_{1n}$ . It follows from Lemma 13 (d) that

$$\begin{aligned} & \frac{n^3}{72} \sum_{ijkqrs} h_{ijk}^*(\hat{\theta}_N) h_{qrs}^*(\hat{\theta}_N) \mu_{ijkqrs}^* - \frac{n^3}{72} \sum_{ijkqrs} h_{ijk}(\hat{\theta}) h_{qrs}(\hat{\theta}) \mu_{ijkqrs} \\ &= \frac{n^3}{72} \sum \left\{ (h_{ijk}^*(\hat{\theta}_N) - h_{ijk}(\hat{\theta})) h_{qrs}^*(\hat{\theta}_N) \mu_{ijkqrs}^* \right. \\ & \quad \left. + h_{ijk}(\hat{\theta}) (h_{qrs}^*(\hat{\theta}_N) - h_{qrs}(\hat{\theta})) \mu_{ijkqrs}^* + h_{ijk}(\hat{\theta}) h_{qrs}(\hat{\theta}) (\mu_{ijkqrs}^* - \mu_{ijkqrs}) \right\} \\ &= \frac{1}{72} \cdot 2 \sum \left( \frac{1}{n} \sum h_{\alpha ijk} h^{\alpha\beta} G_\beta - \frac{1}{n} G_{ijk} \right) h_{qrs} [n^3 \mu_{ijkqrs}^*] + \frac{1}{72} \sum h_{ijk} h_{qrs} n^3 (\mu_{ijkqrs}^* - \mu_{ijkqrs}) \\ & \quad + O(n^{-2}) \end{aligned} \tag{C.11}$$

The left term of the foregoing equation becomes

$$\frac{1}{36n} \sum h_{\alpha ijk} h_{qrs} h^{\alpha\beta} [n^3 \mu_{ijkqrs}^*] G_\beta - \frac{1}{36n} \sum h_{qrs} [n^3 \mu_{ijkqrs}^*] G_{ijk}. \tag{C.12}$$

By using Lemma 14 (b), the right term equation is given by

$$\begin{aligned} & \frac{1}{72} \left\{ -\frac{9}{n} \sum h_{ijk} h_{qrs} h_{l\alpha\beta} h^{jk} h^{rs} h^{i\alpha} h^{\beta q} h^{lm} G_m + \frac{9}{n} \sum h_{ijk} h_{qrs} h^{jk} h^{rs} h^{i\alpha} h^{\beta q} G_{\alpha\beta} \right. \\ & \quad - \frac{18}{n} \sum h_{ijk} h_{qrs} h_{l\alpha\beta} h^{jr} h^{ks} h^{i\alpha} h^{\beta q} h^{lm} G_m + \frac{18}{n} \sum h_{ijk} h_{qrs} h^{jr} h^{ks} h^{i\alpha} h^{\beta q} G_{\alpha\beta} \\ & \quad \left. - \frac{18}{n} \sum h_{ijk} h_{qrs} h_{l\alpha\beta} h^{kq} h^{rs} h^{i\alpha} h^{\beta j} h^{lm} G_m + \frac{18}{n} \sum h_{ijk} h_{qrs} h^{kq} h^{rs} h^{i\alpha} h^{\beta j} G_{\alpha\beta} \right\} \\ &= -\frac{1}{8n} \sum h_{ijk} h_{qrs} h_{l\alpha\beta} h^{jk} h^{rs} h^{i\alpha} h^{\beta q} h^{lm} G_m + \frac{1}{8n} \sum h_{ijk} h_{qrs} h^{jk} h^{rs} h^{i\alpha} h^{\beta q} G_{\alpha\beta} \end{aligned} \tag{C.13}$$

$$-\frac{1}{4n} \sum h_{ijk} h_{qrs} h_{l\alpha\beta} h^{jr} h^{ks} h^{i\alpha} h^{\beta q} h^{lm} G_m + \frac{1}{4n} \sum h_{ijk} h_{qrs} h^{jr} h^{ks} h^{i\alpha} h^{\beta q} G_{\alpha\beta} \tag{C.14}$$

$$-\frac{1}{4n} \sum h_{ijk} h_{qrs} h_{l\alpha\beta} h^{kq} h^{rs} h^{i\alpha} h^{\beta j} h^{lm} G_m + \frac{1}{4n} \sum h_{ijk} h_{qrs} h^{kq} h^{rs} h^{i\alpha} h^{\beta j} G_{\alpha\beta}. \tag{C.15}$$

In contrast, it follows from Lemma 13 (g), and Lemma 13 (e) that

$$\begin{aligned}
& -\frac{1}{8} \left( \sum h_{ijkq}^*(\hat{\boldsymbol{\theta}}_N) h^{*ij}(\hat{\boldsymbol{\theta}}_N) h^{*kq}(\hat{\boldsymbol{\theta}}_N) - \sum h_{ijkq}(\hat{\boldsymbol{\theta}}) h^{ij}(\hat{\boldsymbol{\theta}}) h^{kq}(\hat{\boldsymbol{\theta}}) \right) \\
& = -\frac{1}{8} \sum_{ijkq} \left\{ h_{ijkq}^*(\hat{\boldsymbol{\theta}}_N) h^{*ij}(\hat{\boldsymbol{\theta}}_N) [h^{*kq}(\hat{\boldsymbol{\theta}}_N) - h^{kq}(\hat{\boldsymbol{\theta}})] \right. \\
& \quad \left. + h_{ijkq}^*(\hat{\boldsymbol{\theta}}_N) [h^{*ij}(\hat{\boldsymbol{\theta}}_N) - h^{ij}(\hat{\boldsymbol{\theta}})] h^{kq}(\hat{\boldsymbol{\theta}}) + h^{ij}(\hat{\boldsymbol{\theta}}) h^{kq}(\hat{\boldsymbol{\theta}}) [h_{ijkq}^*(\hat{\boldsymbol{\theta}}_N) - h_{ijkq}(\hat{\boldsymbol{\theta}})] \right\} \\
& = -\frac{1}{8} \left( -\frac{2}{n} \sum h_{ijkq} h^{ij} h^{k\alpha} h_{l\alpha\beta} h^{\beta q} h^{lm} G_m + \frac{2}{n} \sum h_{ijkq} h^{ij} h^{k\alpha} h^{\beta q} G_{\alpha\beta} \right. \\
& \quad \left. + \frac{1}{n} \sum h_{ijkql} h^{ij} h^{kq} h^{lm} G_m - \frac{1}{n} \sum h^{ij} h^{kq} G_{ijkq} \right) + O(n^{-2}) \\
& = \frac{1}{4n} \sum h_{ijkq} h^{ij} h^{k\alpha} h_{l\alpha\beta} h^{\beta q} h^{lm} G_m - \frac{1}{4n} \sum h_{ijkq} h^{ij} h^{k\alpha} h^{\beta q} G_{\alpha\beta} \\
& \quad - \frac{1}{8n} \sum h_{ijkql} h^{ij} h^{kq} h^{lm} G_m + \frac{1}{8n} \sum h^{ij} h^{kq} G_{ijkq} + O(n^{-2}). \tag{C.16}
\end{aligned}$$

Combining (C.12), (C.13), (C.14), (C.15), and (C.16), we have  $a_{1n}^* - a_{1n} = \kappa_n/n$ , where  $\kappa_n$  is of order 1. Next, we evaluate  $a_{2n}^* - a_{2n}$ .

Following the proof of Tierney and Kadane (1986), we have

$$a_{2n}^* - a_{2n} = -\frac{1}{2} \sum_{ijk} h_{ijk}^*(\hat{\boldsymbol{\theta}}_N) (n^2 b_i^*) h^{*jk} + \frac{1}{2} \sum_{ijk} h_{ijk}(\hat{\boldsymbol{\theta}}) (n^2 b_i) h^{jk} + O(n^{-1}). \tag{C.17}$$

Therefore,

$$E[g^+(\boldsymbol{\theta})] = \left( \frac{|D^2 h_n(\hat{\boldsymbol{\theta}})|}{|D^2 h_n^*(\hat{\boldsymbol{\theta}}_N)|} \right)^{1/2} \frac{C_n^*(\hat{\boldsymbol{\theta}}_N) \exp[-nh^*(\hat{\boldsymbol{\theta}}_N)]}{C_n(\hat{\boldsymbol{\theta}}) \exp[-nh(\hat{\boldsymbol{\theta}})]} \left( 1 + \frac{c_n}{n^2} + O(n^{-3}) \right),$$

where  $C_n^*(\hat{\boldsymbol{\theta}}_N) = \exp\{(n/2)D^1 h^*(\hat{\boldsymbol{\theta}}_N)^T [D^2 h^*(\hat{\boldsymbol{\theta}}_N)]^{-1} D^1 h^*(\hat{\boldsymbol{\theta}}_N)\}$  and

$$\begin{aligned}
c_n & = -\frac{n^2}{2} \sum h_{ijk} b_i^* h^{jk} + \frac{n^2}{2} \sum h_{ijk} b_i h^{jk} + \frac{1}{4} \sum h_{ijkq} h_{l\alpha\beta} h^{ij} h^{k\alpha} h^{\beta q} h^{lm} G_m \\
& \quad - \frac{1}{4} \sum h_{ijkq} h^{ij} h^{k\alpha} h^{\beta q} G_{\alpha\beta} - \frac{1}{8} \sum h_{ijkql} h^{ij} h^{kq} h^{lm} G_m + \frac{1}{8} \sum h^{ij} h^{kq} G_{ijkq} \\
& \quad + \frac{1}{36} \sum h_{\alpha ijk} h_{qrs} h^{\alpha\beta} [n^3 \mu_{ijkqrs}] G_\beta - \frac{1}{36} \sum h_{qrs} [n^3 \mu_{ijkqrs}] G_{ijk} \\
& \quad - \frac{1}{8} \sum_{ijkqrs\alpha\beta lm} h_{ijk} h_{qrs} h_{l\alpha\beta} h^{jk} h^{rs} h^{i\alpha} h^{\beta q} h^{lm} G_m + \frac{1}{8} \sum_{ijkqrs\alpha\beta} h_{ijk} h_{qrs} h^{jk} h^{rs} h^{i\alpha} h^{\beta q} G_{\alpha\beta} \\
& \quad - \frac{1}{4} \sum_{ijkqrs\alpha\beta lm} h_{ijk} h_{qrs} h_{l\alpha\beta} h^{jr} h^{ks} h^{i\alpha} h^{\beta q} h^{lm} G_m + \frac{1}{4} \sum_{ijkqrs\alpha\beta} h_{ijk} h_{qrs} h^{jr} h^{ks} h^{i\alpha} h^{\beta q} G_{\alpha\beta} \\
& \quad - \frac{1}{4} \sum_{ijkqrs\alpha\beta lm} h_{ijk} h_{qrs} h_{l\alpha\beta} h^{kq} h^{rs} h^{i\alpha} h^{\beta j} h^{lm} G_m + \frac{1}{4} \sum_{ijkqrs\alpha\beta} h_{ijk} h_{qrs} h^{kq} h^{rs} h^{i\alpha} h^{\beta j} G_{\alpha\beta}
\end{aligned}$$

As an alternative expression of  $-(n^2/2) \sum h_{ijk} b_i^* h^{jk}$  in  $c_n$ , from Lemma 14 (d), we have

$$\begin{aligned} b_i^*(\hat{\boldsymbol{\theta}}_N) &= -\sum_l h^{il} h_l^*(\hat{\boldsymbol{\theta}}_N) + O(n^{-3}) \\ &= -\frac{1}{2n^2} \sum_{\alpha\beta lmr} h_{l\alpha\beta} h^{il} h^{\alpha r} h^{\beta m} G_r G_m + O(n^{-3}). \end{aligned}$$

Thus

$$-\frac{n^2}{2} \sum_{ijk} h_{ijk} b_i^* h^{jk} = \frac{1}{4} \sum_{ijklmr\alpha\beta} h_{ijk} h_{l\alpha\beta} h^{il} h^{jk} h^{\alpha r} h^{\beta m} G_r G_m + O(n^{-1}) \quad (\text{C.18})$$

## Appendix D: Moments of multivariate normal distributions

A  $d \times 1$  random vector  $\mathbf{u}$  is according to  $N(\mathbf{0}, \Sigma)$ , where  $\Sigma \equiv (\mu_{ij})$ , and  $\mathbf{0}$  is a  $d \times 1$  null vector. Let  $\mu_{ijkq}$  and  $\mu_{ijkqrs}$  denote the fourth and sixth central moments of multivariate normal distribution  $N(\mathbf{0}, \Sigma)$ . Then we have the formula concerning the moments:

$$\begin{aligned} \mu_{ijkq} &= \mu_{ij}\mu_{ks} + \mu_{ik}\mu_{js} + \mu_{is}\mu_{jk}, \\ \mu_{ijkqrs} &= \mu_{ij}\mu_{kq}\mu_{rs} + \mu_{ij}\mu_{kr}\mu_{qs} + \mu_{ij}\mu_{ks}\mu_{qr} \\ &\quad + \mu_{ik}\mu_{jq}\mu_{rs} + \mu_{ik}\mu_{jr}\mu_{qs} + \mu_{ik}\mu_{js}\mu_{qr} \\ &\quad + \mu_{iq}\mu_{jk}\mu_{rs} + \mu_{iq}\mu_{jr}\mu_{ks} + \mu_{iq}\mu_{js}\mu_{kr} \\ &\quad + \mu_{ir}\mu_{jk}\mu_{qs} + \mu_{ir}\mu_{jq}\mu_{ks} + \mu_{ir}\mu_{js}\mu_{kq} \\ &\quad + \mu_{is}\mu_{jk}\mu_{qr} + \mu_{is}\mu_{jq}\mu_{kr} + \mu_{is}\mu_{jr}\mu_{kq} \end{aligned}$$

## Appendix E: Auxiliary calculation on the Laplace approximations

(iii) From Lemma 12 (d),

$$\begin{aligned} &E \left[ \frac{n^2}{72} \sum h_{ijk} h_{qrs} z_i z_j z_k z_q z_r z_s \right] \\ &= \frac{n^2}{72} \sum h_{ijk} h_{qrs} E[z_i z_j z_k z_q z_r z_s] \\ &= \frac{n^2}{72} \sum h_{ijk} h_{qrs} \left( \mu_{ijkqrs} + \sum_{[m_1, m_2]_6} b_{m_1} b_{m_2} \mu_{m_3 m_4 m_5 m_6} + \sum_{[l_1, l_2, l_3, l_4]_6} b_{l_1} b_{l_2} b_{l_3} b_{l_4} \mu_{l_5 l_6} + b_i b_j b_k b_q b_r b_s \right) \\ &= \frac{n^2}{72} \sum_{ijkqrs} h_{ijk} h_{qrs} \mu_{ijkqrs} + \frac{n^2}{72} \sum_{ijkqrs} h_{ijk} h_{qrs} \left( \sum_{[m_1, m_2]_6} b_{m_1} b_{m_2} \mu_{m_3 m_4 m_5 m_6} \right) + O(n^{-3}) \quad (\text{E.1}) \end{aligned}$$

Because

$$\begin{aligned} \sum_{[m_1, m_2]_6} b_{m_1} b_{m_2} \mu_{m_3 m_4 m_5 m_6} &= \underline{b_i b_j \mu_{kqrs}} + \underline{b_i b_k \mu_{jqrs}} + b_i b_q \mu_{jkrs} + b_i b_r \mu_{jkqs} + b_i b_s \mu_{jkqr} \\ &\quad + \underline{b_j b_k \mu_{iqrs}} + b_j b_q \mu_{ikrs} + b_j b_r \mu_{ikqs} + b_j b_s \mu_{ikqr} + b_k b_q \mu_{ijrs} \\ &\quad + b_k b_r \mu_{ijqs} + b_k b_s \mu_{ijqr} + \underline{b_q b_r \mu_{ijks}} + \underline{b_q b_s \mu_{ijkr}} + \underline{b_r b_s \mu_{ijkq}}, \end{aligned}$$

$\frac{n^2}{72} \sum h_{ijk} h_{qrs} \left( \sum_{[m_1, m_2]} b_{m_1} b_{m_2} \mu_{m_3 m_4 m_5 m_6} \right)$  is divided into two kinds of terms. Hence, the second term in (E.1) is

$$\begin{aligned} &\frac{n^2}{72} \sum h_{ijk} h_{qrs} \left( \sum_{[m_1, m_2]} b_{m_1} b_{m_2} \mu_{m_3 m_4 m_5 m_6} \right) \\ &= \frac{n^2}{72} \cdot 6 \sum h_{ijk} h_{qrs} b_i b_j \mu_{kqrs} + \frac{n^2}{72} \cdot 9 \sum h_{ijk} h_{qrs} b_i b_q \mu_{jkrs}. \end{aligned}$$

Consequently, we have

$$\begin{aligned} &E \left[ \frac{n^2}{72} \sum h_{ijk} h_{qrs} z_i z_j z_k z_q z_r z_s \right] \\ &= \frac{n^2}{72} \sum h_{ijk} h_{qrs} \mu_{ijkqrs} + \frac{n^2}{12} \sum h_{ijk} h_{qrs} b_i b_j \mu_{kqrs} + \frac{n^2}{8} \sum h_{ijk} h_{qrs} b_i b_q \mu_{jkrs}. \end{aligned}$$

(iv) From Lemma 12 (c),

$$\begin{aligned} E \left[ -\frac{n}{120} \sum h_{ijkqr} z_i z_j z_k z_q z_r \right] &= -\frac{n}{120} \sum h_{ijkqr} E[z_i z_j z_k z_q z_r] \\ &= -\frac{n}{120} \sum_{ijkqr} h_{ijkqr} \left( \sum_{[m_1]_5} b_{m_1} \mu_{m_2 m_3 m_4 m_5} \right) + O(n^{-3}) \\ &= -\frac{n}{120} \cdot 5 \sum_{ijkqr} h_{ijkqr} b_i \mu_{jkqr} + O(n^{-3}) \\ &= -\frac{n}{24} \sum_{ijkqr} h_{ijkqr} b_i \mu_{jkqr} + O(n^{-3}). \end{aligned}$$

(v) From Lemma 12 (d)

$$\begin{aligned} E \left[ -\frac{n}{720} \sum h_{ijkqrs} z_i z_j z_k z_q z_r z_s \right] &= -\frac{n}{720} \sum h_{ijkqrs} E[z_i z_j z_k z_q z_r z_s] \\ &= -\frac{n}{720} \sum h_{ijkqrs} \mu_{ijkqrs} + O(n^{-3}). \end{aligned}$$

(vi) From Lemma 12 (e),

$$\begin{aligned} &E \left[ \frac{n^2}{144} \sum h_{ijk} h_{qrst} z_i z_j z_k z_q z_r z_s z_t \right] \\ &= \frac{n^2}{144} \sum h_{ijk} h_{qrst} E[z_i z_j z_k z_q z_r z_s z_t] \\ &= \frac{n^2}{144} \sum h_{ijk} h_{qrst} \left( \sum_{[m_1]_7} b_{m_1} \mu_{m_2 m_3 m_4 m_5 m_6 m_7} \right) + O(n^{-3}) \\ &= \frac{n^2}{144} \cdot 3 \sum h_{ijk} h_{qrst} b_i \mu_{jkqrst} + \frac{n^2}{144} \cdot 4 \sum h_{ijk} h_{qrst} b_q \mu_{ijkqrst} + O(n^{-3}) \\ &= \frac{n^2}{48} \sum h_{ijk} h_{qrst} b_i \mu_{jkqrst} + \frac{n^2}{36} \sum h_{ijk} h_{qrst} b_q \mu_{ijkqrst} + O(n^{-3}). \end{aligned}$$



(vii) From Lemma 12 (f),

$$\begin{aligned} E \left[ \frac{n^2}{1152} \sum h_{ijkq} h_{rstu} z_i z_j z_k z_q z_r z_s z_t z_u \right] &= \frac{n^2}{1152} \sum h_{ijkq} h_{rstu} E[z_i z_j z_k z_q z_r z_s z_t z_u] \\ &= \frac{n^2}{1152} \sum h_{ijkq} h_{rstu} \mu_{ijkqrstu} + O(n^{-3}). \end{aligned}$$

(viii) From Lemma 12 (f),

$$E \left[ \frac{n^2}{720} \sum h_{ijk} h_{qrst} z_i z_j z_k z_q z_r z_s z_t z_u \right] = \frac{n^2}{720} \sum h_{ijk} h_{qrst} \mu_{ijkqrstu} + O(n^{-3}).$$

(ix) From Lemma 12 (g),

$$\begin{aligned} &E \left[ -\frac{n^3}{1296} \sum h_{ijk} h_{qrs} h_{tuv} z_i z_j z_k z_q z_r z_s z_t z_u z_v \right] \\ &= -\frac{n^3}{1296} \sum h_{ijk} h_{qrs} h_{tuv} \left( \sum_{[m_1]_9} b_{m_1} \mu_{m_2 m_3 m_4 m_5 m_6 m_7 m_8 m_9} \right) + O(n^{-3}) \\ &= -\frac{n^3}{1296} \cdot 9 \sum h_{ijk} h_{qrs} h_{tuv} b_i \mu_{jkqrstuv} + O(n^{-3}) \\ &= -\frac{n^3}{144} \sum h_{ijk} h_{qrs} h_{tuv} b_i \mu_{jkqrstuv} + O(n^{-3}). \end{aligned}$$

(x) From Lemma 12 (h),

$$E \left[ -\frac{n^3}{1728} \sum h_{ijk} h_{qrs} h_{tuv} z_i z_j z_k z_q z_r z_s z_t z_u z_v z_w \right] = -\frac{n^3}{1728} \sum h_{ijk} h_{qrs} h_{tuv} \mu_{ijkqrstuvw} + O(n^{-3})$$

(xi) From Lemma 12 (i),

$$\begin{aligned} &E \left[ \frac{n^4}{31104} \sum h_{ijk} h_{qrs} h_{tuv} h_{wxy} z_i z_j z_k z_q z_r z_s z_t z_u z_v z_w z_x z_y \right] \\ &= \frac{n^4}{31104} \sum h_{ijk} h_{qrs} h_{tuv} h_{wxy} \mu_{ijkqrstuvwxy} + O(n^{-3}). \end{aligned}$$

The inequality in Theorem 5.

$$\frac{1 + \frac{a_{1n}^*}{n} + \frac{a_{2n}^*}{n^2} + \frac{a_{3n}^*}{n^3}}{1 + \frac{a_{1n}}{n} + \frac{a_{2n}}{n^2} + \frac{a_{3n}}{n^3}} = 1 + \frac{a_{1n}^* - a_{1n}}{n} + \frac{a_{2n}^* - a_{2n} - a_{1n}(a_{1n}^* - a_{1n})}{n^2} + O(n^{-3}),$$

where  $O(n^{-3})$  is given by

$$\begin{aligned} &\left[ \frac{a_{3n}^*}{n^3} - \frac{a_{3n}}{n^3} - \left( \frac{a_{1n}}{n} + \frac{a_{2n}}{n^2} + \frac{a_{3n}}{n^3} \right) \left( \frac{a_{2n}^* - a_{2n} - a_{1n}(a_{1n}^* - a_{1n})}{n^2} \right) - \left( \frac{a_{2n}}{n^2} + \frac{a_{3n}}{n^3} \right) \left( \frac{a_{1n}^* - a_{1n}}{n} \right) \right] \\ &\times \frac{1}{1 + \frac{a_{1n}}{n} + \frac{a_{2n}}{n^2} + \frac{a_{3n}}{n^3}} \end{aligned}$$

PROOF.

$$\begin{aligned}
& \frac{1 + \frac{a_{1n}^*}{n} + \frac{a_{2n}^*}{n^2} + \frac{a_{3n}^*}{n^3}}{1 + \frac{a_{1n}}{n} + \frac{a_{2n}}{n^2} + \frac{a_{3n}}{n^3}} - \left( 1 + \frac{a_{1n}^* - a_{1n}}{n} + \frac{a_{2n}^* - a_{2n} - a_{1n}(a_{1n}^* - a_{1n})}{n^2} \right) \\
&= \left[ 1 + \frac{a_{1n}^*}{n} + \frac{a_{2n}^*}{n^2} + \frac{a_{3n}^*}{n^3} - \left( 1 + \frac{a_{1n}^* - a_{1n}}{n} + \frac{a_{2n}^* - a_{2n} - a_{1n}(a_{1n}^* - a_{1n})}{n^2} \right) \left( 1 + \frac{a_{1n}}{n} + \frac{a_{2n}}{n^2} + \frac{a_{3n}}{n^3} \right) \right] \\
&\times \frac{1}{1 + \frac{a_{1n}}{n} + \frac{a_{2n}}{n^2} + \frac{a_{3n}}{n^3}}
\end{aligned}$$

Therefore this inequality is proved.

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