

## Supplementary material for On asymptotic validity of naive inference with an approximate likelihood

BY H. E. OGDEN

*Mathematical Sciences, University of Southampton, Southampton SO17 1BJ, U.K.*

h.e.ogden@soton.ac.uk

5

### 1. FINDING $\delta_i(\theta)$ IN EXAMPLE 3.1

Recall  $Y_i$  is the number of successes out of  $m = m_n$  trials on item  $i$ . We study how  $\delta_i(\theta) = \|(d/d\theta)\epsilon_i(\theta)\|$  varies with  $m$ .

Write  $f(b; y_i) = -y_i \log \{\text{logit}^{-1}(b)\} + (m - y_i) \log \{1 - \text{logit}^{-1}(b)\}$  and  $g(b; \theta, y_i) = f(b; y_i) - \log \phi(b; 0, \theta)$ , so that

10

$$L_i(\theta) = \int_{-\infty}^{\infty} \exp\{-g(b; \theta, y_i)\} db.$$

In the following, we drop the data  $y_i$  from the notation for convenience. Write  $\hat{b}(\theta)$  for the maximizer of  $g(\cdot, \theta)$ , and

$$\hat{g}_r(\theta) = \frac{\partial^r g}{\partial b^k}(\hat{b}(\theta); \theta).$$

By equation (4) of Shun & McCullagh (1995), the error in the Laplace approximation to the log-likelihood  $\ell_i(\theta)$  is

15

$$\epsilon_i(\theta) = \sum_{l=1}^{\infty} \frac{1}{2l!} \sum_{P \in \mathcal{P}_{2l}} n_2(P) (-1)^v \hat{g}_{|p_1|}(\theta) \dots \hat{g}_{|p_v|}(\theta) \{\hat{g}_2(\theta)\}^{-l}, \quad (1)$$

where  $P = p_1 | \dots | p_v$  is a partition of  $2l$  indices into  $v$  blocks of size 3 or more, and  $n_2(P)$  is the number of partitions  $Q$  of  $2l$  indices into  $l$  blocks of size 2, such that  $Q$  is complementary to  $P$ .

Write  $h_P(\theta) = \hat{g}_{|p_1|}(\theta) \dots \hat{g}_{|p_v|}(\theta) \{\hat{g}_2(\theta)\}^{-l}$ . Then  $h_P(\theta) = O_p(m^{v-l})$ , since  $\hat{g}_r(\theta) = O_p(m)$  for each  $r$ .

20

Differentiating (1) gives

$$\frac{d}{d\theta} \epsilon_i(\theta) = \sum_{l=1}^{\infty} \frac{1}{2l!} \sum_{P \in \mathcal{P}_{2l}} n_2(P) (-1)^v \frac{d}{d\theta} h_P(\theta), \quad (2)$$

and

$$\frac{d}{d\theta} h_P(\theta) = \sum_{i=1}^v \left[ \hat{g}'_{|p_i|}(\theta) \prod_{j \neq i} \hat{g}_{|p_j|}(\theta) \{\hat{g}_2(\theta)\}^{-l} - \prod_{j=1}^v l \hat{g}_{|p_j|}(\theta) \hat{g}'_2(\theta) \{\hat{g}_2(\theta)\}^{-(l+1)} \right], \quad (3)$$

where  $\hat{g}'_r(\theta) = (d/d\theta)\hat{g}_r(\theta)$ .

For each  $r$ , we have

$$\begin{aligned} \hat{g}'_r(\theta) &= \frac{d}{d\theta} \left\{ g^{(r)}(\hat{b}(\theta); \theta) \right\} \\ &= \frac{\partial g^{(r)}}{\partial \theta} \{\hat{b}(\theta); \theta\} + \frac{d\hat{b}(\theta)}{d\theta} \hat{g}_{r+1}(\theta). \end{aligned} \quad (4)$$

We now study the size of each of the terms in (4). We have

$$\frac{\partial g^{(r)}}{\partial \theta}(b; \theta) = \frac{\partial}{\partial \theta} \left\{ -\frac{\partial^r}{\partial b^r} \log \phi(b; 0, \theta) \right\} = O_p(1), \quad (5)$$

and

$$\hat{g}_{r+1}(\theta) = O_p(m). \quad (6)$$

For each  $\theta$ ,  $\hat{b}(\theta)$  satisfies  $g_1\{\hat{b}(\theta); \theta\} = 0$ . Differentiating this with respect to  $\theta$ ,

$$\frac{d\hat{b}(\theta)}{d\theta} g_2\{\hat{b}(\theta); \theta\} + \frac{\partial g_1}{\partial \theta}\{\hat{b}(\theta); \theta\} = 0.$$

But

$$\frac{\partial g_1}{\partial \theta}(b; \theta) = -2b\theta^{-3},$$

so

$$\frac{d\hat{b}(\theta)}{d\theta} = 2\hat{b}(\theta)\theta^{-3} \{\hat{g}_2(\theta)\}^{-1} = O_p(m^{-1}). \quad (7)$$

Substituting (5), (6) and (7) into (4) gives that  $\hat{g}'_r(\theta) = O_p(1)$  for each  $r$ . From (3) we then have

$$\frac{d}{d\theta} h_P(\theta) = O_p(m^{v-l-1}).$$

The highest order terms in (2) come from partitions with  $(l, v) = (2, 1)$  or  $(3, 2)$ , and so  $\delta_i(\theta) = O_p(m^{-2})$ .

## 2. FINDING $\delta_m^{(k)}(\beta)$ IN EXAMPLE 3.2

Kaufman (1949) provides an exact expression for the normalizing constant for an Ising model on an  $n \times m$  lattice, with  $\alpha = 0$  and periodic boundary, as

$$Z_{n \times m}(0, \beta) = \{2 \sinh(2\beta)\}^{nm/2} \bar{A}_{n,m}(\beta)/2,$$

where

$$\bar{A}_{n,m}(\beta) = A_{n,m}^{(1)}(\beta) + A_{n,m}^{(2)}(\beta) + A_{n,m}^{(3)}(\beta) + A_{n,m}^{(4)}(\beta),$$

and

$$\begin{aligned} A_{n,m}^{(1)}(\beta) &= \prod_{q=0}^{n-1} 2 \cosh \{m a_{2q+1,n}(\beta)/2\}, & A_{n,m}^{(2)}(\beta) &= \prod_{q=0}^{n-1} 2 \sinh \{m a_{2q+1,n}(\beta)/2\}, \\ A_{n,m}^{(3)}(\beta) &= \prod_{q=0}^{n-1} 2 \cosh \{m a_{2q,n}(\beta)/2\}, & A_{n,m}^{(4)}(\beta) &= \prod_{q=0}^{n-1} 2 \sinh \{m a_{2q,n}(\beta)/2\} \end{aligned}$$

where

$$a_{l,n}(\beta) = \cosh^{-1} \left\{ \cosh(2\beta)^2 / \sinh(2\beta) - \cos(\pi l/n) \right\}$$

for  $l \geq 1$ , and  $a_{0,n}(\beta) = a_0(\beta) = 2\beta + \log \{ \tanh(\beta) \}$ .

Using the approximation  $Z_{m \times m}^{(k)}(\beta)$  to  $Z_{m \times m}(\beta)$ , the error in the log-likelihood is

45

$$\epsilon_m^{(k)}(\beta) = (m - k + 1) \log \bar{A}_{k,m}(\beta) - (m - k) \log \bar{A}_{k-1,m}(\beta) - \log \bar{A}_{m,m}(\beta).$$

Differentiating this with respect to  $\beta$ ,

$$\frac{d}{d\beta} \epsilon_m^{(k)}(\beta) = (m - k + 1) \frac{d}{d\beta} \{ \log \bar{A}_{k,m}(\beta) \} - (m - k) \frac{d}{d\beta} \{ \log \bar{A}_{k-1,m}(\beta) \} - \frac{d}{d\beta} \{ \log \bar{A}_{m,m}(\beta) \}, \quad (8)$$

and

$$\frac{d}{d\beta} \{ \log \bar{A}_{n,m}(\beta) \} = \sum_{i=1}^4 \frac{d}{d\beta} \{ \log A_{n,m}^{(i)}(\beta) \} r_{n,m}^{(i)}(\beta),$$

where  $r_{n,m}^{(i)}(\beta) = A_{n,m}^{(i)}(\beta) / \bar{A}_{n,m}(\beta)$ . We have

$$\begin{aligned} \frac{d}{d\beta} \{ \log A_{n,m}^{(1)}(\beta) \} &= m/2 \sum_{q=0}^n a'_{2q+1,n}(\beta) \tanh \{ m a_{2q+1,n}(\beta) / 2 \} \\ &= m/2 \sum_{q=0}^n a'_{2q+1,n}(\beta) + O[m \exp\{-a_0(\beta)m\}] \end{aligned}$$

50

as  $m \rightarrow \infty$ , since  $\tanh(x) = 1 + O\{\exp(-2x)\}$  as  $x \rightarrow \infty$ , and  $a_{2q+1,n}(\beta) \geq a_0(\beta) > 0$ .

Similar expressions may be obtained for the derivatives of the other  $\{ \log A_{n,m}^{(i)}(\beta) \}$  terms, and combining these gives

$$\frac{d}{d\beta} \{ \log \bar{A}_{n,m}(\beta) \} = m S_n^{(o)}(\beta) r_{n,m}^{(o)}(\beta) + m S_n^{(e)}(\beta) r_{n,m}^{(e)}(\beta) + O[m \exp\{-a_0(\beta)m\}]$$

where  $S_n^{(o)} = \sum_{q=0}^n a'_{2q+1,n}(\beta)$ ,  $S_n^{(e)} = \sum_{q=0}^n a'_{2q,n}(\beta)$ ,  $r_{n,m}^{(o)}(\beta) = r_{n,m}^{(1)}(\beta) + r_{n,m}^{(2)}(\beta)$  and  $r_{n,m}^{(e)}(\beta) = r_{n,m}^{(3)}(\beta) + r_{n,m}^{(4)}(\beta)$ . Define

55

$$f(x; \beta) = d_\beta \{ -1 + c_\beta - \cos(x) \}^{-1/2} \{ 1 + c_\beta - \cos(x) \}^{-1/2}$$

where  $d_\beta = 4 \cosh(2\beta) - 2 \cosh(2\beta) \coth(2\beta)^2$  and  $c_\beta = \cosh(2\beta)^2 / \sinh(2\beta)$ . Then  $a'_{j,n}(\beta) = f(j\pi/n; \beta)$ , and  $n^{-1} S_n^{(o)}(\beta)$  and  $n^{-1} S_n^{(e)}(\beta)$  are both trapezium rule approximations to  $I(\beta) = \frac{1}{2\pi} \int_0^{2\pi} f(x; \beta) dx$ . Write  $R_n^{(o)}(\beta) = n^{-1} S_n^{(o)}(\beta) - I(\beta)$  and  $R_n^{(e)}(\beta) = n^{-1} S_n^{(e)}(\beta) - I(\beta)$  for the error in each of these approximations to the integral.

60

**LEMMA 1.** For each  $\beta < \beta_c$ ,  $R_n(\beta) = \max\{|R_n^{(e)}(\beta)|, |R_n^{(o)}(\beta)|\} = O\{\exp(-b_\beta n)\}$ , where  $b_\beta = 2 \cosh^{-1}\{-1 + \cosh(2\beta)^2 / \sinh(2\beta)\}$ .

*Proof.* We apply the results of Trefethen & Weideman (2014) to show exponentially fast convergence of these trapezium rule approximations to  $I(\beta)$ . These results depend on properties of the integrand  $f(z, \beta)$ , considered as a function of complex-valued  $z$ . There are a branch points of  $f(z, \beta)$  at a distance  $a_\beta = \cosh^{-1}\{-1 + \cosh(2\beta)^2 / \sinh(2\beta)\}$  from the real axis, and the

65

function is analytic for  $-a_\beta < \text{Im } z < a_\beta$ , so by Theorem 3.2 of Trefethen & Weideman (2014),  $|R_n^{(o)}(\beta)| = O\{\exp(-2a_\beta n)\} = O\{\exp(-b_\beta n)\}$ .

The same argument holds with  $R_n^{(e)}(\beta)$  in place of  $R_n^{(o)}(\beta)$ , so  $R_n(\beta) = O\{\exp(-b_\beta n)\}$ , as required.  $\square$

We now prove the main result.

LEMMA 2. *If  $k \rightarrow \infty$  as  $m \rightarrow \infty$ ,  $\delta_m^{(k)}(\beta) = O\{m^2 k \exp(-b_\beta k)\} + o(1)$ .*

*Proof.* We have

$$\frac{d}{d\beta} \{\log \bar{A}_{n,m}(\beta)\} = mnI(\beta) + mnt_{n,m}(\beta) + O[m \exp\{-a_0(\beta)m\}]$$

where  $t_{n,m}(\beta) = R_n^{(o)}(\beta)r_{n,m}^{(o)}(\beta) + R_n^{(e)}(\beta)r_{n,m}^{(e)}(\beta)$ .

Substituting this into (8), the contributions from the  $mnI(\beta)$  terms cancel, and the combined remainder terms are always  $o(1)$ , since  $m^2 \exp\{-a_0(\beta)m\} = o(1)$ . We are left with

$$\frac{d}{d\beta} \epsilon_m^{(k)}(\beta) = (m - k + 1)mt_{k,m}(\beta) - (m - k)mt_{k-1,m}(\beta) - mt_{m,m}(\beta) + o(1).$$

Then

$$\begin{aligned} \delta_m^{(k)}(\beta) &= \left| \frac{d}{d\beta} \epsilon_m^{(k)}(\beta) \right| \\ &\leq (m - k + 1)mk|t_{k,m}(\beta)| + (m - k)m(k - 1)|t_{k-1,m}(\beta)| + m^2|t_{m,m}(\beta)| + o(1) \\ &\leq (m - k + 1)mkR_k(\beta) + (m - k)m(k - 1)R_{k-1}(\beta) + m^2R_m(\beta) + o(1) \end{aligned}$$

since  $|t_{n,m}(\beta)| \leq |R_n^{(o)}(\beta)|r_{n,m}^{(o)}(\beta) + |R_n^{(e)}(\beta)|r_{n,m}^{(e)}(\beta) \leq R_n(\beta)$

$$= O\{m^2 k \exp(-b_\beta k)\} + o(1)$$

by Lemma 1, as required.  $\square$

## REFERENCES

- KAUFMAN, B. (1949). Crystal statistics. II. Partition function evaluated by spinor analysis. *Physical Review* **76**, 1232.
- SHUN, Z. & MCCULLAGH, P. (1995). Laplace approximation of high dimensional integrals. *Journal of the Royal Statistical Society. Series B (Methodological)* **57**, 749–760.
- TREFETHEN, L. N. & WEIDEMAN, J. (2014). The exponentially convergent trapezoidal rule. *SIAM Review* **56**, 385–458.

[Received April 2012. Revised September 2012]