

THE ASYMPTOTIC BEHAVIOUR OF BAYES ESTIMATORS FOR DICHOTOMOUS QUANTAL RESPONSE MODELS*

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SUMMARY. The asymptotic behaviour of Bayes estimators is extended from the iid case to dichotomous quantal response data. The Bayes estimator is shown to be asymptotically equivalent to the maximum likelihood estimator for dichotomous quantal response data under assumptions that are similar to those for the iid case.

1. Introduction

Dichotomous quantal response models have many applications (toxicity studies, econometrics). Frequently, maximum likelihood is used to estimate parameters and the asymptotic properties of maximum likelihood are used for inference. Krewski and Van Ryzin (1981) established the asymptotic normality of the maximum likelihood estimator for dichotomous quantal response models. The asymptotic properties of other estimation procedures such as minimum chi-square and least squares can be found in Neyman (1949) and Schumacher (1980), respectively. Relatively little work has been done with regard to Bayes estimation in this setting (Zellner and Rossi (1984), Stewart (1979)). Bickel and Yahav (1969), and Chao (1970), established the asymptotic equivalence of the Bayes estimator and the maximum likelihood estimator in the case of iid random variables with absolutely continuous probability functions. See also Ibragimov and Has'minskii (1981). In this paper, we establish the asymptotic properties of Bayes estimators in the setting of dichotomous quantal response models.

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2. Setting of the Problem

A sequence of binomial response datasets comprises the setting for the asymptotic results of these models. More specifically, each dataset is indexed by $t = \{1, 2, \dots\}$ and consists of a fixed set of m experimental conditions with N_{it} subjects assigned to the i th condition. We do not consider the case where the number of experimental conditions grow with the sample size (i.e. $m \rightarrow \infty$). Each subject is represented by the Bernoulli distributed random variable $Y_{ijt}, i = 1, 2, \dots, m; j = 1, 2, \dots, N_{it}$ which is equal to 1 if the subject responds and is zero otherwise. The Y_{ijt} 's are independent but not identically distributed.

Let

$$\text{Prob}(Y_{ijt} = 1) = 1 - \text{Prob}(Y_{ijt} = 0) = F(\mathbf{x}'_i \boldsymbol{\theta})$$

be the probability of response for subject j at experimental condition i . This probability is a function of a $p \times 1$ vector ($p \leq m$) of unknown parameters $\boldsymbol{\theta}$ that lie in the parameter space Θ and a vector $\mathbf{x}_i = (x_{i1}, x_{i2}, \dots, x_{ip})'$ of fixed measurements of p variables. Let $X = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m)'$ be the $m \times p$ matrix of measurements of the p variables at each of the m experimental conditions. Let

$$z(y_{ijt}, \boldsymbol{\theta}) = F(\mathbf{x}'_i \boldsymbol{\theta})^{y_{ijt}} [1 - F(\mathbf{x}'_i \boldsymbol{\theta})]^{1 - y_{ijt}}$$

and $\Phi(y, \boldsymbol{\theta}) = \ln z(y, \boldsymbol{\theta})$.

In the most general case, we would be interested in estimating some function of the parameters, say $\mathbf{g}(\boldsymbol{\theta}) = (g_1(\boldsymbol{\theta}), g_2(\boldsymbol{\theta}), \dots, g_h(\boldsymbol{\theta}))'$. For simplicity, we shall present results for the estimation of $\mathbf{g}(\boldsymbol{\theta}) = \boldsymbol{\theta}$.

We make the following assumptions:

(A1) F is a continuous distribution function with continuous first and second derivatives $f(u) = F'(u) > 0$, and $f''(u) = F''(u)$.

(A2) The rank of X is equal to p .

(A3) The parameter space Θ is an open subset of \mathbb{R}^p (usually a Cartesian product of subintervals of \mathbb{R}). The true value of $\boldsymbol{\theta}$ will be denoted by $\boldsymbol{\theta}_0$.

(A4) $\lim_{t \rightarrow \infty} (N_{it}/N_{.t}) = c_i, 0 < c_i < 1, i = 1, 2, \dots, m$. where $N_{.t} = \sum_{i=1}^m N_{it} \rightarrow \infty$ as $t \rightarrow \infty$.

(A5) The loss function is given by

$$L(\boldsymbol{\theta}, \boldsymbol{\delta}) = B(\boldsymbol{\theta}) \ell(\|\boldsymbol{\theta} - \boldsymbol{\delta}\|^2), \boldsymbol{\delta} \in \mathbb{R}^p.$$

$\ell(\cdot)$ is a function from $(0, \infty)$ to $(0, \infty)$ such that

(a) ℓ has a derivative ℓ' on $(0, \infty)$.

(b) there exist $0 < \gamma, \delta < \infty$ and $s > 1$ such that $\ell(u) = \gamma u^s / s$ for all $u, 0 < u < \delta$.

- (c) $\limsup_{u \rightarrow \infty} \ell'(u)u^r < \infty$ for some $r, 0 < r < \infty$.
- (d) $\ell(u)$ is bounded away from 0 for u outside some neighborhood of 0.
- (e) $B(\boldsymbol{\theta})$ is continuous in $\boldsymbol{\theta}$ and $B(\boldsymbol{\theta}) > 0$ for $\boldsymbol{\theta} \in \Theta$.

(A6) The prior measure Λ has continuous density $\lambda(\boldsymbol{\theta})$ which is positive for all $\boldsymbol{\theta}$ with

- (a) $\int_{\Theta} \|\boldsymbol{\theta}\|^k \lambda(\boldsymbol{\theta}) d\boldsymbol{\theta} < \infty$
 - (b) $\int_{\Theta} B(\boldsymbol{\theta})(1 + \|\boldsymbol{\theta}\|^k) \lambda(\boldsymbol{\theta}) d\boldsymbol{\theta} < \infty$
- for some $k < \max\{2s, 2r + 2\}$.

3. Preliminary Results

Based on assumptions (A1) through (A6), the following results can be established (for the sake of brevity, the proofs have been omitted. Details may be found in Messig (1990)). These results provide the basis upon which the more general setup in Chao (1970) can be established in the quantal response case.

RESULT 1. The response model, $F(\mathbf{x}'\boldsymbol{\theta})$ is identifiable.

RESULT 2. For all $\mathbf{x}_k, k = 1, 2, \dots, m$, and $i, j = 1, 2, \dots, p$; $\frac{\partial F(\mathbf{x}'_k \boldsymbol{\theta})}{\partial \theta_i}$ and $\frac{\partial^2 F(\mathbf{x}'_k \boldsymbol{\theta})}{\partial \theta_i \partial \theta_j}$ exist and are continuous for all $\boldsymbol{\theta} \in \Theta$.

RESULT 3. For some $\epsilon(\boldsymbol{\theta})$ and all $i, j = 1, 2, \dots, p$; and all $\boldsymbol{\theta} \in \Theta$,

$$E_{\boldsymbol{\theta}} \left\{ \sup \left(\left| \frac{\partial^2 \Phi(Y, \mathbf{s})}{\partial s_i \partial s_j} \right| : \|\mathbf{s} - \boldsymbol{\theta}\| < \epsilon(\boldsymbol{\theta}), \mathbf{s} \in \Theta \right) \right\} < \infty.$$

RESULT 4. The information matrix

$$-A_{\boldsymbol{\theta}} = X' D_m \left[\frac{c_i [f(\mathbf{x}'_i \boldsymbol{\theta})]^2}{F(\mathbf{x}'_i \boldsymbol{\theta}) [1 - F(\mathbf{x}'_i \boldsymbol{\theta})]} \right] X \quad \dots (1)$$

is positive definite. Where $D_m[a_i]$ is an $m \times m$ matrix with diagonal elements a_i ,

RESULT 5. For any $\delta > 0$, there exists $\epsilon > 0$ such that

$$\text{Prob}_{\boldsymbol{\theta}_0} \left\{ \sup \left(\frac{1}{N_{.t}} [\mathcal{L}_t(\boldsymbol{\theta}) - \mathcal{L}_t(\boldsymbol{\theta}_0)] : \|\boldsymbol{\theta} - \boldsymbol{\theta}_0\| \geq \delta, \boldsymbol{\theta} \in \Theta \right) \leq -\epsilon \right\} \rightarrow 1$$

as $t \rightarrow \infty$. Where $\mathcal{L}_t(\boldsymbol{\theta}) = \sum_{i=1}^m \sum_{j=1}^{N_{it}} \Phi(Y_{ijt}, \boldsymbol{\theta})$.

RESULT 6. Denote the maximum likelihood estimator of $\boldsymbol{\theta}$ as $\hat{\boldsymbol{\theta}}_t^M$, then $\hat{\boldsymbol{\theta}}_t^M \rightarrow \boldsymbol{\theta}_0$ as $t \rightarrow \infty$.

4. The Main Result

The following assertion will be proved. For dichotomous quantal response models, if assumptions (A1) and (A6) are satisfied, the Bayes estimator $\hat{\theta}_t^B$ and the maximum likelihood estimator $\hat{\theta}_t^M$ of θ are asymptotically equivalent. That is,

$$N_t^{\frac{1}{2}}(\hat{\theta}_t^B - \hat{\theta}_t^M) \rightarrow 0 \text{ as } t \rightarrow \infty.$$

Denote the posterior distribution of θ by $\lambda(\theta; t)$; then

$$\lambda(\theta; t) = \lambda(\theta) \prod_{i=1}^m \prod_{j=1}^{N_{it}} z(Y_{ijt}, \theta) \left\{ \int_{\Theta} \lambda(s) \prod_{i=1}^m \prod_{j=1}^{N_{it}} z(Y_{ijt}, s) ds \right\}^{-1}.$$

Let $R_t = \min \left\{ \int_{\Theta} B(\theta) \ell(\|\theta - \delta\|^2) \lambda(\theta; t) d\theta : \delta \in \mathbb{R}^R \right\}.$

Suppose that for each t , a minimum is achieved at $\delta = \hat{\theta}_t^B$. Then $\hat{\theta}_t^B$ is the Bayes estimator of θ .

The following theorem will be used to prove the main result. The proof has been omitted.

THEOREM 1. For $\beta = 0, 1; \alpha = 0, 1, 2, \dots, 2s$; such that $\alpha + \beta \leq 2s$,

$$\int B(N_t^{-\frac{1}{2}} \mathbf{u} + \hat{\theta}_t^M) \|\mathbf{u} - \mathbf{a}_t\|^\alpha (u_i - a_{ti})^\beta \lambda^*(\mathbf{u}; t) du$$

$$\xrightarrow{t \rightarrow \infty} B(\theta_0) E \left\{ \|\mathbf{Z} - \mathbf{a}\|^\alpha (Z_i - a_i)^\beta \right\}$$

where $\lambda^*(\mathbf{u}; t)$ is the posterior density of $\mathbf{u} = N_t^{-\frac{1}{2}}(\theta - \hat{\theta}_t^M)$, $\mathbf{Z} \sim N_p(\mathbf{0}_p, -A_{\theta_0}^{-1})$ and \mathbf{a}_t is any $p \times 1$ vector of constants satisfying $\mathbf{a}_t \xrightarrow{t \rightarrow \infty} \mathbf{a}$ and $N_t^{-\frac{1}{2}} \mathbf{a}_t \xrightarrow{t \rightarrow \infty} \mathbf{0}$.

The following lemma is also used to prove the main result. The proof can be found in the appendix.

LEMMA 1. $\hat{\theta}_t^B - \hat{\theta}_t^M \rightarrow \mathbf{0}$ as $t \rightarrow \infty$.

Now the statement of the main result. The proof can be found in the appendix.

THEOREM 2. $N_t^{\frac{1}{2}}(\hat{\theta}_t^B - \hat{\theta}_t^M) \rightarrow \mathbf{0}$ as $t \rightarrow \infty$.

In dose response modeling, one is frequently interested in estimating the response probability at a given dose or the converse problem of estimating the dose that produces a given response probability. The latter problem produces

estimates of the ED50 which is the dose at which the response probability is equal to $\frac{1}{2}$. These estimates are also used to determine “safe” levels of toxic substances. In these models, the set of measurements at experimental condition i can be expressed as $\mathbf{x}_i = \mathbf{x}(d_i) = (x_1(d_i), x_2(d_i), \dots, x_p(d_i))'$, where $d_i > 0$ is the dose given to N_{it} subjects. We will illustrate these problems by example.

EXAMPLE 1. Consider the one-hit model defined by

$$F(\mathbf{x}'_i \boldsymbol{\theta}) = 1 - \exp(-\theta d_i), \quad \theta > 0.$$

In this case, $p = 1$, $\mathbf{x}_i = (d_i)$ and $\boldsymbol{\theta} = (\theta)$.

Suppose we wish to estimate the probability of response at dose d^* . This is given by

$$g(\theta) = F(\theta d^*) = 1 - \exp(-\theta d^*).$$

Without too much difficulty, the results shown here can be extended to the problem of estimating $\mathbf{g}(\boldsymbol{\theta})$, for “suitable” $\mathbf{g}(\cdot)$. Therefore, the Bayes estimator \hat{p}_t^B of $g(\theta) = F(\theta d^*)$, if it exists, satisfies

$$N_{.t}^{\frac{1}{2}}(\hat{p}_t^B - F(\hat{\theta}_t^M d^*)) \rightarrow 0 \text{ as } t \rightarrow \infty$$

and it follows by Slutsky’s Theorem that,

$$N_{.t}^{\frac{1}{2}}(\hat{p}_t^B - F(\theta_0 d^*)) \xrightarrow{\mathcal{L}} N_{0, \sigma_1^2}$$

where “ $\xrightarrow{\mathcal{L}}$ ” indicates convergence in distribution, $\sigma_1^2 = -[d^* f(\theta_0 d^*)]^2 a_{\theta_0}^{-1}$, and

$$a_{\theta} = \sum_{i=1}^m d_i^2 \left[\frac{c_i [f(\theta d_i)]^2}{F(\theta d_i) [1 - F(\theta d_i)]} \right].$$

EXAMPLE 2. Consider the probit model $F(\mathbf{x}'_i \boldsymbol{\theta}) = \Phi(\theta_1 + \theta_2 \log(d_i))$, where $\Phi(\cdot)$ is the standard normal distribution function.

In this case, $p = 2$, $\mathbf{x}_i = (1, \log(d_i))'$ and $\boldsymbol{\theta} = (\theta_1, \theta_2)'$.

Suppose we wish to estimate the dose $d(\boldsymbol{\theta}, \gamma)$ where the probability of response is equal to γ , $0 < \gamma < 1$, i.e.

$$\Phi(\theta_1 + \theta_2 \log(d(\boldsymbol{\theta}, \gamma))) = \gamma.$$

We find that $d(\boldsymbol{\theta}, \gamma) = \exp \left\{ (\Phi^{-1}(\gamma) - \theta_1) / \theta_2 \right\}$.

Again, it can be shown that the Bayes estimator \hat{d}_t^B of $d(\boldsymbol{\theta}, \gamma)$, if it exists, satisfies

$$N_{.t}^{\frac{1}{2}}(\hat{d}_t^B - d(\hat{\boldsymbol{\theta}}_t^M, \gamma)) \rightarrow 0 \text{ as } t \rightarrow \infty.$$

And again it follows that

$$N_{.t}^{\frac{1}{2}}(\hat{d}_t^B - d(\boldsymbol{\theta}_0, \gamma)) \xrightarrow{\mathcal{L}} N_{0, \sigma_2^2}.$$

Let

$$\text{grad}[d(\boldsymbol{\theta}_0, \gamma)] = \left[\frac{\partial d(\boldsymbol{\theta}, \gamma)}{\partial \theta_1} \Big|_{\boldsymbol{\theta}=\boldsymbol{\theta}_0}, \frac{\partial d(\boldsymbol{\theta}, \gamma)}{\partial \theta_2} \Big|_{\boldsymbol{\theta}=\boldsymbol{\theta}_0}, \dots, \frac{\partial d(\boldsymbol{\theta}, \gamma)}{\partial \theta_p} \Big|_{\boldsymbol{\theta}=\boldsymbol{\theta}_0} \right]';$$

then $\sigma_2^2 = -\text{grad}[d(\boldsymbol{\theta}_0, \gamma)]' A_{\boldsymbol{\theta}_0} \text{grad}[d(\boldsymbol{\theta}_0, \gamma)]$, where $A_{\boldsymbol{\theta}}$ is given by (1).

The following corollary to Theorem 2 covers some special loss functions and simplifies the assumptions that are needed.

COROLLARY 1. *In the asymptotic setting of dichotomous quantal response models such as the Probit, Logistic, Multi-hit, Multi-state, and Weibull (see Krewski and Van Ryzin (1981), Messig (1990) and Messig and Strawderman (1993) for definitions of these models), suppose we wish to estimate $\boldsymbol{\theta}$. Assume*

(i) *The sample sizes N_{it} satisfy*

$$N_{it}/N_{.t} \rightarrow c_i, \quad 0 < c_i < 1, \quad i = 1, 2, \dots, m$$

where $N_{.t} \rightarrow \infty$ as $t \rightarrow \infty$.

(ii) *The loss function is given by either of the following*

(a) *(Squared error)*

$$L(\boldsymbol{\theta}, \boldsymbol{\delta}) = \|\boldsymbol{\theta} - \boldsymbol{\delta}\|^2$$

(b) *(Weighted squared error)*

$$L(\boldsymbol{\theta}, \boldsymbol{\delta}) = W(\boldsymbol{\theta})\|\boldsymbol{\theta} - \boldsymbol{\delta}\|^2$$

for $W(\boldsymbol{\theta}) > 0$ continuous in $\boldsymbol{\theta}$.

(c) *(Huber's loss)*

$$L(\boldsymbol{\theta}, \boldsymbol{\delta}) = \begin{cases} \|\boldsymbol{\theta} - \boldsymbol{\delta}\|^2 & \text{if } \|\boldsymbol{\theta} - \boldsymbol{\delta}\| < k \\ 2k\|\boldsymbol{\theta} - \boldsymbol{\delta}\| - k^2 & \text{if } \|\boldsymbol{\theta} - \boldsymbol{\delta}\| \geq k \end{cases}$$

(iii) *The prior density $\lambda(\boldsymbol{\theta})$ satisfies*

(a) $\int_{\Theta} \theta_i^2 \lambda(\boldsymbol{\theta}) d\boldsymbol{\theta} < \infty, i = 1, 2, \dots, p.$

(b) $\int_{\Theta} W(\boldsymbol{\theta})(1 + \theta_i^2) \lambda(\boldsymbol{\theta}) d\boldsymbol{\theta} < \infty, i = 1, 2, \dots, p$ *(Weighted loss only).*

Then the Bayes estimator $\hat{\boldsymbol{\theta}}_t^B$ of $\boldsymbol{\theta}$ satisfies

$$N_{.t}^{\frac{1}{2}}(\hat{\boldsymbol{\theta}}_t^B - \boldsymbol{\theta}_0) \xrightarrow{\mathcal{L}} N_{0, \Sigma_{\boldsymbol{\theta}_0}}$$

where $\Sigma_{\boldsymbol{\theta}_0} = -A_{\boldsymbol{\theta}_0}^{-1}$ for $A_{\boldsymbol{\theta}}$ defined by (1).

Appendix

PROOF OF LEMMA 1. The proof is sketched out. As in Chao (1970),

$$R_t \leq \int_{\|\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}_t^M\| < \delta} B(\boldsymbol{\theta}) \ell(\|\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}_t^M\|^2) \lambda(\boldsymbol{\theta}; t) d\boldsymbol{\theta} \\ + \int_{\|\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}_t^M\| \geq \delta} B(\boldsymbol{\theta}) \ell(\|\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}_t^M\|^2) \lambda(\boldsymbol{\theta}; t) d\boldsymbol{\theta}.$$

The first term can be made arbitrarily small by (A5) and it can be shown that the second term is $o(N_{\cdot t}^{-\alpha})$ for any $\alpha > 0$ using (A5). Therefore,

$$R_t \rightarrow 0 \text{ as } t \rightarrow \infty. \quad \dots (2)$$

The proof is completed by showing that if $\hat{\boldsymbol{\theta}}_{t_k}^B - \boldsymbol{\theta}_0 \rightarrow \mathbf{c}^* \neq \mathbf{0}$, for some subsequence $\{\hat{\boldsymbol{\theta}}_{t_k}^B\}$ of $\{\hat{\boldsymbol{\theta}}_t^B\}$, then R_{t_k} does not converge to 0. This contradicts (2). Therefore, every convergent subsequence $\{\hat{\boldsymbol{\theta}}_{t_k}^B\}$ of $\{\hat{\boldsymbol{\theta}}_t^B\}$ converges to $\boldsymbol{\theta}_0$ and the result follows.

PROOF OF THEOREM 2. Since $\hat{\boldsymbol{\theta}}_t^B$ minimizes r_t , it follows that $\frac{\partial R_t}{\partial \theta_i} = 0$ for $i = 1, 2, \dots, p$. Applying (A5) and the dominated convergence theorem, this is equivalent to

$$\int_{\Theta} B(\boldsymbol{\theta}) \ell'(\|\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}_t^B\|^2) (\theta_i - \hat{\theta}_{it}^B) \lambda(\boldsymbol{\theta}; t) d\boldsymbol{\theta} = 0$$

for $i = 1, 2, \dots, p$.

It can also be established by (A5) and Lemma 1 that

$$\int_{\Theta} B(\boldsymbol{\theta}) \|\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}_t^B\|^{2(s-1)} (\theta_i - \hat{\theta}_{it}^B) \lambda(\boldsymbol{\theta}; t) d\boldsymbol{\theta} = o(N_{\cdot t}^{-\alpha}) \quad \dots (3)$$

for $i = 1, 2, \dots, p$ and any $\alpha > 0$.

Suppose that $N_{\cdot t_j}^{\frac{1}{2}} (\hat{\boldsymbol{\theta}}_{t_j}^B - \hat{\boldsymbol{\theta}}_{t_j}^M) \rightarrow \mathbf{c}^* \neq \mathbf{0}$ for some subsequence.

Case I. $\|\mathbf{c}^*\| = \infty$. (Assume without loss of generality that $c_1 = -\infty$.) It can be shown that the expression

$$N_{\cdot t_j}^s \int_{\theta_1 > \hat{\theta}_{1t_j}^B} B(\boldsymbol{\theta}) \|\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}_{t_j}^B\|^{2s-1} (\theta_1 - \hat{\theta}_{1t_j}^B) \lambda(\boldsymbol{\theta}; t_j) d\boldsymbol{\theta}$$

is both unbounded and bounded. This contradiction leads to the conclusion that Case II must hold.

Case II. $\|\mathbf{c}^*\| < \infty$. A change of variables to $\mathbf{u} = N_{\cdot t}^{\frac{1}{2}} (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}_t^M)$, and applying Lemma 1 and Theorem 2, establishes for $i = 1, 2, \dots, p$ that

$$N_t^{s-\frac{1}{2}} \int_{\Theta} B(\boldsymbol{\theta}) \|\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}_t^B\|^{2(s-1)} (\theta_i - \hat{\theta}_{it}^B \lambda(\boldsymbol{\theta}; t)) d\boldsymbol{\theta} \xrightarrow{t \rightarrow \infty} B(\boldsymbol{\theta}_0) E \left\{ \|\mathbf{Z} - \mathbf{c}^*\|^{2(s-1)} (Z_i - c_i) \right\}.$$

Which, by (3), implies that $E \left\{ \|\mathbf{Z} - \mathbf{c}^*\|^{2(s-1)} (Z_i - c_i) \right\} = 0$ for $i = 1, 2, \dots, p$.

As shown in Chao (1970), this implies that $\mathbf{c}^* = \mathbf{0}$ which completes the proof.

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