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Using Bootstrap Likelihood Ratios in Finite Mixture Models

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SUMMARY

Statistical inference using the likelihood ratio statistic for the number of components in a mixture model is complicated when the true number of components is less than that of the proposed model since this represents a non-regular problem: the true parameter is on the boundary of the parameter space and in some cases the true parameter is in a non-identifiable subset of the parameter space. The maximum likelihood estimator is shown to converge to the subset characterized by the same density function, and connection is made to the bootstrap method proposed by Aitkin and co-workers and McLachlan for testing the number of components in a finite mixture and deriving confidence regions in a finite mixture.

Keywords: BOOTSTRAP; BOUNDARY; FINITE MIXTURE; IDENTIFIABILITY; LIKELIHOOD RATIO TEST

1. INTRODUCTION

Finite mixture models have been widely used in biology, medicine and engineering (Everitt and Hand, 1981; Titterington et al., 1985; McLachlan and Basford, 1988). Let $X = (x_1, \ldots, x_n)$ be a random sample of size n from a probability distribution with a real-valued density function $f(x_i, \theta_0)$, where x can be univariate or vector valued, discrete or continuous and θ_0 is the unknown true parameter vector of dimension p. Let $l(\theta; x_i)$ denote the log-likelihood. A finite mixture density has the form

$$f(x, \theta) = \sum_{j=1}^{k} \pi_j f_j(x, \psi_j),$$
 (1.1)

where ψ_j is the m_j -dimensional parameter vector for component j, π_j is the mixing probability for component j with restriction $\Sigma_{j=1}^k \pi_j = 1$ and $\pi_j \ge 0$, $\theta = (\pi_1, \ldots, \pi_{k-1}, \psi_1, \ldots, \psi_k)$, and

$$p=k-1+\sum_{j=1}^k m_j.$$

The number of components, k, may be known or unknown. When the number of components is known, statistical inferential procedures about the parameters are well developed, mostly via likelihood-based inference. Although the inferential problem for the number of components in a mixture has wide applications, it is still an open

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question without satisfactory treatment (Titterington, 1990). Suppose that we want to test

$$H_0$$
: $f(x, \theta) = N(0, 1)$ (1.2)

against

$$H_1$$
: $f(x, \theta) = (1 - \pi) N(0, 1) + \pi N(\mu, 1),$ (1.3)

where $N(\mu, \sigma^2)$ is a Gaussian density with mean μ and variance σ^2 . We have $\theta = (\pi, \mu) \in [0, 1] \times (-\infty, \infty)$. The parameter space where H_0 holds is

$$\Omega_0 = ([0] \times (-\infty, \infty)) \bigcup ([0, 1] \times [0]),$$

i.e. the entire μ -axis when $\pi=0$ and the line segment [0, 1] on the π -axis when $\mu=0$. Therefore, the parameter is on the boundary of the parameter space and the null hypothesis corresponds to a non-identifiable subset of the parameter space. The classic assumptions (Cramér, 1946) about the asymptotic properties of the maximum likelihood estimator and the likelihood ratio statistic are not valid under the null hypothesis.

There have only been conjectures and simulation results for the limiting distribution of the likelihood ratio statistic for the mixture models under the null hypothesis (Wolfe, 1971; Hartigan, 1977, 1985; McLachlan, 1987; Thode et al., 1988; Mendell et al., 1991, 1993). Ghosh and Sen (1985) showed that choosing an identifiable parameterization can create a problem of differentiability of the density. Bootstrapping the likelihood ratio to test the number of components of a normal mixture was investigated by Aitken et al. (1981) and McLachlan (1987). McLachlan (1987) used a parametric bootstrap in which the parameter estimate was obtained from the maximum likelihood method under the null hypothesis, bootstrap samples were drawn from the null hypothesis with the estimated parameter and for each bootstrap sample the likelihood ratio was computed to form the reference distribution. Feng and McCulloch (1994) noted that the bootstrap is a preferred method for testing the number of components of a normal mixture with unequal variances. For regular cases, Beran (1988) and Martin (1990) studied level error and coverage probability of the bootstrap likelihood ratio on the testing and confidence region problems respectively. Since the maximum likelihood estimator under the alternative hypothesis is not a consistent estimator when the null hypothesis is true, there are questions about the validity of the bootstrap likelihood ratio test based on this inconsistent estimator, such as whether the observed rejection rates will match the levels hoped for (Titterington, 1990).

This work provides some justification for the bootstrap method by showing that the maximum likelihood estimator converges to the non-identifiable subset to which the true parameter belongs. This property has a natural connection to bootstrap likelihood ratio tests and confidence regions. The test sizes and coverage probabilities of bootstrap methods match the nominal levels well in simulation studies when the null hypothesis is true.

2. MAIN RESULTS

Along with other classic regularity conditions, if the true parameter is an interior

point of the parameter space then standard asymptotic theory applies. We extend the standard results by considering a situation where the true parameter lies in a non-identifiable subset Ω_0 , and this subset may be on the boundary of the parameter space. We first extend the definition of consistency and prove that the unrestricted maxima $\hat{\theta}$ (i.e. maximizing θ without restricting it to Ω) is consistent in the following sense: $\hat{\theta} - \theta_0^*(\hat{\theta}) \to 0$, with probability 1 for some $\theta_0^*(\hat{\theta}) \in \Omega_0$, where Ω_0 identifies a subset of Ω in which the distributions are not distinguishable. Consistency also holds for the maximum likelihood estimator in the same sense. We first extend the definition of $l(\theta; x)$ to \mathcal{R}^p :

$$l^*(\theta; x) \equiv \sum_{i=1}^n \log[f^*(\theta; x_i) I\{f^*(\theta; x_i) > 0\}], \tag{2.1}$$

where I() is an indicator function and $f^*(\theta, x_i)$ is the extension of $f(\theta, x_i)$ to all $\theta \in \mathbb{R}^p$.

We need the following assumptions, with θ_0 an arbitrary fixed point in Ω_0 :

- (a) the parameter space Ω has finite dimension;
- (b) $f(x, \theta_0) = f(x, \theta'_0)$ for all $\theta_0, \theta'_0 \in \Omega_0$;
- (c) there exists an open subset ω_{ϵ} of \mathbb{R}^p containing Ω_0 , such that, for almost all $x, f(\theta; x)$ admits all third derivatives with respect to θ for all $\theta \in \omega_{\epsilon}$, and

$$\left|\frac{\partial^3}{\partial \theta_i \partial \theta_k \partial \theta_l} \left\{ \log f(x; \theta) \right\} \right| \leq M_{jkl}(x, \theta),$$

and $m_{ikl}(\theta_0) = E_{\theta_0}\{M_{ikl}(x, \theta_0)\} < \infty$ for all j, k and l, for any fixed $\theta_0 \in \Omega_0$.

Remark 1. ω_{ϵ} is not necessarily an open ball and can be expressed as

$$\omega_{\epsilon} \equiv \bigcup_{\theta_0 \in \Omega_0} B_{\epsilon(\theta_0)}(\theta_0),$$

for each $\epsilon(\theta_0) > 0$ depending on θ_0 , and $B_{\epsilon}(\theta)$ is an open ball of radius ϵ centred at θ . In the example of expression (1.3) when expression (1.2) is true, ω_{ϵ} is an open stripe with unequal width surrounding Ω_0 with ϵ the maximum of $\epsilon(\theta_0)$ s.

(d)
$$E_{\theta_0} \left[\frac{\partial}{\partial \theta_j} \{ \log f(x, \theta) \} \right] = 0$$
 for $j = 1, ..., p$ and all $\theta_0 \in \Omega_0$.

$$I_{jk}(\theta_0) = E_{\theta_0} \left[\frac{\partial}{\partial \theta_j} \{ \log f(x, \theta) \} \frac{\partial}{\partial \theta_k} \{ \log f(x, \theta) \} \right]$$

$$= -E_{\theta_0} \left[\frac{\partial^2}{\partial \theta_j \partial \theta_k} \{ \log f(x, \theta) \} \right]$$

for any $\theta_0 \in \Omega_0$. Also, for any $\theta \notin \Omega_0$, the $\theta_0 \in \Omega_0$ which is nearest to θ in Euclidean distance (i.e. $|\theta - \theta_0| \le |\theta - \theta_0'|$ for all $\theta_0' \in \Omega_0$) is selected and has the property that $(\theta - \theta_0)^T I(\theta_0)(\theta - \theta_0) > 0$ for all θ in the neighbourhood of θ_0 .

Remark 2. Notice that the above properties need not be held by all $\theta_0 \in \Omega_0$. For those θ_0 which will not be selected by the above rule the assumptions can be relaxed,

i.e. the quadratic form can be 0. It is not difficult to check that, for the maximum likelihood estimator under expression (1.3) when expression (1.2) is true, assumptions (a)-(d) are satisfied.

Theorem 1. Let $X = (x_1, \ldots, x_n)$ be independent, identically distributed observations with density $f(x, \theta)$ satisfying assumptions (a)-(d) above and with the true parameter θ_0 being any point in Ω_0 (the value of θ_0 is not important since all points in Ω_0 identify the same density function). Then, with probability tending to 1 as $n \to \infty$, there exists a $\hat{\theta} \in \mathbb{R}^p$, a local maximum of $l^*(\theta, X)$ as defined in expression (2.1), which has the property that there exists a $\theta_0^*(\hat{\theta}) \in \Omega_0$ which depends on $\hat{\theta}$ such that $\hat{\theta} - \theta_0^*(\hat{\theta}) \to 0$ with probability 1. Moreover, the maximum likelihood estimator $\hat{\theta}_{ml} - \theta_0^*(\hat{\theta}_{ml}) \to 0$ with probability 1.

Proof. The proof is similar to that of Lehmann (1983) with modifications to adapt assumptions (b) and (c). We only need to show that, for sufficiently small $\epsilon(\theta_0) > 0$, $l^*(\theta, X) < l^*(\theta_0, X)$ at all points θ on the boundary of some stripe ω_{ϵ} surrounding Ω_0 , since this means that there is at least a local maximum within ω_{ϵ} . We can choose $\epsilon(\theta_0)$ sufficiently small that $f(x_i, \theta) > 0$ for all x_i in the sample and Taylor expansion of $l^*(\theta, X)$ about θ_0 is justified in ω_{ϵ} . For any fixed θ on the boundary of ω_{ϵ} , we define $\theta_0^*(\theta)$ such that $|\theta - \theta_0^*(\theta)| \le |\theta - \theta_0|$ for all $\theta_0 \in \Omega_0$, i.e. $\theta_0^*(\theta)$ is the point in Ω_0 closest to θ in Euclidean distance. Taylor expansion of $l^*(\theta, X)$ about $\theta_0^*(\theta)$ leads to

$$\frac{1}{n} l^*(\theta, X) - \frac{1}{n} l^*\{\theta_0^*(\theta, X)\} = S_1 + S_2 + S_3,$$

with

$$S_{1} = \frac{1}{n} \sum_{j=1}^{p} \{\theta_{j} - \theta_{0j}^{*}(\theta)\} \frac{\partial}{\partial \theta_{j}} l^{*}(\theta, X)|_{\theta = \theta_{0}^{*}(\theta)},$$

$$S_{2} = \frac{1}{2n} \sum_{j=1}^{p} \sum_{k=1}^{p} \{\theta_{j} - \theta_{0j}^{*}(\theta)\} \{\theta_{k} - \theta_{0k}^{*}(\theta)\} \frac{\partial^{2}}{\partial \theta_{j} \partial \theta_{k}} l^{*}(\theta, X)|_{\theta = \theta_{0}^{*}(\theta)},$$

$$S_{3} = \frac{1}{6n} \sum_{j=1}^{p} \sum_{k=1}^{p} \sum_{l=1}^{p} \{\theta_{j} - \theta_{0j}^{*}(\theta)\} \{\theta_{k} - \theta_{0k}^{*}(\theta)\} \{\theta_{l} - \theta_{0l}^{*}(\theta)\} \sum_{i=1}^{n} \gamma_{jkl}(x_{i}) M_{jkl}(x_{i}, \theta),$$

where $0 \le |\gamma_{ikl}(x)| \le 1$ by assumption (c).

The asterisk on the log-likelihood can be dropped in each term of the Taylor expansion since $\theta_0^*(\theta) \in \Omega$. Therefore, the rest of the proof of $S_1 + S_2 + S_3 < 0$ as $n \to \infty$ follows Lehmann (1983). The proof of convergence of $\hat{\theta}_{ml}$ is the same except that Taylor expansion of $l^*(\theta, X)$ is for any fixed θ on the boundary of the intersection of ω_{ϵ} and Ω .

Remark 3. Redner (1981) proved the strong consistency of the maximum likelihood estimator in the quotient topological space. The above proof is the parallel result expressed in Euclidean space and is therefore easier for practitioners to apply. It is also valid for when the true parameter is on the boundary of the parameter space and in a non-identifiable subset whereas Redner's result dealt with the non-identifiable situation only. If the parameter is identifiable but on the

boundary of the parameter space, Self and Liang (1987) proved the consistency and gave the characteristic of the asymptotic distribution of the maximum likelihood estimator. Feng and McCulloch (1992) proposed an unrestricted maximum likelihood estimator which is consistent and has asymptotic normality. So, theorem 1 is the extension of results of Redner (1981) and Self and Liang (1987). When Ω_0 is a single boundary point, theorem 1 reduces to Self and Liang's consistency result of the maximum likelihood estimator. It reduces to Redner's result when Ω_0 is in the interior of Ω , and to the classic consistency of the maximum likelihood estimator when Ω_0 is a single point in the interior of Ω . It also extends Feng and McCulloch's results to non-identifiable cases.

3. CONNECTION TO BOOTSTRAP LIKELIHOOD RATIO

Following Beran (1988), Martin (1990) and McLachlan (1987), we denote

$$W(\theta, X) \equiv 2\{l(\hat{\theta}, X) - l(\theta, X)\}\$$

and

$$W\{\theta_0, X^*(\theta_0)\} \equiv 2[l\{\hat{\theta}^*, X^*(\theta_0)\} - l\{\theta_0, X^*(\theta_0)\}],$$

where $\hat{\theta}$ and $\hat{\theta}^*$ are the maximum likelihood estimators under Ω from X and X^* respectively, and $X^*(\theta_0)$ means a bootstrap sample under θ_0 , where θ_0 is contained in H_0 . The size α bootstrap likelihood ratio test procedure for simple H_0 : $\theta = \theta_0$ is reject H_0 if

$$W(\theta_0, X) > W_{\alpha}\{\theta_0, X^*(\theta_0)\}$$

where $W_{\alpha}(\ ,\)$ is the upper α -quantile of $W(\ ,\)$.

For $\theta = (\theta_1, \theta_2)$ and a composite H_0 : $\theta_1 = \theta_{01}$, θ_2 unspecified, denote the maximum likelihood estimator under H_0 as $\hat{\theta}_0 = (\theta_{01}, \hat{\theta}_{02})$. The bootstrap test is then reject H_0 : $\theta_1 = \theta_{01}$ if

$$W(\hat{\theta}_0, X) > W_{\alpha}\{\hat{\theta}_0, X^*(\hat{\theta}_0)\}.$$

By theorem 1, when H_0 is true, the likelihood computed under H_1 is based on the maximum likelihood estimate converging to Ω_0 with probability 1. If this convergence does not hold, it is clear that the bootstrap likelihood ratio test is not valid. For example (1.2)–(1.3), Hartigan (1985) pointed out that $W(\theta_0, X)$ is asymptotically unbounded above in probability at a very slow rate $(\frac{1}{2}\log(\log n))$ when the null hypothesis is true. However, the distribution of W or W^* for any finite sample size does exist. Since the likelihood is identifiable whereas the parameters are not, the bootstrap likelihood ratio is a natural candidate for this inference problem as compared with other parameter-based tests (e.g. Wald's test).

We can define a bootstrap confidence region $\hat{\mathcal{R}}_{\alpha}$ as

$$\hat{\mathcal{R}}_{\alpha} \equiv \{\theta \colon W(\theta, X) \leqslant W_{\alpha}\{\hat{\theta}, X^{*}(\hat{\theta})\}\},\$$

where $X^*(\hat{\theta})$ is the bootstrap sample from $F(\hat{\theta})$, i.e. the parametric bootstrap, and $\hat{\theta}$ and $\hat{\theta}^*$ are the maximum likelihood estimates of θ from X and $X^*(\hat{\theta})$ respectively. The validity of $\hat{\mathcal{R}}_{\alpha}$ relies heavily on theorem 1, since the resampling is from $F(\hat{\theta})$,

the maximum likelihood estimate under H_1 , whereas in the hypothesis testing situation the resampling is from the null hypothesis.

For the hypothesis testing in example (1.2)–(1.3), bootstrap samples are generated from the standard normal distribution. The maximum likelihood estimate $(\hat{\pi}, \hat{\mu})$ by theorem 1 will converge to

$$\Omega_0$$
: $([0] \times (-\infty, \infty)) \bigcup ([0, 1] \times [0])$

which identifies the standard normal density. Therefore, we expect the bootstrap test to have a high probability of accepting H_0 when the sample size is sufficiently large and H_0 holds. For the confidence region based on model (1.3) when the unknown true distribution is standard normal, $X^*(\hat{\theta})$ is sampled from expression (1.3) with $\hat{\theta}$ converging to Ω_0 . Therefore, we expect the bootstrap confidence region $\hat{\mathcal{R}}_{\alpha}$ to have a high probability of intersecting Ω_0 for a large sample size. Since the asymptotic normality of the unrestricted maximum likelihood estimator by Feng and McCulloch (1992) does not hold under non-identifiable cases and the asymptotic distribution for the maximum likelihood estimator is unknown, the critical values for tests and confidence regions should come from bootstrapping.

4. SIMULATION STUDIES

We conducted two simulation studies to examine the acceptance probabilities of the bootstrap likelihood tests and the coverage probabilities of the bootstrap likelihood confidence regions under null hypotheses. We focus on the null hypothesis since this is where the classic asymptotic distribution theory for the likelihood ratio fails. Table 1 describes the simulation results of bootstrap likelihood ratio tests using 500 bootstrap replications and 500 simulation replications for a mixture normal alternative, $(1-\pi)N(1, 1) + \pi N(0, 1)$ with the true density standard normal. This is the case where the parameter is on the boundary of Ω . We also included the likelihood ratio test based on the unrestricted maximum by Feng and McCulloch (1992) which has a limiting χ^2 -distribution with 1 degree of freedom. The probabilities of correctly accepting H_0 for both procedures are near the nominal level when the sample size N = 100, but the bootstrap procedure outperforms the likelihood ratio method. This difference is clear for smaller sample sizes. The likelihood ratio method performed poorly when n = 10 with the probability of making a correct conclusion from 0.128 to 0.180 less than that of the nominal level whereas the bootstrap procedure has the probability only 0.010-0.018 away from the nominal level. Table 2 summarizes the coverage probabilities of bootstrap confidence regions for a mixture normal model $(1-\pi) N(0, 1) + \pi N(\mu, 1)$ when the true distribution is a standard normal distribution. This is the case where the parameter is on the boundary of Ω and in a non-identifiable subset Ω_0 . The bootstrap confidence procedure is again clearly better than the confidence region based on χ_1^2 (a χ_2^2 approximation was even worse in this simulation). We should mention that neither χ_1^2 nor χ_2^2 has a theoretical basis for use. The bootstrap confidence region has good coverage probabilities that are very close to the nominal levels in all sample sizes at all nominal levels, whereas the χ^2 -approximation, although not bad in 0.95 and 0.99 nominal levels, performed poorly at the 0.90 nominal level.

TABLE 1
Observed proportions of acceptance (and binomial standard errors) out of 500 simulations of H_0 : N(0, 1) versus H_1 : $(1-\pi)$ $N(0, 1)+\pi$ N(1, 1) when H_0 is true†

Nominal 1–α	Sample size	Bootstrap likelihood ratio	Feng and McCulloch's (1992) likelihood ratio
0.90	10	0.882 (0.014)	0.720 (0.020)
	30	0.892 (0.014)	0.824 (0.017)
	100	0.894 (0.014)	0.864 (0.015)
0.95	10	0.938 (0.011)	0.796 (0.018)
	30	0.950 (0.010)	0.884 (0.014)
	100	0.948 (0.010)	0.924 (0.012)
0.99	10	0.980 (0.006)	0.862 (0.015)
	30	0.998 (0.002)	0.956 (0.009)
	100	0.990 (0.004)	0.982 (0.006)

†The bootstrap used 500 replications. Standard errors are given in parentheses.

TABLE 2 Observed coverage proportions (and binomial standard errors) of bootstrap and likelihood-ratio-based confidence regions for a mixture normal model $(1-\pi)$ $N(0,1)+\pi$ $N(\mu,1)$ when the true distribution is N(0,1) in 500 simulations†

Nominal 1–α	Sample size	Bootstrap likelihood ratio	Likelihood ratio (χ_1^2)
0.90	10	0.916 (0.012)	0.878 (0.015)
	30	0.918 (0.012)	0.856 (0.016)
	100	0.916 (0.012)	0.862 (0.015)
0.95	10	0.946 (0.010)	0.926 (0.012)
	30	0.954 (0.009)	0.924 (0.012)
	100	0.966 (0.008)	0.926 (0.012)
0.99	10	0.988 (0.005)	0.986 (0.005)
	30	0.984 (0.006)	0.970 (0.008)
	100	0.996 (0.003)	0.992 (0.004)

†The bootstrap used 500 replications. Standard errors are given in parentheses.

5. CONCLUSIONS AND OPEN QUESTIONS

This paper provides some justification for the bootstrapping likelihood ratio when the true parameter is on the boundary of the parameter space and in a non-identifiable set. It shows that the maximum likelihood estimate is consistent with the set identifying the true density function. Therefore, a procedure based on the likelihood is justified although its asymptotic distribution may be difficult to obtain and we need to use the bootstrap method to construct tests or confidence regions. The parametric bootstrap confidence region works very naturally under this setting since the bootstrap resamples from a consistently estimated density. Therefore, to a large extent we overcome the difficulties of the fact that the density is characterized by a set of the parameters and this set is on the boundary of the parameter space. The simulations indicate that the bootstrap tests and confidence regions seem to hold the nominal levels and the expected coverage probabilities.

To justify fully the bootstrap likelihood ratio method we need to obtain the exact convergence rate of the bootstrap approximation of the distribution of sample

quantiles. The singular Fisher information is the major difficulty in investigating the error rate of the bootstrap procedure for the non-identifiable case. As in Singh (1981), the proof of the error rate of the bootstrap procedure depends on the existence of an Edgeworth expansion of W. Bhattacharya (1985) proved that, if $W = 2n\{H(\bar{Z}) - H(\mu)\}$ where $\bar{Z} = n^{-1}(Z_1 + \ldots + Z_n)$ with $\mu = EZ_1$ and with some other regularity conditions, the Edgeworth expansion of W is valid. Chandra and Ghosh (1979), p. 42, pointed out that, if the assumptions (A_1) – (A_4) and (A_6) of theorem 3 of Bhattacharya and Ghosh (1978) are satisfied, the Edgeworth expansion of the cumulative density function of W agrees with the true distribution up to $o_p(n^{-1})$. Unfortunately, their assumption (A₄) is that the Fisher information is nonsingular. The importance of assumption (A₄) is that it enables us to apply the implicit function theorem to ensure that there is a uniquely defined real-valued infinitely differentiable function H on the neighbourhood of μ . The difference between $n^{1/2}(\hat{\theta}-\theta_0)$ and its Edgeworth representation is then of order $o(n^{(s-2)/2})$, where s is the positive integer such that the ith derivative of the density function with respect to every θ is continuously differentiable for $1 \le i \le s$. The representation of W as a sum of independent and identically distributed random variables is necessary in all three of the above papers' proofs. Therefore, a possible approach is to develop some non-Edgeworth-expansion method or other criterion to justify the Edgeworth expansion.

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