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## QED

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# Nonparametric Identification and Estimation of Multivariate Mixtures 

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# Nonparametric Identification and Estimation of Multivariate Mixtures 

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#### Abstract

We study nonparametric identifiability of finite mixture models of $k$-variate data with $M$ subpopulations, in which the components of the data vector are independent conditional on belonging to a subpopulation. We provide a sufficient condition for nonparametrically identifying $M$ subpopulations when $k \geq 3$. Our focus is on the relationship between the number of values the components of the data vector can take on, and the number of identifiable subpopulations. Intuition would suggest that if the data vector can take many different values, then combining information from these different values helps identification. Hall and Zhou (2003) show, however, when $k=2$, two-component finite mixture models are not nonparametrically identifiable regardless of the number of the values the data vector can take. When $k \geq 3$, there emerges a link between the variation in the data vector, and the number of identifiable subpopulations: the number of identifiable subpopulations increases as the data vector takes on additional (different) values. This points to the possibility of identifying many components even when $k=3$, if the data vector has a continuously distributed element. Our identification method is constructive, and leads to an estimation strategy. It is not as efficient as the MLE, but can be used as the initial value of the optimization algorithm in computing the MLE. We also provide a sufficient condition for identifying the number of nonparametrically identifiable components, and develop a method for statistically testing and consistently estimating the number of nonparametrically identifiable components. We extend these procedures to develop a test for the number of components in binomial mixtures.


Key words and phrases: finite mixture; binomial mixture; model selection; number of components; rank estimation

[^0]
## 1 Introduction: finite mixture models with independent marginals

Consider the following $M$-component finite mixture model of a $k$-vector $X=\left(X_{1}, \ldots, X_{k}\right)$, where the elements of $X$ are independently distributed within each component:

$$
\begin{equation*}
F(x)=F\left(x_{1}, \ldots, x_{k}\right)=\sum_{m=1}^{M} \pi^{m} \prod_{j=1}^{k} F^{j m}\left(x_{j}\right), \quad \pi^{m}>0, \quad \sum_{m=1}^{M} \pi^{m}=1, \tag{1}
\end{equation*}
$$

where $F(x)$ is the distribution function of $X, \pi^{m}$ is the mixture proportion of the $m$ th subpopulation, and $F^{j m}\left(x_{j}\right)$ is the distribution function of $X_{j}$ conditional on being from the $m$ th subpopulation.

We study the nonparametric identifiability of this mixture model, i.e., whether the information from $F(x)$ can uniquely determine $\pi^{m}$ and $F^{j m}\left(x_{j}\right)$ 's when no parametric restrictions are imposed on them. Analyzing nonparametric identification is relevant for applied work, because there is rarely theory to guide the specification of component distributions. For example, Cruz et al. (2004) report a simulation result in which imposing incorrect parametric restrictions on component distributions leads to erroneous inference. Zhou et al. (2005) develop a nonparametric maximum likelihood method for $M=2$ to estimate ROC curves in the absence of a gold standard.

Nonparametric identifiability of finite mixtures has recently attracted increasing attention. Hall and Zhou (2003) and Hall et al. (2005) analyze nonparametric identifiability of the above mixture model with two components $(M=2)$. Hettmansperger and Thomas (2000) and CruzMedina et al. (2004) analyze nonparametric identification of models analogous to (1). Their approach involves reducing multivariate data to binomial or multinomial variables, and applying the identification theory for binomial and multinomial mixtures of Blischke (1964) and Elmore and Wang (2003).

Hall and Zhou (2003) show that $k \geq 3$ is necessary and sufficient for nonparametric identification when $M=2$. Somewhat surprisingly, the non-identifiability for $k=2$ by Hall and Zhou (2003) holds regardless of the number of values the $X_{j}$ 's can take. If $X_{j}$ takes $J$ different values, then considering $F(x)$ for all possible values of $X$ provides $J^{k}-1$ restrictions, whereas the number of unknowns is $k J M+M-1$. Hence, as $J$ increases, the number of restrictions increases at an exponential rate, whereas the number of unknowns increases only linearly. Intuition would suggest that this additional information helps identification. This is not the case, however, when $k=2$.

When $k \geq 3$, combining information from different $x$ 's changes the picture substantially. Now the model (1) is nonparametrically identifiable. We provide a sufficient condition that enables one to identify up to $M$ components. Furthermore, we show that, when $k \geq 3$, there emerges a link between the variation in $X$ and the number of identifiable components: the number of identifiable components increases as $X$ takes more (different) values. If $X$ is continuously
distributed, one can identify as many components as desired. Hall et al. (2005) show that the model in (1) is nonparametrically identifiable when $k \geq k_{M}=(1+o(1)) 6 M \ln (M)$ as $M \rightarrow \infty$. Our results imply that $k=3$ is sufficient if the $X_{j}$ 's have sufficient variation. Our identification method is constructive, and leads to an estimation strategy. It is not as efficient as the MLE, but can be used as the initial value of the optimization algorithm in computing the MLE.

Testing the number of components in finite mixtures has long been a challenging problem. The asymptotic distribution of the likelihood ratio statistic has been derived recently (DacunhaCastelle and Gassiat, 1999; Liu and Shao, 2003) but is nonstandard, and not easy to tabulate. There is also a growing literature on consistent estimation of the number of components, including Henna (1985), Leroux (1992), Chen and Kalbfleisch (1996), Dacunha-Castelle and Gassiat, (1997, 1999), Keribin (2000), and James et al. (2001). In these papers, the component distributions are assumed to belong to a parametric family. Little is known of identifiability of the number of components in a nonparametric setting.

We provide a sufficient condition for nonparametrically identifying the number of components. This condition is stated in terms of $F(x)$, and hence testable by using empirical distribution functions. Using this fact, we develop a procedure to statistically test, and consistently estimate the number of nonparametrically identifiable components. It is based on an estimate of the rank of a matrix constructed from the empirical distribution of $X$. Since our procedure does not require estimating a mixture model, it is computationally easy to implement. Extending this framework, we also develop a procedure to statistically test and consistently estimate the number of components in mixtures of binomial distributions. Simulations illustrate our procedure performs well.

Kasahara and Shimotsu (2007) study nonparametric identification of finite mixture dynamic discrete choice models widely used in econometrics using a similar approach to this paper. This paper analyzes nonparametric identifiability in a more general context of multivariate mixtures, and provides a clearer intuition behind the identification results.

We assume the elements of $X$ (or blocks of the elements of $X$ ) are independent conditional on being from a subpopulation, as in Hall and Zhou (2003) (and other existing papers on nonparametric identification mentioned above). Hall and Zhou (2003, section 2.3) and Hall et al. (2005, p. 668) discuss the validity of the assumption of independent marginals, and list the body of work that employs it. Elmore et al. (2004) and Zhou et al. (2005) also employ a model with independent marginals.

The reminder of the paper is organized as follows. Section 2 briefly reviews the nonidentifiability for $k=2$ shown by Hall and Zhou (2003). Section 3 discusses the identifiability under $k \geq 3$ and provides a sufficient condition for nonparametric identification. Section 4 gives a sufficient condition for nonparametrically identifying the number of components, and section 5 introduces a test of the number of mixture components. Section 6 reports simulation results, and proofs are collected in the Appendix.

## 2 Non-identifiability of finite mixture models under $k=2$

In this section, we consider a two-component mixture model of a $k$-dimensional variable $X=$ $\left(X_{1}, \ldots, X_{k}\right)$ :

$$
\begin{equation*}
F(x)=F\left(x_{1}, \ldots, x_{k}\right)=\pi \prod_{j=1}^{k} F^{j 1}\left(x_{j}\right)+(1-\pi) \prod_{j=1}^{k} F^{j 2}\left(x_{j}\right), \tag{2}
\end{equation*}
$$

where $\pi \in(0,1) . F(x)$ denotes the distribution function of the observed data, and $F^{j m}\left(x_{j}\right)$ denotes the univariate distribution function of $X_{j}$ conditional on being from the $m$ th subpopulation. Let $Q$ be the primitive parameter of this model; $Q=\left\{\pi,\left\{\left\{F^{j m}\left(x_{j}\right)\right\}_{j=1}^{k}\right\}_{m=1}^{2}\right\} . Q$ is nonparametrically identified if it is uniquely determined from $F(x)$, and its marginals.

Hall and Zhou (2003) show that this model is nonparametrically non-identifiable if $k=2$. Somewhat surprisingly, this non-identifiability for $k=2$ holds regardless of the number of values the $X_{j}$ 's can take. Suppose both $X_{1}$ and $X_{2}$ can take at least $J$ distinct values, $\left\{\xi_{1}, \ldots, \xi_{J}\right\}$. Then, considering $F(x)$ for all possible values of $X$ provides $J^{2}-1$ restrictions, whereas the number of unknowns in $Q=\left\{\pi,\left\{F^{11}\left(\xi_{l}\right), F^{21}\left(\xi_{l}\right), F^{12}\left(\xi_{l}\right), F^{22}\left(\xi_{l}\right)\right\}_{l=1}^{J}\right\}$ is $4 J+1$. This suggests that it may be possible to nonparametrically identify $Q$ if $J$ is sufficiently large. However, the additional restrictions from $F(x)$ at different values of $x$ cancel with each other, and the effective number of restrictions is always smaller than the number of unknowns.

Hall and Zhou (2003) prove the non-identifiability by showing that there exists a continuum of $Q$ 's that satisfy (2) for a given $F(x)$ when $k=2$. In the following, we provide an additional insight to this problem by showing that only $4 J-1$ of these $J^{2}-1$ restrictions are effective.

First, we introduce the irreducibility condition used by Hall and Zhou (2003, p. 215). Let $F^{j}\left(x_{j}\right)$ denote the marginal distribution function of $X_{j}$.
Assumption 1 (irreducibility) $F\left(x_{1}, x_{2}\right)$ is not identical to $F^{1}\left(x_{1}\right) F^{2}\left(x_{2}\right)$ for any $x_{1}$ and $x_{2}$.
Note that if the irreducibility condition fails, then we have $F^{j 1}\left(x_{j}\right)=F^{j 2}\left(x_{j}\right)=F^{j}\left(x_{j}\right)$ in (2), and that the right hand side of (2) is not uniquely determined with respect to $\pi$.

The following proposition shows that all the $J^{2}-1$ restrictions implied by $F\left(x_{1}, x_{2}\right)$ can be constructed from a set of $4 J-1$ restrictions and, therefore, the number of unknowns in $Q$ is strictly larger than the number of effective restrictions when $k=2$.

Proposition 1 Suppose that the distribution function of $\left(X_{1}, X_{2}\right)$ is given by (2) with $k=2$, and $F\left(x_{1}, x_{2}\right)$ satisfies Assumption 1. Suppose $\tilde{Q}=\left\{\tilde{\pi},\left\{\tilde{F}^{11}\left(\xi_{l}\right), \tilde{F}^{21}\left(\xi_{l}\right), \tilde{F}^{12}\left(\xi_{l}\right), \tilde{F}^{22}\left(\xi_{l}\right)\right\}_{l=1}^{J}\right\}$ satisfies

$$
\begin{equation*}
F\left(x_{1}, x_{2}\right)=\tilde{\pi} \prod_{j=1}^{2} \tilde{F}^{j 1}\left(x_{j}\right)+(1-\tilde{\pi}) \prod_{j=1}^{2} \tilde{F}^{j 2}\left(x_{j}\right), \tag{3}
\end{equation*}
$$

for $\left(x_{1}, x_{2}\right)=\left(\xi_{1}, \xi_{1}\right),\left(\xi_{1}, \xi_{2}\right), \ldots,\left(\xi_{1}, \xi_{J}\right)$ and $\left(\xi_{2}, \xi_{1}\right),\left(\xi_{3}, \xi_{1}\right), \ldots,\left(\xi_{J}, \xi_{1}\right)$, and $\tilde{Q}$ satisfies

$$
\begin{equation*}
F^{1}\left(x_{1}\right)=\tilde{\pi} \tilde{F}^{11}\left(x_{1}\right)+(1-\tilde{\pi}) \tilde{F}^{12}\left(x_{1}\right), \quad F^{2}\left(x_{2}\right)=\tilde{\pi} F^{21}\left(x_{1}\right)+(1-\tilde{\pi}) \tilde{F}^{22}\left(x_{2}\right), \tag{4}
\end{equation*}
$$

for $x_{1}=\xi_{1}, \ldots, \xi_{J}$, and $x_{2}=\xi_{1}, \ldots, \xi_{J}$. Then $\tilde{Q}$ satisfies (3) for all $\left(x_{1}, x_{2}\right) \in\left\{\xi_{1}, \ldots, \xi_{J}\right\} \times$ $\left\{\xi_{1}, \ldots, \xi_{J}\right\}$.

## 3 Sufficient conditions for nonparametric identification when $k \geq 3$

When $k \geq 3$, the restrictions from $F(x)$ at different values of $x$ help identification. The number of identifiable components increases as the number of values the $X_{j}$ 's can take increases. We focus on the case $k=3$, but the following argument is also valid for $k \geq 3$. The distribution function of $X$ is

$$
\begin{equation*}
F(x)=\pi^{1} \prod_{j=1}^{k} F^{j 1}\left(x_{j}\right)+\cdots+\pi^{M} \prod_{j=1}^{k} F^{j M}\left(x_{j}\right), \tag{5}
\end{equation*}
$$

where $\pi^{m}>0$ and $\sum_{m=1}^{M} \pi^{m}=1$. Let $\mathcal{X}_{j}$ denote the support of $X_{j}$. Consider a partition of $\mathcal{X}_{j}$ into $M$ subsets, $\Xi_{1}^{j}, \ldots, \Xi_{M}^{j}$. Define, for $a, b, c=1, \ldots, M$,

$$
\begin{align*}
p_{a}^{j m} & =\mathbb{P}\left(X_{j} \in \Xi_{a}^{j} \mid X_{j} \text { is from the } m \text { th subpopulation }\right)=\int 1\left\{x_{j} \in \Xi_{a}^{j}\right\} d F^{j m}\left(x_{j}\right)  \tag{6}\\
P_{a, b}^{12} & =\mathbb{P}\left(X_{1} \in \Xi_{a}^{1}, X_{2} \in \Xi_{b}^{2}\right)=\sum_{m=1}^{M} \pi^{m} p_{a}^{1 m} p_{b}^{2 m}  \tag{7}\\
P_{a, b, c}^{123} & =\mathbb{P}\left(X_{1} \in \Xi_{a}^{1}, X_{2} \in \Xi_{b}^{2}, X_{3} \in \Xi_{c}^{3}\right)=\sum_{m=1}^{M} \pi^{m} p_{a}^{1 m} p_{b}^{2 m} p_{c}^{3 m} \tag{8}
\end{align*}
$$

Arrange the $p^{j m}$, s into two $M \times M$ matrices as

$$
L_{j}=\left[\begin{array}{ccc}
p_{1}^{j 1} & \cdots & p_{M}^{j 1}  \tag{9}\\
\vdots & \ddots & \vdots \\
p_{1}^{j M} & \cdots & p_{M}^{j M}
\end{array}\right], \quad j=1,2
$$

The $m$ th row of $L_{j}$ represents the distribution function of $X_{j}$ conditional on being from the $m$ th subpopulation. Define, for $h \in\{1, \ldots, M\}$, two $M \times M$ matrices as

$$
P=\left[\begin{array}{ccc}
P_{1,1}^{12} & \cdots & P_{1, M}^{12}  \tag{10}\\
\vdots & \ddots & \vdots \\
P_{M, 1}^{12} & \cdots & P_{M, M}^{12}
\end{array}\right], \quad P_{h}=\left[\begin{array}{ccc}
P_{1,1, h}^{123} & \cdots & P_{1, M, h}^{123} \\
\vdots & \ddots & \vdots \\
P_{M, 1, h}^{123} & \cdots & P_{M, M, h}^{123}
\end{array}\right]
$$

Define $V=\operatorname{diag}\left(\pi^{1}, \ldots, \pi^{M}\right)$ and $D_{h}=\operatorname{diag}\left(p_{h}^{31}, \ldots, p_{h}^{3 M}\right)$. Then $P$ and $P_{h}$ are expressed as

$$
\begin{equation*}
P=L_{1}^{\prime} V L_{2}, \quad P_{h}=L_{1}^{\prime} D_{h} V L_{2}=L_{1}^{\prime} V D_{h} L_{2} . \tag{11}
\end{equation*}
$$

The following proposition and corollary provide a sufficient condition for nonparametrically identifying $L_{1}, L_{2}, V$, and $D_{h}$. Here, $P$ and $P_{h}$ are functions of the observables, while $L_{1}, L_{2}$, $V$, and $D_{h}$ are unknowns. The restrictions from $P$ alone are not sufficient to determine $L_{1}, L_{2}$ and $V$ uniquely - additional information from $P_{h}$ enables the identification.

Proposition 2 Suppose $P$ is nonsingular and we can find $h$ such that the characteristic roots of $P_{h} P^{-1}$ are distinct. Then $L_{1}, L_{2}, D_{h}$, and $V$ are uniquely determined from $P$ and $P_{h}$.

Corollary 1 Suppose $L_{1}$ and $L_{2}$ are nonsingular and that there exists $h$ such that $p_{h}^{3 m} \neq p_{h}^{3 n}$ for any $m \neq n$. Then, $L_{1}, L_{2}, D_{h}$, and $V$ are uniquely determined from $P$ and $P_{h}$.

Once $L_{1}$ and $V$ are identified, we can identify

$$
p_{S}^{3 m}=\mathbb{P}\left(X_{3} \in S \mid X_{3} \text { is from the } m \text { th subpopulation }\right)
$$

for any subset $S$ of $\mathcal{X}_{3}$. To see why, define $P_{a, S}^{13}=\mathbb{P}\left(X_{1} \in \Xi_{a}^{1}, X_{3} \in S\right)=\sum_{m=1}^{M} \pi^{m} p_{a}^{1 m} p_{S}^{3 m}$, and

$$
P_{S}=\left[\begin{array}{c}
P_{1, S}^{13} \\
\vdots \\
P_{M, S}^{13}
\end{array}\right], \quad L_{S}=\left[\begin{array}{c}
p_{S}^{31} \\
\vdots \\
p_{S}^{3 M}
\end{array}\right]
$$

Then, $P_{S}=L_{1}^{\prime} V L_{S}$ holds, and $L_{S}$ is determined uniquely by $L_{S}=V^{-1}\left(L_{1}^{\prime}\right)^{-1} P_{S}$. Using the same argument, we can identify $p_{S}^{j m}$ for any subset $S$ of $\mathcal{X}_{j}$ for $j=1,2$.

## Remark 1

1. Identification requires both $L_{1}$ and $L_{2}$ to be nonsingular. Therefore, for identifying $M$ components, all the elements of $X$ need to take at least $M$ distinct values. If $X$ is continuously distributed, it is possible to identify as many components as desired.
2. The sufficient condition of Proposition 2 relaxes the identification condition by Hall et al. (2005), which requires $k \geq k_{M}=(1+o(M)) 6 M \log (M)$ as $M$ increases. As long as $X$ has sufficient variation, and $L_{1}$ and $L_{2}$ are nonsingular, $k=3$ suffices for identification.
3. Hall and Zhou (2003, section 4.2) show the nonparametric non-identifiability of the following model with a continuously distributed random effect: $\psi(x)=\int\left\{\prod_{j=1}^{k} F_{j}\left(x_{j} \mid \lambda\right)\right\} \phi(\lambda) d \lambda$, where $\phi$ is the density of the random effect $\Lambda$, and $F_{j}\left(x_{j} \mid \lambda\right)$ is the distribution function of $X_{j}$ conditional on the realization $\lambda$ of $\Lambda$. Our results show that, if the random effect has a discrete distribution with finite support, then it is possible to nonparametrically identify $F_{j}\left(x_{j} \mid \lambda\right)$, and the distribution function of the random effect.
4. Hettmansperger and Thomas (2000) analyze nonparametric identification and inference of the model (5) with conditionally iid marginals $\left(F^{1 m}\left(x_{1}\right)=\cdots=F^{k m}\left(x_{k}\right)\right)$ by defining $Y=\sum_{j=1}^{k} 1\left\{X_{j} \leq c\right\}$, and reducing the data to a mixture of binomials. Cruz-Medina et al. (2004) consider splitting the support of $X_{j}$ further and reducing the data to a mixture of multinomials. In both cases, identification requires $k \geq 2 M-1$. Our results imply that treating each $X_{j}$ separately, and not reducing the data help identification.
5. When $k \geq 4$, and $X$ can be decomposed into $k^{\prime} \geq 3$ conditionally independent subvectors, we can apply Proposition 2 to these subvectors. For example, assume $k$ is odd, let $Z_{1}=\left(X_{1}, \ldots, X_{(k-1) / 2}\right), Z_{2}=\left(X_{(k-1) / 2+1}, \ldots, X_{k-1}\right)$, and assume $Z_{1}, Z_{2}$, and $X_{k}$ are independent conditional on belonging to a subpopulation. Partition the support of $Z_{1}, Z_{2}$, and $X_{k}$ to construct $P$ and $P_{h}$. When the $X_{j}$ 's have $J$ distinct support points, it is possible to identify up to $J^{(k-1) / 2}$ components.

The proof of Proposition 2 uses a similar idea to that of Proposition 1 of Kasahara and Shimotsu (2007), which in turn is developed starting from the contributions to the analysis of latent class models by Anderson (1954) and Gibson (1955).

In some cases, we have an access to two different samples with different mixing probabilities but the same component distributions. The distribution function of the first and second sample is respectively given by,

$$
F(x)=\sum_{m=1}^{M} \pi^{m} \prod_{j=1}^{k} F^{j m}\left(x_{j}\right), \quad \bar{F}(x)=\sum_{m=1}^{M} \bar{\pi}^{m} \prod_{j=1}^{k} F^{j m}\left(x_{j}\right) .
$$

For example, suppose we have the results of $k$ diagnostic tests from two different groups of patients, whose disease status is unknown. The fraction of patients with disease ( $m=1$ ) differs across two groups of patients, so $\pi^{1} \neq \bar{\pi}^{1}$. But the distributions of the test outcomes are the same across groups once one conditions on the true disease status, so that the $F^{j m}\left(x_{j}\right)$ 's are common.

In this case, we may nonparametrically identify the model even when $k=2$. Define $V=\operatorname{diag}\left(\pi^{1}, \ldots, \pi^{M}\right)$ and $\bar{V}=\operatorname{diag}\left(\bar{\pi}^{1}, \ldots, \bar{\pi}^{M}\right)$, and consider a decomposition similar to (11): $P=L_{1}^{\prime} V L_{2}$ and $\bar{P}=L_{1}^{\prime} \bar{V} L_{2}$. It follows that $P(\bar{P})^{-1}=L_{1}^{\prime} V(\bar{V})^{-1}\left(L_{1}^{\prime}\right)^{-1}$. Consequently, $V(\bar{V})^{-1}$ and $L_{1}^{\prime}$ are identified with the characteristic roots and characteristic vectors of $P(\bar{P})^{-1}$. Similarly, the characteristic vectors of $\bar{P} P^{-1}$ identify $L_{2}$, and we in turn identify $V$ and $\bar{V}$. This result is useful in the context of diagnostic tests (cf., Hall and Zhou, 2003), making it possible to determine the distributional properties of diagnostic tests even when only two tests are available.

## 4 Identifying the number of components

In this section, we provide a sufficient condition to nonparametrically identify the number of mixture components, $M$. Section 4.1 analyzes a general case while Section 4.2 studies binomial mixtures.

### 4.1 General case

In this subsection, we provide a sufficient condition to nonparametrically identify $M$ when the distribution function of $X$ is given by (5). Here, we are interested in identifying $M$, but not the component distributions such as $F^{j m}\left(x_{j}\right)$. The requirement in $k$ becomes weaker than in Section 3: it is possible to identify $M$ even when $k=2$.

Let $R_{1}$ and $R_{2}$ be integers such that $R_{1}, R_{2} \geq M$. We may set $R_{1}$ and $R_{2}$ to be the same, but it is not necessary to do so. For each $j=1,2$, consider a partition of $\mathcal{X}_{j}$ into $R_{j}$ subsets, $\Xi_{1}^{j}, \ldots, \Xi_{R_{j}}^{j}$. Following (6)-(7), define $p_{a}^{1 m}, p_{b}^{2 m}$ and $P_{a, b}^{12}$ for $a=1, \ldots, R_{1}$, and $b=1, \ldots, R_{2}$. Arrange $p_{a}^{1 m}$ 's and $p_{b}^{2 m}$ 's into $M \times R_{1}$ and $M \times R_{2}$ matrices as

$$
L_{1}^{*}=\left[\begin{array}{ccc}
p_{1}^{11} & \cdots & p_{R_{1}}^{11}  \tag{12}\\
\vdots & \ddots & \vdots \\
p_{1}^{1 M} & \cdots & p_{R_{1}}^{1 M}
\end{array}\right], \quad L_{2}^{*}=\left[\begin{array}{ccc}
p_{1}^{21} & \cdots & p_{R_{2}}^{21} \\
\vdots & \ddots & \vdots \\
p_{1}^{2 M} & \cdots & p_{R_{2}}^{2 M}
\end{array}\right] .
$$

Arrange $P_{a b}^{12}$ 's into a $R_{1} \times R_{2}$ matrix as

$$
P^{*}=\left[\begin{array}{ccc}
P_{1,1}^{12} & \cdots & P_{1, R_{2}}^{12}  \tag{13}\\
\vdots & \ddots & \vdots \\
P_{R_{1}, 1}^{12} & \cdots & P_{R_{1}, R_{2}}^{12}
\end{array}\right]
$$

The intuition behind our identification result is simple. Suppose there is only one component, so that $M=1$. Then, the joint distribution of $X_{1}$ and $X_{2}$ is a product of their marginal distributions, and we have $P^{*}=\left(L_{1}^{*}\right)^{\prime} L_{2}^{*}$. Consequently, the rank of $P^{*}$ equals one, which is the number of components. For $M \geq 2$, we may write $P^{*}$ as $P^{*}=\left(L_{1}^{*}\right)^{\prime} V L_{2}^{*}$. Then, the rank of $P^{*}$ provides information on the rank of $L_{1}^{*}$ and $L_{2}^{*}$, which is related to the number of components in our finite mixture model.

Proposition 3 Define $L_{1}^{*}$ and $L_{2}^{*}$ as in (12), and define $P^{*}$ as in (13). Then $M \geq \operatorname{rank}\left(P^{*}\right)$. Furthermore, if both $L_{1}^{*}$ and $L_{2}^{*}$ have rank $M$, then $M=\operatorname{rank}\left(P^{*}\right)$.

The rank of $P^{*}$ corresponds to the number of nonparametrically identifiable components from the joint distribution of $X_{1}$ and $X_{2}$. When $L_{1}^{*}$ has only rank $M-1$, then two components have the same marginal distribution for $X_{1}$ with respect to the partition $\Xi_{1}^{1}, \ldots, \Xi_{R_{1}}^{1}$. Consequently,
the variation of $X_{1}$ is not sufficient to identify $M$. The proof of Proposition 3 is essentially the same as the proof of Proposition 3 of Kasahara and Shimotsu (2007), but we provide it in the Appendix for completeness.

When $k \geq 3$, we can group variables into two groups and apply Proposition 3 , similarly to Remark 1.5. For example, when $k$ is even, we may let $Z_{1}=\left(X_{1}, \ldots, X_{k / 2}\right), Z_{2}=\left(X_{k / 2+1}, \ldots, X_{k}\right)$, and partition the support of $Z_{1}$ and $Z_{2}$ to construct $P^{*}$. Reducing the data into bivariate vectors is another option. For example, as our simulation study illustrates, we may define $Z_{1}=X_{1}+\cdots+X_{k / 2}$ and $Z_{2}=X_{k / 2+1}+\cdots+X_{k}$, and partition the support of $Z_{1}$ and $Z_{2}$ to construct $P^{*}$.

### 4.2 Binomial mixtures

Suppose $X$ follows a mixture of binomial distributions, $B\left(K, p_{m}\right)$, in which $p_{m}$ is the parameter of the $m$ th component distribution:

$$
\begin{equation*}
\mathbb{P}(X=k)=\sum_{m=1}^{M} \pi^{m}\left(1-p_{m}\right)^{K-k} p_{m}^{k}, \quad k=0, \ldots, K \tag{14}
\end{equation*}
$$

where $0<p_{1}<\cdots<p_{M}<1, \pi^{m}>0$, and $\sum_{m=1}^{M} \pi^{m}=1$.
In this subsection, we provide a necessary and sufficient condition to identify $M$. It has been known that $K \geq 2 M-1$ is both necessary and sufficient to identity the parameters of the model, $\left\{\pi^{m}, p^{m}\right\}_{m=1}^{M}$ (Teicher, 1961, 1963; Blischke, 1964). However, little is known about the identifiability of $M$ itself. Provided $K \geq 2 M-1$, it is not clear if we can identify how many components are present in this model. In the following, we show that $M$ is identified as the rank of a matrix of the factorial moments of the data.

Similar to Blischke (1964), define the $k$ th (normalized) population factorial moment as

$$
f(k)=E\left[\frac{X(X-1) \cdots(X-k+1)}{K(K-1) \cdots(K-k+1)}\right]
$$

for $k=1, \ldots, K$, and define $f(0)=1$. Then, as shown in Blischke $(1962,1964)$,

$$
f(k)=\sum_{m=1}^{M} \pi^{m} p_{m}^{k}
$$

Let $K^{*}$ be an even number no larger than $K$. Define the following $\left(K^{*} / 2+1\right) \times\left(K^{*} / 2+1\right)$
matrix

$$
P_{B}=\left[\begin{array}{cccc}
f(0) & f(1) & \cdots & f\left(K^{*} / 2\right)  \tag{15}\\
f(1) & f(2) & \cdots & f\left(K^{*} / 2+1\right) \\
\vdots & \vdots & \ddots & \vdots \\
f\left(K^{*} / 2\right) & f\left(K^{*} / 2+1\right) & \cdots & f\left(K^{*}\right)
\end{array}\right],
$$

as well as $V=\operatorname{diag}\left(\pi^{1}, \ldots, \pi^{M}\right)$ and $^{1}$

$$
L_{B}=\left[\begin{array}{cccc}
1 & p_{1} & \cdots & p_{1}^{K^{*} / 2} \\
\vdots & \vdots & & \vdots \\
1 & p_{M} & \cdots & p_{M}^{K^{*} / 2}
\end{array}\right]
$$

Then, it follows that $P_{B}=L_{B}^{\prime} V L_{B}$, and the rank of $P_{B}$ provides the information on $M$ via the rank of $L_{B}$. Using an analogous argument to the proof of Proposition 3, we obtain the following corollary that identifies $M$. Its proof can be found in the Appendix.

Corollary 2 Suppose $X$ follows (14), and assume $K^{*} \geq 2 M-2$. Define $P_{B}$ as in (15). Then $M=\operatorname{rank}\left(P_{B}\right)$.

Note that the condition on $K$ is $K^{*} \geq 2 M-2$. This condition is weaker than $K \geq 2 M-1$, the necessary and sufficient condition for identifying $\left\{\pi^{m}, p^{m}\right\}_{m=1}^{M}$. Hence, in order to identify only $M$, we need one less variation in $X$.

## 5 Testing the number of identifiable components

Proposition 3 shows that the rank of $P^{*}$ gives the lower bound of the number of mixture components. If, in addition, both $L_{1}^{*}$ and $L_{2}^{*}$ have rank $M$, then the rank of $P^{*}$ equals the number of components. Therefore, we may test the (lower bound of the) number of components by estimating $P^{*}$ and testing its rank.

Several statistics for testing the rank of a matrix have been proposed: the LDU decompositionbased statistic by Gill and Lewbel (1992) and Cragg and Donald (1996), the minimum chisquared type statistic by Cragg and Donald (1997), the characteristic root-based statistics by Robin and Smith (2000), and the statistics using the singular value decomposition by Kleibergen and Paap (2006). We use the test statistic by Robin and Smith (2000), because it does not need the covariance matrix of the estimate of the matrix to be of full rank.

In the following, we review the statistic by Robin and Smith (2000), and discuss two procedures to estimate the rank of a matrix: sequential hypothesis testing, and a model selection approach.

[^1]
### 5.1 Statistic by Robin and Smith (2000)

Let $B$ be a $p \times q$ matrix with $p \geq q$. The matrix $B$ corresponds to $P^{*}$ or $P_{B}$ in Section 4 . Suppose the rank of $B$ is $r_{0}$, where $0 \leq r_{0}<q$. Our interest is to estimate $r_{0}$ and test $H_{0}$ : $\operatorname{rank}(B)=r_{0}$ against $H_{1}: \operatorname{rank}(B)>r_{0}$, using a consistent estimate of $B$.

The procedure by Robin and Smith (2000) is based on the estimates of the characteristic roots of $B B^{\prime}$. Let $\lambda_{1} \geq \cdots \geq \lambda_{r_{0}}>0$ and $\lambda_{r_{0}+1}=\cdots=\lambda_{p}=0$ denote the ordered characteristic roots of $B B^{\prime}$. Let $c_{i}$ denote the characteristic vector of $B B^{\prime}$ associated with $\lambda_{i}$, and collect them into a $p \times p$ matrix $C=\left(c_{1}, \ldots, c_{p}\right)$. For $0 \leq r<p$, partition $C$ as $C=\left(C_{r}, C_{p-r}\right)$, where $C_{r}=\left(c_{1}, \ldots, c_{r}\right)$ and $C_{p-r}=\left(c_{r+1}, \ldots, c_{p}\right)$. An alternative representation for the characteristic roots $\lambda_{1} \geq \cdots \geq \lambda_{r_{0}}>0$ and $\lambda_{r_{0}+1}=\cdots=\lambda_{q}=0$ is obtained as the ordered characteristic roots of $B^{\prime} B$. Let $d_{i}$ denote the characteristic vector of $B^{\prime} B$ associated with $\lambda_{i}$, and collect them into a $q \times q$ matrix $D=\left(d_{1}, \ldots, d_{q}\right)$. For $0 \leq r<q$, partition $D$ as $D=\left(D_{r}, D_{q-r}\right)$, where $D_{r}=\left(d_{1}, \ldots, d_{r}\right)$ and $D_{q-r}=\left(d_{r+1}, \ldots, d_{q}\right)$. For unique characteristic roots, the corresponding characteristic vectors are identified up to a normalization of its length, whereas for multiple roots, including zero roots, the corresponding characteristic vectors are identified up to an orthonormal matrix of dimension equal to the multiplicity of the roots.

Let $\hat{B}$ be a root- $N$ consistent estimator of $B$. The test statistic by Robin and Smith (2000) is based on the characteristic roots of $\hat{B} \hat{B}^{\prime}$. Let $\hat{\lambda}_{1} \geq \cdots \geq \hat{\lambda}_{p}$ be the ordered characteristic roots of $\hat{B} \hat{B}^{\prime}$. Robin and Smith (2000) consider the following test statistic:

$$
C R T(r)=N \sum_{i=r+1}^{q} \hat{\lambda}_{i} .
$$

Following Robin and Smith (2000), we introduce the following assumptions:
Assumption $2 \sqrt{N} \operatorname{vec}(\hat{B}-B) \rightarrow{ }_{d} N(0, \Omega)$ where $\Omega$ is finite and rank $s, 0<s \leq p q$.
Assumption 3 If $r_{0}<q \leq p$, the $\left(p-r_{0}\right)\left(q-r_{0}\right) \times\left(p-r_{0}\right)\left(q-r_{0}\right)$ matrix $\left(D_{q-r_{0}} \otimes\right.$ $\left.C_{p-r_{0}}\right)^{\prime} \Omega\left(D_{q-r_{0}} \otimes C_{p-r_{0}}\right)$ is nonzero; that is, $r k\left[\left(D_{q-r_{0}} \otimes C_{p-r_{0}}\right)^{\prime} \Omega\left(D_{q-r_{0}} \otimes C_{p-r_{0}}\right)\right]>0$.

Assumption 4 There exists $\hat{\Omega}$ such that $\hat{\Omega} \rightarrow_{p} \Omega$.
Assumption 3 requires that at least one column of $D_{q-r_{0}} \otimes C_{p-r_{0}}$ is not in the null space of $\Omega$. If $\Omega$ has full rank, this assumption is automatically satisfied. Assumption 3 is a weak assumption, and we expect it to hold in most cases we consider. ${ }^{2}$ However, in general, this assumption is empirically nonverifiable without an explicit knowledge of $\Omega$ and $D_{q-r_{0}} \otimes C_{p-r_{0}}$.

Robin and Smith (2000) derive the asymptotic distribution of $C R T\left(r_{0}\right)$ when $r_{0}<q$ :

[^2]Proposition 4 (Robin and Smith, 2000, Theorem 3.2 and Corollary 3.2) If $r_{0}<q$ and Assumptions 2-3 hold, $C R T\left(r_{0}\right)$ has an asymptotic distribution described by $\sum_{i=1}^{t} \gamma_{i} Z_{i}^{2}$, where $t \leq \min \left\{s,\left(p-r_{0}\right)\left(q-r_{0}\right)\right\}$, and $\gamma_{1} \geq \cdots \geq \gamma_{t}$ are the nonzero ordered characteristic roots of the matrix $\left(D_{q-r_{0}} \otimes C_{p-r_{0}}\right)^{\prime} \Omega\left(D_{q-r_{0}} \otimes C_{p-r_{0}}\right)$, and $\left\{Z_{i}\right\}_{i=1}^{t}$ are independent standard normal variates.

Let $\hat{C}$ and $\hat{D}$ be the estimates of $C$ and $D$ derived from $\hat{B}$, and let $\hat{\gamma}_{i}$ be the estimate of $\gamma_{i}$ constructed from $\hat{C}, \hat{D}$ and $\hat{\Omega}$. Robin and Smith (2000, Theorem 4.1) show that we can estimate the asymptotic distribution function of $C R T\left(r_{0}\right)$ consistently by $\hat{F}_{r_{0}}^{C R T}(\cdot)$, the distribution function of $\sum_{i=1}^{\left(p-r_{0}\right)\left(q-r_{0}\right)} \hat{\gamma}_{i} Z_{i}^{2}$. We can approximate this distribution function to any desired degree by simulations, and test $H_{0}: \operatorname{rank}(B)=r_{0}$ against $H_{1}: \operatorname{rank}(B)>r_{0}$.

### 5.2 Sequential hypothesis testing

We now discuss estimation of $r_{0}$. Robin and Smith (2000) consider sequential hypothesis testing: we sequentially test $H_{0}: \operatorname{rank}(B)=r$ against $H_{1}: \operatorname{rank}(B)>r$ for $r=0,1, \ldots, q,{ }^{3}$ and stop at the first value for $r$ that leads to a nonrejection of $H_{0} .{ }^{4}$ By allowing the significance level of the test to change with the sample size $N$, it is possible to estimate $r_{0}$ consistently. For $r=0, \ldots, q$, let $\hat{c}_{1-\alpha_{N}}^{r}$ denote the $100\left(1-\alpha_{N}\right)$ percentile of the $\operatorname{cdf} \hat{F}_{r}^{C R T}(\cdot)$, and define

$$
\begin{equation*}
\hat{r}=\min _{r \in\{0, \ldots, q\}}\left\{r: C R T(r) \geq \hat{c}_{1-\alpha_{N}}^{i}, i=0, \ldots, r-1, C R T(r)<\hat{c}_{1-\alpha_{N}}^{r}\right\} . \tag{16}
\end{equation*}
$$

By letting $\alpha_{N}$ go to zero at a sufficiently slow rate as the sample size increases, $\hat{r}$ converges to the rank of $B$.

Proposition 5 (Robin and Smith, 2000, Theorem 5.2) If the conditions of Proposition 4 and Assumption 4 hold, and if $\alpha_{N}=o(1)$ and $-N^{-1} \ln \alpha_{N}=o(1)$ as $N \rightarrow \infty$, then $\hat{r}-r_{0}=o_{p}(1)$.

### 5.3 Model selection procedure

We propose to employ a model selection procedure to estimate $r_{0}$ consistently. Consider the following criterion function

$$
S(r)=C R T(r)-f(N) g(r),
$$

where $g(r)$ is a (possibly stochastic) penalty function, which is bounded in probability. Define

$$
\tilde{r}=\underset{1 \leq r \leq q}{\arg \min } S(r) .
$$

Under a standard condition on $f(N)$ and $g(N)$, this gives a consistent estimate of $r_{0}$ :

[^3]Proposition 6 Suppose that $f(N) \rightarrow \infty, f(N) / N \rightarrow 0$, and $\mathbb{P}\left(g(r)-g\left(r_{0}\right)<0\right) \rightarrow 1$ for all $r>r_{0}$ as $N \rightarrow \infty$. Then $\tilde{r} \rightarrow p r_{0}$.

If the asymptotic distribution of $S\left(r_{0}\right)$ were chi-squared with $\left(p-r_{0}\right)\left(q-r_{0}\right)$ degrees of freedom, then using $f(N)=1$ and $g(r)=2(p-r)(q-r)$ would give an AIC-type criterion, while using $f(N)=\log (N)$ and $g(r)=(p-r)(q-r)$ would give a BIC-type criterion.

In light of the non-standard asymptotic distribution of $\operatorname{CRT}\left(r_{0}\right)$, we propose the following penalty function $g(r)$ for a BIC-type criterion:

$$
\begin{equation*}
g(r)=(p-r)(q-r) \bar{\gamma}(r) \tag{17}
\end{equation*}
$$

where $\bar{\gamma}(r)=\frac{\sum_{i=1}^{(p-r)(q-r)} \hat{\gamma}_{i}}{(p-r)(q-r)}$ is the average of the characteristic roots of $\left(\hat{D}_{q-r} \otimes \hat{C}_{p-r}\right)^{\prime} \hat{\Omega}\left(\hat{D}_{q-r} \otimes\right.$ $\hat{C}_{p-r}$ ). In an AIC-type criterion, $g(r)$ is multiplied by 2 . The term $\bar{\gamma}(r)$ in (17) makes our model selection procedure invariant to a rescaling of $B .{ }^{5}$ Further, the asymptotic distribution of $C R T\left(r_{0}\right) / \bar{\gamma}\left(r_{0}\right)$ has the same mean as a chi-squared random variable with $\left(p-r_{0}\right)\left(q-r_{0}\right)$ degrees of freedom.

To apply Proposition 6 with $g(r)$ defined in (17), we need additional assumptions to guarantee that $g(r)$ becomes strictly decreasing in $r$ as $N \rightarrow \infty$. Using the relation $\operatorname{tr}(A B)=\operatorname{tr}(B A)$, and the properties of the Kronecker product, we obtain

$$
\begin{align*}
g(r)-g(r+1)= & \operatorname{tr}\left[\left(\hat{d}_{r+1} \otimes \hat{c}_{r+1}\right)^{\prime} \hat{\Omega}\left(\hat{d}_{r+1} \otimes \hat{c}_{r+1}\right)\right]+\sum_{j=r+2}^{p} \operatorname{tr}\left[\left(\hat{d}_{r+1} \otimes \hat{c}_{j}\right)^{\prime} \hat{\Omega}\left(\hat{d}_{r+1} \otimes \hat{c}_{j}\right)\right] \\
& +\sum_{i=r+2}^{q} \operatorname{tr}\left[\left(\hat{d}_{i} \otimes \hat{c}_{r+1}\right)^{\prime} \hat{\Omega}\left(\hat{d}_{i} \otimes \hat{c}_{r+1}\right)\right] \tag{18}
\end{align*}
$$

Since $\hat{\Omega}$ is positive semidefinite, it follows that $g(r)$ is nonincreasing in $r$. $g(r)$ becomes strictly decreasing as $N \rightarrow \infty$ if the right hand side of (18) becomes strictly positive for any $r$. This holds, for example, if $\left(d_{r} \otimes c_{r}\right)^{\prime} \Omega\left(d_{r} \otimes c_{r}\right)>0$ for $1 \leq r \leq q$, or if for any $1 \leq r \leq q$ there exists a pair $(i, j)$ such that $\left(d_{i} \otimes c_{j}\right)^{\prime} \Omega\left(d_{i} \otimes c_{j}\right)>0$ where $r+1 \leq i \leq p$ and $r+1 \leq j \leq q$.

## 6 Simulation study

### 6.1 General case: an example with normal mixtures

We conduct Monte Carlo simulation experiments with normal mixtures to assess the finite sample performance of our proposed procedures for selecting the number of components. The

[^4]reported results are based on 10,000 simulated samples. Regarding the number of components, we experiment with $M=2$ and 3 .

While the simulated DGP is a parametric (normal) model, our selection procedures do not assume the knowledge of parametric structures. We partition the support of $X_{j}$ into $R_{j}$ subsets such that $\mathbb{P}\left(X_{j} \in \Xi_{l}^{j}\right)=1 / R_{j}$ for $l=1, \ldots, R_{j}$. Specifically, let $\bar{x}_{\beta}^{j}$ denote the $\beta$ quantiles of $X_{j}$. Let $\beta_{l}=l / R_{j}$ for $l=0,1, \ldots, R_{j}$, and define $\Xi_{l}^{j}=\left(\bar{x}_{\beta_{l-1}}^{j}, \bar{x}_{\beta_{l}}^{j}\right]$ for $l=1, \ldots, R_{j}-1$ and $\Xi_{R_{j}}^{j}=\left(\bar{x}_{\beta_{R_{j}-1}}, \infty\right)$.

We construct a consistent estimator of the covariance matrix of $\sqrt{N} \operatorname{vec}\left(\hat{P}^{*}-P^{*}\right)$ as follows. With a slight abuse of notation, let $X_{1}, \ldots, X_{N}$ denote $N$ iid draws of $X$, and let $X_{t, j}$ denote the $j$ th element of $X_{t}$. Let $\hat{P}^{*}$ be the empirical distribution estimator of $P^{*}$ : for $a=1, \ldots, R_{1}$ and $b=1, \ldots, R_{2}$, the $(a, b)$ th element of $\hat{P}^{*}$ is $\hat{P}_{a, b}^{* 12}=N^{-1} \sum_{t=1}^{N} 1\left\{X_{t, 1} \in \Xi_{a}^{1}, X_{t, 2} \in \Xi_{b}^{2}\right\}$. Because $\left\{N \hat{P}_{a, b}^{* 12}\right\}_{a=1, \ldots, R_{1}, b=1, \ldots, R_{2}}$ follows a multinomial distribution with the parameter $\left\{P_{a, b}^{* 12}\right\}$, we can easily see

$$
\begin{aligned}
E \hat{P}_{a, b}^{* 12} & =P_{a, b}^{* 12}, \quad \operatorname{var}\left(\hat{P}_{a, b}^{* 12}\right)=P_{a, b}^{* 12}\left(1-P_{a, b}^{* 12}\right) / N, \\
\operatorname{cov}\left(\hat{P}_{a, b}^{* 12}, \hat{P}_{c, d}^{* 12}\right) & =-P_{a, b}^{* 12} P_{c, d}^{* 12} / N, \quad(a, b) \neq(c, d) .
\end{aligned}
$$

Let $\Omega$ denote the $\left(R_{1} R_{2}\right) \times\left(R_{1} R_{2}\right)$ covariance matrix of $\sqrt{N} \operatorname{vec}\left(\hat{P}^{*}-P^{*}\right)$. Note that the rank of $\Omega$ is $R_{1} R_{2}-1$ because $\sum_{a=1}^{R_{1}} \sum_{b=1}^{R_{2}} \hat{P}_{a, b}^{* 12}=1$. Let $\theta=\operatorname{vec}\left(P^{*}\right)$, then the $i$ th diagonal element of $\Omega$ is given by $\theta_{i}\left(1-\theta_{i}\right)$, and the $(i, j)$ th off-diagonal element of $\Omega$ is given by $-\theta_{i} \theta_{j}$.

We first consider a bivariate normal mixture

$$
\begin{equation*}
F(x)=\sum_{m=1}^{M} \pi^{m} F^{m}(x) \tag{19}
\end{equation*}
$$

where $x=\left(x_{1}, x_{2}\right)^{\prime}$, and $F^{m}(x)$ is $N_{2}\left(\mu^{m}, I\right)$. We set $\mu^{1}=(0,0)^{\prime}$ and $\mu^{2}=(2.0,1.0)^{\prime}$ for $M=2$. For $M=3$, we set, in addition, $\mu^{3}=(4.0,3.0)^{\prime}$. The mixing probabilities are equal across subpopulations, so that $\pi^{1}=\pi^{2}=1 / 2$ for $M=2$, while $\pi^{1}=\pi^{2}=\pi^{3}=1 / 3$ for $M=3$. $R_{1}$ and $R_{2}$ are chosen to $R_{1}=R_{2}=M+1 .{ }^{6}$ In simulations, we use the sample quantiles of $X_{j}$ 's to determine the boundaries of $\Xi_{l}^{j}$. This introduces additional variation, and may affect the asymptotic distribution of $C R T(r)$ statistic, but the consistency of our procedure is not affected. We experimented bootstrapping $C R T(r)$ statistic, however it did not improve the results substantially.

Table 1 reports the result of experiments when the data is generated from the model with two components $(M=2)$. For the sequential hypothesis testing procedure (SHT), the smaller the significance level $\alpha$ is, the more likely the procedure underestimates the number of components. The performance of the SHT improves at all the significance levels as the sample size increases.

[^5]Furthermore, the "optimal" choice of significance level, i.e., $\alpha$ that selects $M=2$ most frequently, decreases from 0.1 to 0.05 , and then to 0.01 as the sample size increases from $N=50$ to 200 , and then to 1000, respectively. These results are in agreement with Proposition 5. Overall, the SHT performs well in reasonably sized samples. The performance of BIC is somewhat disappointing, despite its theoretic superiority to the AIC.

The lower two panels of Table 1 report the performance of the AIC and BIC. With a small sample size of $N=50$, the AIC performs better than the SHT. With a larger sample size of $N=200$ however, the AIC substantially overestimates the number of components, highlighting its inconsistency. On the other hand, the BIC performs worse than both the SHT and AIC when $N=50$, but the performance of BIC is comparable to that of the SHT when $N=1000$.

Table 2 reports the simulation results when the data is generated from the model with three components $(M=3)$. The overall pattern is similar to Table 1 , but the tendency to underestimate $M$ is more pronounced. For the SHT and BIC, the frequency of choosing $M=3$ approaches one as the sample size increases. The AIC performs better than the SHT and BIC when $N=100$ and $N=400$, but overestimates the number of components more often than the SHT and BIC when $N=2000$.

Next, we consider a trivariate normal mixture of the form (19) where $x=\left(x_{1}, x_{2}, x_{3}\right)^{\prime}$ and $F^{m}(x)$ is $N_{3}\left(\mu^{m}, I\right)$. To apply our selection procedure to trivariate mixtures, we group the second and the third variables into one group as $Z_{2}=\left(X_{2}, X_{3}\right)^{\prime}$. We consider a partition of $\mathcal{X}_{1}$ into $R_{1}=M+1$ subsets while $\mathcal{X}_{2}$ and $\mathcal{X}_{3}$ are partitioned into $R_{2}=R_{3}=M$ subsets and, thus, the support of $Z_{2}$ is partitioned into $M^{2}$ subsets. ${ }^{7}$ For instance, for the model with two components, we estimate the rank of the following matrix (see (13)):

$$
P^{*}=\left[\begin{array}{llll}
P_{1,(1,1)} & P_{1,(1,2)} & P_{1,(2,1)} & P_{1,(2,2)} \\
P_{2,(1,1)} & P_{2,(1,2)} & P_{2,(2,1)} & P_{2,(2,2)} \\
P_{3,(1,1)} & P_{3,(1,2)} & P_{3,(2,1)} & P_{3,(2,2)}
\end{array}\right],
$$

where $P_{a,(b, c)}=\mathbb{P}\left(X_{1} \in \Xi_{a}^{1}, Z_{2} \in \Xi_{b}^{2} \times \Xi_{c}^{3}\right)$.
Table 3 shows the result of trivariate mixtures for a two-components model. ${ }^{8}$ We set the first two variables, $\left(X_{1}, X_{2}\right)$, to have the same distribution as the bivariate case, thus $\mu^{1}=(0,0)^{\prime}$ and $\mu^{2}=(2.0,1.0)^{\prime}$. We experiment with two different distributions of $X_{3}$. The first panel of Table 3 reports the case where $X_{3}$ has the same distribution as $X_{2}$, i.e., $E\left[X_{3} \mid m=1\right]=0$ and $E\left[X_{3} \mid m=2\right]=1$. Comparing the first panel of Table 3 with Table 1, we find that the our selection procedures perform better with trivariate mixtures than with bivariate mixtures across different procedures and sample sizes. Thus, the additional information from the third variable can improve the performance of our selection procedures.

[^6]This is not necessarily the case, however, when the third variable contains little information for distinguishing different subpopulations. The second panel of Table 3 reports the case in which the distribution of the third variable similar across different subpopulations; specifically, $E\left[X_{3} \mid m=1\right]=0$ and $E\left[X_{3} \mid m=2\right]=0.5$. Comparing them with the result of Table 1, we notice that our procedure performs worse with trivariate mixtures than with bivariate mixtures in these cases.

Instead of grouping the second and third variables into one group as $Z_{2}=\left(X_{2}, X_{3}\right)^{\prime}$, we may consider a sum of the second and the third variables: $Z_{2}=X_{2}+X_{3}$. The results are reported in Table 4. Comparing it with the result of Table 1, our procedure now performs better with trivariate mixtures than with bivariate mixtures even under the assumption that $E\left[X_{3} \mid m=1\right]=0$ and $E\left[X_{3} \mid m=2\right]=0.5$. In this case, the means of both $X_{2}$ and $X_{3}$ are higher when $m=2$ than when $m=1$ and, as a result, the information for distinguishing different subpopulations is augmented by summing up $X_{2}$ and $X_{3}$.

We have to be cautious, however, of applying this method blindly because it is possible that the summation operation could reduce the information for distinguishing different subpopulations. The second panel of Table 4 illustrates this point under the alternative assumption that $E\left[X_{3} \mid m=1\right]=0.5$ and $E\left[X_{3} \mid m=2\right]=0$; in this case, if we use $Z_{2}=X_{2}+X_{3}$ instead of grouping variable $Z_{2}=\left(X_{2}, X_{3}\right)^{\prime}$, our procedure performs worse.

### 6.2 Binomial mixtures

We also conduct Monte Carlo simulations for mixtures of binomial distributions, $B\left(K, p_{m}\right)$, as defined in (14) with $M=2,3$, and 4 . We set $\left(p_{1}, p_{2}\right)=(0.2,0.5),\left(p_{1}, p_{2}, p_{3}\right)=(0.2,0.5,0.9)$, and $\left(p_{1}, p_{2}, p_{3}, p_{4}\right)=(0.05,0.3,0.7,0.95)$ for models with two, three and four components, respectively. The value of $K$ is chosen to $K=2 M$ so that the maximum identifiable number of components is the true number of components plus one. As before, the mixing probabilities are set to equal to each other across subpopulations.

For binomial mixtures, we construct a consistent estimate of $\Omega$ from an estimate of the covariance matrix of the sample factorial moments. Define $\nu(X, k)=\frac{X(X-1) \cdots(X-k+1)}{K(K-1) \cdots(K-k+1)}$ so that $f(k)=E(\nu(X, k))$. We estimate $f(k)$ by $\hat{f}(k)=N^{-1} \sum_{i=1}^{N} \nu\left(X_{i}, k\right)$. Hence, $N \operatorname{cov}(\hat{f}(j), \hat{f}(k))$ is equal to $E(\nu(X, j) \nu(X, k))-E(\nu(X, j)) E(\nu(X, k))$, which is a linear function of $E X, \ldots, E X^{j+k}$ and, thus, can be estimated from sample moments of $X$.

Tables 5, 6, and 7 show the results for models with two, three, and four components, respectively. Across three different models, as the sample size increases, the frequency to select the true number of components approaches one in the SHT and BIC; on the other hand, the AIC tends to overestimate the true number of components. It is also seen that a relatively large number of observations is required to estimate $M$ accurately when $M$ is large.

## 7 Appendix

### 7.1 Proof of Proposition 1

First, note that, if the joint distribution function of $\left(X_{1}, X_{2}\right)$ is given by (2) with $k=2$, then the marginal distribution function of $X_{1}$ and $X_{2}$ is given by $F^{1}\left(x_{1}\right)=\pi F^{11}\left(x_{1}\right)+(1-\pi) F^{12}\left(x_{1}\right)$ and $F^{2}\left(x_{2}\right)=\pi F^{21}\left(x_{1}\right)+(1-\pi) F^{22}\left(x_{2}\right)$, respectively. In light of $F\left(x_{1}, x_{2}\right)=\pi F^{11}\left(x_{1}\right) F^{21}\left(x_{2}\right)+$ $(1-\pi) F^{12}\left(x_{1}\right) F^{22}\left(x_{2}\right)$, it follows that

$$
\begin{equation*}
F\left(x_{1}, x_{2}\right)-F^{1}\left(x_{1}\right) F^{2}\left(x_{2}\right)=\pi(1-\pi)\left[F^{11}\left(x_{1}\right)-F^{12}\left(x_{1}\right)\right]\left[F^{21}\left(x_{2}\right)-F^{22}\left(x_{2}\right)\right] . \tag{20}
\end{equation*}
$$

Using the irreducibility, we have, for any $x_{a}, x_{b}, x_{c} \in\left\{\xi_{1}, \ldots, \xi_{J}\right\}$,

$$
F\left(x_{a}, x_{b}\right)-F^{1}\left(x_{a}\right) F^{2}\left(x_{b}\right)=\frac{\left[F\left(x_{a}, x_{c}\right)-F^{1}\left(x_{a}\right) F^{2}\left(x_{c}\right)\right]\left[F\left(x_{c}, x_{b}\right)-F^{1}\left(x_{c}\right) F^{2}\left(x_{b}\right)\right]}{F\left(x_{c}, x_{c}\right)-F^{1}\left(x_{c}\right) F^{2}\left(x_{c}\right)} .
$$

Let $\left(x_{a}, x_{b}, x_{c}\right)=\left(\xi_{i}, \xi_{j}, \xi_{1}\right)$, then

$$
\begin{equation*}
F\left(\xi_{i}, \xi_{j}\right)-F^{1}\left(\xi_{i}\right) F^{2}\left(\xi_{j}\right)=\frac{\left[F\left(\xi_{i}, \xi_{1}\right)-F^{1}\left(\xi_{i}\right) F^{2}\left(\xi_{1}\right)\right]\left[F\left(\xi_{1}, \xi_{j}\right)-F^{1}\left(\xi_{1}\right) F^{2}\left(\xi_{j}\right)\right]}{F\left(\xi_{1}, \xi_{1}\right)-F^{1}\left(\xi_{1}\right) F^{2}\left(\xi_{1}\right)} \tag{21}
\end{equation*}
$$

Since $\tilde{Q}$ satisfies (3) and (4) for $\left(x_{1}, x_{2}\right)=\left\{\left(\xi_{1}, \xi_{1}\right),\left(\xi_{1}, \xi_{i}\right),\left(\xi_{j}, \xi_{1}\right)\right\}$, the relation (20) holds for these pairs of $\left(x_{1}, x_{2}\right)$. Therefore, the right hand side of (21) equals $\tilde{\pi}(1-\tilde{\pi})\left[\tilde{F}^{11}\left(\xi_{i}\right)-\right.$ $\left.\tilde{F}^{12}\left(\xi_{i}\right)\right]\left[\tilde{F}^{21}\left(\xi_{j}\right)-\tilde{F}^{22}\left(\xi_{j}\right)\right]$, and hence $\tilde{Q}$ satisfies (3) for $\left(x_{1}, x_{2}\right)=\left(\xi_{i}, \xi_{j}\right)$. Repeating the above for all pairs of $\left(\xi_{i}, \xi_{j}\right)$ gives the stated result.

### 7.2 Proof of Proposition 2 and Corollary 1

Since $P$ is nonsingular, we can construct a matrix $B_{h}=P_{h} P^{-1}=L_{1}^{\prime} D_{h}\left(L_{1}^{\prime}\right)^{-1}$. Because $B_{h} L_{1}^{\prime}=L_{1}^{\prime} D_{h}$, the characteristic roots of $B_{h}$ determine the diagonal elements of $D_{h}$, and the characteristic vectors of $B_{h}$ determine the columns of $L_{1}^{\prime}$ uniquely up to multiplicative constants. Since $p_{1}^{1 m}+\cdots+p_{M}^{1 m}=1$ for each $m$, each column of $L_{1}^{\prime}$ must sum to one, and hence the columns of $L_{1}^{\prime}$ are uniquely determined. Having determined $L_{1}^{\prime}$, we can recover the rows of $L_{2}$ uniquely up to multiplicative constants from $\left(L_{1}^{\prime}\right)^{-1} P$ because $\left(L_{1}^{\prime}\right)^{-1} P=V L_{2}$. Since $p_{1}^{2 m}+\cdots+p_{M}^{2 m}=1$ for each $m$, each row of $L_{2}$ must sum to one, and hence the rows of $L_{2}$ are uniquely determined. Then $V$ is determined as $V=\left(L_{1}^{\prime}\right)^{-1} P\left(L_{2}\right)^{-1}$.

Corollary 1 is proven by observing that $P$ is nonsingular and the characteristic roots of $P_{h} P^{-1}$ are distinct when the conditions of Corollary 1 are satisfied.

### 7.3 Proof of Proposition 3

Let $V=\operatorname{diag}\left(\pi^{1}, \ldots, \pi^{M}\right)$, then $P^{*}=\left(L_{1}^{*}\right)^{\prime} V L_{2}^{*}$. It follows that $\operatorname{rank}\left(P^{*}\right) \leq \min \left\{\operatorname{rank}\left(L_{1}^{*}\right)\right.$, $\left.\operatorname{rank}\left(L_{2}^{*}\right), \operatorname{rank}(V)\right\}$. Since $\operatorname{rank}(V)=M$, it follows that $\operatorname{rank}\left(P^{*}\right) \leq M$ where the inequality becomes strict when $\operatorname{rank}\left(L_{1}^{*}\right)$ or $\operatorname{rank}\left(L_{2}^{*}\right)$ is smaller than $M$.

When $\operatorname{rank}\left(L_{1}^{*}\right)=\operatorname{rank}\left(L_{2}^{*}\right)=M$, multiplying both sides of $P^{*}=\left(L_{1}^{*}\right)^{\prime} V L_{2}^{*}$ from the right by $\left(L_{2}^{*}\right)^{\prime}\left(L_{2}^{*}\left(L_{2}^{*}\right)^{\prime}\right)^{-1}$ gives $P^{*}\left(L_{2}^{*}\right)^{\prime}\left(L_{2}^{*}\left(L_{2}^{*}\right)^{\prime}\right)^{-1}=\left(L_{1}^{*}\right)^{\prime} V$. There are $M$ linearly independent columns in $\left(L_{1}^{*}\right)^{\prime} V$, because $\left(L_{1}^{*}\right)^{\prime}$ has $M$ linearly independent columns while $V$ is a diagonal matrix with strictly positive elements. Thus, $\operatorname{rank}\left(P^{*}\left(L_{2}^{*}\right)^{\prime}\left(L_{2}^{*}\left(L_{2}^{*}\right)^{\prime}\right)^{-1}\right)=M$. Hence, $M \leq \min \left\{\operatorname{rank}\left(P^{*}\right)\right.$, $\left.\operatorname{rank}\left(L_{2}^{*}\right), \operatorname{rank}\left(L_{2}^{*}\left(L_{2}^{*}\right)^{\prime}\right)^{-1}\right\} \leq \operatorname{rank}\left(P^{*}\right)$, and it follows that $\operatorname{rank}\left(P^{*}\right)=M$.

### 7.4 Proof of Corollary 2

Since $P_{B}=L_{B}^{\prime} V L_{B}$, if follows from the proof of Proposition 3 that $\operatorname{rank}\left(P_{B}\right) \leq M$. In view of the proof of Proposition 3, $\operatorname{rank}\left(P_{B}\right)=M$ follows if we show $\operatorname{rank}\left(L_{B}\right)=M$.

First, $\operatorname{rank}\left(L_{B}\right) \leq M$ because $L_{B}$ is a $M \times\left(K^{*} / 2+1\right)$ matrix. To show $\operatorname{rank}\left(L_{B}\right) \geq M$, first note that the condition $K^{*} \geq 2 M-2$ guarantees that $K^{*} / 2 \geq M-1$. Consider the following $M \times M$ submatrix of $L_{B}$ :

$$
L_{B}^{*}=\left[\begin{array}{cccc}
1 & p_{1} & \cdots & p_{1}^{M-1} \\
\vdots & \vdots & & \vdots \\
1 & p_{M} & \cdots & p_{M}^{M-1}
\end{array}\right]
$$

Since $L_{B}^{*}$ is a Vendermonde matrix, its determinant is given by $\prod_{i<j}\left(p_{j}-p_{i}\right)$, which is nonzero by definition. Hence, $\operatorname{rank}\left(L_{B}^{*}\right)=M$. Since $L_{B}^{*}$ is a submatrix of $L_{B}, \operatorname{rank}\left(L_{B}\right) \geq \operatorname{rank}\left(L_{B}^{*}\right)=M$. It follows that $\operatorname{rank}\left(L_{B}\right)=M$.

### 7.5 Proof of Proposition 6

First, we show $\mathbb{P}\left(\tilde{r}<r_{0}\right) \rightarrow 0$. If $\tilde{r}<r_{0}$, this implies $S(r)<S\left(r_{0}\right)$ for some $r<r_{0}$. Thus $\mathbb{P}\left(\tilde{r}<r_{0}\right) \leq \sum_{r=1}^{r_{0}-1} \mathbb{P}\left(S(r)<S\left(r_{0}\right)\right)$. Now, for any $r<r_{0}$,

$$
\begin{aligned}
\mathbb{P}\left(S(r)<S\left(r_{0}\right)\right) & =\mathbb{P}\left(C R T(r)-C R T\left(r_{0}\right)-f(N) g(r)+f(N) g\left(r_{0}\right)<0\right) \\
& \leq \mathbb{P}\left(N \sum_{i=r+1}^{r_{0}} \hat{\lambda}_{i}+f(N)\left[g\left(r_{0}\right)-g(r)\right]<0\right)
\end{aligned}
$$

This probability tends to 0 as $N \rightarrow \infty$ because $f(N) / N \rightarrow 0$ and $\sum_{i=r+1}^{r_{0}} \hat{\lambda}_{i} \rightarrow_{p} \sum_{i=r+1}^{r_{0}} \lambda_{i}>0$ since the $\lambda_{i}$ 's are continuous functions of the elements of $B$.

Second, we show $\mathbb{P}\left(\tilde{r}>r_{0}\right) \rightarrow 0$. Similarly as above, we have $\mathbb{P}\left(\tilde{r}>r_{0}\right) \leq \sum_{r=r_{0}+1}^{q} \mathbb{P}(S(r)<$
$\left.S\left(r_{0}\right)\right)$. Now, for any $r>r_{0}$,

$$
\mathbb{P}\left(S(r)<S\left(r_{0}\right)\right) \leq \mathbb{P}\left(-N \sum_{i=r_{0}+1}^{r} \hat{\lambda}_{i}+f(N)\left[g\left(r_{0}\right)-g(r)\right]<0\right)
$$

This probability tends to 0 as $N \rightarrow \infty$ because $N \sum_{i=r_{0}+1}^{r} \hat{\lambda}_{i}$ converges to a weighted sum of chi-squared variables, $f(N) \rightarrow \infty$, and $\mathbb{P}\left(g\left(r_{0}\right)-g(r)>0\right) \rightarrow 1$ as $N \rightarrow \infty$.

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Table 1: Selection Frequency for the Number of Components: Bivariate Normal with $M=2$

|  |  | $N=50$ |  | $N=200$ |  | $N=1000$ |  |  |  |  |
| :--- | :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | Significance level $\alpha$ |  | Significance level $\alpha$ |  | Significance level $\alpha$ |  |  |  |  |
|  | .10 | 05 | .01 | .10 | .05 | .01 | .10 | .05 | .01 |  |
| SHT | $M=1$ | 0.4936 | 0.6394 | 0.8544 | 0.0245 | 0.0494 | 0.1528 | 0.0000 | 0.0000 | 0.0000 |
|  | $M=2$ | 0.4480 | 0.3403 | 0.1437 | 0.8896 | 0.9083 | 0.8389 | 0.9023 | 0.9527 | 0.9902 |
|  | $M \geq 3$ | 0.0584 | 0.0203 | 0.0019 | 0.0859 | 0.0423 | 0.0083 | 0.0977 | 0.0473 | 0.0098 |
| AIC | $M=1$ |  | 0.3956 |  |  | 0.0125 |  | 0.0000 |  |  |
|  | $M=2$ |  | 0.5128 |  |  | 0.8474 |  | 0.8448 |  |  |
|  | $M \geq 3$ |  | 0.0916 |  |  | 0.1401 |  | 0.1552 |  |  |
| BIC | $M=1$ |  | 0.7887 |  |  | 0.2807 |  | 0.0000 |  |  |
|  | $M=2$ |  | 0.2010 |  |  | 0.7044 |  | 0.9921 |  |  |
|  | $M \geq 3$ |  | 0.0103 |  |  | 0.0149 |  | 0.0079 |  |  |

Notes: The parameter values are: $\pi^{1}=\pi^{2}=1 / 2, \mu^{1}=(0,0)^{\prime}$ and $\mu^{2}=(2,1)$.

Table 2: Selection Frequency for the Number of Components: Bivariate Normal with $M=3$

|  |  | $N=100$ |  |  | $N=400$ |  |  | $N=2000$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | Significance level $\alpha$ |  |  | Significance level $\alpha$ |  |  | Significance level $\alpha$ |  |  |
|  |  | . 10 | 05 | . 01 | . 10 | . 05 | . 01 | . 10 | . 05 | . 01 |
| SHT | $M=1$ | 0.0000 | 0.0001 | 0.0002 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
|  | $M=2$ | 0.7090 | 0.8184 | 0.9462 | 0.1650 | 0.2590 | 0.5148 | 0.0000 | 0.0000 | 0.0000 |
|  | $M=3$ | 0.2610 | 0.1713 | 0.0522 | 0.7663 | 0.7090 | 0.4811 | 0.9039 | 0.9538 | 0.9900 |
|  | $M \geq 4$ | 0.0300 | 0.0102 | 0.0014 | 0.0687 | 0.0320 | 0.0041 | 0.0961 | 0.0462 | 0.0100 |
| AIC | $M=1$ |  | 0.0000 |  |  | 0.0000 |  |  | 0.0000 |  |
|  | $M=2$ |  | 0.5759 |  |  | 0.0941 |  |  | 0.0000 |  |
|  | $M=3$ |  | 0.3747 |  |  | 0.7935 |  |  | 0.8456 |  |
|  | $M \geq 4$ |  | 0.0494 |  |  | 0.1124 |  |  | 0.1544 |  |
| BIC | $M=1$ |  | 0.0006 |  |  | 0.0000 |  |  | 0.0000 |  |
|  | $M=2$ |  | 0.9453 |  |  | 0.7275 |  |  | 0.0022 |  |
|  | $M=3$ |  | 0.0517 |  |  | 0.2685 |  |  | 0.9920 |  |
|  | $M \geq 4$ |  | 0.0024 |  |  | 0.0040 |  |  | 0.0058 |  |

Notes: The parameter values are: $\pi^{1}=\pi^{2}=\pi^{3}=1 / 3, \mu^{1}=(0,0)^{\prime}, \mu^{2}=(2,1)$, and $\mu^{3}=(4,3)$.

Table 3: Selection Frequency for the Number of Components: Trivariate Normal with $M=2$

| $E\left[x_{3} \mid m=1\right]=0$ and $E\left[x_{3} \mid m=2\right]=1$ |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $N=50$ |  |  | $N=200$ |  |  | $N=1000$ |  |  |
|  |  | Significance level $\alpha$ |  |  | Significance level $\alpha$ |  |  | Significance level $\alpha$ |  |  |
|  |  | . 10 | 05 | . 01 | . 10 | . 05 | . 01 | . 10 | . 05 | . 01 |
| SHT | $M=1$ | 0.3864 | 0.5284 | 0.7809 | 0.0020 | 0.0052 | 0.0298 | 0.0000 | 0.0000 | 0.0000 |
|  | $M=2$ | 0.5448 | 0.4410 | 0.2149 | 0.8942 | 0.9396 | 0.9582 | 0.8880 | 0.9396 | 0.9863 |
|  | $M \geq 3$ | 0.0688 | 0.0306 | 0.0042 | 0.1038 | 0.0552 | 0.0120 | 0.1120 | 0.0604 | 0.0137 |
| AIC | $M=1$ | 0.3084 |  |  | 0.0011 |  |  | 0.0000 |  |  |
|  | $M=2$ | 0.5988 |  |  | 0.8570 |  |  | 0.8501 |  |  |
|  | $M \geq 3$ | 0.0928 |  |  | 0.1419 |  |  | 0.1499 |  |  |
| BIC | $M=1$ | 0.7792 |  |  | 0.1342 |  |  | 0.0000 |  |  |
|  | $M=2$ | 0.2130 |  |  | 0.8600 |  |  | 0.9990 |  |  |
|  | $M \geq 3$ | 0.0078 |  |  | 0.0058 |  |  | 0.0010 |  |  |
| $E\left[x_{3} \mid m=1\right]=0$ and $E\left[x_{3} \mid m=2\right]=0.5$ |  |  |  |  |  |  |  |  |  |  |
|  |  | $N=50$ |  |  | $N=200$ |  |  | $N=1000$ |  |  |
|  |  | Significance level $\alpha$ |  |  | Significance level $\alpha$ |  |  | Significance level $\alpha$ |  |  |
|  |  | . 10 | 05 | . 01 | . 10 | . 05 | . 01 | . 10 | . 05 | . 01 |
| SHT | $M=1$ | 0.5766 | 0.7135 | 0.9065 | 0.0384 | 0.0746 | 0.2170 | 0.0000 | 0.0000 | 0.0000 |
|  | $M=2$ | 0.3671 | 0.2625 | 0.0905 | 0.8503 | 0.8681 | 0.7719 | 0.8692 | 0.9296 | 0.9822 |
|  | $M \geq 3$ | 0.0563 | 0.0240 | 0.0030 | 0.1113 | 0.0573 | 0.0111 | 0.1308 | 0.0704 | 0.0178 |
| AIC | $M=1$ |  | 0.4910 |  |  | 0.0230 |  |  | 0.0000 |  |
|  | $M=2$ |  | 0.4356 |  |  | 0.8251 |  |  | 0.8288 |  |
|  | $M \geq 3$ |  | 0.0734 |  |  | 0.1519 |  |  | 0.1712 |  |
| BIC | $M=1$ |  | 0.9144 |  |  | 0.5183 |  |  | 0.0000 |  |
|  | $M=2$ |  | 0.0816 |  |  | 0.4774 |  |  | 0.9976 |  |
|  | $M \geq 3$ |  | 0.0040 |  |  | 0.0043 |  |  | 0.0024 |  |

Notes: The parameter values are: $\pi^{1}=\pi^{2}=1 / 2, \mu^{1}=(0,0)^{\prime}$ and $\mu^{2}=(2,1)^{\prime}$.

Table 4: Selection Frequency for the Number of Components: Trivariate Normal with $M=2$ and using $Z_{2}=X_{2}+X_{3}$

|  |  | $E\left[x_{3} \mid m=1\right]=0$ and $E\left[x_{3} \mid m=2\right]=0.5$ using $Z_{2}=X_{2}+X_{3}$ |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $N=50$ |  |  | $N=200$ |  |  | $N=1000$ |  |  |
|  |  | Significance level $\alpha$ |  |  | Significance level $\alpha$ |  |  | Significance level $\alpha$ |  |  |
|  |  | . 10 | 05 | . 01 | . 10 | . 05 | . 01 | . 10 | . 05 | . 01 |
| SHT | $M=1$ | 0.4483 | 0.5922 | 0.8170 | 0.0132 | 0.0315 | 0.1060 | 0.0000 | 0.0000 | 0.0000 |
|  | $M=2$ | 0.4896 | 0.3853 | 0.1799 | 0.8987 | 0.9271 | 0.8875 | 0.9030 | 0.9481 | 0.9899 |
|  | $M \geq 3$ | 0.0621 | 0.0225 | 0.0031 | 0.0881 | 0.0414 | 0.0065 | 0.0970 | 0.0519 | 0.0101 |
| AIC | $M=1$ |  | 0.3538 |  |  | 0.0062 |  |  | 0.0000 |  |
|  | $M=2$ |  | 0.5464 |  |  | 0.8515 |  |  | 0.8425 |  |
|  | $M \geq 3$ |  | 0.0998 |  |  | 0.1423 |  |  | 0.1575 |  |
| BIC | $M=1$ |  | 0.7498 |  |  | 0.2030 |  |  | 0.0000 |  |
|  | $M=2$ |  | 0.2372 |  |  | 0.7843 |  |  | 0.9921 |  |
|  | $M \geq 3$ |  | 0.0130 |  |  | 0.0127 |  |  | 0.0079 |  |


|  |  | $E\left[x_{3} \mid m=1\right]=0.5$ and $E\left[x_{3} \mid m=2\right]=0$ using $Z_{2}=X_{2}+X_{3}$ |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $N=50$ |  |  | $N=200$ |  |  | $N=1000$ |  |  |
|  |  | Significance level $\alpha$ |  |  | Significance level $\alpha$ |  |  | Significance level $\alpha$ |  |  |
|  |  | . 10 | 05 | . 01 | . 10 | . 05 | . 01 | . 10 | . 05 | . 01 |
| SHT | $M=1$ | 0.8316 | 0.9096 | 0.9775 | 0.6838 | 0.7899 | 0.9255 | 0.1163 | 0.1920 | 0.4018 |
|  | $M=2$ | 0.1467 | 0.0840 | 0.0221 | 0.2832 | 0.1982 | 0.0734 | 0.8052 | 0.7731 | 0.5926 |
|  | $M \geq 3$ | 0.0217 | 0.0064 | 0.0004 | 0.0330 | 0.0119 | 0.0011 | 0.0785 | 0.0349 | 0.0056 |
| AIC | $M=1$ |  | 0.7537 |  |  | 0.5823 |  |  | 0.0720 |  |
|  | $M=2$ |  | 0.2118 |  |  | 0.3642 |  |  | 0.7994 |  |
|  | $M \geq 3$ |  | 0.0345 |  |  | 0.0535 |  |  | 0.1286 |  |
| BIC | $M=1$ |  | 0.9651 |  |  | 0.9738 |  |  | 0.7829 |  |
|  | $M=2$ |  | 0.0324 |  |  | 0.0254 |  |  | 0.2153 |  |
|  | $M \geq 3$ |  | 0.0025 |  |  | 0.0008 |  |  | 0.0018 |  |

Notes: The parameter values are: $\pi^{1}=\pi^{2}=1 / 2, \mu^{1}=(0,0)^{\prime}$ and $\mu^{2}=(2,1)^{\prime}$.

Table 5: Selection Frequency for the Number of Components: Binomial with $M=2$

|  |  | $N=50$ |  |  | $N=200$ |  |  | $N=1000$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | Significance level $\alpha$ |  |  | Significance level $\alpha$ |  |  | Significance level $\alpha$ |  |  |
|  |  | . 10 | 05 | . 01 | . 10 | . 05 | . 01 | . 10 | . 05 | . 01 |
| SHT | $M=1$ | 0.7494 | 0.8752 | 0.9763 | 0.2423 | 0.4083 | 0.7493 | 0.0000 | 0.0001 | 0.0013 |
|  | $M=2$ | 0.1887 | 0.0960 | 0.0189 | 0.6860 | 0.5633 | 0.2471 | 0.9104 | 0.9586 | 0.9907 |
|  | $M \geq 3$ | 0.0619 | 0.0288 | 0.0048 | 0.0717 | 0.0284 | 0.0036 | 0.0896 | 0.0413 | 0.0080 |
| AIC | $M=1$ |  | 0.6279 |  |  | 0.1564 |  |  | 0.0000 |  |
|  | $M=2$ |  | 0.2748 |  |  | 0.7181 |  |  | 0.8554 |  |
|  | $M \geq 3$ |  | 0.0973 |  |  | 0.1255 |  |  | 0.1446 |  |
| BIC | $M=1$ |  | 0.9051 |  |  | 0.6644 |  |  | 0.0025 |  |
|  | $M=2$ |  | 0.0754 |  |  | 0.3290 |  |  | 0.9904 |  |
|  | $M \geq 3$ |  | 0.0195 |  |  | 0.0066 |  |  | 0.0071 |  |

Notes: The parameter values are $\pi^{1}=\pi^{2}=1 / 2,\left(p^{1}, p^{2}\right)=(0.2,0.5)$, and $K=4$.

Table 6: Selection Frequency for the Number of Components: Binomial with $M=3$

|  |  | $N=100$ |  |  | $N=400$ |  |  | $N=2000$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | Significance level $\alpha$ |  |  | Significance level $\alpha$ |  |  | Significance level $\alpha$ |  |  |
|  |  | . 10 | 05 | . 01 | . 10 | . 05 | . 01 | . 10 | . 05 | . 01 |
| SHT | $M=1$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
|  | $M=2$ | 0.6918 | 0.7867 | 0.9202 | 0.1949 | 0.2918 | 0.5148 | 0.0000 | 0.0000 | 0.0008 |
|  | $M=3$ | 0.2813 | 0.2042 | 0.0791 | 0.7327 | 0.6750 | 0.4810 | 0.9061 | 0.9541 | 0.9910 |
|  | $M \geq 4$ | 0.0269 | 0.0091 | 0.0007 | 0.0724 | 0.0332 | 0.0042 | 0.0939 | 0.0459 | 0.0082 |
| AIC | $M=1$ |  | 0.0000 |  |  | 0.0000 |  |  | 0.0000 |  |
|  | $M=2$ |  | 0.6176 |  |  | 0.1447 |  |  | 0.0000 |  |
|  | $M=3$ |  | 0.3286 |  |  | 0.7305 |  |  | 0.8492 |  |
|  | $M \geq 4$ |  | 0.0538 |  |  | 0.1248 |  |  | 0.1508 |  |
| BIC | $M=1$ |  | 0.0000 |  |  | 0.0000 |  |  | 0.0000 |  |
|  | $M=2$ |  | 0.8635 |  |  | 0.5155 |  |  | 0.0019 |  |
|  | $M=3$ |  | 0.1322 |  |  | 0.4778 |  |  | 0.9941 |  |
|  | $M \geq 4$ |  | 0.0043 |  |  | 0.0067 |  |  | 0.0040 |  |

Notes: The parameter values are $\pi^{1}=\pi^{2}=\pi^{3}=1 / 3,\left(p^{1}, p^{2}, p^{3}\right)=(0.2,0.5,0.9)$, and $K=6$.

Table 7: Selection Frequency for the Number of Components: Binomial with $M=4$

|  |  | $N=200$ |  |  | $N=800$ |  |  | $N=4000$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | Significance level $\alpha$ |  |  | Significance level $\alpha$ |  |  | Significance level $\alpha$ |  |  |
|  |  | . 10 | 05 | . 01 | . 10 | . 05 | . 01 | . 10 | . 05 | . 01 |
| SHT | $M=1$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
|  | $M=2$ | 0.0061 | 0.0145 | 0.0504 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
|  | $M=3$ | 0.6625 | 0.7405 | 0.8378 | 0.1919 | 0.2816 | 0.4917 | 0.0000 | 0.0000 | 0.0004 |
|  | $M=4$ | 0.3017 | 0.2338 | 0.1108 | 0.7463 | 0.6933 | 0.5042 | 0.9093 | 0.9575 | 0.9916 |
|  | $M \geq 5$ | 0.0297 | 0.0112 | 0.0010 | 0.0618 | 0.0251 | 0.0041 | 0.0907 | 0.0425 | 0.0080 |
| AIC | $M=1$ |  | 0.0000 |  |  | 0.0000 |  |  | 0.0000 |  |
|  | $M=2$ |  | 0.0032 |  |  | 0.0000 |  |  | 0.0000 |  |
|  | $M=3$ |  | 0.5997 |  |  | 0.1393 |  |  | 0.0000 |  |
|  | $M=4$ |  | 0.3440 |  |  | 0.7515 |  |  | 0.8491 |  |
|  | $M \geq 5$ |  | 0.0531 |  |  | 0.1092 |  |  | 0.1509 |  |
| BIC | $M=1$ |  | 0.0000 |  |  | 0.0000 |  |  | 0.0000 |  |
|  | $M=2$ |  | 0.0325 |  |  | 0.0000 |  |  | 0.0000 |  |
|  | $M=3$ |  | 0.8222 |  |  | 0.5257 |  |  | 0.0024 |  |
|  | $M=4$ |  | 0.1426 |  |  | 0.4706 |  |  | 0.9945 |  |
|  | $M \geq 5$ |  | 0.0027 |  |  | 0.0037 |  |  | 0.0031 |  |

Notes: The parameter values are $\pi^{1}=\pi^{2}=\pi^{3}=\pi^{4}=1 / 4,\left(p^{1}, p^{2}, p^{3}, p^{4}\right)=(0.05,0.3,0.7,0.095)$, and $K=8$.


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[^1]:    ${ }^{1} F_{B}, V$, and $L_{B}$ corresponds to $D, A$, and $P$ in Blischke (1964, pp. 513-514).

[^2]:    ${ }^{2}$ Kleibergen and Paap (2006) need a stronger assumption (Assumption 2, p.104) on the rank of a matrix involving $\Omega$, which may be violated, for instance, when we apply it to binomial mixtures.

[^3]:    ${ }^{3}$ Robin and Smith (2000) propose to test the null for $r=0,1, \ldots, p$, but it is not necessary to test the null for $r>q$ because $\operatorname{rank}(B)$ cannot be larger than $q$.
    ${ }^{4}$ Cragg and Donald (1997) also use sequential hypothesis testing with their estimator.

[^4]:    ${ }^{5}$ Alternatively, we may consider a BIC-type criterion function of the form $S(r)=C R T(r) / \bar{\gamma}(r)-f(N) g(r)$ with $f(N)=\log (N)$ and $g(r)=(p-r)(q-r)$. These two versions of $S(r)$ performed similarly in simulations that are not reported here.

[^5]:    ${ }^{6}$ We also experimented with $R_{1}=R_{2}=M+2$ (not reported here) and found that the procedures with $R_{1}=R_{2}=M+1$ performed better than those with $R_{1}=R_{2}=M+2$.

[^6]:    ${ }^{7}$ We also experimented a partition of $\mathcal{X}_{2}$ and $\mathcal{X}_{3}$ into $M-1$ or $M+1$ subsets, but the results did not improve for either two components models or three components models.
    ${ }^{8}$ The results of trivariate mixtures for three components model are similar and, thus, not reported here.

