

MARGINAL DISTRIBUTIONS OF FINITE MIXTURES OF MULTIVARIATE NORMAL DISTRIBUTIONS

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We give a transformation such that, for a k -dimensional finite normal mixture, the number of components and the mixing ratios are preserved on each marginal density through the transformation. Furthermore, under the only assumption of a k -dimensional finite normal mixture, we construct a one-dimensional random variable with a finite normal mixture of the true number of components and the true mixing ratios.

Key words and phrases: Finite mixture, k -dimensional distribution, One-dimensional distribution, Orthogonal matrix.

1. Introduction

Let $n(\mathbf{x} | \boldsymbol{\mu}, \boldsymbol{\Sigma})$ be a k -dimensional normal probability density function (pdf) with mean vector $\boldsymbol{\mu}$ and variance-covariance matrix $\boldsymbol{\Sigma}$. The pdf

$$(1.1) \quad f(\mathbf{x}) = \sum_{i=1}^m \alpha_i n(\mathbf{x} | \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$$

will be called a finite mixture of $n(\mathbf{x} | \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$ ($i = 1, 2, \dots, m$), where $0 < \alpha_i < 1$ and $\sum_{i=1}^m \alpha_i = 1$. The usefulness of the mixture model is explained in McLachlan and Basford (1988) and Titterton *et al.* (1985). Even if \mathbf{X} has a finite mixture (1.1), the marginal pdf of the j -th coordinate X_j of \mathbf{X} is not necessarily a finite mixture of m pdf's. A simple example is given as follows:

$$(1.2) \quad f(\mathbf{x}) = \alpha_1 n(\mathbf{x} | \boldsymbol{\mu}_1, I) + \alpha_2 n(\mathbf{x} | \boldsymbol{\mu}_2, I) + \alpha_3 n(\mathbf{x} | \boldsymbol{\mu}_3, I),$$

which is a finite mixture of three pdf's, where $\boldsymbol{\mu}_1 = (0, 0)'$, $\boldsymbol{\mu}_2 = (0, 1)'$, $\boldsymbol{\mu}_3 = (1, 1)'$ and I is the 2×2 identity matrix. Then the pdf of X_1 is given as follows:

$$(1.3) \quad g_1(x_1) = (\alpha_1 + \alpha_2)n(x_1 | 0, 1) + \alpha_3 n(x_1 | 1, 1),$$

which is a finite mixture of two one-dimensional normal pdf's. This can be similarly said for X_2 .

Now let us consider transformation $\mathbf{Y} = \mathbf{M}\mathbf{X} + \boldsymbol{\rho}$, where \mathbf{M} is a $k \times k$ orthogonal matrix and $\boldsymbol{\rho}$ a vector. From a property of normal pdf (Anderson (1984)), it can be seen that a necessary and sufficient condition for \mathbf{X} to have a finite mixture (1.1) is for \mathbf{Y} to have a finite mixture

$$(1.4) \quad g(\mathbf{y}) = \sum_{i=1}^m \alpha_i n(\mathbf{y} | \mathbf{M}\boldsymbol{\mu}_i + \boldsymbol{\rho}, \mathbf{M}\boldsymbol{\Sigma}_i\mathbf{M}').$$

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Taking into account of the above example, it is valuable to find an \mathbf{M} such that the marginal pdf of the j -th coordinate Y_j of \mathbf{Y} is a finite mixture of m one-dimensional normal pdf's. The purpose of this paper is to find the orthogonal matrix \mathbf{M} and then obtain \mathbf{Y} . For the purpose, we give a statement which can be obtained easily from the theory of linear algebra (Gantmacher (1977)).

STATEMENT 1.1. *Let μ_{j1} and μ_{j2} be the j -th coordinates, referred to the orthogonal coordinate system (x_1, x_2, \dots, x_k) , of $\boldsymbol{\mu}_1$ and $\boldsymbol{\mu}_2$, respectively. Then $\mu_{j1} = \mu_{j2}$ is equivalent to the fact that the j -th coordinate axis lies on the $(k - 1)$ -dimensional hyperplane π going through the origin and perpendicular to the straight line going through the points $(\mu_{11}, \mu_{21}, \dots, \mu_{k1})$ and $(\mu_{12}, \mu_{22}, \dots, \mu_{k2})$.*

In Section 2, we construct \mathbf{Y} such that, when \mathbf{X} has the pdf (1.1) with known mean vectors, the number of components and the mixing ratios are preserved on each marginal density through the transformation. In Section 3, when \mathbf{X} has the pdf (1.1) with unknown mean vectors, we construct a one-dimensional random variable $Y_j^{(\gamma)}$ with a finite normal mixture of the true number of components and the true mixing ratios, and then give an example to construct such random variable.

2. Construction of \mathbf{Y} when $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \dots, \boldsymbol{\mu}_m$ are known

We first need to obtain an \mathbf{M} to give a transformation which satisfies our demand under the assumption that the mean vectors of component pdf's of (1.1) are known. For this purpose, we give the following lemma.

LEMMA 2.1. *For any different $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \dots, \boldsymbol{\mu}_m$ and any $\boldsymbol{\rho}$, there exists an \mathbf{M} such that $\nu_{j1}, \nu_{j2}, \dots, \nu_{jm}$ are different for $j = 1, 2, \dots, k$, where ν_{ji} is the j -th coordinate of $\boldsymbol{\nu}_i = \mathbf{M}\boldsymbol{\mu}_i + \boldsymbol{\rho}$ ($i = 1, 2, \dots, m$).*

PROOF. Without loss of generality, we assume that $\boldsymbol{\rho} = \mathbf{0}$, the zero vector. Referring to the orthogonal coordinate system (x_1, x_2, \dots, x_k) , the $(k - 1)$ -dimensional hyperplane π_{st} going through the origin and perpendicular to the straight line going through the points $(\mu_{1s}, \mu_{2s}, \dots, \mu_{ks})$ and $(\mu_{1t}, \mu_{2t}, \dots, \mu_{kt})$ is determined uniquely by $\boldsymbol{\mu}_s$ and $\boldsymbol{\mu}_t$ ($s < t$ and $s, t = 1, 2, \dots, m$). Consider a new orthogonal coordinate system (z_1, z_2, \dots, z_k) which has the origin in common with the coordinate system (x_1, x_2, \dots, x_k) and neither coordinate axis of which lies on any π_{st} for $s < t$ and $s, t = 1, 2, \dots, m$. Then the j -th coordinates $\nu_{j1}, \nu_{j2}, \dots, \nu_{jm}$ ($j = 1, 2, \dots, k$), referred to the coordinate system (z_1, z_2, \dots, z_k) , of $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \dots, \boldsymbol{\mu}_m$, respectively, are different by Statement 1.1. Let $\boldsymbol{\nu}_i = \mathbf{M}\boldsymbol{\mu}_i$ ($i = 1, 2, \dots, m$), where \mathbf{M} is the orthogonal matrix which transforms the coordinate system (z_1, z_2, \dots, z_k) to the coordinate system (x_1, x_2, \dots, x_k) . Then we can see that $\nu_{j1}, \nu_{j2}, \dots, \nu_{jm}$ ($j = 1, 2, \dots, k$) are equal to the j -th coordinates of $\boldsymbol{\nu}_1, \boldsymbol{\nu}_2, \dots, \boldsymbol{\nu}_m$, respectively. This completes the proof.

THEOREM 2.1. *Suppose that \mathbf{X} has the finite mixture (1.1) with different $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \dots, \boldsymbol{\mu}_m$. Then, for any $\boldsymbol{\rho}$, there exists an \mathbf{M} such that the j -th coordinate*

Y_j of $\mathbf{Y} = \mathbf{M}\mathbf{X} + \boldsymbol{\rho}$ has also a finite mixture of m one-dimensional normal pdf's such as

$$(2.1) \quad g_j(y_j) = \sum_{i=1}^m \alpha_i n(y_j \mid \nu_{ji}, \sigma_{ji}^2) \quad (j = 1, 2, \dots, k),$$

where ν_{ji} is the j -th coordinate of $\boldsymbol{\nu}_i = \mathbf{M}\boldsymbol{\mu}_i + \boldsymbol{\rho}$, σ_{ji}^2 the (j, j) -th element of $\mathbf{M}\boldsymbol{\Sigma}_i\mathbf{M}'$ ($i = 1, 2, \dots, m$), and $\nu_{j1}, \nu_{j2}, \dots, \nu_{jm}$ are different.

PROOF. By the last lemma, there exists an \mathbf{M} such that $\nu_{j1}, \nu_{j2}, \dots, \nu_{jm}$ are different for $j = 1, 2, \dots, k$, where ν_{ji} is the j -th coordinate of $\boldsymbol{\nu}_i = \mathbf{M}\boldsymbol{\mu}_i + \boldsymbol{\rho}$ ($i = 1, 2, \dots, m$). The pdf of \mathbf{Y} is given by (1.4). Hence, the marginal pdf of Y_j is given by (2.1) and the means $\nu_{j1}, \nu_{j2}, \dots, \nu_{jm}$ of m normal pdf's are different. Accordingly, each Y_j has a finite mixture of m components. This completes the proof.

3. Construction of $Y_j^{(\gamma)}$ when $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \dots, \boldsymbol{\mu}_m$ are unknown

The last theorem guarantees the existence of an \mathbf{M} we hope. However, as can be seen from the proof, we use a knowledge of $\boldsymbol{\mu}_i$ ($i = 1, 2, \dots, m$) to give an \mathbf{M} . We want to obtain actually a one-dimensional random variable Y_j with a finite mixture of m one-dimensional pdf's under the only assumption that \mathbf{X} has a k -dimensional finite normal mixture. Hence, we need to construct an \mathbf{M} with no knowledge of $\boldsymbol{\mu}_i$ ($i = 1, 2, \dots, m$) other than a fact that m is finite. This difficulty can be solved by constructing matrices \mathbf{M}_γ ($\gamma = 1, 2, \dots$) sequentially by the following.

A procedure of construction of \mathbf{M}_γ :

- (i) For $\gamma = 1$, $\mathbf{M}_1 = (\mathbf{e}_1^{(1)}, \mathbf{e}_2^{(1)}, \dots, \mathbf{e}_k^{(1)})$ is the $k \times k$ identity matrix.
- (ii) For $\gamma \geq 2$, $\mathbf{M}_\gamma = (\mathbf{e}_1^{(\gamma)}, \mathbf{e}_2^{(\gamma)}, \dots, \mathbf{e}_k^{(\gamma)})$ is a $k \times k$ orthogonal matrix such that $\mathbf{e}_1^{(\gamma)}$ is linearly independent of any $k-1$ vectors in $\{\mathbf{e}_i^{(\delta)} : 1 \leq i \leq k, 1 \leq \delta \leq \gamma-1\}$, and $\mathbf{e}_j^{(\gamma)}$ is linearly independent of any $k-1$ vectors in $\{\mathbf{e}_i^{(\delta)} : 1 \leq i \leq k, 1 \leq \delta \leq \gamma-1\} \cup \{\mathbf{e}_1^{(\gamma)}, \mathbf{e}_2^{(\gamma)}, \dots, \mathbf{e}_{j-1}^{(\gamma)}\}$ when $2 \leq j \leq k$.

Let $\{\mathbf{M}_\gamma : \gamma = 1, 2, \dots, \ell\}$ be a set of matrices obtained by the procedure above, then we have the following lemma which shows that an \mathbf{M}_γ which satisfies our demand can be obtained.

LEMMA 3.1. For any different $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \dots, \boldsymbol{\mu}_m$ and any $\boldsymbol{\rho}$, if $m(m-1)(k-1) < 2\ell k$, then there exist a γ and a j such that $\nu_{j1}^{(\gamma)}, \nu_{j2}^{(\gamma)}, \dots, \nu_{jm}^{(\gamma)}$ are different, where $\nu_{ji}^{(\gamma)}$ is the j -th coordinate of $\boldsymbol{\nu}_i^{(\gamma)} = \mathbf{M}_\gamma\boldsymbol{\mu}_i + \boldsymbol{\rho}$ ($i = 1, 2, \dots, m$).

PROOF. Without loss of generality, we assume again that $\boldsymbol{\rho} = \mathbf{0}$. Let us consider ℓ new orthogonal coordinate systems $(z_1^{(\gamma)}, z_2^{(\gamma)}, \dots, z_k^{(\gamma)})$ ($\gamma = 1, 2, \dots, \ell$) which have the origin in common with the orthogonal coordinate system (x_1, x_2, \dots, x_k) . Suppose that the coordinate system $(z_1^{(\gamma)}, z_2^{(\gamma)}, \dots, z_k^{(\gamma)})$ is transformed to the coordinate system (x_1, x_2, \dots, x_k) by \mathbf{M}_γ , then all of coordinate

axes are different and any k coordinate axes can not lie on the same $(k - 1)$ -dimensional hyperplane as can be seen from the construction of the new coordinate systems. Therefore, the number of coordinate axes lying on a hyperplane π_{st} is $k - 1$ at most. The total number of coordinate axes lying on some hyperplane π_{st} , for $s < t, s = 1, 2, \dots, m$, then is half of $m(m - 1)(k - 1)$ at most. On the other hand, the total number of coordinate axes is ℓk . So, if $m(m - 1)(k - 1) < 2\ell k$, then there exists at least one coordinate axis $z_j^{(\gamma)}$ which does not lie on any π_{st} . Accordingly, the j -th coordinates $\nu_{j1}^{(\gamma)}, \nu_{j2}^{(\gamma)}, \dots, \nu_{jm}^{(\gamma)}$, referred to the coordinate system $(z_1^{(\gamma)}, z_2^{(\gamma)}, \dots, z_k^{(\gamma)})$, of $\mathbf{M}_\gamma \boldsymbol{\mu}_1, \mathbf{M}_\gamma \boldsymbol{\mu}_2, \dots, \mathbf{M}_\gamma \boldsymbol{\mu}_m$, respectively, are different by Statement 1.1. This completes the proof.

Let $\{\mathbf{Y}_\gamma : \gamma = 1, 2, \dots, \ell\}$ be a set of k -dimensional random vectors, where $\mathbf{Y}_\gamma = \mathbf{M}_\gamma \mathbf{X} + \boldsymbol{\rho}$ and \mathbf{M}_γ is an orthogonal matrix obtained by the procedure above. Then we can prove the following theorem in the same way to the proof of Theorem 2.1 by substituting \mathbf{M}_γ for \mathbf{M} .

THEOREM 3.1. *Suppose that \mathbf{X} has a finite mixture (1.1) with different $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \dots, \boldsymbol{\mu}_m$. If $m(m - 1)(k - 1) < 2\ell k$, then, for any $\boldsymbol{\rho}$, there exist a γ and a j such that the j -th coordinate $Y_j^{(\gamma)}$ of $\mathbf{Y}_\gamma = \mathbf{M}_\gamma \mathbf{X} + \boldsymbol{\rho}$ also has a finite mixture of m one-dimensional normal pdf's such as*

$$(3.1) \quad g_j(y_j) = \sum_{i=1}^m \alpha_i n(y_j \mid \nu_{ji}^{(\gamma)}, (\sigma_{ji}^{(\gamma)})^2),$$

where $\nu_{ji}^{(\gamma)}$ is the j -th coordinate of $\boldsymbol{\nu}_i^{(\gamma)} = \mathbf{M}_\gamma \boldsymbol{\mu}_i + \boldsymbol{\rho}$, $(\sigma_{ji}^{(\gamma)})^2$ the (j, j) -th element of $\mathbf{M}_\gamma \boldsymbol{\Sigma}_i \mathbf{M}'_\gamma$ ($i = 1, 2, \dots, m$), and $\nu_{j1}^{(\gamma)}, \nu_{j2}^{(\gamma)}, \dots, \nu_{jm}^{(\gamma)}$ are different.

The last theorem guarantees that if we construct a sequence of k -dimensional random vectors $\{\mathbf{Y}_\gamma\}$ sequentially by the method above, then we will eventually obtain a one-dimensional random variable $Y_j^{(\gamma)}$ which has a finite normal mixture with the true number of components and the true mixing ratios.

Example. Let the pdf of \mathbf{X} be

$$(3.2) \quad f(\mathbf{x}) = \alpha_1 n(\mathbf{x} \mid \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) + \alpha_2 n(\mathbf{x} \mid \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) + \alpha_3 n(\mathbf{x} \mid \boldsymbol{\mu}_3, \boldsymbol{\Sigma}_3),$$

where $\boldsymbol{\mu}_i$ ($i = 1, 2, 3$) are those of (1.2). By the last theorem, we can construct a univariate random variable which satisfies our demand for $\ell = 2$. So, any orthogonal matrix \mathbf{M}_2 other than the identity matrix satisfies this requirement. Let us have a try with

$$\mathbf{M}_2 = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix}.$$

Then the pdf of $\mathbf{Y}_2 = \mathbf{M}_2 \mathbf{X}$ is

$$(3.3) \quad g(\mathbf{y}) = \alpha_1 n(\mathbf{y} \mid \boldsymbol{\eta}_1, \boldsymbol{\Sigma}_1^*) + \alpha_2 n(\mathbf{y} \mid \boldsymbol{\eta}_2, \boldsymbol{\Sigma}_2^*) + \alpha_3 n(\mathbf{y} \mid \boldsymbol{\eta}_3, \boldsymbol{\Sigma}_3^*),$$

where $\boldsymbol{\eta}_1 = (0, 0)'$, $\boldsymbol{\eta}_2 = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})'$, $\boldsymbol{\eta}_3 = (\sqrt{2}, 0)'$ and $\boldsymbol{\Sigma}_i^* = \mathbf{M}_2 \boldsymbol{\Sigma}_i \mathbf{M}_2'$ ($i = 1, 2, 3$). Accordingly, the pdf of the first coordinate $Y_1^{(2)}$ of \mathbf{Y}_2 is given as follows:

$$(3.4) \quad g_1(y_1) \\ = \alpha_1 n(y_1 \mid 0, (\sigma_{11}^{(2)})^2) + \alpha_2 n\left(y_1 \mid \frac{1}{\sqrt{2}}, (\sigma_{12}^{(2)})^2\right) + \alpha_3 n(y_1 \mid \sqrt{2}, (\sigma_{13}^{(2)})^2).$$

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