On Mixtures of Factor Mixture Analyzers

Cinzia Viroli cinzia.viroli@unibo.it

Department of Statistics, University of Bologna, Italy

Compstat 2010

Paris August 22-27 - slide 1

 \succ State of the art

 \succ State of the art

MFMA

An empirical illustration

In model based clustering the data are assumed to come from a finite mixture model (McLachlan and Peel, 2000) with each component corresponding to a cluster.

≻State of the art

- \succ State of the art
- \succ State of the art
- \succ State of the art
- \succ State of the art

MFMA

An empirical illustration

- In model based clustering the data are assumed to come from a finite mixture model (McLachlan and Peel, 2000) with each component corresponding to a cluster.
- For quantitative data each mixture component is usually modeled as a multivariate Gaussian distribution (Fraley and Raftery, 2002):

$$f(\mathbf{y}; \boldsymbol{\theta}) = \sum_{i=1}^{k} w_i \phi^{(p)}(\mathbf{y}; \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$$

≻State of the art

- \succ State of the art
- \succ State of the art
- \succ State of the art
- \succ State of the art

MFMA

An empirical illustration

- In model based clustering the data are assumed to come from a finite mixture model (McLachlan and Peel, 2000) with each component corresponding to a cluster.
- For quantitative data each mixture component is usually modeled as a multivariate Gaussian distribution (Fraley and Raftery, 2002):

$$f(\mathbf{y}; \boldsymbol{\theta}) = \sum_{i=1}^{k} w_i \phi^{(p)}(\mathbf{y}; \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$$

However when the number of observed variables is large, it is well known that Gaussian mixture models represent an over-parameterized solution.

Model based clustering

Dimensionally reduced model based clustering

Model based clustering

Banfield and Raftery (1993): proposed a parameterization of the generic componentcovariance matrix based on its spectral decomposition: $\Sigma_i = \lambda_i \mathbf{A}_i^\top \mathbf{D}_i \mathbf{A}_i$

Bouveyron et al. (2007): proposed a different parameterization of the generic componentcovariance matrix Dimensionally reduced model based clustering

Model based clustering

Banfield and Raftery (1993): proposed a parameterization of the generic componentcovariance matrix based on its spectral decomposition: $\Sigma_i = \lambda_i \mathbf{A}_i^\top \mathbf{D}_i \mathbf{A}_i$

Bouveyron et al. (2007): proposed a different parameterization of the generic componentcovariance matrix

Dimensionally reduced model based clustering

 Ghahrami and Hilton (1997) and McLachlan et al. (2003): Mixtures of Factor Analyzers (MFA)

Model based clustering

Banfield and Raftery (1993): proposed a parameterization of the generic componentcovariance matrix based on its spectral decomposition: $\Sigma_i = \lambda_i \mathbf{A}_i^\top \mathbf{D}_i \mathbf{A}_i$

Bouveyron et al. (2007): proposed a different parameterization of the generic componentcovariance matrix

Dimensionally reduced model based clustering

- Ghahrami and Hilton (1997) and McLachlan et al. (2003): Mixtures of Factor Analyzers (MFA)
- Yoshida et al. (2004), Baek and McLachlan (2008), Montanari and Viroli (2010) : Factor Mixture Analysis (FMA)

Dimensionality reduction is performed through k factor models with Gaussian factors Dimensionality reduction is performed through k factor models with Gaussian factors

The distribution of each observation is modelled, with probability π_j (j = 1, ..., k), according to an ordinary factor analysis model $\mathbf{y} = \boldsymbol{\eta}_j + \boldsymbol{\Lambda}_j \mathbf{z} + \mathbf{e}_j$, with $\mathbf{e}_j \sim \phi^{(p)}(\mathbf{0}, \Psi_j)$, where Ψ_j is a diagonal matrix and $\mathbf{z}_j \sim \phi^{(q)}(\mathbf{0}, \mathbf{I}_q)$ Dimensionality reduction is performed through k factor models with Gaussian factors

The distribution of each observation is modelled, with probability π_j (j = 1, ..., k), according to an ordinary factor analysis model $\mathbf{y} = \boldsymbol{\eta}_j + \boldsymbol{\Lambda}_j \mathbf{z} + \mathbf{e}_j$, with $\mathbf{e}_j \sim \phi^{(p)}(\mathbf{0}, \Psi_j)$, where Ψ_j is a diagonal matrix and $\mathbf{z}_j \sim \phi^{(q)}(\mathbf{0}, \mathbf{I}_q)$

In the observed space we obtain a finite mixture of multivariate Gaussians with heteroscedastic components:

$$f(\mathbf{y}) = \sum_{j=1}^{k} \pi_j \phi^{(p)}(\boldsymbol{\eta}_j, \boldsymbol{\Lambda}_j \boldsymbol{\Lambda}_j^{\top} + \boldsymbol{\Psi}_j)$$

Dimensionality reduction is performed through a single factor model with factors modelled by a multivariate Gaussian mixture

- Dimensionality reduction is performed through a single factor model with factors modelled by a multivariate Gaussian mixture
- The observed centred data are described as $\mathbf{y} = \mathbf{\Lambda}\mathbf{z} + \mathbf{e}$ with $\mathbf{e} \sim \phi^{(p)}(\mathbf{0}, \Psi)$ where Ψ is diagonal.

- Dimensionality reduction is performed through a single factor model with factors modelled by a multivariate Gaussian mixture
- The observed centred data are described as $\mathbf{y} = \mathbf{\Lambda}\mathbf{z} + \mathbf{e}$ with $\mathbf{e} \sim \phi^{(p)}(\mathbf{0}, \Psi)$ where Ψ is diagonal.
- The q factors are assumed to be standardized and are modelled as a finite mixture of multivariate Gaussians

$$f(\mathbf{z}) = \sum_{i=1}^{k} \gamma_i \phi_i^{(q)}(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i).$$

- Dimensionality reduction is performed through a single factor model with factors modelled by a multivariate Gaussian mixture
- The observed centred data are described as $\mathbf{y} = \mathbf{\Lambda}\mathbf{z} + \mathbf{e}$ with $\mathbf{e} \sim \phi^{(p)}(\mathbf{0}, \Psi)$ where Ψ is diagonal.
- The q factors are assumed to be standardized and are modelled as a finite mixture of multivariate Gaussians

$$f(\mathbf{z}) = \sum_{i=1}^{k} \gamma_i \phi_i^{(q)}(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i).$$

In the observed space we obtain a finite mixture of multivariate Gaussians with heteroscedastic components:

$$f(\mathbf{y}) = \sum_{i=1}^{k} \gamma_i \phi_i^{(p)} (\mathbf{\Lambda} \boldsymbol{\mu}_i, \mathbf{\Lambda} \boldsymbol{\Sigma}_i \mathbf{\Lambda}^\top + \boldsymbol{\Psi}).$$

MFA

FMA

- k factor models with q Gaussian factors;
- one factor model with q non Gaussian factors (distributed as a multivariate mixture of Gaussians);

MFA

■ k factor models with q Gaussian factors;

■ The number of clusters corresponds to the number of factor models; ⇒ 'local' dimension reduction within each group

FMA

- one factor model with q non Gaussian factors (distributed as a multivariate mixture of Gaussians);
- The number of clusters is defined by the number of components of the Gaussian mixture; ⇒ 'global' dimension reduction and clustering is performed in the latent space.

MFA

■ k factor models with q Gaussian factors;

■ The number of clusters corresponds to the number of factor models; ⇒ 'local' dimension reduction within each group

A flexible solution with less parameters than model based clustering;

FMA

- one factor model with q non Gaussian factors (distributed as a multivariate mixture of Gaussians);
- The number of clusters is defined by the number of components of the Gaussian mixture; ⇒ 'global' dimension reduction and clustering is performed in the latent space.
- A flexible solution with less parameters than model based clustering;

MFMA

>Definition (1)

≻Definition (2)

≻A note

An empirical illustration

Mixtures of Factor Mixture Analyzers

Introduction

MFMA

≻Definition (1)

≻Definition (2)

≻A note

An empirical illustration

We assume the data can be described by k_1 factor models with probability π_j $(j = 1, ..., k_1)$:

$$\mathbf{y} = \boldsymbol{\eta}_j + \boldsymbol{\Lambda}_j \mathbf{z} + \mathbf{e}_j. \tag{1}$$

Introduction

MFMA

 \succ Definition (1)

≻Definition (2)

≻A note

An empirical illustration

We assume the data can be described by k_1 factor models with probability π_j $(j = 1, ..., k_1)$:

$$\mathbf{y} = \boldsymbol{\eta}_j + \boldsymbol{\Lambda}_j \mathbf{z} + \mathbf{e}_j.$$
 (1)

Within all the factor models, the factors are assumed to be distributed according to a finite mixture of k_2 Gaussians:

$$f(\mathbf{z}) = \sum_{i=1}^{k_2} \gamma_i \phi^{(q)}(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i), \qquad (2)$$

with mixture parameters supposed to be equal across the factor models $j = 1, \ldots, k_1$.

Introduction

MFMA

≻Definition (1)

≻Definition (2)

≻A note

An empirical illustration

From the previous assumptions it follows that the distribution of the observed variables becomes a '*double*' mixture of Gaussians:

$$f(\mathbf{y};\boldsymbol{\theta}) = \sum_{j=1}^{k_1} \pi_j \sum_{i=1}^{k_2} \gamma_i \phi^{(p)}(\boldsymbol{\eta}_j + \boldsymbol{\Lambda}_j \boldsymbol{\mu}_i, \boldsymbol{\Lambda}_j \boldsymbol{\Sigma}_i \boldsymbol{\Lambda}_j^\top + \boldsymbol{\Psi}_j). \quad (3)$$

which leads to a '*double*' interpretation:

(1) a mixture of k_1 factor analyzers with non-Gaussian factors, jointly modelled by a mixture of k_2 Gaussians, or (2) a non-linear factor mixture analysis model.

Introduction

MFMA

≻Definition (1)

≻Definition (2)

≻A note

An empirical illustration

From the previous assumptions it follows that the distribution of the observed variables becomes a '*double*' mixture of Gaussians:

$$f(\mathbf{y};\boldsymbol{\theta}) = \sum_{j=1}^{k_1} \pi_j \sum_{i=1}^{k_2} \gamma_i \phi^{(p)}(\boldsymbol{\eta}_j + \boldsymbol{\Lambda}_j \boldsymbol{\mu}_i, \boldsymbol{\Lambda}_j \boldsymbol{\Sigma}_i \boldsymbol{\Lambda}_j^\top + \boldsymbol{\Psi}_j). \quad (3)$$

which leads to a '*double*' interpretation:

(1) a mixture of k_1 factor analyzers with non-Gaussian factors, jointly modelled by a mixture of k_2 Gaussians, or (2) a non-linear factor mixture analysis model.

Moreover it coincides with MFA when $k_2 = 1$ and with FMA when $k_1 = 1$. Thus the method includes MFA and FMA as special cases.

| Introduction | | |
|------------------------------|--|--|
| MFMA | | |
| ≻Definition (1) | | |
| ≻Definition (2) | | |
| ≻A note | | |
| An empirical illustration | | |
| | | |

| Introduction |
|---------------------------|
| MFMA |
| ≻Definition (1) |
| ≻Definition (2) |
| ≻A note |
| An empirical illustration |
| |

(1) units may be described by one out of the k_1 different factor models;

| Introduction | |
|-----------------|--|
| MFMA | |
| ≻Definition (1) | |
| ≻Definition (2) | |
| ≻A note | |
| An empirical | |
| illustration | |
| | |

(1) units may be described by one out of the k_1 different factor models;

(2) then units (within each factor model) may belong to different k_2 sub-populations (defined by the k_2 components of the multivariate factor distribution.)

| Introduction | |
|-----------------|--|
| MFMA | |
| ≻Definition (1) | |
| ≻Definition (2) | |
| ≻A note | |
| An empirical | |
| illustration | |
| | |
| | |
| | |

(1) units may be described by one out of the k_1 different factor models;

(2) then units (within each factor model) may belong to different k_2 sub-populations (defined by the k_2 components of the multivariate factor distribution.)

■ The question is: k₁, k₂ or k₁ × k₂ groups? *i.e.* k₁ or k₂ non-Gaussian sub-populations or k₁ × k₂ Gaussian ones?

The data set contains 569 clinical cases of benignant (62.7%) and malignant (37.3%) diagnoses of breast cancer. Cluster analysis is based on p = 3 attributes: extreme area, extreme smoothness, and mean texture.

(ARI by Mclust, k=4 groups: 0.55)

| | MFA | FMA | MFMA |
|------------------|-------|-------|-------|
| k_1 | 2 | 1 | 2 |
| k_2 | 1 | 3 | 3 |
| q | 1 | 1 | 1 |
| h | 16 | 12 | 22 |
| logL | -2174 | -2167 | -2139 |
| BIC | 4449 | 4410 | 4418 |
| AIC | 4379 | 4385 | 4323 |
| $ARI_{(k_1)}$ | 0.73 | 0.00 | 0.80 |
| $ARI_{(k_2)}$ | 0.00 | 0.64 | 0.05 |
| $ARI_{(k_1k_2)}$ | 0.73 | 0.64 | 0.52 |

The data set contains 569 clinical cases of benignant (62.7%) and malignant (37.3%) diagnoses of breast cancer. Cluster analysis is based on p = 3 attributes: extreme area, extreme smoothness, and mean texture.

(ARI by Mclust, k=4 groups: 0.55)

| | MFA | FMA | MFMA |
|------------------|-------|-------|-------|
| k_1 | 2 | 1 | 2 |
| k_2 | 1 | 3 | 3 |
| q | 1 | 1 | 1 |
| h | 16 | 12 | 22 |
| logL | -2174 | -2167 | -2139 |
| BIC | 4449 | 4410 | 4418 |
| AIC | 4379 | 4385 | 4323 |
| $ARI_{(k_1)}$ | 0.73 | 0.00 | 0.80 |
| $ARI_{(k_2)}$ | 0.00 | 0.64 | 0.05 |
| $ARI_{(k_1k_2)}$ | 0.73 | 0.64 | 0.52 |

MFMA: 2, 3 or 6 groups?

Compstat 2010

Some indicators to measure the separation of the estimated clusters have been computed:

| | k | avg. dist. between | avg. dist. within | avg. silhouette width |
|-------------------|---|--------------------|-------------------|-----------------------|
| $MFMA_{(k_1)}$ | 2 | 2.71 | 1.77 | 0.32 |
| $MFMA_{(k_2)}$ | 3 | 2.67 | 1.88 | 0.15 |
| $MFMA_{(k_1k_2)}$ | 6 | 2.57 | 1.47 | 0.19 |
| MFA | 2 | 2.68 | 1.73 | 0.32 |
| FMA | 3 | 2.72 | 1.76 | 0.26 |
| MCLUST | 4 | 2.60 | 1.41 | 0.27 |

Some indicators to measure the separation of the estimated clusters have been computed:

| | k | avg. dist. between | avg. dist. within | avg. silhouette width |
|-------------------|---|--------------------|-------------------|-----------------------|
| $MFMA_{(k_1)}$ | 2 | 2.71 | 1.77 | 0.32 |
| $MFMA_{(k_2)}$ | 3 | 2.67 | 1.88 | 0.15 |
| $MFMA_{(k_1k_2)}$ | 6 | 2.57 | 1.47 | 0.19 |
| MFA | 2 | 2.68 | 1.73 | 0.32 |
| FMA | 3 | 2.72 | 1.76 | 0.26 |
| MCLUST | 4 | 2.60 | 1.41 | 0.27 |

 $k_1 = 2$ factor models with $k_2 = 3$ components for modeling the factor

... a mixture of factor analyzers with non-Gaussian components

■ MFMA is a double mixture model which extends and combines MFA and FMA

- I MFMA is a double mixture model which extends and combines MFA and FMA
- A MFMA model with k_1 and k_2 components may be interpreted in three different ways:
 - as a double mixture which performs clustering into $k = k_1 \times k_2$ groups,
 - as a mixture of factor mixture analysis models which performs clustering into $k = k_2$ groups
 - or as a mixture of factor analyzers with non-Gaussian components which classifies units into $k = k_1$ groups.

- I MFMA is a double mixture model which extends and combines MFA and FMA
- A MFMA model with k_1 and k_2 components may be interpreted in three different ways:
 - as a double mixture which performs clustering into $k = k_1 \times k_2$ groups,
 - as a mixture of factor mixture analysis models which performs clustering into $k = k_2$ groups
 - or as a mixture of factor analyzers with non-Gaussian components which classifies units into $k = k_1$ groups.
- In the last two perspectives the proposed model represents a powerful tool for modelling non-Gaussian latent variables.

- I MFMA is a double mixture model which extends and combines MFA and FMA
- A MFMA model with k₁ and k₂ components may be interpreted in three different ways:
 - as a double mixture which performs clustering into $k = k_1 \times k_2$ groups,
 - as a mixture of factor mixture analysis models which performs clustering into $k = k_2$ groups
 - or as a mixture of factor analyzers with non-Gaussian components which classifies units into $k = k_1$ groups.
- In the last two perspectives the proposed model represents a powerful tool for modelling non-Gaussian latent variables.
- Some references:
 - A. Montanari and C. Viroli (2010), *Heteroscedastic Factor Mixture Analysis*, Statistical Modelling, forthcoming
 - C. Viroli (2011), Dimensionally reduced model-based clustering through Mixtures of Factor Mixture Analyzers, Journal of Classification, forthcoming