Clustering of non-Gaussian data by variational Bayes for normal inverse Gaussian mixture models

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Abstract

Finite mixture models, typically Gaussian mixtures, are well known and widely used as model-based clustering. In practical situations, there are many non-Gaussian data that are heavy-tailed and/or asymmetric. Normal inverse Gaussian (NIG) distributions are normal-variance-mean which mixing densities are inverse Gaussian distributions and can be used for both heavy-tail and asymmetry. For NIG mixture models, both expectation-maximization method and variational Bayesian (VB) algorithms have been proposed. However, the existing VB algorithm for NIG mixture have a disadvantage that the shape of the mixing density is limited. In this paper, we propose another VB algorithm for NIG mixture that improves on the shortcomings. We also propose an extension of Dirichlet process mixture models to overcome the difficulty in determining the number of clusters in finite mixture models. We evaluated the performance with artificial data and found that it outperformed Gaussian mixtures and existing implementations for NIG mixtures, especially for highly non-normative data.

Keywords: unsupervised learning, density estimation, tail-heavy, asymmetry, normal-variance mean, Dirichlet process mixture

1 Introduction

Finite mixture models are commonly used for density estimation or data clustering in a variety of fields (Melnykov and Maitra 2010, McLachlan et al. 2019). Finite mixture models are known
as model-based unsupervised learning that does not use label information. Historically, Gaussian mixture models are most popular for model-based clustering (Celeux and Govaert, 1995; Fraley and Raftery, 1998). However, there are many heavy-tailed and/or asymmetric cases where normality cannot be assumed in the actual data. Therefore, in recent years, there has been increasing attention on the use of non-normal models in model-based clustering. Specifically, mixture models of $t$-distributions (Shoham, 2002; Takekawa and Fukai, 2009), skew $t$-distributions (Lin et al., 2007), normal inverse Gaussian distributions (Karlis and Santourian, 2009; Subedi and McNicholas, 2014; O’Hagan et al., 2016; Fang et al., 2020) and generalized hyperbolic distributions (Browne and McNicholas, 2015) have been proposed.

For parameter estimation of the mixture distribution, the expectation-maximization (EM) algorithm based on the maximum likelihood inference was classically used and is still in use today (Dempster et al., 1977). In the maximum likelihood method, it is impossible to determine the number of clusters in principle. Therefore, it is necessary to apply the EM method under the condition of multiple number of clusters and then determine it using some information criteria like Baysian information criteria (BIC). Bayesian inferences make use of prior knowledge about clusters in the form of prior distributions. Therefore, we can evaluate the estimation results for different numbers of clusters based on the model evidence. In Bayesian inference, it is natural and common to use the Dirichlet distribution, which is a conjugate prior of the categorical distribution, as a prior for cluster concentration. Since the Dirichlet distribution is defined based on the number of clusters, the disadvantage is that the prior distribution is affected by the number of clusters. Dirichlet process mixture (DPM) models can be used as a solution to this problem (Antoniak, 1974; MacEachern, 1994; Neal, 2000). DPM is a model that divides data into infinite number of clusters.

There are two methods for parameter estimation based on Bayesian inference, one is Monte Carlo Markov chane (MCMC) sampling and the other is variational Bayesian (VB) (Ghahramani and Beal, 2001; Jordan et al., 1999). MCMC has the advantage of being a systematic approach to various problems. However, it has the problem of slow convergence and difficulty in finding convergence. These shortcomings have a large impact particularly on large scale problems (Blei et al., 2017). On the other hand, VB, in which the independence between variables is assumed,
allow us to solve the relaxed problems faster. VB algorithm is similar to EM algorithm, it eliminates solves the disadvantage of the slow and unstable convergence of EM algorithm (Renshaw et al., 1987). In addition, automatic relevance determination eliminates unnecessary clusters during the iteration, and the number of clusters can be determined in a natural way (Neal, 1996).

Normal inverse Gaussian (NIG) distribution, a subclass of generalized hyperbolic distributions, is mathematically tractable and open used to treat a tail-heaviness and skewness of data. NIG distribution is defined as the normal variance-mean mixture with the inverse Gaussian mixing density. An expectation-maximization (EM) framework for mixtures of NIG was proposed by Karlis and Santourian (2009). And a VB framework for NIG mixtures was also proposed by Subedi and McNicholas (2014). Recently, Fang et al. (2020) introduced Dirichlet process mixture to framework by Subedi and McNicholas (2014). Fang et al. (2020) introduce Dirichlet process mixture models to Subedi’s implementation. However, as pointed out in this paper, the implementation of Subedi and McNicholas (2014) and Fang et al. (2020) have the drawback of fixing the shape of the mixing density, which represents the non-normality.

In this paper, we introduce an approximate Bayes inference for mixture models of NIG by VB without fixing the shape of the mixing density. In this formulation, the conjugate prior of the shape of the mixing density is a generalized inverse normal distribution, and we propose to use inverse normal distributions or gamma distributions as a prior, both of these are a subclass of generalized inverse Gaussian. For the concentration parameter, we propose both Dirichlet distribution model and DPM model. Finally, the proposed method was evaluated with artificial data. As a result, the The proposed method is based on the non-normality of mixed distribution data. Compared to VB for GMM and past VB for NIGMM implementations, the Estimating the number of clusters and clustering comprehensively The results were significantly better in terms of both the quality and aduative rank index (ARI) (Hubert and Arabie, 1985).

2 Methods

In this section, we described another variational Bayes implementation for finite mixture of NIG distributions, in which the prior of mixing density’s shape parameter \( \lambda \) obeys generalized inverse
Gaussian distribution. First, the Dirichlet distribution version of VB for mixture of NIG is described in 2.1-2.4. Then, we introduce the Dirichlet process mixture framework in 2.5. We also discuss the policy for setting hyperparameters in 2.6. The difference between Subedi and McNicholas (2014) and the proposed model is described in Appendix B. The details of the distributions shown in this section are described in Appendix A.

2.1 Multivariate normal inverse Gaussian distribution

NIG distribution is defined as the normal variance-mean mixture with the inverse Gaussian mixing density (Barndorff-Nielsen, 1997). The mixing density \( y' \in \mathbb{R} \) arises from an inverse Gaussian distribution \( \mathcal{N}^{-1} \) with the mean \( y_0 \in \mathbb{R} \) and the shape \( \lambda \in \mathbb{R} \) and the observation \( x \in \mathbb{R}^D \) arises from an \( D \)-dimensional multivariate normal distribution \( \mathcal{N}_D \) with the mean \( \mu + y' \beta' \in \mathbb{R}^D \) and the precision matrix \( y' \tau' \in \mathbb{R}^{D \times D} \):

\[
p(x \mid y') = \mathcal{N}_D \left( x \mid \mu + y' \beta', y'^{-1} \tau' \right) \quad \text{and} \quad p(y') = \mathcal{N}^{-1} \left( y' \mid y_0, \lambda \right),
\]

where \( \mu \in \mathbb{R}^D \) and \( \beta' \in \mathbb{R}^D \) is the center and the drift parameter, respectively. Originally, it is assumed that \(|\tau'| = 1\) should be satisfied to eliminate redundancy. However, the restriction \(|\tau'| = 1\) make the parameter inference difficult (Protassov, 2004).

To avoid the difficulty, we introduce an alternative representation which fix the mean of \( \lambda \):

\[
p(x \mid y) = \mathcal{N} \left( x \mid \mu + y \beta, y^{-1} \tau \right) \quad \text{and} \quad p(y \mid \lambda) = \mathcal{N}^{-1} \left( y \mid 1, \lambda \right).
\]

The representation can be easily available by the scale change \( \beta = y_0 \beta', \tau = y_0^{-1} \tau' \) and the property of the distribution:

\[
\text{if} \quad y' \sim \mathcal{N}^{-1} \left( y' \mid y_0, \lambda \right), \quad \text{then} \quad y = \frac{y'}{y_0} \sim \mathcal{N}^{-1} \left( y \mid 1, \lambda \right).
\]

The mean and the precision matrix of normal inverse Gaussian are \( \mu + \beta \) and \( \tau \), respectively. The larger the normality \( \lambda \), the closer NIG distribution approaches the normal distribution. A large
bias $\beta$ results in an asymmetric distribution (see Fig. 1).

Subedi and McNicholas (2014) also proposed a similar representation. However, as a result, their proposal fixed the mean rather than the shape of $\lambda$. Then, they conclude that the conjugate prior should obey truncated normal distributions (see Appendix B). As a results, their representation lose the flexibility of NIG distribution. Moreover, the redundancy and difficulty of truncated process still remain. On the other hand, our representation could deal the entire NIG and the conjugate prior of $\lambda$ which obey generalized inverse Gaussian distributions do not need additional process such as truncation.
Figure 2: Example of data generated by the NIG mixture model: The normality parameter $\lambda$ is set around 1 and the asymmetry parameter $\beta$ around a half of standard deviation. Using the parameters described in section 2.6, this can be describe as $\lambda_\ast = 1$ and $\sigma_\beta = 0.5$. 
2.2 Variational Bayes for mixture of MNIG

The probability distribution function for the mixture of $M$ NIG is defined as:

$$p(x_i \mid \alpha, \lambda, \mu, \beta, \tau) = \sum_{j=1}^{M} \alpha_j \int N^{-1}(y_i \mid 1, \lambda_j) N(x_{ij} \mid \mu_j + y_i \beta_j, y_i^{-1} \tau_j) \, dy_i,$$  \hspace{1cm} (4)$$

where $\alpha_j$ are the concentration parameters of mixture and its satisfied $p(z_i \mid \alpha) = \prod_{j=1}^{M} \alpha_{ij}$. An example of the data generated by NIG mixture is shown in Fig[2]. Here, we introduce the component indicator vector $z_i; z_i = G_j$ if the subject belongs to group $j$ and $G_j$ is a one-hot encoded $D$-dimensional vector which only the $j$-th element is 1. The joint probability of the observed data $x_i$, the mixing densities $y_i$ and the component indicators $z_i$ is described as following:

$$p(x_i, y_i, z_i \mid \alpha, \lambda, \mu, \beta, \tau) = \prod_{j=1}^{M} [\alpha_j N^{-1}(y_i \mid 1, \lambda_j) N(x_i \mid \mu_j + y_i \beta_j, y_i^{-1} \tau_j)]^{z_{ij}}. \hspace{1cm} (5)$$

In the variational Bayesian (VB) algorithm, the test function $q(y, z, \alpha, \lambda, \mu, \beta, \tau)$ which approximates the posterior $p(y, z, \alpha, \lambda, \mu, \beta, \tau \mid x)$ should be optimized in the sense of minimizing the KL divergence $KL[q(y, z, \alpha, \lambda, \mu, \beta, \tau), p(y, z, \alpha, \lambda, \mu, \beta, \tau \mid x)]$. VB introduce the approximation of assuming the independence between hidden variables and parameters:

$$q(y, z, \alpha, \lambda, \mu, \beta, \tau) = q_{\zeta}(y, z) q_{\theta}(\alpha, \lambda, \mu, \beta, \tau). \hspace{1cm} (6)$$

In the VB algorithm, M-step update the parameter test function $q(\alpha, \lambda, \mu, \beta, \tau)$ by fixing the test function of hidden variable $q(y, z)$ the as following:

$$\log q(\alpha, \lambda, \mu, \beta, \tau) = \text{const} + \log p(\alpha, \lambda, \mu, \beta, \tau) + \langle \log p(x, y, z \mid \alpha, \lambda, \mu, \beta, \tau) \rangle_{q_{\zeta}}. \hspace{1cm} (7)$$

And E-step update the test function of hidden variable $q(y, z)$ by fixing the parameter test function $q(\alpha, \lambda, \mu, \beta, \tau)$ as following:

$$q(y_i, z_i) \propto \exp \langle \log p(x_i, y_i, z_i \mid \alpha, \lambda, \mu, \beta, \tau) \rangle_{q_{\theta}}. \hspace{1cm} (8)$$
The convergence of E-step and M-step iteration can be evaluated by the evidence lower bound (ELBO):

\[ L = \log p(x) - KL[q_\theta(\alpha, \lambda, \mu, \beta, \tau), p(\alpha, \lambda, \mu, \beta, \tau | x)]. \]  

(9)

2.3 M-step

If we have the values of the expected value of hidden variables:

\[ \bar{z}_{ij} = \langle z_{ij} \rangle_{q(\alpha, \lambda, \mu, \beta, \tau | z_i = G_j)}, \quad \bar{y}_{ij} = \langle y_{ij} \rangle_{q(\alpha, \lambda, \mu, \beta, \tau | y_i | z_i = G_j)}, \quad \hat{y}_{ij} = \langle y_{ij}^{-1} \rangle_{q(\alpha, \lambda, \mu, \beta, \tau | y_i | z_i = G_j)}, \]  

(10)

the statics of data can be also available:

\[
\begin{align*}
Z^*_j &= \sum_{i=1}^{N} \bar{z}_{ij}, \\
Z^+_j &= \sum_{i=1}^{N} \bar{y}_{ij} \bar{z}_{ij}, \\
Z^-_j &= \sum_{i=1}^{N} \hat{y}_{ij} \bar{z}_{ij}, \\
X^*_j &= \sum_{i=1}^{N} \bar{z}_{ij} x_i, \\
X^-_j &= \sum_{i=1}^{N} \hat{y}_{ij} \bar{z}_{ij} x_i, \\
S^-_j &= \sum_{i=1}^{N} \hat{y}_{ij} \bar{z}_{ij} x_i x_i^\top,
\end{align*}
\]

(11)

Using these values, the expectation term with respect to the parameters \( \alpha, \lambda, \mu, \beta \) and \( \tau \) in Eq. (7) can be rearranged:

\[
\langle \log p(x, y, z | \alpha, \lambda, \mu, \beta, \tau) \rangle_{q_\xi} = \text{const} + \sum_{j=1}^{M} Z^*_j \log \alpha_j \\
+ \sum_{j=1}^{M} \left\{ \frac{Z^*_j}{2} \log \lambda_j - \frac{Z^+_j + Z^-_j - 2Z^*_j}{2} \lambda_j - \frac{0}{2} \lambda_j^{-1} \right\} + \sum_{j=1}^{M} \frac{1}{2} \left\{ Z^*_j \log \det \tau_j - \text{tr} S^-_j \tau_j \right\} \\
+ \sum_{j=1}^{M} \frac{1}{2} \text{tr} \left\{ -Z^-_j \mu_j \mu_j^\top - Z^+_j \beta_j \beta_j^\top + Z^*_j \left( \mu_j \beta_j^\top + \beta_j \mu_j^\top \right) + X^-_j \mu_j^\top + X^*_j \beta_j^\top \right\} \tau_j. \]  

(12)
The prior to correspond to the form of the posterior test function could be defined as

\[
\log p(\alpha, \lambda, \mu, \beta, \tau) = \text{const} + \sum_{j=1}^{M} (l_j - 1) \log \alpha_j \\
+ \sum_{j=1}^{M} \left\{ (h_0 - 1) \log \lambda_j - \frac{f_0}{2} \lambda_j - \frac{g_0}{2} \lambda_j^{-1} \right\} + \sum_{j=1}^{M} \frac{1}{2} \left\{ s_0 \log \det \tau_j - \text{tr} t'_0 \tau_j \right\} \\
+ \sum_{j=1}^{M} \frac{1}{2} \text{tr} \left\{ -u_0 \mu_j \beta_j^\top - v_0 \beta_j \beta_j^\top - w_0 \left( \mu_j \beta_j^\top + \beta_j \mu_j^\top \right) + \mu_j^\top m'_0 + \beta_j^\top n'_0 \right\} \tau_j. \tag{13}
\]

Here, we can find that Eq. (13) represent the combination of Dirichlet \( D \), generalized inverse Gaussian \( N^{-1} \), Wishart \( W \) and multivariate normal distribution as the following:

\[
p(\alpha, \lambda, \mu, \beta, \tau) = p(\alpha_1, \alpha_2, \cdots, \alpha_M) \prod_{j=1}^{M} p(\lambda_j) p(\tau_j) p(\mu_j, \beta_j | \tau_j), \tag{14}
\]

\[
p(\alpha_1, \alpha_2, \cdots, \alpha_M) = D(\alpha_1, \alpha_2, \cdots, \alpha_M | l_0, \cdots, l_0),
\]
\[
p(\lambda_j) = N^{-1}(\lambda_j | f_0, g_0, h_0),
\]
\[
p(\tau_j) = W(\tau_j | s_0, t_0), \tag{15}
\]
\[
p(\mu_j, \beta_j | \tau_j) = N\begin{pmatrix}
\mu_j \\
\beta_j
\end{pmatrix}
\begin{pmatrix}
m_0 & u_0 \tau_j & w_0 \tau_j \\
n_0 & w_0 \tau_j & v_0 \tau_j
\end{pmatrix},
\]

where

\[
t'_0 = t_0 + u_0 m_0 m_0^\top + w_0 m_0 n_0^\top + w_0 n_0 m_0^\top + w_0 n_0 n_0^\top,
\]
\[
m'_0 = u_0 m_0 + w_0 n_0, \quad n'_0 = w_0 m_0 + v_0 n_0. \tag{16}
\]

The hyper parameters can be described that \( m_0, n_0 \) and \( t_0/s_0 \) are the mean of \( \mu, \beta \) and \( \tau \), respectively; \( l_0 \) and \( s_0 \) are the precision (degree of freedom) of \( \alpha \) and \( \tau \), respectively; \( u_0, v_0 \) and \( w_0 \) are the co-variance scale of \( \mu, \beta \) and correlation between \( \mu \) and \( \beta \). We will discuss the hyper parameter for mixing density \( f_0, g_0, h_0 \) in subsection.
Finally, the formula to update hyper parameters of posterior is described as

\[ q_\theta (\alpha, \lambda, \mu, \beta, \tau) = q_\alpha (\alpha_1, \alpha_2, \cdots, \alpha_M) \prod_{j=1}^{M} q_\lambda (\lambda_j) q_\tau (\tau_j) q_\mu (\mu_j, \beta_j | \tau_j), \quad (17) \]

where

\[ q_\alpha (\alpha_1, \alpha_2, \cdots, \alpha_M) = \mathcal{D} (\alpha_1, \alpha_2, \cdots, \alpha_M | l_1, l_2, \cdots, l_M), \]

\[ q_\lambda (\lambda_j) = \mathcal{N}^{-1} (\lambda_j | f_j, g_j, h_j), \]

\[ q_\tau (\tau_j) = \mathcal{W} (\tau_j | s_j, t_j), \]

\[ q_\mu (\mu_j, \beta_j | \tau_j) = \mathcal{N} \left( \begin{array}{c} m_j \\ n_j \end{array} \bigg| m_j, u_j \tau_j, w_j \tau_j, v_j \tau_j \right). \]

The hyper parameters of the test function \( l_j, f_j, g_j, h_j, s_j, t_j, u_j, v_j \) and \( w_j \) are the sum of the prior hyper parameter and the statistical value of observed and hidden variables. The hyper parameter of the mean \( m_j \) and bias \( n_j \) can be calculated as

\[
\begin{bmatrix}
m_j \\
n_j
\end{bmatrix} = \begin{bmatrix}
u_j & w_j \\
w_j & v_j
\end{bmatrix}^{-1} \begin{bmatrix}
m_0' + X_j^- \\
n_0' + X_j^*
\end{bmatrix} = \begin{bmatrix}
u_j & -w_j \\
-u_j v_j - w_j & u_j v_j - w_j
\end{bmatrix} \begin{bmatrix}
m_0' + X_j^- \\
n_0' + X_j^*
\end{bmatrix}.
\]

\[ (20) \]

2.4 E-step

By calculating the expectations and organizing for \( y \) in Eq. (8), we obtain the following equation:

\[
\langle \log p (x_i, y_i, z_i | \alpha, \lambda, \mu, \beta, \tau) \rangle_{q_\theta} = \sum_{j=1}^{M} z_{ij} \left[ \log \rho_{ij} + \log \mathcal{N}^{-1} (y_j | a_j, b_{ij}, c) \right],
\]

\[ (21) \]
where \( c = -\frac{D+1}{2} \),

\[
a_j = \langle \lambda_j \rangle_{q_0} + \text{tr} \langle \tau_j \beta_j \beta_j^\top \rangle_{q_0} + \text{tr} \langle \tau_j \rangle_{q_0} \langle \lambda_j \rangle_{q_0} \langle \beta_j \rangle_{q_0}^\top,
\]

\[
b_{ij} = \langle \lambda_j \rangle_{q_0} + \text{tr} \langle \tau_j \mu_j \mu_j^\top \rangle_{q_0} + \text{tr} \langle \tau_j \rangle_{q_0} \left( x_i - \langle \mu_j \rangle_{q_0} \right) \left( x_i - \langle \mu_j \rangle_{q_0} \right)^\top,
\]

and

\[
\log \rho_{ij} = -\frac{D+1}{2} \log 2\pi + \langle \log \alpha_j \rangle_{q_0} + \frac{1}{2} \langle \log \lambda_j \rangle_{q_0} + \langle \lambda_j \rangle_{q_0} + \frac{1}{2} \langle \log \det \tau_j \rangle_{q_0}
- \text{tr} \langle \tau_j \mu_j \beta_j \rangle_{q_0} + \text{tr} \langle \tau_j \rangle_{q_0} \left( x_i - \langle \mu_j \rangle_{q_0} \right) \langle \beta_j \rangle_{q_0}^\top - \log \Delta \left( a_j, b_{ij}, c \right). \tag{23}
\]

The integral constant of generalized inverse Gaussian distribution \( \Delta \left( a_j, b_{ij}, c \right) \) and the expectations of parameters are described in Appendix A.

From Eq. (8) and (21), the test function of hidden variables can be written with generalized inverse Gaussian and categorical distributions:

\[
q_\zeta \left( y_i, z_i \right) = q_\zeta \left( y_i \mid z_i \right) q_\zeta \left( z_i \right), \quad q_\zeta \left( y_i \mid z_i = G_j \right) = \mathcal{N}^{-1}_{*} \left( y_i \mid a_j, b_{ij}, c \right), \quad q_\zeta \left( z_i = G_j \right) \propto \rho_{ij}. \tag{24}
\]

We can finally calculate expectation value of \( y_i, z \) which is used in M-step:

\[
\bar{z}_{ij} = \frac{\rho_{ij}}{\sum_{j' = 1}^{M} \rho_{ij'}}, \quad \bar{y}_{ij} = \langle y_j \rangle_{\mathcal{N}^{-1}_{*} \left( y_j \mid a_j, b_{ij}, c \right)} , \quad \hat{y}_{ij} = \langle y_j^{-1} \rangle_{\mathcal{N}^{-1}_{*} \left( y_j \mid a_j, b_{ij}, c \right)}. \tag{25}
\]

### 2.5 Dirichlet process mixtures

In Dirichlet process mixture models, the concentration parameters \( \alpha \) can be represented by the stick-breaking process using the collections of independent random variables \( \gamma \) as follow:

\[
\alpha_j = \gamma_j \prod_{j' = 1}^{j-1} \left( 1 - \gamma_{j'} \right). \tag{26}
\]
Then, the term corresponding to $\alpha$ in Eq. (13) can be re-written by $\gamma$ as

$$
\sum_{j=1}^{M} Z_j^* \log \alpha_j = \sum_{j=1}^{M} Z_j^* \left[ \log \gamma_j + \sum_{j'=1}^{j-1} \log (1 - \gamma_{j'}) \right] \\
= \sum_{j=1}^{M} \left[ Z_j^* \log \gamma_j + \sum_{j'=j+1}^{M} Z_{j'}^* \log (1 - \gamma_j) \right].
$$

(27)

Since Eq. (27) consist of $\log \gamma_j$ and $\log (1 - \gamma_j)$, the conjugate prior of $\gamma_j$ should be beta distributions $B$. The prior and test function in the case of Dirichlet distribution which described in Eq. (14) and (17) are replaced for DPM by

$$
p(\gamma, \lambda, \mu, \beta, \tau) = \prod_{j=1}^{M} p(\gamma_j) p(\lambda_j) p(\tau_j) p(\mu_j, \beta_j | \tau_j)
$$

(28)

and

$$
q_{\theta}(\gamma, \lambda, \mu, \beta, \tau) = \prod_{j=1}^{M} q(\gamma_j) q(\lambda_j) q(\tau_j) q(\mu_j, \beta_j | \tau_j),
$$

(29)

where

$$
p(\gamma_j) = B(\gamma_j | l_0, r_0), \quad q_{\gamma}(\gamma_j) = B(\gamma_j | l_j, r_j).
$$

(30)

$p(\lambda_j), p(\tau_j), p(\mu_j, \beta_j | \tau_j), q(\lambda_j)$, $q(\tau_j)$ and $q(\mu_j, \beta_j | \tau_j)$ are the same in Eq. (15) and (18).

The M-step for DPM is the same as the M-step for Dirichlet distribution model expect for the update rule of $r$:

$$
l_j = l_0 + Z_j^*, \quad r_j = r_0 + \sum_{j'=j+1}^{M} Z_{j'}^*.
$$

(31)

In the E-step for DPM, the only difference from Dirichlet distribution models is the expectation
values of $\log \alpha$ in Eq. (23):

$$
\langle \log \alpha_j \rangle_{q_\theta} = \langle \log \gamma_j \rangle_{\mathcal{B}(\alpha_j|l_j, r_j)} + \sum_{j'=1}^{j-1} \langle \log (1 - \gamma_{j'}) \rangle_{\mathcal{B}(\gamma_{j'}|l_{j'}, r_{j'})}.
$$

(32)

2.6 Priors

In this paper, we define the prior by the hyper-parameters using the mean $\mu_x$ and co-variance matrix $\Sigma_x$ of data. The mean of cluster centers is same as the center of data; $m_0 = \mu_x$. The mean of bias is zero vector; $n_0 = 0$. Basically, an uninformed prior is defined for the concentration parameter $\alpha$: $l_0 = 1$ for Dirichlet distribution and $l_0 = r_0 = 1$ for Dirichlet process mixtures. Increasing $l$ in the case of DD and $r$ in the case of DPM favors small clusters and increases the overall number of clusters.

Here, we consider how to set parameters that reflect the structure of the data as much as possible. An overview of the structure is shown in Fig.3. We first assume that $\eta_r$ is the ratio of the size of the cluster defined by the co-variance matrix $\tau^{-1}$ to the size of the whole data defined by $\Sigma_x$:

$$
\langle \tau_j \rangle_p^{-1} = s_0^{-1} l_0 = \eta_r^2 \Sigma_x,
$$

(33)

The range of $\mu$ present is shown as a ratio $\eta_\mu$ to the total data $\Sigma_x$, and the range of $\beta$ is shown as
a ratio $\eta_\beta$ to $\tau$. The correlation between $\mu$ and $\beta$ is defined by $\xi \in [-1, 1]$. In other words, from the prior distribution of $\alpha$ and $\beta$, the following equation holds:

$$\begin{bmatrix}
u_0 \langle \tau_j \rangle_p & w_0 \langle \tau_j \rangle_p \\
w_0 \langle \tau_j \rangle_p & v_0 \langle \tau_j \rangle_p
\end{bmatrix}^{-1} = \begin{bmatrix}
\eta_\mu^2 \Sigma_x & \eta_\mu \eta_\beta \xi \Sigma_x^{\frac{1}{2}} \langle \tau_j \rangle_p^{-\frac{1}{2}} \\
\eta_\mu \eta_\beta \xi \Sigma_x^{\frac{1}{2}} \langle \tau_j \rangle_p^{-\frac{1}{2}} & \eta_\beta^2 \langle \tau_j \rangle_p
\end{bmatrix}. \quad (34)$$

Finally, we set the degree of freedom (confidence level) of $\tau$ as $s_0 = \nu_\tau$. To summarize the above equations, $s_0$, $t_0$, $u_0$, $w_0$ and $v_0$ can be expressed using $\eta_\mu$, $\eta_\tau$ and $\eta_\beta$,

$$s_0 = \nu_\tau, \quad t_0 = \nu_\tau \eta_\tau^2 \Sigma_x, \quad u_0 = \frac{\eta_\tau^2}{\eta_\mu (1 - \xi^2)}, \quad w_0 = \frac{\eta_\tau \xi}{\eta_\mu \eta_\beta (1 - \xi^2)}, \quad v_0 = \frac{1}{\eta_\beta^2 (1 - \xi^2)}. \quad (35)$$

For the shape of mixing density (normality) is $\lambda_0$, the mean $\lambda_0 = \langle \lambda \rangle_p$ and the shape $\nu_\lambda = \lambda_0^2 \langle (\lambda - \lambda_0)^2 \rangle_p^{-1}$ are used to define the hyper-parameters. The conjugate prior is generalized inverse Gaussian, but its special cases inverse Gaussian and Gamma were used for the prior distribution. The hyper-parameters of $\lambda$ are defined for inverse Gaussian prior as

$$f_0 = \nu_\lambda \lambda_0^{1}, \quad g_0 = \nu_\lambda \lambda_0, \quad h_0 = -\frac{1}{2}. \quad (36)$$

On the other hand, Gamma distribution with the mean $\lambda_0$ and shape $\nu_\lambda$ can be defined as

$$f_0 = 2\nu_\lambda \lambda_0^{1}, \quad g_0 = 0, \quad h_0 = \nu_\lambda. \quad (37)$$

In this paper, we basically set $\eta_\mu = 1$, $\eta_\tau = 0.3$, $\eta_\beta = 0.3$, $\xi = 0$, $\lambda_0 = 5$, $\nu_\tau = D + 1$ and $\nu_\lambda = 1$. Since the spatial size of the cluster and the nature of the bias varies from data to data, it is useful to set the parameters appropriately. However, setting $nu_\tau$ to a small value can reduce the influence of the parameters. If the nature of the data is actually known, a larger $nu_\tau$ will give more appropriate results. Similarly, for normality $\lambda$, it is important to set appropriately $\lambda_0$ and its influence $\nu_\lambda$.
2.7 Initial and convergence conditions

The initial conditions are set to $\bar{y} = \hat{y} = 1$, with $z$ being the one hot representation based on the clusters obtained by the K-means algorithm. Then, apply M-step first, then the E-step. If the estimated number in cluster $Z_j^*$ shrinks less than $\varepsilon_z = 2$ during the iteration, the corresponding cluster is removed and the algorithm proceeds.

If the change in ELBO $L$ is smaller than $\varepsilon_{dL} = 10^{-5}N$ five times in a row, algorithm is terminated. After finding $\rho_{ij}$ in E-step, ELBO is evaluated by the following equation (Takekawa and Fukai 2009):

$$L = \sum_i \log \sum_j \rho_{ij} - \text{KL} [q_\theta (\alpha, \lambda, \mu, \beta, \tau), p (\alpha, \lambda, \mu, \beta, \tau)].$$

3 Results

As simulation data, the $M$ centers $\mu_1, \cdots, \mu_M$ are generated from the normal distribution of the average 0 and covariance matrix $I$. Similarly, we generate the bias $\beta_1, \cdots, \beta_M$ from the normal distribution of mean 0 and covariance matrix $\sigma^2 I$. The precision matrix $\tau_1, \cdots, \tau_M$ are also generated from a Wishart distribution with mean $\sigma^{-2} I$ and degrees of freedom $D + 5$. The normalities $\lambda_1, \cdots, \lambda_M$ are generated from an inverse normal distribution with mean $\lambda_*$ and shape parameter $5$. Finally, a sample data with $N = 1000$ is generated using the above parameters. The number of data in the cluster was prepared for two cases: the uniform case and the non-uniform case. In the uniform case, each cluster contains 100 data. In the non-uniform case, there are two large clusters with 400 and 200 data and eight small clusters with 50 data. An example of 3D data generated in Fig. 2 is shown.

In the following, we control the normality $\lambda_j$ by $\lambda_*$ and the asymmetry by $\sigma_\beta$. In addition, we adjust the difficulty by approaching the relative distance between clusters by $\sigma$. Basically, algorithms are applied 10 times per dataset with different initial conditions. Initial number of the cluster $M_0$ is set to 50. We evaluate the performance of the clustering using ARI. Hereafter, we name that VB for Gaussian mixture models as GMM, VB for NIG mixture models with $\lambda$ shape.
Figure 4: ARI score of simulation data.
Figure 5: Estimate number of clustering. The truth is $M = 10$. 

$\lambda^* = 10$ 
$\lambda^* = 1$ 
$\lambda^* = 0.1$ 

$\sigma_\theta = 0$ 
$\sigma_\theta = 0.5$ 
$\sigma_\theta = 1$ 

GMM 
trun 
gam 
invG 

0.1 0.2 0.3

difficulty 

difficulty
Figure 6: Relationship between ELBO and ARI in the proposed algorithms.

fixed as trun, the proposed model with gamma prior as gam and the proposed model with inverse Gaussian prior as invG, respectively.

For the case of high normality ($\lambda^* = 10$; see left columns of Fig. 4 and 5), the results of four algorithms were almost identical. Although the ARI decreased with increasing difficulty (Fig. 4), the estimate of the number of clusters was generally close to correct answer $M = 10$ (Fig. 4). For the case of $\lambda^* = 1$, the ARI of the proposed models (gam and invG) are slightly higher than the ARI of GMM and trun. This tendency is especially strong when the asymmetry $\sigma_\beta$ is large. In most cases, GMM fails to estimate the number of clusters. For the case of highly non-normal and tail-heavy ($\lambda^* = 0.1$), the ARI of the proposed models (gam and invG) are significantly higher than the ARI of GMM and trun. In particular, the results of trun have a large variation and low values. This is because trun assumes that $\lambda = 1$. It can be interpreted as not being able to cope with different situations than expected. Overall, the proposed model estimates the correct number of clusters in all cases and obtains a high ARI score. The proposed method showed higher AIR and less variability especially when the normality was lower.

The relationship between ELBO and ARI for the proposed method shows a strong correlation (Fig. 6). This shows that selecting a large ELBO result from multiple output with different initial
Figure 7: Comparison between finite (Dirichlet distribution) and infinite (Dirichlet process mixture) model in estimation number of clusters for unbaranced population data.

conditions yields a better performance. In the relationship between the ELBO and the ARI, There was no difference between the finite (Dirichlet distribution) model and the infinite (Dirichlet process mixture) model (Fig. 6). In the non-uniform population case, the estimate of the number of clusters is slightly worse than that in the uniform case (Fig. 5). The estimation by the infinite model is a slightly better estimate than that of the finite model, but it is not significantly different (Fig. 5).

4 Discussion

We proposed a variational Bayesian clustering method for heavy tailed and/or asymmetric data based on a variational Bayes algorithm for NIG mixture models as an improvement of an existing model. In addition to the finite mixture model with Dirichlet distributions, Dirichlet process mixture were also derived. In the evaluation by artificial data, the proposed method performed much better than the Gaussian and existing NIG distribution models, especially in the case of normality $\lambda$ small.

In this paper, in addition to the infinite and finite implementations we have two prior distributions of non-normality: the gamma distribution and the inverse gamma distribution. None of the implementation combinations showed significant differences for artificial data. If we have some prior knowledge of the data, we can set each hyperparameter more appropriately. The adjustment of hyperparameters by empirical Bayesian methods is also a topic worthy of further study.
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A Distributions

In this section, we use the modified Bessel function of the third kind $K_c(\cdot)$ of order $c$ the gamma function $\Gamma$, the $D$-dimensional gamma function $\Gamma_D$ and the digamma function $\psi$.

A.1 Definitions

The generalized inverse Gaussian distribution is defined as

$$
\log \mathcal{N}^{-1}_s \left( x \mid a, b, c \right) = \Delta (a, b, c) + (c - 1) \log x - \frac{a}{2} - \frac{b}{2} x^{-1},
$$

(39)

$$
\Delta (a, b, c) = -\log 2 + \frac{c}{2} \log \frac{a}{b} - \log K_c \left( \sqrt{ab} \right).
$$

(40)

The generalized inverse Gaussian with $c = -\frac{1}{2}$ is inverse Gaussian distribution

$$
\log \mathcal{N}^{-1}_s \left( x \mid a, b, -\frac{1}{2} \right) = \log \mathcal{N}^{-1} \left( x \mid \mu = \sqrt{\frac{b}{a}}, \lambda = \sqrt{ac} \right)
$$

$$
= -\frac{1}{2} \log 2\pi + \frac{1}{2} \log \lambda + \lambda - \log \mu - \frac{3}{2} \log \frac{x}{\mu} - \frac{\lambda x}{2 \mu} - \frac{\lambda \mu}{2 x},
$$

(41)

and the generalized inverse Gaussian with $b = 0$ is Gamma distribution

$$
\log \mathcal{N}^{-1}_s \left( x \mid a, 0, c \right) = \log \mathcal{G} \left( x \mid \alpha = \sqrt{c}, \beta = \frac{a}{2} \right)
$$

$$
= -\log \Gamma (\alpha) + \alpha \log \beta - (\alpha - 1) \log x - \beta x.
$$

(42)
Dirichlet, Beta, Wishart and normal distribution are respectively defined as

\[
\log \mathcal{D} (\alpha_1, \cdots \alpha_M \mid l_1, \cdots, l_M) = \log \Gamma \left( \sum_{j=1}^{M} l_j \right) - \sum_{j=1}^{M} \log \Gamma (l_j) + \sum_{j=1}^{M} (l_j - 1) \log \alpha_j, \tag{43}
\]

\[
\log \mathcal{B} (x \mid \alpha, \beta) = \Gamma (\alpha + \beta) - \Gamma (\alpha) - \Gamma (\beta) + (\alpha - 1) \log x + (\beta - 1) \log (1 - x), \tag{44}
\]

\[
\log \mathcal{W} (x \mid \alpha, \beta) = \frac{\alpha}{2} \log \det \beta - \log \Gamma_D (\frac{\alpha}{2}) + \frac{\alpha - D - 1}{2} \log \det x - \frac{1}{2} \tr \beta x, \tag{45}
\]

\[
\log \mathcal{N} (x \mid \mu, \tau) = -\frac{d}{2} \log 2\pi + \frac{1}{2} \log \det \tau - \frac{1}{2} \tr \tau (x - \mu) (x - \mu)\top. \tag{46}
\]

A.2 The mixing density

In the definition of the proposed model, the mixing density obey the inverse Gaussian which mean is 1:

\[
\log \mathcal{N}^{-1} (y \mid y_0 = 1, \lambda) = \log \mathcal{N}_*^{-1} \left( y \mid \lambda, \lambda, -\frac{1}{2} \right) = -\frac{1}{2} \log 2\pi + \frac{1}{2} \log \lambda + \lambda - \frac{3}{2} \log y - \lambda \frac{y}{2} - \lambda \frac{y^{-1}}{2}. \tag{47}
\]

And the expectation values of the posterior \( q (y \mid z) = \mathcal{N}_*^{-1} (y \mid a, b, c) \) are calculated as

\[
\langle y \rangle_{\mathcal{N}_*^{-1}(y/a,b,c)} = \sqrt{\frac{b}{a}} K_{c+1} \left( \sqrt{ab} \right), \quad \langle y^{-1} \rangle_{\mathcal{N}_*^{-1}(y/a,b,c)} = \sqrt{\frac{a}{b}} K_{c-1} \left( \sqrt{ab} \right). \tag{48}
\]

A.3 Expectations for posteriors

For Dirichlet distribution models, the conjugate prior of \( \alpha \) is \( q (\alpha) = \mathcal{D} (\alpha \mid l) \) and the expectation values are

\[
\langle \log \alpha_j \rangle_{\mathcal{D}(\alpha \mid l)} = \psi (l_j) - \psi \left( \sum_{j'=1}^{M} l_{j'} \right). \tag{49}
\]
For DPM, the conjugate prior of $\gamma$ is beta distribution $q(\gamma) = \mathcal{B}(\gamma | l, r)$ and the expectation values are

$$\langle \log \gamma_j \rangle_{\mathcal{B}(\gamma | l, r)} = \psi(l) - \psi(l + r),$$  \hspace{1cm} (50)

$$\langle \log (1 - \gamma_j) \rangle_{\mathcal{B}(\gamma | l, r)} = \psi(r) - \psi(l + r).$$ \hspace{1cm} (51)

The posterior of $\lambda$ obey the generalized inverse Gaussian $q(\lambda) = \mathcal{N}_s^{-1}(\lambda | f, g, h)$ and the expectation values are

$$\langle \lambda \rangle_{\mathcal{N}_s^{-1}(\lambda | f, g, h)} = \sqrt{\frac{g}{f}} K_{h+1}(\sqrt{fg})^s,$$

$$\langle \log \lambda \rangle_{\mathcal{N}_s^{-1}(\lambda | f, g, h)} = \log \sqrt{\frac{g}{f}} + \frac{\partial \log K_h}{\partial h}(\sqrt{fg})$$ \hspace{1cm} (53)

In the case that $\lambda$ obey Gamma distribution $q(\lambda) = \mathcal{N}_s^{-1}(\lambda | f, 0, h) = \mathcal{G}(\lambda | h, f/2)$, which is the special case of the generalized inverse Gaussian with $g = 0$, the expectation values are

$$\langle \lambda \rangle_{\mathcal{G}(\lambda | h, f/2)} = \frac{2h}{f},$$ \hspace{1cm} (54)

$$\langle \log \lambda \rangle_{\mathcal{G}(\lambda | h, f/2)} = \psi(h) - \log f + \log 2$$ \hspace{1cm} (55)

The posterior of $\tau$ obey Wishart distribution $q(\tau) = \mathcal{W}(\tau | s, t)$ and the expectation values are

$$\langle \tau \rangle_{\mathcal{W}(\tau | s, t)} = st^{-1},$$ \hspace{1cm} (56)

$$\langle \log \det \tau \rangle_{\mathcal{W}(\tau | s, t)} = \psi_d\left(\frac{s}{2}\right) - \log \det \frac{t}{2}.$$ \hspace{1cm} (57)

The posterior of $\mu$ and $\beta$ obey Normal distribution:

$$q_{\mu}(\mu, \beta | \tau) = \mathcal{N}\left(\begin{array}{c}
\mu \\
\beta
\end{array} \middle| \begin{array}{cc}
m & u\tau & w\tau \\
n & w\tau & v\tau
\end{array}\right).$$ \hspace{1cm} (58)
and the expectation values are

$$
\langle \mu \rangle_{q(\mu,\beta\mid \tau)} = m, \quad \langle \beta \rangle_{q(\mu,\beta\mid \tau)} = n, \quad (59)
$$

$$
\langle \tau \mu \mu^\top \rangle_{q(\mu,\beta\mid \tau)} = u^{-1}I, \quad \langle \tau \mu \beta^\top \rangle_{q(\mu,\beta\mid \tau)} = w^{-1}I, \quad \langle \tau \beta \beta^\top \rangle_{q(\mu,\beta\mid \tau)} = v^{-1}I. \quad (60)
$$

### A.4 Prior setting

The inverse Gaussian distribution is a special case of generalized inverse Gaussian with $c = -1/2$ and described by mean $\mu$ and shape $\lambda$ parameter

$$
\mathcal{N}_x^{-1} \left( \lambda \mid f, g, -\frac{1}{2} \right) = \mathcal{N}^{-1} \left( \lambda \mid \sqrt{\frac{g}{f}}, \sqrt{fg} \right), \quad (61)
$$

$$
\lambda_0 = \langle \lambda \rangle_{\mathcal{N}_x^{-1}(\lambda\mid f, g, -\frac{1}{2})} = \sqrt{\frac{g}{f}}, \quad \nu_{\lambda} = \lambda_0^2 \langle (\lambda - \lambda_0)^2 \rangle_{\mathcal{N}_x^{-1}(\lambda\mid f, g, -\frac{1}{2})} = \sqrt{fg} \quad (62)
$$

The gamma distribution is also special case of generalized inverse Gaussian with $c = 0$ and described by shape $\alpha$ and rate $\beta$ parameter

$$
\mathcal{N}_x^{-1} \left( x \mid f, 0, h \right) = \mathcal{G} \left( x \mid \frac{h}{f^2} \right), \quad (63)
$$

$$
\lambda_0 = \langle \lambda \rangle_{\mathcal{N}_x^{-1}(\lambda\mid f, 0, h)} = \frac{2h}{f}, \quad \nu_{\lambda} = \lambda_0^2 \langle (\lambda - \lambda_0)^2 \rangle_{\mathcal{N}_x^{-1}(\lambda\mid f, 0, h)} = h \quad (64)
$$

### B Difference between the previous and the proposed model

Main difference between the previous model [Subedi and McNicholas, 2014] and the proposed model is limitation to the mixing density. The inverse Gaussian distribution has the mean and the shape parameters. The previous model fix the shape parameter and it conclude the truncated normal distribution $\mathcal{N}_{>0}$ for the conjugate prior.

They defined that the probability of the mixing density $y$ obey

$$
p(y) = \mathcal{N}^{-1} \left( y \mid \frac{1}{\lambda}, 1 \right). \quad (65)$$
In this condition, the terms of $\lambda'$ in the expectation of joint model can be written as

$$\langle \log p(x, y, z \mid \alpha, \lambda, \mu, \beta, \tau) \rangle_{q_c} = \sum_{j=1}^{M} \left\{ -\frac{Z_j^+}{2} \lambda_j^2 + Z_j^+ \lambda_j \right\} + \cdots$$  \hspace{1cm} (66)

And the conjugate prior and the update rules in M-step can be described as

$$p(\lambda_0) = \mathcal{N}_{>0}(\lambda_j \mid f_0, g_0), \quad q(\lambda_j) = \mathcal{N}_{>0}(\lambda_j \mid f_j, g_j)$$  \hspace{1cm} (67)

and

$$f_j = \frac{f_0 g_0 + Z_j^*}{g_0 + Z_j^+}, \quad g_j = g_0 + Z_j^+.$$  \hspace{1cm} (68)

In E-step, Eq. (22) and (23) are replaced by the following equations:

$$a_j = \langle \lambda_j^2 \rangle_{q_0} + \text{tr} \langle \tau_j \beta_j \beta_j^T \rangle_{q_0} + \text{tr} \langle \tau_j \beta_j \rangle_{q_0} \langle \beta_j \rangle_{q_0} \langle \beta_j \rangle_{q_0}^T,$$

$$b_{ij} = 1 + \text{tr} \langle \tau_j \mu_j \mu_j^T \rangle_{q_0} + \text{tr} \langle \tau_j \mu_j \rangle_{q_0} \left(x_i - \langle \mu_j \rangle_{q_0}\right) \left(x_i - \langle \mu_j \rangle_{q_0}\right)^T$$  \hspace{1cm} (69)

and

$$\log \rho_{ij} = -\frac{D + 1}{2} \log 2\pi + \langle \log \alpha_j \rangle_{q_0} + \langle \lambda_j \rangle_{q_0} + \frac{1}{2} \langle \log \det \tau_j \rangle_{q_0}$$

$$- \text{tr} \langle \tau_j \mu_j \beta_j \rangle_{q_0} + \text{tr} \langle \tau_j \beta_j \rangle_{q_0} \left(x_i - \langle \mu_j \rangle_{q_0}\right) \langle \beta_j \rangle_{q_0}^T - \log \Delta(a_j, b_{ij}, c).$$  \hspace{1cm} (70)
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