A Bayesian Mixture Model for Clustering on the Stiefel Manifold

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Abstract: Analysis of a Bayesian mixture model for the Matrix Langevin distribution on the Stiefel manifold is presented. The model exploits a particular parametrization of the Matrix Langevin distribution, various aspects of which are elaborated on. A general, and novel, family of conjugate priors, and an efficient Markov chain Monte Carlo (MCMC) sampling scheme for the corresponding posteriors is then developed for the mixture model. Theoretical properties of the prior and posterior distributions, including posterior consistency, are explored in detail. Extensive simulation experiments are presented to validate the efficacy of the framework. Real-world examples, including a large scale neuroimaging dataset, are analyzed to demonstrate the computational tractability of the approach.

Keywords and phrases: Matrix Langevin Mixture model, Mixture model, Orthonormal vectors, Parametric model, Stiefel manifold.

1. Introduction

Analysis of directional data comprises a major sub-field of study in Statistics. Directional data range from unit vectors in the simplest examples, to sets of ordered orthonormal frames in the general case. Since the associated sample space is not the Euclidean space, standard statistical methods developed for the Euclidean space for the analysis of univariate or multivariate data cannot be easily adapted for directional data. For example, it is often desirable to account for the geometric structure underlying the sample space in statistical inference. Beyond those fashioned for simpler non-Euclidean spaces like the circle or the sphere, there is a pressing need for methodology development for general sample spaces such as the Stiefel or the Grassmann manifold to support modern
applications, increasingly seen in the fields of computer vision (Turaga, Veeraraghavan and Chellappa, 2008; Turaga et al., 2011; Anand, Mittal and Meer, 2016; Lui and Beveridge, 2008; Zeng et al., 2015), medical image analysis (Lui, 2012), astronomy (Mardia and Jupp, 2009; Lin, Rao and Dunson, 2017), and, biology (Downs, 1972; Mardia and Khatri, 1977), to name but a few. In this article, we present a framework for Bayesian inference of a mixture model on the Stiefel manifold (James, 1976; Chikuse, 2012) that remains computationally tractable even at large data sizes. With ever-growing computational power, we argue that it is now feasible to apply Bayesian methods to real world large and directional data.

One of the most commonly used distributions on the Stiefel manifold is an exponential family distribution known as the Matrix Langevin ($\mathcal{ML}$) or the Von-Mises Fisher matrix distribution (Mardia and Jupp, 2009; Khatri and Mardia, 1977), introduced first by Downs (1972). In early work Mardia and Khatri (1977) and Jupp and Mardia (1980) studied the properties of the maximum likelihood estimators for this distribution in the classical setting. In large measure, subsequent efforts at exploring the $\mathcal{ML}$ distribution (Chikuse, 1991a,b, 1998) were limited to asymptotic results on distributional or inferential problems. More recently, Hoff (2009) has developed a rejection sampling based method to sample from a matrix Bingham-Von Mises-Fisher distribution on the Stiefel manifold. To date, Bayesian analysis on these general sample spaces have been very limited. A major obstacle for the development of efficient inference techniques for this family of distributions has been the intractability of the corresponding normalizing constant, a hypergeometric function of matrix argument.

The article that is most aligned to our overall objective is Lin, Rao and Dunson (2017), where the authors have developed a rejection sampling based data augmentation strategy for Bayesian inference with the mixture of $\mathcal{ML}$ distribution. However, it is well known that sampling techniques based on a data augmentation strategy often suffer from slow rates of convergence. With the additional detrimental impact of the rejection ratio, convergence can become painfully slow. Applicability of their MCMC technique is therefore limited, particularly in terms of scalability to large datasets.

Our contribution begins with an exploration of the properties of the $\mathcal{ML}$ distribution, followed by the construction of a family of conjugate priors for $\mathcal{ML}$ distribution, which we then analyze in considerable detail. In the context of the natural exponential family, Diaconis and Ylvisaker (Diaconis and Ylvisaker, 1979) laid the foundations for constructing conjugate prior distributions (the DY class) for natural exponential family models. In our case, however, the DY construction can not be directly applied, and we therefore derive a modified construction. The resultant prior is flexible in the sense that one can incorporate information from data via appropriate hyperparameter selection, and furthermore, there is the provision to set the hyperparameters in the absence of any prior knowledge to a weakly non-informative prior. For the latter, the prior might become improper in which case we adopt a constrained mixture model. Using this novel prior we implement a scalable posterior inference scheme by designing an efficient Gibbs sampler. We note in passing that in the expression for
the posterior, the presence of $_0F_1(\cdot,\cdot)$ in the denominator make the inference procedure challenging. We also explore the weak and strong posterior consistency under the new class of priors. Finally, we extend the proposed framework for a single $\mathcal{ML}$ distribution to a finite mixture of $\mathcal{ML}$'s.

To identify the optimum number of clusters, often times deviance information criterion (DIC) has been used in the literature (Gelman et al., 2003; Spiegelhalter et al., 2002). However, several studies have pointed to the weakness of the standard DIC measure in mixture models and have proposed alternatives. We perform extensive simulations to identify alternative schemes to computing DIC that would work best for a mixture of $\mathcal{ML}$ distributions. In order to demonstrate the scalability of our inference scheme, we then analyze a large-scale DT-MRI dataset. Real datasets that have been analyzed in the literature come from astronomy (near-earth objects) or vectorcardiography. In both cases the data is drawn from a matrix valued manifold where each element is a collection of two orthonormal vectors in $\mathbb{R}^3$. Realizing that most of the existing applications rely on an efficient computation of the matrix hypergeometric function on a $2 \times 2$ matrix, we have also optimized our inference technique for this class of matrices. We have tested our method on a moderate sized dataset of near earth objects (NEO) with the goal of clustering the data. Obtained results are very similar to that reported in the literature.

In summary, we aim to achieve three objectives: (i) the construction of a new class of distributions for conjugate priors for ML distributions and the development of their theoretical properties, (ii) the design of an efficient MCMC sampling algorithm, and finally, (iii) successful application of the framework to a large-scale (DTI) dataset.

The remainder of the paper is organized as follows. In Section 2, we introduce the $\mathcal{ML}$ distribution defined on the Stiefel manifold ($\mathcal{V}_{n,p}$) and explore its theoretical properties as well as properties of the corresponding hypergeometric constant. In Section 3, we present the construction of the conjugate prior and the posterior for a single $\mathcal{ML}$ distribution, properties of which are then analyzed in considerable detail. Generalization to a finite mixture model and inference are presented in Section 4, as well as extended theoretical properties such as the weak and strong posterior consistency. Extensive simulation studies are presented and summarized in Section 5. In Section 6, we provide experimental results from two real-world datasets. Conclusions and future work in presented in Section 7.

Notational Convention

- $\mathbb{R}^k$ = The $k$-dimensional real space.
- $\mathcal{S}_p = \{(d_1, \ldots, d_p) \in \mathbb{R}_+^p : 0 < d_p < \cdots < d_1 < \infty\}$.
- $\mathbb{R}^{n \times p}$ = Space of all $n \times p$ real-valued matrices.
- $\mathcal{V}_{n,p}$ = Stiefel Manifold.
- $\mathcal{V}_{n,p} = \{X \in \mathcal{V}_{n,p} : X_{1,j} > 0 \ \forall j = 1, 2, \cdots, p\}$.
- $\mathcal{V}_{p,p} = O(p)$ = Space of Orthogonal matrices.
- $\Upsilon(\cdot)$ = Product measure defined on $\mathcal{V}_{n,p} \times \mathbb{R}^p_+ \times \mathcal{V}_{p,p}$. 
• $I_p = p \times p$ identity matrix.
• $f(\cdot, \cdot) =$ Probability density function.
• $g(\cdot, \cdot) =$ Unnormalized version of the probability density function.
• $tr(A) =$ Trace of a square matrix $A$.
• $etr(A) =$ Exponential of $tr(A)$.
• $\mathbb{E}(X) =$ Expectation of the random variable $X$.
• $\mathbb{1}(\cdot) =$ Indicator function.
• We use $d$ and $D$ interchangeably. $D$ is the diagonal matrix with diagonal $d$. We use matrix notation $D$ in the place of $d$ wherever needed, and vector $d$ otherwise.
• $\| \cdot \|_2 =$ Matrix operator norm.

2. $\mathcal{ML}$ distribution on the Stiefel manifold ($\mathcal{V}_{n,p}$)

The Stiefel manifold, $\mathcal{V}_{n,p}$ is the space of all $p$ ordered orthonormal vectors (also known as $p$-frames) in $\mathbb{R}^n$ and is defined as

$$\mathcal{V}_{n,p} = \{ X \in \mathbb{R}^{n \times p} : X^T X = I_p \},$$

where $\mathbb{R}^{n \times p}$ is the space of all $n \times p$ real-valued matrices and $I_p$ is the $p \times p$ identity matrix (Mardia and Jupp, 2009; Absil, Mahony and Sepulchre, 2009; Chikuse, 2012; Edelman, Arias and Smith, 1998; Downs, 1972). $\mathcal{V}_{n,p}$ is a compact Riemannian manifold of dimension $np - p(p+1)/2$. For $p = 1$, $\mathcal{V}_{n,p}$ is the $(n-1)$ hypersphere $\mathbb{S}^{n-1}$ and for $p = n$, $\mathcal{V}_{n,p} = O(p)$, the orthogonal group consisting all orthogonal $p \times p$ real-valued matrices, with the group operation being matrix multiplication. $\mathcal{V}_{n,p}$ may be embedded in the $np$-dimensional Euclidean space of $n \times p$ real-valued matrices with the inclusion map as a natural embedding, and is thus a submanifold of $\mathbb{R}^{np}$. Since $\mathcal{V}_{n,p}$ is an embedded submanifold of $\mathbb{R}^{np}$, its topology is the subset topology induced by $\mathbb{R}^{np}$ (Absil, Mahony and Sepulchre, 2009; Edelman, Arias and Smith, 1998).

The differential form $(H_1^T dH_1) = \bigwedge_{i=1}^p \bigwedge_{j=i+1}^n h_i^T d h_i$ where $H_1 \in \mathcal{V}_{n,p}$, is invariant under the transforms $H_1 \rightarrow QH_1$ and $H_1 \rightarrow PH_1$ where $Q \in \mathcal{V}_{n,n}$ and $P \in \mathcal{V}_{p,p}$, respectively. This defines an invariant measure on $\mathcal{V}_{n,p}$. The surface area or volume of $\mathcal{V}_{n,p}$ is $Vol(\mathcal{V}_{n,p}) := \int_{\mathcal{V}_{n,p}} (H_1^T dH_1) = 2^n (\sqrt{\pi})^{np} / \Gamma_p(n/2)$ where $\Gamma_p(\cdot)$ is the multivariate Gamma function (page 70 in Muirhead (2009)).

The measure defined in this manner is called the invariant unnormalized or the Haar measure. This measure can be normalized to a probability measure by setting $\int_{\mathcal{V}_{n,p}} [dH] = 1$ where $[dH] = (H_1^T dH_1) / Vol(\mathcal{V}_{n,p})$. Uniform distribution on $\mathcal{V}_{n,p}$ is denoted by $[dH]$ and is the unique probability measure which is invariant under rotations and reflections. For detail description of construction of the Haar measure on $\mathcal{V}_{n,p}$ and its properties please refer to Muirhead (2009).

$\mathcal{ML}$ distribution (Mardia and Jupp 2009) is a widely used non-uniform distribution on $\mathcal{V}_{n,p}$ (Khatri and Mardia, 1977; Mardia and Jupp, 2009; Chikuse, 2012; Lin, Rao and Dunson, 2017). This distribution is also known as Von Mises-Fisher Matrix Distribution (Khatri and Mardia, 1977). The density function of
the $\mathcal{ML}$ distribution with respect to the normalized Haar measure $[dX]$ and parametrized by $F \in \mathbb{R}^{n \times p}$, defined in Chikuse (2012), is given by

$$f_{\mathcal{ML}}(X; F) = \frac{etr(F^T X)}{0 F_1 \left( \frac{n}{2}, \frac{F^T F}{4} \right)},$$  \hspace{1cm} (1)$$

where $etr(Z) = \exp(\text{trace}(Z))$ for any square matrix $Z$ and the normalizing constant, $0 F_1(n/2, F^T F/4)$, is a hypergeometric function with a matrix argument (Herz, 1955; James, 1964; Muirhead, 1975; Gupta and Richards, 1985; Gross and Richards, 1987, 1989; Butler and Wood, 2003; Koev and Edelman, 2006; Chikuse, 2012). We consider a particular form of the unique singular value decomposition (SVD) (as defined in Equation 1.5.8 in Chikuse (2012)) of the $n \times p$ parameter matrix $F = MDV^T$ where $M \in \tilde{V}_{n,p}$, $V \in V_{p,p}$ and the diagonal entries of $D$, $d = (d_1, d_2, \cdots, d_p) \in S_p$ where $0 < d_p < \cdots < d_2 < d_1 < \infty$ (Chikuse, 2012). See Notation for definitions of $\tilde{V}_{n,p}, V_{p,p}$ and $S_p$. Here, $\tilde{V}_{n,p}$ denotes the a subspace of $V_{n,p}$ consisting of matrices in $V_{n,p}$ whose elements of the first row of are positive. Note that, being a closed subspace of $V_{n,p}$, $\tilde{V}_{n,p}$ is also a compact space.

Plugging in the SVD form of $F$, we rewrite the $\mathcal{ML}$ density function as

$$f_{\mathcal{ML}}(X; (M, d, V)) = \frac{etr(VDM^T X)}{0 F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right)} \mathbb{1}(M \in \tilde{V}_{n,p}, d \in S_p, V \in V_{p,p}).$$

This parametrization ensures identifiability of all the parameters $(M, d$ and $V$). For notational convenience we omit the indicator function part and use the following form of the $\mathcal{ML}$ density for rest of the article

$$f_{\mathcal{ML}}(X; (M, d, V)) = \frac{etr(VDM^T X)}{0 F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right)},$$  \hspace{1cm} (2)$$

with respect to the normalized Haar measure $[dX]$ (Muirhead, 2009). From Khatri and Mardia (1977) (page 96) note that the normalizing constant can be simplified as follows –

$$0 F_1 \left( \frac{n}{2}, \frac{F^T F}{4} \right) = 0 F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right).$$

Thus $0 F_1(\cdot)$ only depends on the eigenvalues of the matrix $F^T F$, which are the diagonal elements of the matrix $D^2$. The parametrization with $M, D$ and $V$ enables us to represent the intractable hypergeometric function of matrix argument as a function of vector $d$, diagonal entries of $D$, paving a path for an efficient posterior inference. This makes posterior inference computationally tractable. Note that an alternative parametrization through polar decomposition with $M$ and $K$ (Mardia and Jupp, 2009) may pose computational challenges since the elliptical part $K$ lies on a positive semi-definite cone and inference on positive semi-definite cone is not that straightforward (Hill and Waters, 1987; Bhatia,
In this article, we use $M$, $D$ and $V$ parameters based representation for $\mathcal{ML}$ distribution for most part of our theory. In the following subsection we study a few important properties of the hypergeometric function of matrix argument $\mathbf{0}_F^1\left(\frac{n}{2}, D^2/4\right)$, which are required for subsequent sections.

### 2.1. Properties of $\mathbf{0}_F^1\left(\frac{n}{2}, D^2/4\right)$

**Lemma 1.** For any $p \times p$ diagonal matrix $D$ with positive elements, $\mathbf{0}_F^1\left(\frac{n}{2}, D^2/4\right) \leq \text{etr}(D)$ when $n \geq p$.

**Proof of Lemma 1.**
From Equation 2, we have

$$
\int_{\mathcal{V}_{n,p}} f_{\mathcal{ML}}(X; (M, d, V)) [dX] = 1
$$

$$
\Rightarrow \int_{\mathcal{V}_{n,p}} \frac{\text{etr}(VDM^T X)}{\mathbf{0}_F^1\left(\frac{n}{2}, D^2/4\right)} [dX] = 1
$$

$$
\Rightarrow \mathbf{0}_F^1\left(\frac{n}{2}, D^2/4\right) = \int_{\mathcal{V}_{n,p}} \text{etr}(VDM^T X) [dX].
$$

(3)

We know that $f_{\mathcal{ML}}(X; (M, d, V))$ has the unique modal orientation $MV^T$ (page 32 in Chikuse (2012)). Hence it follows from Equation 3 that

$$
\mathbf{0}_F^1\left(\frac{n}{2}, D^2/4\right) \leq \int_{\mathcal{V}_{n,p}} \text{etr}(VDM^T MV^T) [dX]
$$

$$
= \text{etr}(D) \int_{\mathcal{V}_{n,p}} [dX] = \text{etr}(D),
$$

(4)

where $[dX]$ is the normalized Haar measure on $\mathcal{V}_{n,p}$.

**Lemma 2.** Let $A$ be a $n \times p$ real matrix with $n \geq p$. If $\|A\|_2 \leq \delta (< \delta)$ for some $\delta > 0$ then $|A_{j,j}| \leq \delta(< \delta)$ for $j = 1, \ldots, p$. Here $A_{j,j}$ denotes the $(j, j)$-th entry of the matrix $A$ and $\|A\|_2$ is the spectral norm of the matrix $A$.

**Proof of Lemma 2.**
From the assumptions of the Lemma 2 along with the definition of the spectral norm, it follows that $l^T A^T A l \leq \delta^2(< \delta^2)$ for all $l \in \mathbb{R}^p$ with $l^T l = 1$. In particular, $e^T_j A^T A e_j \leq \delta^2(< \delta^2)$ where $e_j \in \mathbb{R}^p$ such that its $j$-th entry equals 1 while rest of its entries are 0. Hence we have that $\sum_{k=1}^n A^2_{k,j} \leq \delta^2(< \delta)$ implying the fact that $|A_{j,j}| \leq \delta(< \delta)$.
Lemma 3. Let $D$ be a $p \times p$ diagonal matrix with positive diagonal elements $d = \{d_1, d_2, \ldots, d_p\}$. Then for any $\delta > 0$ and $n \geq p$, there exists a positive constant, $K_{n,p,\delta}$, depending on $n, p$ and $\delta$, such that
\[
_0 F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) > K_{n,p,\delta} \text{etr} \left( (1-\delta)D \right).
\]

Proof of Lemma 3.
Note that, $D$ is a $p \times p$ diagonal matrix with positive diagonal elements $d_1, \ldots, d_p$. For the case $n \geq p$, define
\[
\widetilde{M} = \begin{bmatrix} I_p & 0_{p \times (n-p)} \\ 0_{(n-p) \times p} & 0_{(n-p) \times (n-p)} \end{bmatrix}, \quad \widetilde{V} = I_p \quad \text{and} \quad I^* := \begin{bmatrix} I_p & 0_{p \times (n-p)} \\ 0_{(n-p) \times p} & 0_{(n-p) \times (n-p)} \end{bmatrix},
\]
where $I_p$ denotes the $p \times p$ identity matrix and $0_{a \times b}$ represents the zero matrix of dimension $a \times b$. For arbitrary given positive constant $\delta > 0$, consider
\[
B_{\delta} := \{ X \in \mathcal{V}_{n,p}, \text{ such that } \|X - I^*\|_2 < \delta \},
\]
where $\|\cdot\|_2$ denotes the spectral norm of a matrix. Let $\mu$ denotes the normalized Haar measure on the $\mathcal{V}_{n,p}$. Clearly, $0 < \mu(B_{\delta}) < \infty$, as $B_{\delta}$ is a non-empty open subset of $\mathcal{V}_{n,p}$. Now from Equation 2 we have,
\[
_0 F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) = \int_{\mathcal{V}_{n,p}} \text{etr} \left( \widetilde{V}D\widetilde{M}^T X \right) d\mu(X).
\]
\[
\geq \int_{B_{\delta}} \text{etr} \left( \widetilde{V}D\widetilde{M}^T X \right) d\mu(X).
\]
(6)
Using Lemma 2 we know that $X_{j,j} > (1 - \delta)$ for $j = 1, 2, \ldots, p$ where $X \in B_{\delta}$. Note that, $X_{j,j}$ denotes the $(j,j)$-th entry of the matrix $X$. Hence from Equation 5 and 6 it follows that,
\[
_0 F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) \geq \int_{B_{\delta}} \exp \left( \sum_{j=1}^{p} X_{j,j} d_j \right) d\mu(X),
\]
\[
> \mu(B_{\delta}) \text{etr} \left( (1-\delta)D \right),
\]
(7)
where the last inequality uses the fact that $d_j > 0$ for all $j = 1, \ldots, p$. Finally we denote $K_{n,p,\delta} := \mu(B_{\delta}) > 0$ as it depends on $n, p$ along with $\delta$, to conclude that
\[
_0 F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) > K_{n,p,\delta} \text{etr} \left( (1-\delta)D \right).
\]

□

Lemma 4. For any $p \times p$ diagonal matrix $D$ with positive elements $d \in \mathcal{S}_p$, the hypergeometric function of matrix argument denoted by $_0 F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right)$ is log-convex with respect to $d$ where $n \geq p$. 
Proof of Lemma 4.

From Equation 2, we have

$$0F1\left(\frac{n}{2}, D^2, 4\right) = \int_{\mathcal{V}_{n,p}} e^{tr(VDM^TX)} [dX],$$

(8)

for arbitrary $M \in \mathcal{V}_{n,p}$ and $V \in \mathcal{V}_{n,p}$ where $n \geq p$. Without loss of generality, we can take $M = \tilde{M} = \begin{bmatrix} I_p \\ 0_{(n-p),p} \end{bmatrix}$ and $V = I_p$.

Let $D_1$ and $D_2$ be two $p \times p$ diagonal matrix with positive diagonal entries $d_1$ and $d_2$, respectively and $d_1 \neq d_2$. From Equation 8, we have

$$0F1\left(\frac{n}{2}, \frac{D_1^2}{4}\right) = \int_{\mathcal{V}_{n,p}} e^{tr(D_1\tilde{M}^TX)} [dX]$$

and

$$0F1\left(\frac{n}{2}, \frac{D_2^2}{4}\right) = \int_{\mathcal{V}_{n,p}} e^{tr(D_2\tilde{M}^TX)} [dX].$$

(9)

Let $\lambda \in [0, 1]$ be any real number. We have

$$0F1\left(\frac{n}{2}, \frac{\lambda D_1 + (1 - \lambda) D_2}{4}\right)$$

$$= \int_{\mathcal{V}_{n,p}} e^{tr(\lambda D_1 + (1 - \lambda) D_2\tilde{M}^TX)} [dX]$$

$$= \int_{\mathcal{V}_{n,p}} \left( e^{tr(D_1\tilde{M}^TX)} \right)^\lambda \left( e^{tr(D_2\tilde{M}^TX)} \right)^{1-\lambda} [dX]$$

$$< \left( \int_{\mathcal{V}_{n,p}} e^{tr(D_1\tilde{M}^TX)} [dX] \right)^\lambda \left( \int_{\mathcal{V}_{n,p}} e^{tr(D_2\tilde{M}^TX)} [dX] \right)^{1-\lambda}$$

$$= \left( 0F1\left(\frac{n}{2}, \frac{D_1^2}{4}\right) \right)^\lambda \left( 0F1\left(\frac{n}{2}, \frac{D_2^2}{4}\right) \right)^{1-\lambda}. \quad (10)$$

Note that the inequality is due to Hölder (Hardy, Littlewood and Pólya, 1952) and note that in this case $d_1 \neq d_2$. Therefore from Equation 10 we have,

$$\log 0F1\left(\frac{n}{2}, \left(\frac{\lambda D_1^2}{4} + (1 - \lambda) \frac{D_2^2}{4}\right)\right) < \lambda \log 0F1\left(\frac{n}{2}, \frac{D_1^2}{4}\right) + (1 - \lambda) \log 0F1\left(\frac{n}{2}, \frac{D_2^2}{4}\right). \quad (11)$$

Hence $0F1\left(\frac{n}{2}, D^2\right)$ is a convex function or equivalently $0F1\left(\frac{n}{2}, D^2\right)$ is a log-convex function of the diagonal entries $d$ of matrix $D$. \qed
Lemma 5. For any $p \times p$ ($p \geq 2$) diagonal matrix $D$ with positive elements $d \in S_p$, then for $i = 1, 2, \cdots, p$ we have

$$0 < \frac{\partial}{\partial d_i} \left[ aF_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) \right] < aF_1 \left( \frac{n}{2}, \frac{D^2}{4} \right)$$

where $n \geq p$.

Proof of Lemma 5.

Right hand side inequality: Proceeding similar way as Lemma 4 we have

$$aF_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) = \int_{V_{n,p}} \text{etr} (D \tilde{M}^T X) [dX], \text{ where } \tilde{M} = \left[ \begin{array}{c} I_p \\ 0_{(n-p),p} \end{array} \right].$$

From Equation 12, we have

$$aF_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) = \int_{V_{n,p}} \exp \left( \sum_{j=1}^{p} d_j X_{j,j} \right) [dX].$$

Consider the set $V_0 := \{ X \in V_{n,p} : X_{i,i} = 1 \}$. Note that $V_0$ is isomorphic to the lower dimensional Stiefel manifold, $V_{n,p-1}$. $V_0$, being a lower dimensional subspace of $V_{n,p}$, has measure zero i.e. $\int_{V_{n,p}} I(X \in V_0) [dX] = 0$, where $I(X \in V_0)$ is the indicator function for $X$ to be in the set $V_0$. From Equation 13, we have

$$aF_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) = \int_{V_{n,p}} \exp \left( \sum_{j=1}^{p} d_j X_{j,j} \right) I(X \in V_0^c) [dX],$$

where $V_0^c$ is the complement of $V_0$. Hence,

$$\frac{\partial}{\partial d_i} \left[ aF_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) \right] = \int_{V_{n,p}} X_{i,i} I(X \in V_0^c) \exp \left( \sum_{j=1}^{p} d_j X_{j,j} \right) [dX].$$

Observe that, $\|X\|_2 = 1$ on $V_{n,p}$. Hence from Lemma 2 we have $|X_{i,i}| \leq 1$. Also, $X_{i,i} \neq 1$ when $X \in V_0^c$. As a result, we conclude that $X_{i,i} < 1$ on $V_{n,p} \cap V_0^c$. Subsequently, it follows from Equations 14 and 15 that,

$$\frac{\partial}{\partial d_i} \left[ aF_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) \right] < \int_{V_{n,p}} \exp \left( \sum_{j=1}^{p} d_j X_{j,j} \right) I(X \in V_0^c) [dX]
= aF_1 \left( \frac{n}{2}, \frac{D^2}{4} \right).$$
Left hand side inequality: Consider $V_{n,p}^{i,+} := \{ X \in V_{n,p} : X_{i,i} > 0 \}$, $V_{n,p}^{i,-} := \{ X \in V_{n,p} : X_{i,i} < 0 \}$ and $V_{n,p}^{i,0} := \{ X \in V_{n,p} : X_{i,i} = 0 \}$. Clearly, $V_{n,p}^{i,+}$, $V_{n,p}^{i,0}$ and $V_{n,p}^{i,-}$ forms a partition of $V_{n,p}$. Hence from equation 13 we have,

$$
\frac{\partial}{\partial d_i} \left[ \binom{\alpha}{\frac{n}{2}} \left( \frac{D^2}{4} \right) \right] = \int_{V_{n,p}^{i,+}} X_{i,i} \exp \left( \sum_{j=1}^{p} d_j X_{j,j} \right) \left[ dX \right] + \int_{V_{n,p}^{i,0}} X_{i,i} \exp \left( \sum_{j=1}^{p} d_j X_{j,j} \right) \left[ dX \right] + \int_{V_{n,p}^{i,-}} X_{i,i} \exp \left( \sum_{j=1}^{p} d_j X_{j,j} \right) \left[ dX \right].
$$

(17)

Let $\Gamma$ be the $n \times n$ diagonal matrix such that $\Gamma_{i,j} = 1$ for $j = 1, \ldots, n, j \neq i$ and $\Gamma_{i,i} = -1$. $\Gamma$ is an orthogonal matrix as $\Gamma^T \Gamma = I_n$. It is easy to show that $V_{n,p}^{i,+} = \{ \Gamma X : X \in V_{n,p}^{i,-} \}$.

Consider the change of variable $Y := \Gamma X$. Using standard algebra we can show that $X_{i,i} = -Y_{i,i}$ and $X_{j,j} = Y_{j,j}$ for $j = 1, \ldots, p, j \neq i$. As the normalized Haar measure on $V_{n,p}$ is invariant under orthogonal transformation from Left i.e. $[dX] = [dY]$ Chikuse (2012), we get that

$$
\int_{V_{n,p}^{i,-}} X_{i,i} \exp \left( \sum_{j=1}^{p} d_j X_{j,j} \right) \left[ dX \right] = -\int_{V_{n,p}^{i,+}} Y_{i,i} \exp \left( -d_{i,i} + \sum_{j=1, j \neq i}^{p} d_j Y_{j,j} \right) \left[ dY \right] = -\int_{V_{n,p}^{i,+}} X_{i,i} \exp \left( -d_{i,i} + \sum_{j=1, j \neq i}^{p} d_j X_{j,j} \right) \left[ dX \right].
$$

(18)

From Equations 17 and 18 we have,

$$
\frac{\partial}{\partial d_i} \left[ \binom{\alpha}{\frac{n}{2}} \left( \frac{D^2}{4} \right) \right] = \int_{V_{n,p}^{i,+}} X_{i,i} \exp \left( \sum_{j=1, j \neq i}^{p} d_j X_{j,j} \right) \left[ \exp (d_i X_{i,i}) - \exp (-d_i X_{i,i}) \right] \left[ dX \right] = \int_{V_{n,p}^{i,+}} X_{i,i} \exp \left( \sum_{j=1, j \neq i}^{p} d_j X_{j,j} \right) 2 \sinh (d_i X_{i,i}) \left[ dX \right].
$$

(19)
where sinh is the hyperbolic sin function. Note that sinh \((d_i X_{i,i}) > 0\) as \(d_i > 0\) and \(X_{i,i} > 0\) on \(\mathbb{V}_{n,p}^i\). Hence from Equation 19 it follows that,

\[
\frac{\partial}{\partial d_i} \left[ \, _0F_1 \left( -\frac{1}{2}, \frac{D^2}{4} \right) \right] > 0.
\]  

(20)

From Equations 16 and 20, we have the result. □

All five lemmas will be used for a theoretical development of a conjugate prior family for \(\mathcal{ML}\) distributions, which we discuss next.

3. Bayesian framework for \(\mathcal{ML}\) distribution

In this section we develop a comprehensive Bayesian framework related to \(\mathcal{ML}\) distribution. We construct a novel class of conjugate priors and study their properties. We also derive the posterior form and comment on hyperparameter settings.

3.1. Prior construction

In the context of the exponential family of distributions, Diaconis and Ylvisaker (1979) (DY) provides a standard procedure to obtain a class of conjugate priors when the distribution is represented through natural parametrization Casella and Berger (2002). But we realize that for the \(\mathcal{ML}\) distribution DY theorem could not be applied directly. We postpone the discussion on the DY theory later in Section 3.4 since a direct application of their construction is not possible. Instead, we propose two different conjugate priors next aiming for scalable and flexible posterior inference.

In this context, we would also like to mention that the construction of the class of priors in Hornik and Grün (2013) is based on the direct application of DY, which is also not quite appropriate for \(\mathcal{ML}\) distribution. The idea of constructing a conjugate prior on the natural parameter \(F\) and using a transformation afterwards involves calculation of complicated Jacobean term Hornik and Grün (2013). Hence the corresponding class of prior obtained by this transformation would lack the interpretation of the corresponding hyperparameters. As the DY theorem is not directly applicable, an appropriate modification is required in order to use with \(\mathcal{ML}\) distribution (see details in Section 3.4). In this section we construct a new class of conjugate prior for \(\mathcal{ML}\) density. We then show that the hyperparameters of the constructed class of priors are easily interpretable from practitioners point of view. We further extend our investigation to study properties that are essential for the hyperparameter selection and posterior inference. In the following paragraphs we design both joint and independent prior structures for the parameters of the \(\mathcal{ML}\) distribution.
Definition 1. The probability density function of the joint conjugate prior with respect to the appropriate product measure $\Upsilon$ on $V_{n,p} \times \mathbb{R}^p_+ \times V_{p,p}$ on the parameters $M, D$ and $V$ for $\mathcal{M}L$ distribution is proportional to

$$g(M, d, V; \nu, \Psi) = \frac{\text{etr} \left( \nu V D M^T \Psi \right)}{[\text{$_0F_1$} \left( \frac{n}{2}, \frac{D}{4} \right)]^{\nu}}, \quad (21)$$

as long as $g(M, d, V; \nu, \Psi)$ can be integrable. Here $\nu > 0$ and $\Psi \in \mathbb{R}^{n \times p}$.

Although joint prior structure has some desirable properties (see Theorem 4 and Section 3.3), it sometimes difficult to incorporate strength of prior belief which could differ for different parameters. For example, if a practitioner has strong prior belief on $M$ but has very less knowledge about parameters $D$ and $V$, then $JMDY$ may not be the optimal choice for prior structure. We design a class of conditional conjugate prior which would be better suited for this type of situation due to flexibility. Also, it is customary to come up with independent prior structure (Gelman et al., 2014; Khare, Pal and Su, 2017) for parameters of curved exponential family (Casella and Berger, 2002), where the parametrization differs from the natural parametrization. In order to develop conditional conjugate prior structure we assume independent priors on $M, d$ and $V$. It is easy to see that conditional conjugate priors for both $M$ and $V$ are $\mathcal{M}L$ distribution whereas the following definition is used to construct the conditional conjugate prior for $D$.

Definition 2. The probability density function of the conditional conjugate prior for $D$ with respect to the Lebesgue measure on $\mathbb{R}^p_+$ is proportional to

$$g(d; \nu, \eta) = \frac{\exp(\nu \eta^T d)}{[\text{$_0F_1$} \left( \frac{n}{2}, \frac{D}{4} \right)]^{\nu}}, \quad (22)$$

as long as $g(d; \nu, \eta)$ can be integrable. Here $\nu > 0$, $\eta \in \mathbb{R}^p$ and $n \geq p$.

Note that, $g(d; \nu, \eta)$ is a function of $n$ as well, however we do not vary $n$ anywhere in our construction and thus we omit the symbol $n$ from the notation of $g(d; \nu, \eta)$.

We refer this particular class of distributions defined in Definition 1 and Definition 2 as joint modified Diaconis-Ylvisaker ($JMDY$) and independent modified Diaconis-Ylvisaker ($IMDY$) class, respectively for subsequent discussions.

Theorem 1 and Theorem 2 provides conditions on $\nu, \Psi$ and $\eta$ so that $g(M, d, V; \nu, \Psi)$ and $g(M, d, V; \nu, \eta)$ are integrable, respectively. We state and prove the following lemma which is necessary to prove these theorems.

Lemma 6. Let $\Psi \in \mathbb{R}^{n \times p}$ and $D$ be a diagonal matrix with positive diagonal entries. If $\|\Psi\|_2 < 1$, then for arbitrary $M \in V_{n,p}, V \in V_{p,p}$,

$$\frac{\text{etr} \left( V D M^T \Psi \right)}{[\text{$_0F_1$} \left( \frac{n}{2}, \frac{D}{4} \right)]^{\nu}} < \frac{\text{etr} (-\epsilon_0 D)}{K_{n,p,\epsilon_0}}, \quad (23)$$

where $\epsilon_0 = \frac{1}{2} (1 - \|\Psi\|_2)$ and $K_{n,p,\epsilon_0} > 0$ is a constant depending on $n, p$ and $\epsilon_0$. 
Proof of Lemma 6.
Note that, $0 < \epsilon_0 < \frac{1}{2}$ as $\|\Psi\|_2 < 1$. Assume $Y_0 = M^T \Psi V \in \mathbb{R}^{p \times p}$. For arbitrary $l \in \mathbb{R}^p$ with $\|l\| = 1$, we have

$$l^T Y_0^T Y_0 l = (V l)^T \Psi^T (V l) - l^T V^T \Psi^T (I_n - MM^T) \Psi V l \leq (1 - 2\epsilon_0)^2.$$  \hspace{1cm} (24)

The last inequality follows as $\|\Psi\|_2 = 1 - 2\epsilon_0$ and $(I_n - MM^T)$ is a non-negative definite matrix. From Equation 24 it follows that $\|Y_0\|_2 \leq 1 - 2\epsilon_0$. Hence, we can apply Lemma 2 we obtain that $|Y_{0,j,j}| < 1 - 2\epsilon_0$ for $j = 1, \cdots, p$, where $Y_{0,j}$ is the $j$-th diagonal element of the matrix $Y_0$. Now applying Lemma 3 we have,

$$etr(VDM^T \Psi) < \frac{etr(DY_0 - (1 - \epsilon_0)D)}{K_{n,p,\epsilon_0}} < \frac{etr(-\epsilon_0 D)}{K_{n,p,\epsilon_0}}.$$  \hspace{1cm} \blacksquare

Theorem 1. Let $M \in \mathcal{V}_{n,p}$ and $V \in \mathcal{V}_{p,p}$ and $D$ be a diagonal matrix with positive diagonal elements $d \in \mathbb{R}^p_+$. Let $\Psi \in \mathbb{R}^{n \times p}$ with $n \geq p$, then for any $\nu > 0$,

(a) if $\|\Psi\|_2 < 1$, we have

$$\int_{\mathcal{V}_{n,p}} \int_{\mathcal{V}_{p,p}} \int_{\mathbb{R}^p_+} g(M, d, V; \nu, \Psi) \, dd \, d\mu(V) \, d\mu(M) < \infty,$$

(b) if $\|\Psi\|_2 > 1$, we have

$$\int_{\mathcal{V}_{n,p}} \int_{\mathcal{V}_{p,p}} \int_{\mathbb{R}^p_+} g(M, d, V; \nu, \Psi) \, dd \, d\mu(V) \, d\mu(M) = \infty,$$

where $g(M, d, V; \nu, \Psi)$ is defined in Definition 1.

Proof of Theorem 1.

(a) When $\|\Psi\|_2 < 1$: The function $g(M, d, V; \nu, \Psi)$ can be normalized to construct a probability den-
sity function with respect to the product measure \( \Upsilon \). Consider that
\[
\int_{V_{n,p}} \int_{V_{p,p}} \int_{\mathbb{R}_+^p} g(M, d, V; \nu, \Psi) \, dd \, d\mu(V) \, d\mu(M)
\]
\[
= \int_{V_{n,p}} \int_{V_{p,p}} \int_{\mathbb{R}_+^p} \frac{\text{etr} \left( \nu V D M^T \Psi \right)}{\left[ 0 \, F_1 \left( \frac{\nu D}{2}, \frac{D^2}{4} \right) \right]^p} \, dd \, d\mu(V) \, d\mu(M)
\]
\[
< \infty,
\]
where the inequality (i) is due to Lemma 6 while (ii) follows as \( \mu \) is the normalized Haar measure. Note that, here we write \( [dV] = d\mu(V) \) and \( [dM] = d\mu(M) \).

(b) When \( \|\Psi\|_2 > 1 \):
Let \( \Psi := M_\Psi D\Psi V_\Psi^T \) be the the unique SVD (Chikuse, 2012) decomposition for the matrix \( \Psi \). Note that, using sub-multiplicativity
\[
\|\Psi\|_2 \leq \|M_\Psi\|_2 \|D\Psi\|_2 \|V_\Psi^T\|_2 = \|D\Psi\|_2 = D_{\Psi,1}.
\]
Hence there exists an \( \epsilon_0 > 0 \) such that, \( D_{\Psi,1} > (1 + \epsilon_0) \) where \( D_{\Psi,1} \) denotes the first diagonal element of the diagonal matrix \( D\Psi \). Now consider the fact that
\[
\int_{V_{n,p}} \int_{V_{p,p}} \int_{\mathbb{R}_+^p} g(M, d, V; \nu, \Psi) \, dd \, d\mu(V) \, d\mu(M)
\]
\[
\geq \int_{V_{n,p}} \int_{V_{p,p}} \int_{S_p} g(M, d, V; \nu, \Psi) \, dd \, d\mu(V) \, d\mu(M)
\]
\[
= \int_{V_{n,p}} \int_{V_{p,p}} \int_{S_p} \frac{\text{etr} \left( \nu V D M^T \Psi \right)}{\left[ 0 \, F_1 \left( \frac{\nu D}{2}, \frac{D^2}{4} \right) \right]^p} \, dd \, d\mu(V) \, d\mu(M)
\]
\[
= \int_{V_{n,p}} \int_{V_{p,p}} \int_{S_p} \frac{\text{etr} \left( \nu D M^T M_\Psi D\Psi V_\Psi^T V \right)}{\left[ 0 \, F_1 \left( \frac{\nu D}{2}, \frac{D^2}{4} \right) \right]^p} \, dd \, d\mu(V) \, d\mu(M). \quad (25)
\]
Consider the change of variable via the following orthogonal transformations
\[
M^* = [ M_\Psi \ , \ M_\Psi ] M, \quad V^* = V_\Psi^T V,
\]
where \( M_\Psi \) is matrix containing the bases for the orthogonal complement of the column space of \( M_\Psi \). Note that \( [ M_\Psi \ , \ M_\Psi ]^T M_\Psi = (I^*)^T \) where \( I^* := [ I_p \ , \ 0_{n-p,p} ]^T \). As the Haar measure on the Stiefel manifold is invariant
under the orthogonal transformations (Chikuse, 2012), from Equation 25 we get that,

\[

\begin{align*}
\int_{V_{n,p}} \int_{V_{p,p}} \int_{\mathbb{R}^n_{+}} g(M, d, V; \nu, \Psi) \, d\mu(V) \, d\mu(M) \\
\geq \int_{V_{n,p}} \int_{V_{p,p}} \int_{S_p} \text{etr}\left(\nu DM^* J* D_\Psi V^*\right) \, d\mu(V^*) \, d\mu(M^*).
\end{align*}
\]

(26)

Consider

\[
V_{n,p}^\dagger := \left\{ M \in V_{n,p} : \| I^* - M \|_2 < \frac{\delta_0}{2} \right\}, \quad V_{p,p}^\dagger := \left\{ V \in V_{p,p} : \| I_p - V \|_2 < \frac{\delta_0}{2} \right\},
\]

where \( \delta_0 = \epsilon_0/(2 \| D_\Psi \|_2) \). Note that \( \delta_0 > 0 \) as \( 0 < \| D_\Psi \|_2 < \infty \). Clearly \( V_{n,p}^\dagger \) and \( V_{p,p}^\dagger \) are open subsets of \( V_{n,p} \) and \( V_{p,p} \) respectively. Hence, \( \mu(V_{n,p}^\dagger) > 0 \) and \( \mu(V_{p,p}^\dagger) > 0 \).

If \( M \in V_{n,p}^\dagger \) and \( V \in V_{p,p}^\dagger \), then using sub-multiplicativity of \( \| \cdot \|_2 \) (Conway, 1990) and triangle inequality, we get

\[
\| M^T I^* D_\Psi V - D_\Psi \|_2 \\
\leq \| M^T I^* D_\Psi V - D_\Psi V \|_2 + \| D_\Psi V - D_\Psi \|_2 \\
\leq \| (M - I^*)^T I^* \|_2 \| D_\Psi V \|_2 + \| D_\Psi \|_2 \| V - I_p \|_2 \\
\leq \| (M - I^*)^T I^* \|_2 \| I^* \|_2 \| D_\Psi \|_2 \| V \|_2 + \| D_\Psi \|_2 \| V - I_p \|_2 \\
\leq \delta_0 \| D_\Psi \|_2 \\
= \frac{\epsilon_0}{2}.
\]

(27)

Let \( \lambda_1, \ldots, \lambda_p \) be diagonal elements of the matrix \( M^T I^* D_\Psi V \). From Lemma 2 we get that \( |\lambda_j - D_{\Psi,j}| \leq \epsilon_0/2 \) for \( j = 1, \ldots, p \). Here \( D_{\Psi,j} \) denotes the \( j \)-th diagonal element of the matrix \( D_\Psi \). Hence for arbitrary \( M \in V_{n,p}^\dagger \) and \( V \in V_{p,p}^\dagger \), we have

\[
\text{tr} \left( M^T I^* D_\Psi V \right) = \sum_{j=1}^{p} \lambda_j \geq \sum_{j=1}^{p} \left( D_{\Psi,j} - \frac{\epsilon_0}{2} \right),
\]

(28)

as \( \lambda_j \geq \left( D_{\Psi,j} - \frac{\epsilon_0}{2} \right) \) for all \( j = 1, 2, \ldots, p \).
Now from Equation 26, we have

\[
\int_{V_n,p} \int_{V_{p,p}} \int_{\mathbb{R}_+^p} g(M, d, V; \nu, \Psi) dd \ d\mu(V) \ d\mu(M) \\
\geq \int_{V_{n,p}^+} \int_{V_{p,p}^+} \int_{S_p} \text{etr} \left( \nu DM^*TI^*D\Psi V^* \right) \ 
\left[ \frac{\left[ F_1 \left( \frac{\nu}{2}, \frac{D^*}{4} \right) \right]^p}{e^{\nu \sum_{j=1}^p d_j (D\Psi, j - \frac{\epsilon_0}{2})}} \right] \ d\mu(V^*) \ d\mu(M^*),
\]

\[(iii) \geq \int_{V_{n,p}^+} \int_{V_{p,p}^+} \int_{S_p} \exp \left( \nu \sum_{j=1}^p d_j (D\Psi, j - \frac{\epsilon_0}{2}) \right) \ d\mu(V^*) \ d\mu(M^*),
\]

\[(iv) \geq \mu(V_{n,p}^+ \mu(V_{p,p}^+) \int_{S_p} \exp \left( \nu \sum_{j=1}^p d_j (D\Psi, j - \frac{\epsilon_0}{2}) \right) \ d\mu(V^*) \ d\mu(M^*),
\]

\[(v) \geq \mu(V_{n,p}^+ \mu(V_{p,p}^+) \int_{S_p} \exp \left( \nu \frac{\epsilon_0}{2} d_1 \prod_{j=2}^p \exp \left( \nu d_j (D\Psi, j - \frac{\epsilon_0}{2}) \right) \right) \ d\mu(V^*) \ d\mu(M^*),
\]

\[\geq \infty, \quad (29)\]

where \((iii)\) and \((iv)\) follow from Equation 28 and Lemma 1, respectively. Finally, \((v)\) follows as \(D\Psi, 1 > (1 + \epsilon_0)\).

\[\square\]

**Remark for Theorem 1.** One could notice that the conditions mentioned in this theorem is not entirely necessary and sufficient conditions. We have not addressed the case where \(\|\Psi\|_2 = 1\). This scenarios could be broken into two cases (a) all the eigenvalues of \(\Psi\) are equal to 1 and (b) only a few eigenvalues are equal to 1 and rest are strictly less than 1. In both the cases, it seems that the problem is more involved than the current one and we have not investigated the finiteness of the corresponding integral in detail for those cases. For now, we leave those for future work.

**Theorem 2.** Let \(D\) be diagonal matrix with diagonal elements \(d \in \mathbb{R}_+^p\). Let \(\eta = (\eta_1, \ldots, \eta_p) \in \mathbb{R}^p\) and \(n\) be any integer with \(n \geq p\). Then for any \(\nu > 0\),

\[
\int_{\mathbb{R}_+^p} g(d; \nu, \eta, n) \ dd < \infty, \]

if and only if \(\max_{1 \leq j \leq p} \eta_j < 1\), where \(g(d; \nu, \eta, n)\) is defined in Definition 2.

**Proof of Theorem 2.**
Sufficient condition: For any $\eta := (\eta_1, \ldots, \eta_p) \in \mathbb{R}^p$, define $\eta^+ := (\eta_1^+, \ldots, \eta_p^+)$ where $\eta_j^+$ equals $\eta_j$ when $\eta_j > 0$ and zero otherwise. Define $D_{\eta}$ to be the diagonal matrix with diagonal elements $\eta$. Let us consider the following matrices

$$
\Psi = \begin{bmatrix} D_{\eta} & 0 \\ 0_{n-p,p} & 0 \end{bmatrix}, \quad M^* = \begin{bmatrix} I_{p,p} \\ 0_{n-p,p} \end{bmatrix} \quad \text{and} \quad V^* = I_p.
$$

Note that $\tilde{M} \in \tilde{V}_{n,p}$, $\tilde{V} \in V_{p,p}$ and $D_{\eta} = \tilde{M}^T \Psi \tilde{V}$. Now from Definition 2 we get that

$$
\int_{\mathbb{R}^n_+} g(d; \nu, \eta, n) \, dd = \int_{\mathbb{R}^n_+} \frac{\exp(\nu \sum_{j=1}^p \eta_j d_j)}{\left[ \frac{\nu}{\eta} \right]^{\eta_j} \Gamma \left( \frac{\eta_j}{\eta} \right)} \, dd
$$

$$
\leq \int_{\mathbb{R}^n_+} \frac{\exp(\nu \sum_{j=1}^p \eta_j^+ d_j)}{\left[ \frac{\nu}{\eta} \right]^{\eta_j^+} \Gamma \left( \frac{\eta_j^+}{\eta} \right)} \, dd
$$

$$
= \int_{\mathbb{R}^n_+} \frac{\text{etr}(\nu DD_{\eta})}{\left[ \frac{\nu}{\eta} \right]^{\eta_j} \Gamma \left( \frac{\eta_j}{\eta} \right)} \, dd
$$

$$
= \int_{\mathbb{R}^n_+} \frac{\text{etr}(\nu \tilde{V} \tilde{D} \tilde{M}^T \Psi)}{\left[ \frac{\nu}{\eta} \right]^{\eta_j} \Gamma \left( \frac{\eta_j}{\eta} \right)} \, dd
$$

$$
< \int_{\mathbb{R}^n_+} \frac{\text{etr}(-\nu \epsilon_0 D)}{(K_{n,p,\epsilon_0})^{\nu}} \, dd
$$

$$
= \frac{1}{(K_{n,p,\epsilon_0})^{\nu}} \prod_{j=1}^p \int_{\mathbb{R}^n_+} \exp(-\nu \epsilon_0 d_j) \, dd_j
$$

$$
< \infty,
$$

(30)

where the inequality at step (vi) follows from Lemma 6 with appropriate $\epsilon_0 > 0$.

Necessary condition: Let $\eta \in \mathbb{R}^p$ be such that $\max_{j=1,\ldots,p} \eta_j \geq 1$. There exist at least one $j \in \{1, \ldots, p\}$ such that $\eta_j \geq 1$. Without loss of generality, let us assume that $\eta_1 \geq 1$. From Definition 2, we have
\[
\int_{\mathbb{R}^n_+} g(d; \nu, \eta, n) \, dd \\
= \int_{\mathbb{R}^n_+} \frac{\exp(\nu \sum_{j=1}^p \eta_j d_j)}{\left[ \text{e}^{\nu \left( \frac{n}{2} \right)} \right]^p} \, dd \\
\geq \int_{\mathbb{R}^n_+} \frac{\exp(\nu \sum_{j=1}^p \eta_j d_j)}{\text{etr}(\nu D)} \, dd \\
= \prod_{j=1}^p \int_{\mathbb{R}^n_+} \exp(\nu(\eta_j - 1)d_j) \, dd_j \\
= \int_{\mathbb{R}^n_+} \exp(\nu(\eta_1 - 1)d_1) \, dd_1 \prod_{j=2}^p \int_{\mathbb{R}^n_+} \exp(\nu(\eta_j - 1)d_j) \, dd_j \\
= \infty,
\]
where the inequality is due to Lemma 1.

\[ \square \]

**Remark for Theorem 2.** We could alternatively parametrize IMDY in the following way:

\[ g(d; \nu, \eta) \propto \exp \left( \sum_{j=1}^p \eta_j d_j \right) \left[ \frac{0}{\text{F}_1 \left( \frac{n}{2}, D \right)} \right]^\nu \]

when \( \max_{1 \leq j \leq p} \eta_j < \nu \).

In this parametrization if we set \( \nu = 0 \) and \( \beta := -\eta \) then \( g(d; \nu, \eta) \) refers to the Exponential distribution with parameter \( \beta \).

### 3.2. Properties of IMDY and JMDY class of distributions

The following lemmas are essential to study theoretical properties of the conjugate prior mentioned in Section 3.1.

**Lemma 7.** The probability density function for the prior distribution of \( d \sim \text{IMDY}(d; \nu, \eta) \) denoted by \( g(d; \nu, \eta) := \exp(\nu \eta^T d) / \left[ \text{e}^{\nu \left( \frac{n}{2} \right)} \right] \), is log-concave as a function of \( d \) where \( D \) is the diagonal matrix with diagonal elements \( d \), \( \max_{1 \leq j \leq p} \eta_j < 1 \), \( \nu > 0 \) and \( n \geq p \).

**Proof of Lemma 7.**

From Definition 2 we have,

\[ g(d; \nu, \eta) := \frac{\exp(\nu \eta^T d)}{\left[ \text{e}^{\nu \left( \frac{n}{2} \right)} \right]^p}, \]

\[ \implies \log g(d; \nu, \eta) := \nu \eta^T d - \nu \log \left( \text{e}^{\nu \left( \frac{n}{2} \right)} \right) \]

From Lemma 4, it follows that \( -\nu \log \left( \text{e}^{\nu \left( \frac{n}{2} \right)} \right) \) is concave function of \( d \).

Also, \( \nu \eta^T d \) is a linear function of \( d \). Therefore from Equation 31 it is clear that \( \log g(d; \nu, \eta) \) is a concave function of \( d \).
Lemma 8. The distribution of $d$ is unimodal if $0 < \eta_j < 1$ for all $j = 1, 2, \cdots, p$. The mode of the distribution is characterized by the parameter $\eta$ and it does not dependent on the parameter $\nu$.

Proof of Lemma 8.
Let $l(d, \nu, \eta) = \log(g(d; \nu, \eta))$. If $\hat{d}$ is the mode of the distribution then

$$
\frac{\partial}{\partial d} l(d, \nu, \eta) \bigg|_{d=\hat{d}} = 0,
$$

$$
\Rightarrow \nu \eta - \nu \frac{\partial}{\partial d} \log \left( _0F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) \right) \bigg|_{d=\hat{d}} = 0,
$$

$$
\Rightarrow \frac{\partial}{\partial d} \log \left( _0F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) \right) \bigg|_{d=\hat{d}} = \eta,
$$

$$
\Rightarrow h(\hat{d}) = \eta,
$$

(32)

where $h(d) := (h_1(d), h_2(d), \cdots, h_p(d))$ with $h_j(d) := \left( \frac{\partial}{\partial d_j} _0F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) \right) / \left. _0F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) \right|_{d=\hat{d}}$ for $j = 1, 2, \cdots, p$. The function $h_j(d)$ is strictly increasing as the function $_0F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right)$ is log-convex (see Lemma 4). Also, it follows from Lemma 5 that $0 < h_j(d) < 1$ for all $d \in S_p$. Hence the Equation 32 has a unique solution when $0 < \eta_j < 1$ for all $j = 1, 2, \cdots, p$. Also it is clear that the solution does not depend on $\nu$. On the other hand, given any $\hat{d} \in S_p$ we can always find a $\eta$ satisfying Equation 32 such that $0 < \max_{1 \leq j \leq p} \eta_j < 1$. \qed

Remark: In the case of $\eta_j \leq 0$, the density defined in 2 is decreasing as a function of $d_j$ on the set $\mathbb{R}_+$. Therefore, mode does not exist.

In order to introduce the notion of “concentration” for IMDY class of distributions we require the concept of level set. Let unnormalized probability density function for IMDY class of distributions, $g(x; \nu, \eta)$, achieves the maximum value at $m_{\eta}$ and let

$$
S_l = \{ x \in \mathbb{R}_+^p : g(x; 1, \eta)/g(m_{\eta}; 1, \eta) > l \}
$$

be the level set of order $l$ containing the mode $m_{\eta}$ where $0 \leq l < 1$. Note that, to define the level set we could have used any fixed value of $\nu_0 > 0$ in $g(x; \nu_0, \eta)$ instead of $g(x; 1, \eta)$, however without loss of generality we choose $\nu_0 = 1$.

Lemma 9. Let $\eta \in \mathbb{R}^p$ be a fixed vector such that $0 < \max_{1 \leq j \leq p} \eta_j < 1$. Whenever $d \sim$ IMDY$(d; \nu, \eta)$, we have

(a) $P_{\nu}(S_l)$ is an increasing function of $\nu$.

(b) For any open set $S \subset \mathbb{R}_+^p$ containing $m_{\eta}$, $P_{\nu}(d \in S)$ goes to 1 as $\nu \rightarrow \infty$. 

where \( P_\nu(\cdot) \) denotes the probability distribution corresponding to \( d \sim \text{IMDY}(d; \nu, \eta) \).

**Proof of Lemma 9.**

(a) Note that, from definitions of unimodality and level set we have

\[
\left[ \frac{g(y; \nu, \eta)}{g(x; \nu, \eta)} \right] > 1 \text{ for all } y \in S \text{ and for all } x \in S^c. \tag{33}
\]

Consider the function

\[
r(\nu, x) := \int_S \frac{g(y; \nu, \eta)}{g(x; \nu, \eta)} dy = \int_S \left[ \frac{g(y; 1, \eta)}{g(x; 1, \eta)} \right]^{\nu} dy, \tag{34}
\]

where \( x \in S^c \). Using equation 33 it is easy to see that \( \left[ \frac{g(y; 1, \eta)}{g(x; 1, \eta)} \right]^{\nu} \) is monotonically increasing in \( \nu \) for all \( y \in S \). Hence \( r(\nu, x) \) is increasing function in \( \nu \) for any \( x \in S^c \).

Note that,

\[
\frac{P_\nu(d \in S^c)}{P_\nu(d \in S)} = \frac{\int_{S^c} g(x; \nu, \eta) dx}{\int_S g(y; \nu, \eta) dy} = \int_{S^c} \frac{1}{\int_S \frac{g(y; \nu, \eta)}{g(x; \nu, \eta)} dy} dx = \int_{S^c} \frac{1}{r(\nu, x)} dx. \tag{35}
\]

Hence \( P_\nu(d \in S^c)/P_\nu(d \in S) \) is a decreasing function of \( \nu \) as \( \frac{1}{r(\nu, x)} \) is a decreasing function in \( \nu \) for every \( x \in S^c \) or equivalently \( P_\nu(d \in S) \) increasing function in \( \nu \).

□

(b) Let \( d \sim \text{IMDY}(\cdot; \nu, \eta) \) with \( 0 < \eta_j < 1 \) for \( j = 1, \ldots, p \). Let \( m_\eta \) be the mode the distribution. Note that the value of \( m_\eta \) only depends on the parameter \( \eta \) and does not depend on the parameter \( \nu \). Let \( f(d; \nu, \eta) \) be the corresponding probability density function. Hence for the class of distribution function defined in Definition 2, it follows that,

\[
f(d; \nu, \eta) = \frac{1}{K_{\nu, \eta} \left[ \frac{n}{\tau}, \frac{D^2}{1} \right]} \exp(\nu^T d), \tag{36}
\]

where \( K_{\nu, \eta} \) is the appropriate normalizing constant.

Let us define the function \( g(d; \eta) = \exp(\eta^T d)/\left[ \frac{n}{\tau}, \frac{D^2}{1} \right] \). Let \( S \) be any open set containing \( m_\eta \), the mode of the density function \( f(d; \nu, \eta) \). Consider, the set \( S^* := \{ d : g(d; \eta) \leq \zeta \} \), where \( \zeta = \sup_{d \in S^c} g(d; \eta) \). It is easy to show that \( S^c \subseteq S^* \).
Consider the fact that,

\[
g(d; \eta) \quad \text{where } \lambda \in (0, 1)
\]

\[
= \exp(\eta^T d) \quad \text{and}\quad \eta^T (\lambda m_\eta + (1 - \lambda)d)
\]

\[
\leq \left[ \frac{\exp(\eta^T d)}{\lambda F_1 \left( \frac{\eta^T d}{\lambda}, \frac{D^2}{\lambda} \right)} \right]^{\lambda} \leq \left[ \frac{\exp(\eta^T d)}{\lambda F_1 \left( \frac{\eta^T d}{\lambda}, \frac{D^2}{\lambda} \right)} \right]^{\lambda}
\]

where \( D_m \) is the diagonal matrix with diagonal \( m_\eta \). Note that, inequality \((vii)\) follows from the fact that \( F_1(\cdot) \) is a log-convex function.

Hence we have,

\[
f(d; \nu, \eta) = \left[ \frac{g(d; \eta)}{g(m_\eta; \eta)} \right]^\lambda
\]

\[
f(\lambda m_\eta + (1 - \lambda)d; \nu, \eta) \leq \left[ \frac{g(d; \eta)}{g(m_\eta; \eta)} \right]^\lambda
\]

\[
\leq \left[ \frac{\exp(\eta^T d)}{\lambda F_1 \left( \frac{\eta^T d}{\lambda}, \frac{D^2}{\lambda} \right)} \right]^{\lambda}
\]

\[
= \left[ \frac{g(d; \eta)}{g(m_\eta; \eta)} \right]^{\nu \lambda}
\]

\[
\text{(37)}
\]

where \( D_m \) is the diagonal matrix with diagonal \( m_\eta \). Note that, inequality \((vii)\) follows from the fact that \( F_1(\cdot) \) is a log-convex function.

Hence we have,

\[
P_\nu(S^\star) = \int_{S^*} f(d; \nu, \eta) \, d d
\]

\[
= \int_{S^*} \frac{f(d; \nu, \eta)}{f(\lambda m_\eta + (1 - \lambda)d; \nu, \eta)} \, f(\lambda m_\eta + (1 - \lambda)d; \nu, \eta) \, d d
\]

\[
\leq \int_{S^*} \left[ \frac{g(d; \eta)}{g(m_\eta; \eta)} \right]^{\nu \lambda} \, f(\lambda m_\eta + (1 - \lambda)d; \nu, \eta) \, d d
\]

\[
\leq \int_{S^*} \left[ \frac{\zeta}{g(m_\eta; \eta)} \right]^{\nu \lambda} \, f(\lambda m_\eta + (1 - \lambda)d; \nu, \eta) \, d d
\]

\[
= \left[ \frac{\zeta}{g(m_\eta; \eta)} \right]^{\nu \lambda} \int_{S^*} \, f(\lambda m_\eta + (1 - \lambda)d; \nu, \eta) \, d d
\]

\[
\text{(39)}
\]

Hence we have,

\[
\lim_{\nu \to \infty} P_\nu(S) \geq 1 - \lim_{\nu \to \infty} P_\nu(S^\star) \geq 1 - \lim_{\nu \to \infty} \left[ \frac{\zeta}{g(m_\eta; \eta)} \right]^{\nu \lambda} = 1
\]

as \( \zeta < g(m_\eta; \eta) \).
The following two theorems establishes few important properties of \( \text{IMDY} \) and \( \text{JMDY} \) class of distributions.

**Theorem 3.** Let \( d \sim \text{IMDY}(\cdot; \nu, \eta) \) for some \( \nu > 0 \) and \( \max_{1 \leq j \leq p} \eta_j < 1 \) where \( \eta = (\eta_1, \ldots, \eta_p) \). Then

(a) The distribution of \( d \) is log-concave.

(b) The distribution of \( d \) is unimodal if \( \eta_j > 0 \) for all \( j = 1, 2, \ldots, p \). The mode of the distribution is characterized by the parameter \( \eta \) and it does not dependent on the parameter \( \nu \).

(c) The parameter \( \nu \) relates to the concentration of the probability around mode of the distribution. Larger values of \( \nu \) implies larger concentration of probability near the mode of the distribution.

**Proof of Theorem 3.**

Proof of part (a), (b) and (c) follow from Lemma 7, 8 and 9, respectively.

We call the parameter \( \eta \) as modal parameter and \( \nu \) as Concentration parameter.

**Definition 3.** The parameter \( \eta \) in the distribution that belongs to the class of distributions \( \text{IMDY} \) is defined as “modal parameter”.

**Definition 4.** The scalar parameter \( \nu \) in the distribution that belongs to the class of distributions \( \text{IMDY} \) is defined as “concentration parameter”.

**Theorem 4.** Let \( (M, d, V) \sim \text{JMDY}(\cdot; \nu, \Psi) \) for some \( \nu > 0 \) and \( \|\Psi\|_2 < 1 \). Then

(a) The distribution has unique mode. The mode is characterized by the parameter \( \Psi \) and it does not dependent on the parameter \( \nu \).

(b) Conditional distribution of \( M \) given \( (d, V) \) and \( V \) given \( (M, d) \) are \( \mathcal{MCL} \) distributions whereas conditional distribution of \( d \) given \( (M, V) \) is \( \text{IMDY} \) class of distribution.

**Proof of Theorem 4.**

The joint density is proportional to

\[
g(M, d, V; \nu, \Psi) = \frac{\text{etr}(\nu VDM^T \Psi)}{[\text{B}^T]^{\nu}},
\]

\[
(40)
\]

(a) Let us write the SVD (Chikuse, 2012) of \( \Psi = M\Psi D^T \). We have,

\[
\text{etr}(\nu VDM^T \Psi) = \text{etr}(\nu M^T \Psi D^T V) = \text{etr}(\nu V^T \Psi D^T U_M D_M V^T \Psi D^T)
\]

\[
\text{etr}(\nu V^T \Psi D^T U_M D_M V^T D) = \text{etr}(\nu V^T D^T U_M D_M V^T D)
\]

\[
(41)
\]
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where SVD of is written as \( M^T M = U_M D_M V_M^T \) and \( V_1 = V_M D_M \) is an orthogonal matrix. Therefore we have,

\[
\text{etr}(\nu VDM^T \Psi) = \text{etr}(\nu V_1 D U_M D_M V_M^T D_\Psi) \\
\leq \text{etr}(\nu D D_M D_\Psi),
\]

where the inequality \((\text{viii})\) follows from Kristof (1969) (see Theorem on page 5) as \( V_1, U_M \) and \( V_M \) are orthogonal matrices while \( D, D_M \) and \( D_\Psi \) are diagonal matrices with nonnegative diagonal entries. Note that, using sub-multiplicativity of the \( \| \cdot \|_2 \) (Conway, 1990), we have

\[
\|D_M\|_2 = \|U_M^T M^T M_\Psi V_M\|_2 \leq \|U_M^T\|_2 \|M^T\|_2 \|M_\Psi\|_2 \|V_M\|_2 \leq 1.
\]

Therefore, using Lemma 2, we infer that all the diagonal entries of \( D_M \) is less than or equal to 1. Hence from Equation 42, we get that

\[
\text{etr}(\nu VDM^T \Psi) \leq \text{etr}(\nu DD_\Psi).
\]

Therefore, it follows from Kristof (1969) that \( M = M_\Psi \) and \( V = V_\Psi \) are unique maximizers when \( M_\Psi \in \tilde{\mathcal{V}}_{n,p} \) and \( V_\Psi \in \mathcal{V}_{p,p} \). Note that, this does not depend on the choice of \( \nu \).

Now putting back the value of \( M \) and \( V \), we write the expression given in the Equation 40 which can now be seen as \( \text{etr}(\nu DD_\Psi)/\left[0 F_1 \left(\frac{n}{2}, \frac{D^2}{4}\right)\right]^{\nu} \). Note that, the diagonal elements of \( D_\Psi \) is between 0 and 1 as \( \|\Psi\|_2 < 1 \). Hence using part \((\text{b})\) of Theorem 3 we know that \( \text{etr}(\nu DD_\Psi)/\left[0 F_1 \left(\frac{n}{2}, \frac{D^2}{4}\right)\right]^{\nu} \) has a unique maximizer which also does not depend on the choice of \( \nu \).

\[
\square \]

\((b)\) For \( JMDY \) prior structure, the conditional distribution of \( M \) given \((d, V)\) is proportional to

\[
\text{etr} \left( \nu (\Psi V D)^T M \right).
\]

This distribution is an \( \mathcal{MC} \) distribution with parameters \( M_\Psi^M, D_\Psi^M, V_\Psi^M \) where SVD decomposition (Chikuse, 2012) of \( \nu (\Psi V D) = M_\Psi^M D_\Psi^M (V_\Psi^M)^T \).

Similarly, the conditional distribution of \( V \) given \( M \) and \( d \) is proportional to

\[
\text{etr} \left( \nu (\Psi^T M D)^T V \right).
\]

Therefore, it is another \( \mathcal{MC} \) distribution with parameters \( M_\Psi^V, D_\Psi^V, V_\Psi^V \) where SVD decomposition of \( \nu (\Psi^T M D) = M_\Psi^V D_\Psi^V (V_\Psi^V)^T \).

Finally, the conditional distribution of \( d \) given \((M, V)\) is a distribution that belongs to \( IMDY \) class of distributions with parameters \( \nu \) and \( \eta_\Psi \), where \( \eta_\Psi = \{\eta_{\Psi 1}, \eta_{\Psi 2}, \cdots, \eta_{\Psi p}\} \) and \( \eta_{\Psi j} \) is the \( j \)-th diagonal element of the matrix \( M^T \Psi V \).
In next subsection (Section 3.3) we show that the posterior “modal parameter” is a linear combination of the prior “modal parameter” and a function of sample mean.

The following lemmas are useful from the practitioner viewpoint. The result will help to truncate the right tail of the distribution at an appropriate point according to a criteria involving only the unnormalized density function.

**Lemma 10.** Let \( \mathbf{d} \sim \text{IMDY}(\cdot; \nu, \mathbf{\eta}) \) for some \( \nu > 0 \) and \( \max_{1 \leq j \leq p} \eta_j < 1 \) where \( \mathbf{\eta} = (\eta_1, \ldots, \eta_p) \). Let \( m \) be the mode of the conditional distribution, \( g_1(\cdot) := g(\cdot; \nu, \mathbf{\eta} | (d_2, \ldots, d_p)) \), of the variable \( d_1 \) given \( (d_2, \ldots, d_p) \). Then \( Q(d_1) = g_1(d_1 + b)/g_1(d_1) \) is strictly decreasing when \( b > 0 \) and \( d_1 > m \) where \( m \) is the mode of the density function given in Definition 2.

**Proof of Lemma 10.**
We have,

\[
\log(g_1(d_1)) = \nu \eta_1 d_1 - \log \left( \frac{n}{2} F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) \right)
\]

\[
\Rightarrow \frac{\partial^2}{\partial d_1^2} \log(g_1(d_1)) = -\frac{\partial^2}{\partial d_1^2} \left( \log \left( \frac{n}{2} F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) \right) \right) < 0, \quad (44)
\]

as \( \log \left( \frac{n}{2} F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) \right) \) is a strictly convex function (from Lemma 4). Therefore \( \frac{\partial}{\partial d_1} (\log g_1(d_1)) = g_1'(d_1)/g_1(d_1) \) is a strictly decreasing function in \( d_1 \).

\[
\log(Q(d_1)) = \log(g_1(d_1 + b)) - \log(g_1(d_1))
\]

\[
\Rightarrow \frac{\partial}{\partial d_1} (\log Q(d_1)) = \frac{g_1'(d_1 + b)}{g_1(d_1 + b)} - \frac{g_1'(d_1)}{g_1(d_1)} < 0,
\]

as \( g_1'(d_1)/g_1(d_1) \) is a strictly decreasing function. Therefore, \( Q(d_1) \) is also a strictly decreasing function in \( d_1 \). \( \square \)

**Lemma 11.** Let \( \mathbf{d} \sim \text{IMDY}(\cdot; \nu, \mathbf{\eta}) \) for some \( \nu > 0 \) and \( \max_{1 \leq j \leq p} \eta_j < 1 \) where \( \mathbf{\eta} = (\eta_1, \ldots, \eta_p) \). Let \( m \) be the mode of the conditional distribution, \( g_1(\cdot) := g(\cdot; \nu, \mathbf{\eta} | (d_2, \ldots, d_p)) \), of the variable \( d_1 \) given \( (d_2, \ldots, d_p) \). Let \( B > m \), be such that \( \frac{g_1(B)}{g_1(m)} < \epsilon \) for some \( \epsilon > 0 \), then \( P(d_1 > B | d_2, \ldots, d_p) < \epsilon \).

**Proof of Lemma 11.**
The unnormalized conditional density of the random variable \( d_1 \) is proportional to

\[
g_1(d_1) = \frac{\exp(\nu \eta_1 d_1)}{\frac{n}{2} F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right)}.
\]
Let \( f(d_1; \nu, \eta | (d_2, \ldots, d_p)) \) be the density function for the conditional distribution of \( d_1 \) given \((d_2, \ldots, d_p)\). For notational convenience, for rest of this lemma we use \( f_1(\cdot) \) as the conditional probability density function. Hence we have,

\[
f_1(d_1) = \frac{1}{K_{\nu, \eta}^1} \exp(\nu \eta d_1) \int_0^{F_1(n_2, D_2^4)} \nu \frac{1}{\gamma} \text{d}y,
\]

where \( K_{\nu, \eta}^1 \) is an appropriate normalizing constant. From Lemma 10, it follows that \( f_1(B + x) / f_1(m + x) \) is a decreasing function of \( x \) when \( B > m \). Hence for all \( x > 0 \),

\[
f_1(B + x) / f_1(m + x) < g_1(B) / g_1(m) < \epsilon,
\]

where the inequality at (viii) follows due to the assumption of the lemma. Therefore,

\[
P(d_1 > B \mid (d_2, \ldots, d_p)) = \int_B^\infty f_1(y)dy = \int_0^\infty \frac{f_1(B + x)}{f_1(m + x)} f_1(m + x) dx < \epsilon P(d_1 > m \mid (d_2, \ldots, d_p)) < \epsilon.
\]

\[
\square
\]

3.3. Linearity for posterior modal parameter

Let \( W_i \) for \( i = 1, 2, \cdots, N \) be the samples drawn from \( \mathcal{M}_{\nu, \Psi} \) distribution with parameters \( \mu, d, V \). If we consider a Bayesian analysis with the prior class \( \text{JMDY} \) with parameters \( \nu \) and \( \Psi \), then the probability density for the joint posterior distribution of \( M, d \) and \( V \) given \( \{W_i\}_{i=1}^N \) is proportional to

\[
g(M, d, V; \nu, \Psi) \propto \prod_{i=1}^N \text{etr}(VDM^TW_i) / \sum_{i=1}^N \text{etr}(VDM^TW_i) \]

\[
= \text{etr}\left(\nu VDM^T \Psi\right) / \sum_{i=1}^N \text{etr}(VDM^TW_i) \]

\[
= \text{etr}\left((\nu + N) VDM^T \left(\frac{\nu}{\nu + N} \Psi + \frac{N}{\nu + N} \tilde{W}\right)\right) / \sum_{i=1}^N \text{etr}(VDM^TW_i),
\]

(45)

where \( \tilde{W} = \sum_{i=1}^N W_i / N \) and \( N \) is the number of data points. Observe that, the posterior distribution is also in \( \text{JMDY} \) class with concentration parameter \( (\nu + N) \) and modal parameter \( \left(\frac{\nu}{\nu + N} \Psi + \frac{N}{\nu + N} \tilde{W}\right) \).
On the other hand, when we consider a Bayesian analysis with the prior class IMDY with parameters $\nu$ and $\eta$, then the conditional probability density for posterior distribution of $d$ given $M, V, \{W_i\}_{i=1}^N$ is proportional to

$$
g(d; \nu, \eta) \times \prod_{i=1}^N \text{etr}(V D M^T W_i) \frac{\nu}{\nu + N} \eta^T d \quad \frac{\nu}{\nu + N} \eta^T d = \exp\left(\nu \eta^T d \left[\frac{\nu}{\nu + N} \eta^T d + \frac{1}{\nu + N} \eta Y\right]^T\right)$$

Here the conditional posterior distribution of $d$ is in IMDY class with concentration parameter $\frac{(\nu + N)}{\nu + N}$ and modal parameter $\left(\frac{\nu}{\nu + N} \eta^T d + \frac{N}{\nu + N} \eta Y\right)$. (46)

Finally, in the following subsection we talk about the several reasons for not being able to use DY theorem directly in our case.

3.4. Inapplicability of DY theorem to construct prior for $\mathcal{M}$ distribution

According to the assumption of DY, for a $d$-dimensional exponential family distribution, $\mu$ be the measure defined on the Borel sets of $\mathbb{R}^d$. In the context of the $\mathcal{M}$ distribution $\mu$ is the measure defined on the Stiefel manifold. The symbol $\mathcal{X}$ is used to denote the interior of the support of the measure $\mu$. As showed in Hornik and Grün (2013) $\mathcal{X} := \{X : \|X\|_2 < 1\}$. According to the assumptions of DY $\int_X dP_\theta(X) = 1$ (See the paragraph after equation (2.1) on page 271 in Diaconis and Ylvisaker (1979)). On the contrary for matrix Langevin distribution

$$
\int_X dP_\theta(X) = \int_X f_{\mathcal{M}}(X) |dX| = 0.
$$

During the proof of Theorem 1 in Diaconis and Ylvisaker (1979) Dy constructs
a probability measure restricted on set $A$ as follows.

$$
\mu_A(B) = \frac{\mu(A \cap B)}{\mu(A)}, \text{ where } \mu(A) > 0.
$$

Also, $x_A = \int Z d\mu_A(Z)$. In the context of the proof of Theorem 1 in Diaconis and Ylvisaker (1979) uses the crucial fact that $x_A$ are dense in $\text{supp}(\mu)$ (See the line after Equation (2.4) on page 272 in Diaconis and Ylvisaker (1979)).

In the context of the $\mathcal{ML}$ distribution $\text{supp}(\mu)$ is the Stiefel manifold. It can be shown that similar construction in the case of $\mathcal{ML}$ distribution would lead to $x_A$ where $x_A$ does not belong to the Stiefel manifold i.e. $x_A \notin \text{supp}(\mu)$. Hence $x_A$ will not be dense $\text{supp}(\mu)$. As a result, Theorem 1 in (Diaconis and Ylvisaker, 1979) is not applicable for $\mathcal{ML}$ distribution. Note that a modified DY construction can be formulated that would enable us constructing prior on $F$. However, our parametrization is different than the natural parametrization, therefore we require a new approach to construct the prior distribution on $M, d$ and $V$.

**Plots for conditional prior of $d$ given $M$ and $V$** Figure 1 shows plots for prior densities for different values of $\nu$ and $\eta$. Note that, with the same value of $\eta$ the location of the mode remain the same for different values of $\nu$ (see each row of Figure 1). As $\nu$ increases, the probability concentration around the mode of the distribution increases.

**Finding the modal parameter from the mode** We have given an example when the practitioner wants to set a particular mode denoted by $d_{\text{mode}}$. We solve for the corresponding $\eta_{\text{mode}}$ from Equation 32. For example, let us denote the mode by $(5, 7)$ and after solving for $\eta_{\text{mode}}$, we have $\eta_{\text{mode}} = (0.85, 0.88)$. In the Figure 2, we see that the mode is shown by $(5, 7)$ for two different setting of $\nu$ which incorporates the strength of the belief in the value of the mode. Here we take $\nu = 10$ and $\nu = 20$.

### 3.5. Hyperparameter selection procedure

For both $JMDY$ and $IMDY$ class of distributions, we have uniform prior over respective parameters whenever the probability density function is proportional to 1. For $JMDY$, it can be achieved by setting $\nu = 0$ in Definition 1. For $IMDY$, $\nu = 0$ provides the uniform prior on parameter $d$. The resulting priors would be improper as in this case, the integral over the entire space becomes infinite. However, in this case, it is necessary to check the propriety of posterior distributions.

In order to incorporate the prior belief for $IMDY$ class of distributions, one can find the appropriate value of hyperparameter $\eta$ from Equation 32 once mode of $d$ (denoted by $d_{\text{mode}}$) is given. Note that, we get a feasible $\eta$ for every real $d_{\text{mode}} \in \mathcal{S}_p$. The other parameter $\nu$ sets the strength of one’s prior belief. It is important to realize that there is a strong relationship between $\nu$ and number
Fig 1: Prior density plots for different values of $\nu$ and $\eta$
of data samples. For setting the hyperparameters of the prior distribution for \( M \) and \( V \), one can use \( M_{\text{mode}} \) and \( V_{\text{mode}} \), respectively with the appropriate parameters for \( \mathcal{M} \mathcal{L} \) distribution.

On the other hand for \( JMDY \) class of distribution, we set appropriate value of hyperparameter \( \eta \) from Equation 32 when mode of \( d \) is given. Next, we construct a diagonal matrix, \( D_{\eta} \) with the diagonal entries \( \eta \). The hyperparameter \( \Psi \) can be constructed in the following way, \( \Psi = M_{\text{mode}} D_{\eta} V_{\text{mode}}^T \), where \( M_{\text{mode}} \) and \( V_{\text{mode}} \) are the choices for the modes of their respective distributions.

In order to setup an empirical prior framework, one could obtain the maximum likelihood estimator (MLE) using the technique described in Chikuse (2012). We could set the hyperparameters in such a way that the mode of the prior distribution is same as MLE. Also note that, the “Empirical Bayesian” procedure (Robbins, 1985; Casella, 1985) is out of scope of this study.

### 4. Bayesian framework for Mixture of \( \mathcal{M} \mathcal{L} \) distributions

In this section, we develop a framework for a finite mixture of \( \mathcal{M} \mathcal{L} \) distributions. We talk about posterior form and consistency. We also elaborate on sampling technique.

#### 4.1. Mixture model

Cluster analysis helps to determine the internal structure of data in an unsupervised way when no information other than the observed values of data is available (Picard, 2007). Finite mixture model allows us to cluster data points...
by assuming that each component of the mixture comes from a suitable parametric distribution and the mixture distribution is constructed by a convex combination of a number of individual component distributions. This number of components is typically specified initially.

We describe our framework as a finite mixture of $ML$ distribution with a fixed number of mixture component $C$. Details on the selection number of mixture component is described in Section 4.5. One of the popular techniques of clustering data is to model the data by a mixture of appropriate distributions. For example Gaussian mixture model is one of the most popular methods which has been used in numerous application spanning from computer vision to computational neuroscience (Stauffer and Grimson, 1999; McKenna, Raja and Gong, 1999; KaewTraKulPong and Bowden, 2002; Lewicki, 1998; Wood et al., 2004), in the context of directional data mixture of Von Mises (McGraw et al., 2006; Mardia, Taylor and Subramaniam, 2007; Tang, Chu and Huang, 2009; Bangert, Hennig and Oelfke, 2010; Reisinger et al., 2010; Hornik and Grün, 2014) or mixture of $ML$ distributions used in Lin, Rao and Dunson (2017).

Consider a product parameter space denoted by $\Theta := \tilde{V}^C_{n,p} \times S^C_p \times V^C_{p,p}$. Let $\theta := \{\theta_c\}_{c=1}^C$ denote any point in $\Theta$. Let $S_{\pi} := \{\langle \pi_1, \pi_2, \cdots, \pi_C \rangle \in (0,1)^C : \sum_{c=1}^C \pi_c = 1 \}$ be the $C$-Simplex, and $\pi \in S_{\pi}$ be any point in it. Let us also denote $\Xi := \Theta \times S_{\pi}$. Now consider a class of finite mixture of $ML$ densities denoted by $C_{\text{ML}} := \{f(X; \theta, \pi) = \sum_{c=1}^C \pi_c f_{ML}(X; \theta_c) : (\theta, \pi) \in \Xi \}$. Let $X_i \in V_{n,p}$ ($i = 1, 2, \cdots, N$) be the observed data from mixture of $ML$ distributions.

$$f(X; (\theta, \pi)) = \sum_{c=1}^C \pi_c f_{\text{ML}}(X; \theta_c) \text{ as } f \in C_{\text{ML}}.$$ 

For convenience it is customary to introduce latent cluster assignment variable to make sampling easier (McLachlan and Peel, 2004; Bishop, 2006). Therefore this mixture model can be described as the following

$$X_i \mid (Z_i = c) \sim f_{\text{ML}}(X_i; \theta_c) \text{ with } P(Z_i = c) = \pi_c \text{ for } c = 1, \cdots, C,$$

where $\pi_c > 0$ and $\sum_{c=1}^C \pi_c = 1$ and $Z_i$ is the latent cluster assignment for $i$-th data point, $X_i$. The likelihood function for the parameter $\theta$ is given by

$$L(\theta) = \prod_{i=1}^N \prod_{c=1}^C [\pi_c f_{\text{ML}}(X_i \mid \theta_c)]^{I(Z_i = c)}$$

In Section 3 we talk about the prior structure and its properties in detail. We assume two different class of prior structures. In the first one, we have

$$(M_c, D_c, V_c) \sim JMDY(\nu_c, \Psi_c)\pi \sim \text{Dir}(\alpha_1, \alpha_2, \cdots, \alpha_C),$$
while in the second one, we have
\[
\begin{align*}
M_c & \sim \mathcal{ML}(\cdot; \xi^M, \xi^D, \xi^V) \\
D_c & \sim \text{IMDY}(\cdot; \nu_c, \eta_c) \\
V_c & \sim \mathcal{ML}(\cdot; \gamma^M_c, \gamma^D_c, \gamma^V_c) \\
\pi & \sim \text{Dir}(\cdot; (\alpha_1, \alpha_2, \cdots, \alpha_C)).
\end{align*}
\tag{50}
\]

For both the prior structures the conditional posterior distributions of the parameters would be similar. Therefore, we choose to use independent prior structure given in Equation 50 to demonstrate the posterior computation described in Section 4.4.

The posterior density of \((\theta, \pi, Z_i)\) given \(\{X_i\}_{i=1}^N\) is proportional to
\[
\left\{ \prod_{i=1}^N \prod_{c=1}^C [\pi_c f_{\mathcal{ML}}(X_i \mid \theta_c)]^{I(Z_i=c)} \right\} f_{\text{prior}}(\pi, \theta) \tag{51}
\]

From Equation 51 it follows that the posterior density is proportional to
\[
\prod_{c=1}^C \left\{ \pi_c^{(\alpha_c+N_c-1)} \text{etr} \left( \left( V_c D_c M_c^T \right) N_c \bar{X}_c + G^0_c M_c + H^0_c V_c \right) \right. \\
\left. \quad \frac{\text{etr}(\nu_c \eta_c^T d_c)}{\Gamma(\nu_c + N_c)} \right\},
\tag{52}
\]

where \(N_c = \sum_{i=1}^N I(Z_i = c)\) and \(\bar{X}_c = \frac{1}{N_c} \sum_{i=1}^N X_i I(Z_i = c)\) for \(c = 1, \cdots, C\). Also we have,
\[
G^0_c = \xi^V_c \xi^D_c (\xi^M_c)^T \quad \text{and} \quad H^0_c = \gamma^V_c \gamma^D_c (\gamma^M_c)^T.
\tag{53}
\]

### 4.2. Hyperparameter selection for mixture model

The class of prior distributions specified in Equations 50 and 49 are flexible in the sense, empirical information and/or prior knowledge about any parameters can be incorporated in the model via appropriate hyper-parameter choices. On the other hand, in the absence of prior knowledge, one can specify hyper-parameters values such that the corresponding prior distributions becomes weakly informative or vague. In the following section we note down two specific procedures to select the value of hyper-parameters focusing independent prior structure in Equation 50 in mind. Similar procedure can easily be developed to select hyper-parameters for the joint prior structure described in Equation 49.

**Weakly informative prior** If the prior probability density function is proportional to 1 then we refer the corresponding prior as uniform prior. We can construct uniform prior using the prior structure defined in Equation 50 by
choosing $\alpha_c = 1$, $\nu_c = 0$, $\xi^D_c = 0_{p,p}$ and $\xi^D_c = 0_{p,p}$ for $c = 1, \ldots, C$. Here $0_{p,p}$ denotes the zero matrix of dimension $p \times p$. Note that, the other hyperparameters, $\eta_c, \xi^M_c, \xi^V_c, \gamma^M_c, \gamma^D_c$, are not required to be specified in this case. Note that the uniform prior designed here is improper in nature and the improper priors are not allowed for mixture models as it leads to invalid posterior. As a remedy one may construct “constrained mixture model” (Diebolt and Robert, 1994) by introducing some additional constraint to ensure propriety for corresponding posterior. As it is tangential to the current discussion, we avoid the detailed construction on ‘constrained mixture model’ for the current model in this article. Without going into the additional complexity, one may construct weakly informative, proper prior by choosing $\eta_c$ to be very close to zero (such as 0.01) instead of zero.

**Empirical prior** We first gather the empirical information by fitting a EM based algorithm to the data to obtain the maximum likelihood estimator of the parameters (see Section 4.6). Once we have a basic basic estimates of the cluster assignments, we compute number of points, $n^*_c$, assigned to the various clusters and rough estimates of the cluster specific parameters, $M^1_c, d^1_c, V^1_c$, for $c \in \{1, \ldots, C\}$. The idea is to choose appropriate hyper-parameter values in Equation 50, so that the corresponding prior distributions have modes at the values $M^1_c, D^1_c, V^1_c$. For the prior distribution of $d_c$ use the procedure described in Section 3.5 to set appropriate value of $\eta_c$. For $c = 1\ldots C$, we set $\xi^M_c = M^1_c, \xi^V_c = I_p$ and $\gamma^M_c = V^1_c, \gamma^V_c = I_p$. The choice for $\nu_c$ and $\xi^D_c, \xi^D_c$ are crucial and it may not desired to set very high values for these parameters. We set $\nu_c = n^*_c/K^1$ and the values for $\xi^D_c, \xi^D_c$ to be close to $n^*_c/K^1$. Here $K^1$ determines the relative strength of the prior distribution appropriately. To select hyperparameters from the parameter $\pi$ we set $\alpha_c = n^*_c/K^1$ for $c = 1, \ldots, C$.

In any Bayesian model, consistency of the posterior distribution is a desirable property. In the following subsection we establish posterior consistency for our mixture model.

### 4.3. Weak and Strong Posterior Consistency

Consider a product parameter space denoted by $\Theta := V^C_{p,n^p} \times S^C_p \times V^C_{p,p}$. Let $\theta := \{\theta_c\}^C_{c=1} = \{M_c, d_c, V_c\}^C_{c=1}$ denote any point in $\Theta$, and $\theta_0 := \{M^0_c, d^0_c, V^0_c\}^C_{c=1} \in \Theta$ a particular point. Let $S_\pi := \{(\pi_1, \pi_2, \cdots, \pi_C) \in (0, 1)^C : \sum_{c=1}^C \pi_c = 1\}$ be the $C$-Simplex, and $\pi \in S_\pi$ be any point in it.

Consider the distance metric $d(\cdot, \cdot)$ on the parameter space $\Xi := \Theta \times S_\pi$ constructed from appropriate distance metrics in the respective parameter spaces:

$$d(\theta_1, \theta_2) := \sqrt{\sum_{c=1}^C [d^2_{S_p}(M^1_c, M^2_c) + d^2_{S_p}(d^1_c, d^2_c) + d^2_{S_p}(V^1_c, V^2_c)]}$$

$$d((\theta_1, \pi_1), (\theta_2, \pi_2)) := \sqrt{d^2_{S_\pi}(\pi_1, \pi_2) + d^2(\theta_1, \theta_2)}$$ (54)
We alternatively denote \( \Pi(\theta) \) by \( \Pi((\theta, \pi)) \) where \( \Pi(\theta, \pi) \) is defined on \( \Xi \). Let \( C \) be a class of finite mixture of \( \mathcal{MC} \) densities denoted by \( \mathcal{C}_{\mathcal{MC}} := \{ f(X; (\theta, \pi)) = \sum_{c=1}^{C} \pi_c f_{\mathcal{MC}}(X; \theta_c) : (\theta, \pi) \in \Xi \} \).

We alternatively denote \( f(X; (\theta, \pi)) \) by \( f_{\theta, \pi}(X) \) when we wish to emphasize the parametrization. \( f_{\theta, \pi} : \mathcal{V}_{n,p} \to \mathbb{R}^+ \) is a family of probability density functions with respect to the normalized Haar measure \( dX \) on \( \mathcal{V}_{n,p} \). Observe that \( \Xi \) and \( \mathcal{V}_{n,p} \) are complete separable metric spaces and that \( (\theta, \pi) \sim f_{\theta, \pi} \) is one-to-one and \( (X, \theta, \pi) \sim f(X; (\theta, \pi)) \) is measurable. The prior \( \Pi \) is defined on \( \Xi \). Let \( X_1, X_2, \ldots, X_N \) be independent and identically distributed with probability density function \( f_{\theta_0, \pi_0} \). The posterior distribution \( \Pi(A \mid X_1, X_2, \ldots, X_N) \) for any measurable subset \( A \) of \( \Xi \) is given by

\[
\Pi(A \mid X_1, X_2, \ldots, X_N) = \frac{\int_A R_n((\theta, \pi))d\Pi((\theta, \pi))}{\int_{\Xi} R_n((\theta, \pi))d\Pi((\theta, \pi))} \tag{56}
\]

where

\[
R_n((\theta, \pi)) = \prod_{i=1}^{N} \frac{f(X_i; (\theta, \pi))}{f(X_i; (\theta_0, \pi_0))} . \tag{57}
\]

In our model, \( \Pi((\theta, \pi)) \) in Equation (56) is defined with respect to the appropriate product measure on \( \Theta \) and the Lebesgue measure on \( \mathbb{S}_\pi \). The prior \( \Pi \) is given by the Equation (50).

For \( \epsilon > 0 \) define, respectively, a neighborhood in parameter space, a Kullback-Leibler (KL) neighborhood, a weak neighborhood, and a Hellinger neighborhood of \( (\theta_0, \pi_0) \) (corresponding to the true density \( f_{\theta_0, \pi_0} \)) in \( \Xi \) as

\[
N_\epsilon((\theta_0, \pi_0)) = \left\{ (\theta, \pi) \in \Xi : d((\theta, \pi), (\theta_0, \pi_0)) < \epsilon \right\} ,
\]

\[
KL_\epsilon((\theta_0, \pi_0)) = \left\{ (\theta, \pi) \in \Xi : \int_{\mathcal{V}_{n,p}} f_{\theta_0, \pi_0}(X) \log \left( \frac{f_{\theta, \pi}(X)}{f_{\theta_0, \pi}(X)} \right) dX < \epsilon \right\} ,
\]

\[
\mathcal{U}_\epsilon((\theta_0, \pi_0)) = \left\{ (\theta, \pi) \in \Xi : \left| \int_{\mathcal{V}_{n,p}} g(X) f_{\theta_0, \pi_0}(X) dX - \int_{\mathcal{V}_{n,p}} g(X) f_{\theta_0, \pi}(X) dX \right| < \epsilon \right\} ,
\]

\[
\mathcal{W}_\epsilon((\theta_0, \pi_0)) = \left\{ (\theta, \pi) \in \Xi : \left( \int_{\mathcal{V}_{n,p}} \left( \sqrt{f_{\theta_0, \pi_0}(X)} - \sqrt{f_{\theta, \pi}(X)} \right)^2 dX \right)^{1/2} < \epsilon \right\} .
\]

The weak neighborhood definition holds if the corresponding equation is satisfied for all bounded and continuous functions \( g \) on \( \mathcal{V}_{n,p} \).

**Lemma 12.** A finite mixture of \( \mathcal{MC} \) densities is strictly positive, bounded away from zero and bounded from above.
Proof of Lemma 12.
Let \( f(X; \theta, \pi) \in C_{ML} \) be a density function that is a \( C \)-component mixture of \( ML \) distributions parametrized by \((\theta, \pi) \in \Xi \), that is,

\[
f(X; \theta, \pi) = \sum_{c=1}^{C} \pi_c f_{ML}(X; \theta_c).
\] (58)

Since the density function \( f_{ML}(\cdot; \theta_c) : V_{n,p} \to \mathbb{R}^+ \) is continuous on the compact manifold \( V_{n,p} \), the extreme value theorem (Rudin et al., 1964) dictates that \( f_{ML}(\cdot; \theta_c) \) is bounded and attains at least one minima and maxima. In particular, \( f_{ML}(X; \theta_c) \) has the unique modal orientation \( M_c V^T_c \) (page 32 in Chikuse (2012)) where \( \theta_c = (M_c, d_c, V_c) \). Likewise, it is easy to see that the minimum value of the density function occurs at \(-M_c V^T_c \). Hence for any \( X \in V_{n,p} \), we have

\[
\frac{\text{etr} \left( V_c D_c M_c^T \left( M_c V^T_c \right) \right)}{\eta F_{1}(n/2; D_c^2/4)} \geq f_{ML}(X; \theta_c) \geq \frac{\text{etr} \left( -V_c D_c M_c^T \left( M_c V^T_c \right) \right)}{\eta F_{1}(n/2; D_c^2/4)},
\]

\[
\Rightarrow \frac{\text{etr} \left( D_c \right)}{\eta F_{1}(n/2; D_c^2/4)} \geq f_{ML}(X; \theta_c) \geq \frac{\text{etr} \left( -D_c \right)}{\eta F_{1}(n/2; D_c^2/4)},
\]

\[
\Rightarrow \frac{\exp(\sum_{i=1}^{p} d_{ic})}{\eta F_{1}(n/2; D_c^2/4)} \geq f_{ML}(X; \theta_c) \geq \frac{\exp(-\sum_{i=1}^{p} d_{ic})}{\eta F_{1}(n/2; D_c^2/4)} > 0.
\] (59)

Let \( UB = \max_{1 \leq c \leq C} \frac{\exp(\sum_{i=1}^{p} d_{ic})}{\eta F_{1}(n/2; D_c^2/4)} \) and \( LB = \min_{1 \leq c \leq C} \frac{\exp(-\sum_{i=1}^{p} d_{ic})}{\eta F_{1}(n/2; D_c^2/4)} \). Using Equations 58 and 59, we get

\[
0 < LB \leq f(X; (\theta, \pi)) \leq UB < \infty.
\] (60)

\[\square\]

Lemma 13. Let \((\theta, \pi), (\theta_0, \pi_0) \in \Xi \). Then for any \( \epsilon > 0 \), there exists a \( \delta > 0 \) such that

\[
d((\theta, \pi), (\theta_0, \pi_0)) < \delta \implies \sup_{X \in V_{n,p}} \left| \log \frac{f(X; (\theta_0, \pi_0))}{f(X; (\theta, \pi))} \right| < \epsilon,
\]

where \( f(X; (\theta, \pi)), f(X; (\theta_0, \pi_0)) \in C_{ML} \).

Proof of Lemma 13.
Let \( f(X; (\theta, \pi)) \in C_{ML} \), that is, let \( f(X; (\theta, \pi)) = \sum_{c=1}^{C} \pi_c f_{ML}(X; \theta_c) \). Note that for all \( c = 1, \ldots, C \), the function \( f_{ML}(X; \theta_c) \) is continuous in \( X \) and \( \theta_c \).

Since \( f(X; (\theta, \pi)) \) is a linear combination of functions \( \{f_{ML}(X; \theta_c)\}_{c=1}^{C} \) with weights \( \{\pi_c\}_{c=1}^{C} \), it too is continuous in \( X \in V_{n,p} \) and \((\theta, \pi) \in \Xi \). Moreover, from Lemma 12, \( f(X; (\theta, \pi)) \) is bounded away from 0 and \( \infty \). Hence log \( f(X; (\theta, \pi)) \) is continuous in \( X \in V_{n,p} \) and \((\theta, \pi) \in \Xi \), since log is continuous and well defined over the range.
Let $B(\theta_0, \pi_0) \subset \Xi$ be a compact ball around $(\theta_0, \pi_0)$ with strictly positive, bounded radius.

Now, consider the function $f(X; (\theta, \pi))$, restricted to the domain $\mathcal{V}_{n,p} \times B(\theta_0, \pi_0)$. Within both $\mathcal{V}_{n,p}$ and $B(\theta_0, \pi_0)$, $f$ is continuous in each argument $\theta$, $\pi$ and $X$. The compactness of both these spaces ensures uniform continuity individually in each argument. The latter ensures uniform continuity of the joint function within the joint space $\mathcal{V}_{n,p} \times B(\theta_0, \pi_0)$.

Now, since $\mathcal{V}_{n,p} \times B(\theta_0, \pi_0)$ is compact, the function restricted to this domain is uniformly continuous. Therefore for any $\epsilon > 0$, there exists a $\delta > 0$, such that

\[
d \left( (X_1, \theta_0, \pi_0), (X_2, \theta, \pi) \right) < \delta \implies | \log f(X_1; (\theta_0, \pi_0)) - \log f(X_2; (\theta, \pi)) | < \epsilon,
\]

for arbitrary $(X_1, \theta_0, \pi_0), (X_2, \theta, \pi) \in \mathcal{V}_{n,p} \times B(\theta_0, \pi_0)$. In particular, setting $X_1 = X_2 = X$, and using the fact that $d \left( (\theta, \pi), (\theta_0, \pi_0) \right) = d \left( (X, \theta_0, \pi_0), (X, \theta, \pi) \right) < \delta$ for all $X$ (clear from Equations 54 and 55), we have

\[
d \left( (\theta, \pi), (\theta_0, \pi_0) \right) < \delta \implies \sup_{X \in \mathcal{V}_{n,p}} | \log f(X; (\theta_0, \pi_0)) - \log f(X; (\theta, \pi)) | < \epsilon,
\]

\[
\implies \sup_{X \in \mathcal{V}_{n,p}} \left| \frac{\log f(X; (\theta_0, \pi_0))}{f(X; (\theta, \pi))} \right| < \epsilon. \quad (61)
\]

\[\square\]

**Theorem 5. (Weak Consistency)** For our prior $\Pi$ (defined in Definition 2 in Section 3)

\[\Pi(\mathcal{U}^c \mid X_1, X_2, \cdots, X_N) \to 0 \quad \text{a.s.} \quad F_{\theta_0, \pi_0}^\infty,\]

for any weak neighborhood $\mathcal{U}$ of $(\theta_0, \pi_0)$. $F_{\theta_0, \pi_0}$ is the probability distribution function corresponding to the density $f_{\theta_0, \pi_0}$, and $F_{\theta_0, \pi_0}^\infty$ is the corresponding infinite product measure.

**Proof of Theorem 5.**

For every $\epsilon > 0$ there exists a $\delta > 0$ such that

\[
d \left( (\theta, \pi), (\theta_0, \pi_0) \right) < \delta \implies \sup_{X \in \mathcal{V}_{n,p}} \left| \frac{\log f(X; (\theta_0, \pi_0))}{f(X; (\theta, \pi))} \right| < \epsilon, \quad \text{[from Lemma 13]},
\]

\[
\implies \int_{\mathcal{V}_{n,p}} f(X; (\theta_0, \pi_0)) \left| \log \frac{f(X; (\theta_0, \pi_0))}{f(X; (\theta, \pi))} \right| dX < \epsilon,
\]

\[
\implies \int_{\mathcal{V}_{n,p}} f(X; (\theta_0, \pi_0)) \log \frac{f(X; (\theta_0, \pi_0))}{f(X; (\theta, \pi))} dX < \epsilon.
\]

Hence, $N_3((\theta_0, \pi_0)) \subset KL_e((\theta_0, \pi_0))$. It is easy to see that $\Pi$ puts strictly positive measure on $N_3((\theta_0, \pi_0))$ for all $\delta > 0$, because by the definition of distance metric given in Equation 54, any neighborhood around $(\theta_0, \pi_0)$ has a positive measure. It follows that $\Pi$ puts strictly positive measure on $KL_e((\theta_0, \pi_0))$ for all $\epsilon > 0$. The theorem then follows from Schwartz (1965).
Theorem 6. (Strong/Hellinger Consistency) For our prior $\Pi$

$$\Pi(\mathcal{W}^c \mid X_1, X_2, \cdots, X_N) \to 0 \quad \text{a.s.} \quad F_{\theta_0,\pi_0}^\infty,$$

for any Hellinger neighborhood $\mathcal{W}$ of $(\theta_0, \pi_0)$.

Proof of Theorem 6.

For any $\epsilon > 0$ consider the weak neighborhood

$$\mathcal{U}_\epsilon((\theta_0, \pi_0)) = \left\{(\theta, \pi) \in \Xi : \left| \int_{\mathcal{V}_{n,p}} g(X)f_{\theta,\pi_0}(X)[dX] - \int_{\mathcal{V}_{n,p}} g(X)f_{\theta,\pi}(X)[dX] \right| < \epsilon^2 \right\},$$

for all bounded and continuous functions $g$ on $\mathcal{V}_{n,p}$.

For each $(\theta, \pi) \in \mathcal{U}_\epsilon((\theta_0, \pi_0))$ choose

$$g(X) := \left( \frac{\sqrt{f_{\theta,\pi_0}(X)} - \sqrt{f_{\theta,\pi}(X)}}{\sqrt{f_{\theta,\pi_0}(X)} + \sqrt{f_{\theta,\pi}(X)}} \right)^2.$$

Now from Lemma 12, the functions $f_{\theta,\pi}$ are bounded away from 0, ensuring a positive lower bound for the denominator. The upper bound for the denominator is guaranteed from the upper bound property that follows from the same Lemma.

A similar argument holds for the numerator as well. This ensures boundedness of the function $g(X)$ and the continuity follows from the continuity of $f(X)$ (from Lemma 12). Thus $g(X)$ is a bounded and continuous function. Hence,

$$\left| \int \left( \frac{\sqrt{f_{\theta,\pi_0}(X)} - \sqrt{f_{\theta,\pi}(X)}}{\sqrt{f_{\theta,\pi_0}(X)} + \sqrt{f_{\theta,\pi}(X)}} \right)^2 f_{\theta,\pi}(X)[dX] \right| < \epsilon^2,$$

$$\Rightarrow \left| \int \left( \sqrt{f_{\theta,\pi_0}(X)} - \sqrt{f_{\theta,\pi}(X)} \right)^2 [dX] \right| < \epsilon^2,$$

$$\Rightarrow \left( \left( \sqrt{f_{\theta,\pi_0}(X)} - \sqrt{f_{\theta,\pi}(X)} \right)^2 \right)^{1/2} < \epsilon. \quad (62)$$

Hence $\mathcal{U}_\epsilon((\theta_0, \pi_0)) \subset \mathcal{W}_\epsilon((\theta_0, \pi_0))$. The Theorem now follows from an application of Theorem 5. \qed

4.4. Sampling procedure

In order to perform Bayesian inference, it is important to compute statistics related to the posterior distribution e.g. the posterior mean or posterior quantiles. The posterior density, defined in Equation 52, is intractable in the sense that it is not possible to compute these quantities analytically by performing integration or to generate i.i.d. samples from the posterior distribution.
However we can design a Gibbs sampling Markov chain to generate samples from the posterior distribution. It is known that the Markov chain corresponding to Gibbs samplers would converge to the desired stationary distribution.

In order to implement the Gibbs sampler, we sample cluster specific parameters along with the latent indicator \( Z_i \) for cluster assignment for each data point \( X_i \) where \( i = 1, 2, \ldots, N \). The conditional distribution of \( Z_i \) given all other parameters follows

\[
P(Z_i = c \mid M_c, d_c, V_c, \pi, \{X_i\}_i^N) = \frac{\pi_c f_{\mathcal{ML}}(X_i \mid M_c, d_c, V_c)}{\sum_c \pi_c f_{\mathcal{ML}}(X_i \mid M_c, d_c, V_c)} \tag{63}
\]

for \( c = 1, 2, \ldots, C \). The conditional posterior distribution of \( \pi \) is given as

\[
\pi \mid \{M_c, d_c, V_c\}_{c=1}^C, \{X_i, Z_i\}_i^N \sim \text{Dir}(\alpha_1 + N_1, \alpha_1 + N_2, \ldots, \alpha_C + N_C), \tag{64}
\]

where \( N_c = \sum_{i=1}^N \mathbb{I}(Z_i = c) \) for \( c = 1, \ldots, C \). Given the latent cluster assignments, the conditional posterior distribution of cluster specific parameters are independent. Due to conditional functional conjugacy for \( M_c \) and \( V_c \), it is straightforward to show that the full conditional of the corresponding posterior would belong to the \( \mathcal{ML} \) class of distribution. In particular,

\[
M_c \mid \{d_c, V_c, \{X_i, Z_i\}_i^N, \pi\} \sim \mathcal{ML} \left( \cdot \mid (S^M_G, S^D_G, S^V_G) \right) \tag{65}
\]

\[
V_c \mid \{M_c, d_c, \{X_i, Z_i\}_i^N, \pi\} \sim \mathcal{ML} \left( \cdot \mid (S^M_H, S^D_H, S^V_H) \right), \tag{66}
\]

where \((S^M_G, S^D_G, S^V_G)\) and \((S^M_H, S^D_H, S^V_H)\) are SVD decompositions of matrices \((D_c V_c^T N_c \bar{X}_c^T + G_c^0)\) and \((D_c V_c^T N_c \bar{X}_c^T + H_c^0)\), respectively. Observe that

\[
\bar{X}_c = \frac{1}{N_c} \sum_{i=1}^N X_i \mathbb{I}(Z_i = c).
\]

Efficient sampling from \( \mathcal{ML} \) distribution is done using algorithm developed in Hoff (2009).

The conditional posterior distribution for \( d_c \) given other parameters has the following density

\[
f(d_c \mid M_c, V_c, \{X_i, Z_i\}_i^N, \pi) \propto \exp \left( \left( \nu_c \eta_c^T + N_c \phi_c^T \right) d_c \right) \left( 0F_1 \left( \frac{n_2}{2}; D_c^2/4 \right) \right) \mathbb{I}(d_c \in S_p) \tag{67}
\]

\[
d_c \mid \{M_c, V_c, \{X_i, Z_i\}_i^N, \pi\} \sim \text{IMDY} \left( \cdot \mid (\nu_c + N_c), \frac{\nu_c \eta_c + N_c}{\nu_c + N_c} \right),
\]

where \( \phi_c = \{\phi_c, \phi_{i2}, \ldots, \phi_{ip}\} \) with \( \phi_{cj} \) is the \( j \)-th diagonal element of the matrix \( M_c^T \bar{X}_c V_c \) for \( j = 1, 2, \ldots, p \). Note that, this can also be verified from the Equation 46 in Section 3.3. Due to non-standard form of the posterior distribution given in Equation 67, sampling of \( d_c \) is challenging.
The density corresponding to the full conditional distribution of \(d_{cj}\), the \(j\)-th diagonal entry of \(D_c\) for \(j = 1, 2, \ldots, p\), is given below,

\[
f \left( d_{cj} \mid d_{-cj}, M_c, V_c, \{X_i, Z_i\}_i^N, \pi \right) \propto \exp(d_{cj} (\nu_c \eta_{cj} + N_c \phi_{cj})) \_0\text{F}_1(n/2, D_c^2/4)^{\nu_c+N_c} \_I(d_{cj+1} < d_{cj} < d_{cj-1}) . \tag{68}
\]

Also let \(F_{cj}(\cdot)\) is the corresponding distribution function of conditional distribution of \(d_{cj}\). We describe the detailed implementation of sampling from this conditional distribution in the following paragraph after this subsection. For a generic representation of posterior distribution for \(d_{cj}\) for all \(j = 1, \cdots, p\), we define \(d_{c0} = \infty\) and \(d_{cp+1} = 0\). We also write

\[
d_{-cj} := \{d_{c1}, \cdots, d_{cj-1}, d_{cj+1}, \cdots, d_{cp}\} . \tag{69}
\]

We have designed an efficient sampling scheme to sample \(d_c\) using the set of \(p\) distributions given in Equation 68. Observe that support of the distribution for \(d_{c1}\) is \([d_{c2}, \infty)\) while that of the others are bounded. Note that the posterior distribution of \(d_{c1}\) is unimodal (see Theorem 3) and we exploit that fact to design an efficient sampler for \(d_c\). A description of the sampling steps is given in Algorithm 1 below. Note that, because of log-concavity nature of the conditional distribution function for \(d_{cj}\), we could have implemented adaptive rejection sampler (ARS) for it. However, the standard ARS algorithm can not be immediately implemented in this context because of involved computation with \(0\_F_1(\cdot)\) function. So we reserved this development for our future work.

**Gibbs algorithm** The following algorithm outlines the steps of the Gibbs sampling algorithm which shows the full conditional distribution of the parameters at \(k\)-th step based on the samples drawn at \((k-1)\)-th step and data.
Algorithm 1 Algorithm for MCMC method

for $c = 1, 2, \cdots, C$ do
    initialize the MCMC chain with $M_c^{(0)}$, $D_c^{(0)}$, $V_c^{(0)}$ and $\pi^{(0)}$
end for

$k = 0$
repeat
    $k = k + 1$
    for $i = 1, 2, \cdots, N$ do
        $Z_i^{(k)} \sim \text{Categorical} \left( \cdot ; \{1, 2, \cdots, C\}, \pi^{(k-1)} \right)$
    end for
    for $c = 1, 2, \cdots, C$ do
        \[ N_c^{(k)} = \sum_{i=1}^{N} \mathbb{1}(Z_i^{(k)} = c) \]
        \[ \bar{N}_c^{(k)} = \frac{1}{N_c} \sum_{i=1}^{N} X_i \mathbb{1}(Z_i^{(k)} = c) \]
        \[ M_c^{(k)} \sim \mathcal{ML} \left( \cdot ; \left( S_{CM}^{(k-1)}, S_{CD}^{(k-1)}, S_{CV}^{(k-1)} \right) \right) \]
        \[ V_c^{(k)} \sim \mathcal{ML} \left( \cdot ; \left( S_{CH}^{(k)}, S_{DH}^{(k-1)}, S_{VH}^{(k-1)} \right) \right) \]
        \[ d_{cj}^{(k)} \sim F_{cj} \left( \cdot ; \left( d_{cj}^{(k)}, M_c^{(k)}, V_c^{(k)}, \{X_i, Z_i\}_i^N, \pi^{(k-1)} \right) \right) \text{ for all } j = 1, 2, \cdots, p \]
    end for
    $\pi^{(k)} \sim \text{Dir} \left( \cdot ; \alpha_1 + N_1^{(k)}, \cdots, \alpha_C + N_C^{(k)} \right)$
until convergence

Note that, $(d_{cj}^{(k)})$ is given by the following set
\[ (d_{cj}^{(k)}) := \left\{ (d_{cj})^{(k)}, \cdots, (d_{cj-1})^{(k)}, (d_{cj+1})^{(k-1)}, \cdots, (d_{cp})^{(k-1)} \right\} \]

The stationary distribution of the Gibbs sampling Markov chain is the posterior distribution corresponding to Equation 52. Convergence to this stationary distribution does not on the choice of the initial point. However, in order to run the MCMC method it is required to initialize Algorithm 1 with certain values (e.g. $M_c^{(0)}$, $D_c^{(0)}$, $V_c^{(0)}$ and $\pi^{(0)}$). In practice, specifically in the case of large-scale dataset, it is often seen that bad choice of initial value might lead to slow convergence of the MCMC method. In order to come up with a reasonable choice of initial value, we first run a hierarchical clustering (Lattin, Carroll and Green, 2003; Rokach and Maimon, 2005) on the entire dataset with a fixed number of clusters, $C$ (for selection of optimal $C$ see Section 4.5) to get a initial cluster assignments for the data points. Based on the initial assignment, we adopt a
maximum likelihood based technique described in Chikuse (2012) to obtain the initial value of the cluster specific parameters. This initial point selection procedure has worked well for our simulated dataset. We notice that the selection of initial point may not be crucial for small datasets. However, for large dataset choice of suitable initial point could save significant amount of time by reducing number of burn-in steps.

**Efficient Rejection Sampler** In this section we describe the rejection sampling procedure from the conditional distribution of \((d_1 \mid (d_2, \cdots, d_p))\) when \(d \sim IMDY(\cdot; \nu, \eta)\) for some \(\nu > 0\) and \(\max_{1 \leq j \leq p} \eta_j < 1\). Here \(\eta = (\eta_1, \ldots, \eta_p)\). Let \(m\) be the mode of the conditional distribution, \(g_1(\cdot) := g(\cdot; \nu, \eta \mid (d_2, \ldots, d_p))\), of the variable \(d_1\) given \((d_2, \ldots, d_p)\) when \(\eta_1 > 0\). In case, \(\eta_1 < 0\), we explicitly set \(m\) to be 0.

Using property of the conditional distribution described Lemma 11 the we compute a critical point \(RT_{crit}\) so that \(P(d_1 > RT_{crit} \mid (d_2, \cdots, d_p), \{X_j\}_{j=1}^N) < \epsilon\) with the choice of \(\epsilon = 0.0001\).

We restrict the support of the conditional posterior distribution for \(d_1\) to the bounded interval \((0, RT_{crit})\]. We employ a efficient rejection sampling scheme to sample from the desired distribution in the following way.

Let \(\delta = RT_{crit}/N_{bin}\) where \(N_{bin}\) is the total number of partitions for the interval \((0, RT_{crit})\]. Consider, \(k = \lceil m/\delta\rceil + 1\) where \(\lceil m/\delta\rceil\) denotes the greatest integers less that or equal to \(m/\delta\). Now define the function

\[
\bar{g}_1(x) := \sum_{j=1}^{k-1} g_1(j\delta) \cdot \mathbb{I}_{((j-1)\delta, j\delta)}(x) + g_1(m) \cdot \mathbb{I}_{((k-1)\delta, k\delta)}(x) + \sum_{j=k+1}^{N_{bin}} g_1((j-1)\delta) \cdot \mathbb{I}_{((j-1)\delta, j\delta)}(x).
\]

Note that \(\bar{g}_1(x) \geq g_1(x)\) for all \(x \in (0, RT_{crit})\] as \(g_1(\cdot)\) unimodal log-concave function with maxima \(m\). To sample from the distribution with density corresponding to the function \(\bar{g}_1(\cdot)\) we consider, \(p_j = q_j / \sum_{j=1}^{N_{bin}} q_j\) for \(j = 1, 2, \cdots, N_{bin}\) where,

\[
q_j = \begin{cases} 
  g_1(j\delta) & \text{if } 1 \leq j < \left\lceil \frac{m}{\delta} \right\rceil + 1, \\
  g_1(m) & \text{if } j = \left\lceil \frac{m}{\delta} \right\rceil + 1, \\
  g_1((j-1)\delta) & \text{if } \left\lceil \frac{m}{\delta} \right\rceil + 1 < j \leq M.
\end{cases}
\]

The steps of the rejection samplers are given below

- Sample \(Z\) from the discrete distribution with the support \(\{1, 2, \ldots, N_{bin}\}\) corresponding probability \(\{p_j\}_{j=1}^M\).
- Sample \(y \sim Uniform((Z-1)\delta, Z\delta)\).
- Sample \(U \sim Uniform(0, 1)\).
- Accept \(y\) if \(U \leq \frac{\bar{g}_1(y)}{\bar{g}_1(y)}\).
Note that the efficiency of the sampler increases when we choose larger values for $N_{bin}$.

**Posterior summary** There are multiple ways to summarize the posterior distribution for the estimates of the parameters. We choose to use the parametrization given in Equation 1 for posterior summary. This parametrization enables us to report the error in a more interpretable way. Using $M, d, V$, it is challenging to report the error as $M$ and $V$ lie on a non-euclidean space. Generating summary of results for different parameters on $V_{n,p}$ is not straightforward. Some generalized version of mean like Karcher mean could be investigated. Note that we can directly compare true $F$ and $\hat{F}$ as there is no constraint on the elements of $F$. This direct comparison is not immediately possible for $M, d, V$ parametrization given in Equation 2 which is mainly done to achieve computational tractability.

### 4.5. Model selection

In order to identify the optimum number of clusters we use Deviance Information Criteria for Bayesian model selection (DIC) (Gelman et al., 2003; Spiegelhalter et al., 2002). It has been successfully used as a model selection criteria in in various Bayesian models (Berg, Meyer and Yu, 2004; François and Laval, 2011; Khare, Pal and Su, 2017). To explain the DIC criterion in the context of the current model, let $\theta^{(C)} = \{M_c, d_c, V_c\}^c_{c=1}$ denote all the parameter vectors and the *deviance function* is defined as $Dev(\theta^{(C)}) := -2 \log L(\theta^{(C)})$ where $L(\cdot)$ is the likelihood function defined in Equation 48. Let $\{\theta^{(C,i)}\}^S_{i=1}$ be $S$ values of the parameters, sampled from the appropriate posterior distribution in Equation 52. The DIC score with a given choice for $C$, is computed as $DIC^{(C)} := \overline{Dev}^{(C)}(\theta^{(C)}) + \sum_{i=1}^{S} \left( Dev(\theta^{(C,i)}) - \overline{Dev}^{(C)} \right)^2 \big/ (2(S-1))$ where $\overline{Dev}^{(C)} = \sum_{i=1}^{S} Dev(\theta^{(C,i)}) / S$ (Gelman et al. (2003), page 185). To infer the number of clusters, samples are generated from different Markov chain assuming different values of $C$. The optimum number of cluster is given by $C_{opt} = \arg\max_C DIC^{(C)}$. For detailed discussion on DIC see DeIorio and Robert (2002); Gelman et al. (2003); Titterington et al. (2006). Specifically, in the context of the mixture model, DeIorio and Robert (2002) described possible limitations for the standard DIC criterion. Following the alternative criteria proposed in Titterington et al. (2006), we considered several score functions (i.e. $DIC_2, DIC_3, DIC_4, DIC_5, DIC_6, DIC_7, DIC_8$ as defined in Titterington et al. (2006)). We conducted an extensive numerical study with several simulated data sets. We found that the score function $DIC_5$ outperforms other alternative criteria in terms of efficiency for the model. Also, the computation of $DIC_5$ takes significantly less time than that of standard DIC. Therefore one may use $DIC_5$ instead of standard DIC whenever computation of standard DIC takes significantly longer time particularly for any large dataset. Additional details along with a table comparing the performance of different DIC scores in our simulation study is given in Section 5) where we observe that
DIC\textsubscript{5} score can identify the correct number of clusters in most of the cases in our model.

### 4.6. Iterative method to find posterior mode

In this section, we develop an iterative optimization technique to obtain point estimator for the parameters specified in the model given by Equation 49. Specifically, we employ expectation maximization (EM) algorithm (Dempster, Laird and Rubin, 1977) to obtain mode of the posterior distribution for the parameters in the model specified in Equation 49. Note that the algorithm is computationally fast and can be useful to get some rough estimates of the parameter specially for large data-sets. Also, we may use this algorithm in specific way to select appropriate values of the hyperparameters (See Section 3.5) in the case of MCMC based posterior inference. Note that the rough estimates can also help find suitable initial values for the MCMC procedures, particularly for analyzing massive data. To describe the procedure, let us consider complete data log-likelihood (From Equation 52) as follows

\[
\begin{align*}
\sum_{i=1}^{N} \sum_{c=1}^{C} Z_{ic} \log f_{ML}(X_i \mid \theta_c) + Z_{ic} \log \pi_c + \\
+ \sum_{c=1}^{C} \alpha_c \log \pi_c + \text{tr} (\nu_c V_c D_c M_c M_c^T \Psi) - \nu_c \log \left( F_{1 \nu/2} \left( \frac{n}{2}, \frac{D^2}{4} \right) \right),
\end{align*}
\]

(70)

where \( Z_{ic} = \mathbb{I}(Z_i = c) \) and

\[
\log f_{ML}(X_i \mid \theta_c) = \text{tr}((V_c D_c M_c^T) X_i)) - \log \left( F_{1 \nu/2} \left( \frac{n}{2}, \frac{D^2}{4} \right) \right).
\]

Let we start the iterative algorithm at an initial point \((\theta^{(0)}, \pi^{(0)})\). We construct a sequence of parameter values \(\{ (\theta^{(t)}, \pi^{(t)}) \}_{t \geq 1}\) where we move from \((\theta^{(t)}, \pi^{(t)})\) to \((\theta^{(t+1)}, \pi^{(t+1)})\) using the “E-step” and “M-step” described below.

**E-step:** We construct the objective function

\[
\begin{align*}
Q(\theta, \pi \mid X, \theta^{(t)}, \pi^{(t)}) \\
:= \sum_{i=1}^{N} \sum_{c=1}^{C} \langle Z_{ic} \rangle \log f_{ML}(X_i \mid \theta_c) + \langle Z_{ic} \rangle \log \pi_c + \\
+ \sum_{c=1}^{C} \alpha_c \log \pi_c + \text{tr} (\nu_c V_c D_c M_c M_c^T \Psi) - \nu_c \log \left( F_{1 \nu/2} \left( \frac{n}{2}, \frac{D^2}{4} \right) \right),
\end{align*}
\]

(71)

where

\[
\langle Z_{ic} \rangle := \mathbb{E}(Z_{ic} \mid X, \theta^{(t)}) = \frac{\pi_c^{(t)} f_{ML}(X_i \mid \theta_c^{(t)})}{\sum_{k=1}^{C} \pi_k^{(t)} f_{ML}(X_i \mid \theta_k^{(t)})}
\]
M-step: In this step, we maximize $Q(\theta, \pi \mid X, \theta^{(t)}, \pi^{(t)})$ with respect to the $\theta, \pi$. It is easy to see that, $Q(\theta, \pi \mid X, \theta^{(t)}, \pi^{(t)})$ is maximized when we set $\pi = \hat{\pi}$ where the $c$-th component of the vector $\hat{\pi}_c$,

$$\hat{\pi}_c = \frac{\alpha_c + \sum_{i=1}^{N} (z_{ic})}{N + \sum_{c=1}^{C} \alpha_c}$$ for $c = 1, \ldots, C$.

Note that $\theta := \{\theta_c\}_{c=1}^{C}$ where $\theta_c = \{M_c, d_c, V_c\}$. Hence, the function $Q(\theta, \pi \mid X, \theta^{(t)}, \pi^{(t)})$ can be maximized by maximizing the function

$$tr \left( V_c D_c M_c^T \left[ \hat{X}^{(c)} + \Psi \right] \right) - \nu_c \log \left( _0 F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) \right), \quad (72)$$

with respect to the variables $M_c \in \hat{\mathcal{V}}_{n,p}, V_c \in \mathcal{V}_{p,p}$ and $d_c \in \mathcal{S}_p$ for each $c = 1, \ldots, C$ separately where $\hat{X}^{(c)} = \sum_{i=1}^{N} \frac{(z_{i,c}) X}{\sum_{c=1}^{C} (z_{i,c})}$.

Let $\hat{M}^{(c)}, \hat{D}^{(c)}$ and $\hat{V}^{(c)}$ be the unique singular value decomposition (Chikuse, 2012) for the matrix $[\hat{X}^{(c)} + \Psi]$. Let $\hat{d}^{(c)}$ be the diagonal elements of the matrix $\hat{D}^{(c)}$ and $\hat{d}_c$ be the solution of the set of equations $h(\hat{d}_c) = \hat{d}^{(c)}$ where $h(d) := \left( \frac{\partial \nu}{\partial d} \right)_{\nu} F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right) / \nu F_1 \left( \frac{n}{2}, \frac{D^2}{4} \right)$. Standard Newton-Raphson (NR) (Wright and Nocedal, 1999) method can be used to solve for $\hat{d}_c$ from the equation $h(\hat{d}_c) = \hat{d}^{(c)}$. In the case of $p = 2$, we derive the explicit expression of the Hessian matrix and show the steps by NR to solve for $\hat{d}_c$ in Section 4.6.1.

From Chikuse (2012) we get that the objective function in Equation 72 is maximized at $\hat{M}_c = \hat{M}^{(c)}$, $\hat{V}_c = \hat{V}^{(c)}$ and $\hat{D}_c$ where $\hat{D}_c$ is the diagonal matrix with diagonal elements $\hat{d}_c$.

Finally we move to the values $(\theta^{(t+1)}, \pi^{(t+1)})$ by the setting,

$$\theta^{(t+1)} := \left\{ \left( \hat{M}_c, \hat{d}_c, \hat{V}_c \right) \right\}_{c=1}^{C}$$ and $\pi^{(t+1)} := \hat{\pi}$.

We stop the iteration when we achieve convergence, i.e. the values of the parameters in the two consecutive iterations are very close.

4.6.1. Hessian computation and NR method

For this subsection we omit the subscript $c$ for ease of notation. Now observe that,

$$_0 F_1 \left( p + 2k, \frac{d_1^2 + d_2^2}{4} \right) = \frac{\Gamma (p + 2k)}{4^{-\nu \frac{p+2k-1}{2}}} \left( \sqrt{d_1^2 + d_2^2} \right)^{(p+2k-1)} I_{p+2k-1} \left( \sqrt{d_1^2 + d_2^2} \right).$$

where $I_{\nu}(\cdot)$ is the modified Bessel function of first kind with order $\nu$. Taking partial derivative with respect to $d_1$ we have,

$$\frac{\partial}{\partial d_1} _0 F_1 \left( p + 2k, \frac{d_1^2 + d_2^2}{4} \right) = \frac{d_1}{2(p+2k)} _0 F_1 \left( p + 2k + 1, \frac{d_1^2 + d_2^2}{2} \right).$$
Consider the expression for the hypergeometric function of the Matrix argument with $2 \times 2$ matrix (Muirhead, 1975)

$$\binom{0}{p} \left( \frac{D^2}{4} \right) = \sum_{k=0}^{\infty} \frac{d_1^{2k} d_2^{2k}}{2k (p - \frac{1}{2}) k!} \binom{0}{p + 2k} \left( \frac{d_1^2 + d_2^2}{4} \right).$$

(73)

This representation is also useful as we can get a good idea on error bound by approximating the number of terms for this infinite series.
Let us use the following notations

$$T_0 = \binom{d_1^2}{(p - \frac{1}{2}) k} \binom{d_2^2}{(p + 2k)} \binom{0}{p} \left( \frac{d_1^2 + d_2^2}{4} \right),$$

$$T_1 = \binom{0}{p + 2k} \left( \frac{d_1^2 + d_2^2}{4} \right),$$

$$T_2 = \binom{0}{p + 2k + 1, \frac{d_1^2 + d_2^2}{4}} \binom{0}{p + 2k + 2, \frac{d_1^2 + d_2^2}{4}}.$$

We derive

$$\frac{\partial}{\partial d_1} \left( \binom{0}{p} \left( \frac{D^2}{4} \right) \right) = \sum_{k=0}^{\infty} T_0 \left\{ \frac{2k}{d_1^2} T_1 + \frac{d_1}{2(p + 2k)} T_2 \right\},$$

$$\frac{\partial}{\partial d_2} \left( \binom{0}{p} \left( \frac{D^2}{4} \right) \right) = \sum_{k=0}^{\infty} T_0 \left\{ \frac{2k}{d_2^2} T_1 + \frac{d_2}{2(p + 2k)} T_2 \right\},$$

$$\frac{\partial}{\partial d_1} \frac{\partial}{\partial d_2} \left( \binom{0}{p} \left( \frac{D^2}{4} \right) \right) = \sum_{k=0}^{\infty} T_0 \left\{ \frac{2k}{d_1^2} \frac{2k}{d_2^2} T_1 + \frac{k (\frac{d_1}{d_2} + \frac{d_2}{d_1})}{(p + 2k)} T_2 \right\} + \frac{d_1}{2(p + 2k)} \frac{d_2}{2(p + 2k + 1)} T_3,$$

$$\frac{\partial^2}{\partial d_1^2} \left( \binom{0}{p} \left( \frac{D^2}{4} \right) \right) = \sum_{k=0}^{\infty} T_0 \left\{ \frac{2k}{d_1^2} \frac{2k - 1}{d_1} T_1 + \frac{4k + 1}{2(p + 2k)} T_2 \right\} + \frac{d_1}{2(p + 2k)} \frac{d_1}{2(p + 2k + 1)} T_3,$$

$$\frac{\partial^2}{\partial d_2^2} \left( \binom{0}{p} \left( \frac{D^2}{4} \right) \right) = \sum_{k=0}^{\infty} T_0 \left\{ \frac{2k}{d_2^2} \frac{2k - 1}{d_2} T_1 + \frac{4k + 1}{2(p + 2k)} T_2 \right\} + \frac{d_2}{2(p + 2k)} \frac{d_2}{2(p + 2k + 1)} T_3.$$

(74)

Denoting $R(d_1, d_2) = \binom{0}{p} \left( \frac{D^2}{4} \right)$, the Hessian matrix is written with the
help of set of Equations in 74 as 
\[ H = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix}, \]

where

\[ H_{11} = \frac{\partial}{\partial d_1} \left( \frac{\partial R}{\partial R} \right) = \left( \frac{\partial^2 R}{\partial R^2} \right) - \left( \frac{\partial R}{\partial R} \right)^2, \]

\[ H_{12} = \frac{\partial}{\partial d_1} \left( \frac{\partial R}{\partial d_2} \right) = \left( \frac{\partial R}{\partial d_1} \frac{\partial R}{\partial d_2} \right) - \left( \frac{\partial R}{\partial d_1} \right) \left( \frac{\partial R}{\partial d_2} \right), \]

\[ H_{21} = H_{12}, \]

\[ H_{22} = \frac{\partial}{\partial d_2} \left( \frac{\partial R}{\partial R} \right) = \left( \frac{\partial^2 R}{\partial R^2} \right) - \left( \frac{\partial R}{\partial R} \right)^2. \]

where \( R \) is used in the places of \( R(d_1, d_2) \) for brevity of symbol.

Now, the update equation for NR method is given below

\[ \begin{bmatrix} \hat{d}_{1\text{new}} \\ \hat{d}_{2\text{new}} \end{bmatrix} = \begin{bmatrix} \hat{d}_{1\text{old}} \\ \hat{d}_{2\text{old}} \end{bmatrix} - H^{-1} \begin{bmatrix} \frac{\partial R}{\partial d_1} \frac{\partial d_{1\text{old}}}{\partial d_{2\text{old}}} \\ \frac{\partial R}{\partial d_2} \frac{\partial d_{2\text{old}}}{\partial d_{2\text{old}}} \end{bmatrix}. \]

5. Experiments with simulated data

We carry out two sets of simulation to investigate the clustering framework with our proposed Bayesian mixture model. In order to evaluate the performance of our clustering method, we consider the following three criteria –

(a) identification of the correct number of clusters,

(b) correct assignment for each data point to the appropriate cluster and thus evaluate a measure of goodness for clustering using some well established metrics,

(c) accuracy in estimation of cluster specific parameters.

In order to evaluate the criterion (a), we start with two simulation scenarios where the true numbers of clusters are three and four, respectively. In each case, we have 50 individual datasets where number of data points is 400 and 500, respectively. For rest of the section we refer the these two simulation scenarios as simulation (i) and simulation (ii). In simulation (i), three parameter matrices are set

We select appropriate values of hyperparameters for prior distributions in 50 empirically using the procedure developed in Section 4.2. Note that, the value of \( K^\dagger \) is set to 20 to reflect the concentration similar to 5% of the size of the respective cluster.

In general, for MCMC procedure, choice of a good initial point expedite the convergence for practical purposes. Therefore, we use the procedure described in Section 4.6 to set the initial value of the parameters \( M, d \) and \( V \).

Optimal number of cluster is chosen based on \( DIC \) criteria described in Section 4.5. We performed numerous experiments with several score functions for
DIC (Titterington et al., 2006) apart from standard definition of DIC. We run our model with number of clusters equal to 2, 3, 4 and 5 for simulation (i) and 2, 3, 4, 5 and 6 for simulation (ii). We present a summary of our result (see Table 1) for DIC and DIC5 values, where we have shown that in almost all the cases (94% for original DIC, 95% for original DIC5) we are able to select the correct number of clusters. The computation time for DIC5 is significantly less than that of original DIC.

| Method | True number of clusters | Total number of datasets | Number of datasets with correct number of estimated clusters |
|--------|-------------------------|--------------------------|-------------------------------------------------------------|
| DIC    | 3                       | 50                       | 48                                                          |
| DIC    | 4                       | 50                       | 46                                                          |
| DIC5   | 3                       | 50                       | 47                                                          |
| DIC5   | 4                       | 50                       | 48                                                          |

*Table 1*

Number of datasets where correct number of clusters is identified with DIC and DIC5.

We notice that in simulation, whenever the model fails to identify the true number of clusters, it always overestimates the number of clusters. Realizing this, we appropriately design a penalized version of the standard DIC criterion with which we significantly improve the estimation of correct model.

**Common metrics for evaluating clustering methods** It is important to measure the assignment of each data point to the appropriate cluster. Note that, even if the number of clusters is right, the performance of the clustering method could be low because of incorrect cluster assignments. In order to evaluate clustering efficiency one could calculate several external cluster evaluation metrics. Here in this study we compute purity, Normalized mutual information (NMI), rand index (RI), adjusted rand index (ARI), Jaccard Index (JI) and F-measure (Rand, 1971; Vinh, Epps and Bailey, 2010).

We build up some notations for introducing those metric briefly. Let us assume we have N data points denoted \( \{X_j\}_{j=1}^N \). Set of \( C \) true classes is given by \( A = \{A_1, A_2, \ldots, A_C\} \) where \( A_c = \{X_j : X_j \text{ belongs to } c\text{-th cluster}\} \) for \( c = 1, 2, \ldots, C \) and clustering method returns \( K \) number of clusters and the set of clusters is given by \( B = \{B_1, B_2, \ldots, B_K\} \) where \( B_k = \{X_j : X_j \text{ assigned to } k\text{-th cluster}\} \) for \( k = 1, 2, \ldots, K \). Note that we use \( |·| \) to denote the number of elements in a set.

- Purity is defined (see Rand (1971); Vinh, Epps and Bailey (2010)) as
  \[
  \text{purity}(A, B) = \frac{\sum_k \max_c |B_k \cap A_c|}{N}.
  \]

It is the most simple evaluation measure. To compute purity each cluster is assigned to the class which is most prevalent in the cluster and the accuracy of the assignment is measured by counting the number of correctly assigned data to the cluster and dividing by total number of data in the
dataset. Clearly, Purity lies between 0 and 1 where perfect clustering has a purity of 1.

- NMI is an information-theoretic measure which is defined as

\[
\text{NMI}(A, B) = \frac{I(A, B)}{\frac{H(A) + H(B)}{2}}
\]

where, \(I(\cdot, \cdot)\) and \(H(\cdot)\) stand for mutual information and entropy, respectively with

\[
I(A, B) = \sum_k \sum_c \frac{|B_k \cap A_c|}{N} \log \frac{N |B_k \cap A_c|}{|B_k| |A_c|},
\]

and

\[
H(A) = -\sum_k \frac{|B_k|}{N} \log \frac{|B_k|}{N}; \quad H(M) = -\sum_c \frac{|A_c|}{N} \log \frac{|A_c|}{N}.
\]

NMI reaches its maximum value 1 only when the two sets \(A\) and \(B\) have a perfect one-to-one correspondence.

- RI is written as

\[
\text{RI} = \frac{TP + TN}{TP + FP + TN + FN},
\]

where TP is the number of true positives, TN is the number of true negatives, FP is the number of false positives, and FN is the number of false negatives. This can be viewed as a measure of the percentage of correct decisions. Note that, here false positives and false negatives are equally weighted. The Rand index also lies between 0 and 1. When clustering results agree with the class perfectly, the Rand index is 1.

- ARI is a chance-corrected version of RI. A problem with RI is that the expected value of the RI between two random clustering methods is not a constant. This problem is corrected in ARI which assumes the generalized hyper-geometric distribution as the model of randomness. The ARI has the maximum value 1, and its expected value is 0 in the case of random clusters. A larger ARI means a higher agreement between two clustering methods.

- JI is defined by the following formula –

\[
\text{JI} = \frac{TP}{TP + FP + FN}.
\]

It is also known as intersection over union used to quantify the similarity between two sets. It takes a value between 0 and 1. Index value 1 or 0 means two sets are identical or two sets have no common elements, respectively.

- F-measure is defined by

\[
F_\beta = \frac{(\beta^2 + 1) \cdot \text{Precision} \cdot \text{Recall}}{\beta^2 \cdot \text{Precision} + \text{Recall}},
\]
where
\[
\text{Precision} = \frac{TP}{TP + FP} \quad \text{and} \quad \text{Recall} = \frac{TP}{TP + FN}.
\]

F-measure can be used to penalize false negatives more strongly than false positives by selecting \( \beta > 1 \). On the other hand, when \( \beta = 0 \), recall has no impact on F-measure.

We summarize all the evaluation metrics for the two simulation scenarios in the following Table 2 and 3. We observe that most of the metrics are close to the maximum possible value 1, which indicates an overall success of our clustering method.

| Metrics | PUR | RI | ARI | JI | NMI | F05 | F1 | F2 | F5 |
|---------|-----|----|-----|----|-----|-----|----|----|----|
| Mean    | 0.984 | 0.979 | 0.952 | 0.938 | 0.923 | 0.968 | 0.968 | 0.968 | 0.968 |
| Std. dev. | 0.008 | 0.010 | 0.023 | 0.028 | 0.031 | 0.015 | 0.015 | 0.015 | 0.015 |

Table 2
Clustering evaluation metrics when true number of clusters equal to three

| Metrics | PUR | RI | ARI | JI | NMI | F05 | F1 | F2 | F5 |
|---------|-----|----|-----|----|-----|-----|----|----|----|
| Mean    | 0.978 | 0.978 | 0.942 | 0.918 | 0.921 | 0.957 | 0.957 | 0.957 | 0.957 |
| Std. dev. | 0.008 | 0.008 | 0.020 | 0.027 | 0.024 | 0.015 | 0.015 | 0.015 | 0.015 |

Table 3
Clustering evaluation metrics when true number of clusters equal to four

In order to evaluate parameter values for each clusters let us denote the true parameter set for \( C \) classes by \( \{F_1, F_2, \cdots, F_C\} \) where \( F_c = M_c D_c V_c^T \). We find out \( d_{MSE} = \sum_c \| \hat{F}_c - F_c \|_F \), where \( \hat{F}_c \) is the estimate of the parameter matrix for the \( c \)-th cluster, where \( \| \cdot \|_F \) denotes the matrix Frobenious norm.

We plot below (in Figure 3) the relative error (in percentage) in estimating the true parameter \( F \). From the plot we observe that procedure is efficient in estimating the parameter as the maximum relative error is below 4\%. We show the simulation results for one particular dataset from simulation (i) and (ii) for both the eigenvectors in Figures 4 and 5, respectively.

As our Bayesian inference technique involves MCMC sampling scheme, it is customary to check the standard MCMC convergence and efficiency diagnostics (Cowles and Carlin, 1996). We investigate the convergence by carefully observing the MCMC cumulative average plot and auto-correlation function (ACF) plot for one of the elements of parameter \( F \) for one of the clusters in the dataset. Here in Figure 6, we show both the plots for the simulation scenario (i). By looking at the cumulative average (Figure 6(b)) we set the value for number of burn-in iteration to 800. The small values in the ACF plot (Figure 6(a)) indicates high efficiency for parameter estimation based on the MCMC
Fig 3: Relative error (in percentage) for parameter $F$ in simulation (i) (left panel) and simulation (ii) (right panel).

samples. Note that, these plots have very similar characteristics for all the other scenarios.

6. Application

In this section we show two real data based applications with our model. The first one is associated with medical image analysis while the second one is related to astronomical data. We present each application in different subsections below.

6.1. Diffusion tensor imaging data

The human brain consists of more than 100 billion neurons, and it is arguably the most complex structure in our body (Basser and Jones, 2002; Mori and Zhang, 2006). Magnetic resonance imaging (MRI) is powerful noninvasive and three-dimensional imaging technique to characterize the entire brain anatomy. Diffusion tensor imaging (DTI) is a relatively new MRI technique which helps to reconstruct the underlying 3D structures of axonal bundles in the brain. Using a technique called tractography using the data collected by DTI the voxels that belong to the same white matter tract are grouped together. This is
Fig 4: First and second eigenvectors using one of the datasets in simulation (i).

Fig 5: First and second eigenvectors using one of the datasets in simulation (ii).
used to investigate brain connectivity, for example, cortex-white matter connectivity (Catani et al., 2002; Lazar and Alexander, 2005) or corticothalamic connectivity (Guy M Mckhann, 2004).

DTI technique was introduced in the mid 1990s (Basser, Mattiello and LeBihan, 1994). The diffusion term represents translational motion of water molecules and this motions is used as a probe to estimate the axonal organization of the brain. The water molecules move relatively easily along the axonal bundles compared to the perpendicular to these bundles because there are fewer obstacles to prevent movement along the fibers which carry rich anatomical information about the white matter (Mori and Zhang, 2006). Fiber orientations are estimated from three independent diffusion measurements along the $x$, $y$ and $z$ axes. However, these three measurements are not enough as the fiber orientation is not always along one of these three axes. But to accurately construct apparent diffusion coefficient where the intensity of each voxel is proportional to the extent of diffusion, we need to measure diffusion along many directions, which is difficult. In order to give a practical solution to this, the concept of DT was introduced (Basser, Mattiello and LeBihan, 1994).

In this model, measurements along different axes (see Figure 7a) are fitted to a 3D ellipsoid shown in Figure 7b, which represents average diffusion distance in each direction (Mori and Zhang, 2006). Note that the properties of a 3D ellipsoid can be defined by six parameters – three of its eigenvalues and corresponding eigenvectors (mutually perpendicular), which can compactly represented by a $3 \times 3$ symmetric, positive-definite matrix (SPD) and this is known as DT. In anisotropic fibrous tissues the major eigenvector also defines the fiber tract axis of the tissue. The three positive eigenvalues of DT ($\lambda_1, \lambda_2$ and $\lambda_3$) give the diffusivity in the direction of each eigenvector, denoted by $E_1, E_2$ and $E_3$ in Figure 7c.
According to our knowledge, this is the very first work with DTI data which is modeled with a mixture of $\mathcal{M}\mathcal{L}$ distributions. Also, we consider a final dataset after selecting the voxels in the white matter region of the brain containing information from almost 63,000 voxels. Our implementation is very efficient in handling this large amount of data. We model diffusion tensors by elements in $\mathcal{V}_{n,p}$. Note that, for the scope of this project we are only interested in the direction of the eigenvectors of DT. Also, we only need to model $E_1$ and $E_2$ as direction of $E_3$ will be totally governed by the rest of the two eigenvectors. Therefore, we have two orthonormal eigenvectors in three dimensions i.e. a $3 \times 2$ matrix which has two orthonormal vectors as columns - this is precisely the space of $3 \times 2$ orthonormal matrices i.e. $\mathcal{V}_{n,p}$.

In practice, Wishart distribution is commonly used to analyze DT, a $3 \times 3$ positive definite matrix. It could be argued that one can use a mixture of Wishart distributions directly on the space of SPD matrices. However, note that, in the case of Wishart distribution the sense of directionality is difficult to comprehend. The directional aspect of eigenvectors from DTI data can be therefore better suited to model by using a mixture of $\mathcal{M}\mathcal{L}$ distributions. It is easier to find interpretations of the parameters for $\mathcal{M}\mathcal{L}$ distribution in terms of direction of the data. Therefore our Bayesian mixture model is relatively more flexible in terms of handling DTI data which have directional components. Also our inference mechanism can handle a very large number of DTI data from each voxels. To the extent of our knowledge, this is the first paper that develops the
Before presenting the results, we would like to point out that our results could be improved by incorporating eigenvalues along with the eigenvectors. However, that requires more complicated statistical model which we currently reserve for our future work and it is outside of the scope of current paper as we mainly focusing on building the appropriate framework for analyzing DTI data. Nevertheless, we show in in Section 6.1.2 that we have found evidences of meaningful clusters by only investigating the directional part of the data.

### 6.1.1. Data source and pre-processing

The Philadelphia Neurodevelopmental Cohort (PNC) is a large-scale initiative to understand how genetics impact trajectories of brain development and cognitive functioning in adolescence, and understand how abnormal trajectories of development are associated with psychiatric symptomatology (Satterthwaite et al., 2014). As part of the PNC, 1,445 children ages 8-21 received multi-modal neuroimaging in order to evaluate with a detailed cognitive and psychiatric assessment. Data is pre-processed with the comprehensive DTI data processing software library FSL (Woolrich et al., 2009).

Some of the important features of this dataset is that all imaging data was acquired at a single site, on a single scanner, in a short period of time that did not span any software or hardware upgrades. Quality of the images of the DTI data was primarily assessed by visual inspection and rarely, two artifacts were noted in the DTI data (Satterthwaite et al., 2014).

### 6.1.2. Results

We take one anonymous subject from this dataset consisting of 62,667 measurements. We use a finite mixture of $\mathcal{M}\mathcal{L}$ distributions to cluster this large dataset.

We use conditional conjugate prior distributions defined in Equation 50. We select appropriate values of hyperparameters using the procedure developed for empirical prior in Section 4.2. Note that, the value of $K^\dagger$ is set to 100 as we expect relatively large number of data points in each cluster. Here we use the procedure described in Section 4.6 to set the initial value of the parameters $M$, $d$ and $V$ for the MCMC algorithm. First 1000 MCMC samples are discarded as burn-in samples.

We use different number of clusters to fit the dataset with our Bayesian model and choose 12 as the estimated number of clusters by DIC criterion described in Section 4.5.

In Figure 8 we present the top three clusters with their voxel locations mapped inside the anatomical structure of brain (see [http://www.compgenome.org/stiefel](http://www.compgenome.org/stiefel) for 3D version of these figures). Note that in this figure, panel (a), (b) and (c) represent top, side and front view, respectively. It is important to notice that we are successfully able to locate few important fiber structures in the dataset from the sample.
Fig 8: DTI clustering results for three major clusters
6.2. Near Earth comet dataset

The Near Earth Object (NEO) population is defined as a group of small bodies with perihelion distance less than 1.3 astronomical unit (AU) and aphelion distance greater than 0.983 AU (Donnison, 2006). NEOs are NEAs (near-Earth asteroids) and NECs (near-Earth comets). NEAs are asteroids whose perihelion distance is less than 1.3 AU. NECs are comets whose perihelion distance is less than 1.3 AU and whose orbital period is less than 200 years (https://cneos.jpl.nasa.gov/faq/). A detailed categorization of NEO can also be found in https://cneos.jpl.nasa.gov/about/neo_groups.html. They are also called short-period (SP) comets, which are generally confined to direct orbits with angle of inclination with respect to a reference plane, less than approximately 35°. The SP comets are in well determined orbits with modest eccentricities and inclinations. This make them a possible resource for space developments (Lewis, Matthews and Guerrieri, 1993).

The NEC dataset was built by the Near Earth Object Program of the National Aeronautics and Space Administration (NASA). Each data point characterizes the orientation of a two-dimensional elliptical orbit in three-dimensional space, and thus lies on the Stiefel manifold $V_{3,2}$. For our experiment we have downloaded NEC dataset containing 175 entries. Orientation of SP comet’s orbit can be specified by the following quantities. We could find the definition of these three important quantities in https://ssd.jpl.nasa.gov/?glossary.

- Celestial longitude ($L$)
- Latitude of the perihelion ($\theta$)
- Longitude of the ascending node ($\Omega$)

Celestial longitude of the comet ($L$) (Hughes, 1985) and latitude of the perihelion ($\theta$) (Yabushita, Hasegawa and Kobayashi, 1979) are computed by the following formula, respectively.

$$L = \Omega + \tan^{-1}\left(\frac{\sin \omega \cos i}{\cos \omega}\right)$$

$$\sin \theta = \sin i \sin \omega$$

From the dataset we could find the values of orbital inclination ($i$), longitude of the ascending node ($\Omega$), argument of periapsis (perihelion)($\omega$) as shown in Figure 9 Using the appropriate transformations given in Jupp and Mardia (1979); Yabushita, Hasegawa and Kobayashi (1979) we find $L$, $\theta$, and $\Omega$ for each comet. The direction of the perihelion is $\mathbf{x}_1 = (\cos \theta \cos L, \cos \theta \sin L, \sin \theta)$ and the directed unit normal to the orbit given by the right hand rule is

$$\mathbf{x}_2 = (\sin \theta \sin \Omega - \sin \theta \cos \Omega - \cos \theta \sin (\Omega - L)) / r$$

where $r^2 = \sin^2 \theta + \cos^2 \theta \sin^2 (\Omega - L)$. The orientation of the orbit therefore can be represented by the matrix $X \in V_{3,2}$ given by $X = [\mathbf{x}_1^T \mathbf{x}_2^T]$. An appropriate model for the distribution of these matrices is the $ML$ family (Jupp and Mardia, 1979).
Here we model NEC dataset as a finite mixture of $\mathcal{M}_L$ distributions. We ran our model for number of clusters equals to 3, 4, 5, 6. In each situation we use 2000 MCMC samples out of which we set initial 1000 iterations as burn-ins. We select appropriate values of hyperparameters for prior distributions in Equation 50 empirically using the procedure developed in Section 4.2. We choose number of burn-in iterations (1000 in this case) by observing the MCMC convergence diagnostic plot. Below we report the DIC for selecting the model. Our DIC (shown in Table 4) is minimized at number of clusters equals to four. Note that, also from the reported results in Lin, Rao and Dunson (2017), four seems to be the most likely number of clusters.

| Number of Clusters | DIC Value |
|--------------------|-----------|
| 3                  | 3074.91   |
| 4                  | 2607.04   |
| 5                  | 2712.96   |
| 6                  | 2685.94   |

**Table 4**

DIC table for NEC dataset

We compute the probabilities for any two NEC data to belong to the same cluster for all the NEC data. This is also called as cluster co-occurrence probability matrix (Hofmann and Puzicha, 1998). We draw the corresponding heatmap in Figure 10 to show this.

Finally, we plot each eigenvector from a data point of $V_{3,2}$ in a sphere (Figure 11 and 12). We use different color (red, blue, green, black) to represent four different clusters. The NECs denoted by the points with same color indicates the group of comets with similar orbital characteristics.
7. Discussions and Future directions

In this paper, we build a Bayesian framework for a mixture of \( \mathcal{MC} \) distributions which could be applied to real world directional data. We construct two special families of distributions to be used as prior distributions following the original conjugate prior construction in Diaconis and Ylvisaker (1979). We discuss few important properties for our prior class of distributions. For the mixture model we computed the posterior and also give insights on selection of hyperparameters, which should be helpful for practitioners. Finally, we are able to handle a large amount of DTI data in the real data application and results look quite promising.

For our future extension, instead of selecting the number of clusters by DIC criterion, we would like the number of clusters to be a random variable. A fully Bayesian model-based approach which assumes a parametric prior (e.g. Poisson) on the number of clusters, could be employed. The next natural step in this direction is to extend the existing model to a non-parametric framework. In fact, non-parametric version is more flexible in terms of modeling and experimenting with different types of underlying clustering structure. Note that, though Lin, Rao and Dunson (2017) opened the doors to such modeling, their model space
differs from ours in various respects.

On a separate direction, we also plan to explore in depth the analytical properties of the hypergeometric function of matrix argument function \( _pF_1(\cdot) \) for \( p \geq 2 \). Direct computation, as is done in our case studies, could create bottlenecks for data coming from higher dimension. Analytical bounds could help either in approximation or designing a good MCMC sampler. For example, one could borrow the importance sampling approach used for evaluating the normalizing constants in Mitra et al. (2013). This would primarily rely on the ability to simulate efficiently from \( \mathcal{M} \mathcal{L} \) distributions, which is already ensured by Hoff (2009). Along this line, it would be nice to study the theoretical properties, particularly ergodicity of the MCMC schemes rigorously.

The coming together of state-of-the-art Bayesian methods incorporating topological properties of the space is a rich area that has been initiated only recently by Bhattacharya and Dunson (2012) and Lin, Rao and Dunson (2017). We plan to continue along this direction and contribute to the Bayesian methodolog-
Fig 12: Second eigenvector of a data point is embedded in a sphere.

cal development on general analytic manifolds, which would be appropriate to analyze large-scale data with complex structure.

References

Absil, P.-A., Mahony, R. and Sepulchre, R. (2009). *Optimization algorithms on matrix manifolds*. Princeton University Press.

Anand, S., Mittal, S. and Meer, P. (2016). Robust Estimation for Computer Vision Using Grassmann Manifolds. In *Riemannian Computing in Computer Vision* 125–144. Springer.

Bangert, M., Hennig, P. and Oelfke, U. (2010). Using an infinite von Mises-Fisher mixture model to cluster treatment beam directions in external radiation therapy. In *Machine Learning and Applications (ICMLA), 2010 Ninth International Conference* on 746–751. IEEE.

Basser, P. J. and Jones, D. K. (2002). Diffusion-tensor MRI: theory, experimental design and data analysis—a technical review. *NMR in Biomedicine* 15 456–467.
Basser, P. J., Mattiello, J. and LeBihan, D. (1994). MR diffusion tensor spectroscopy and imaging. *Biophysical journal* **66** 259–267.

Berg, A., Meyer, R. and Yu, J. (2004). Deviance information criterion for comparing stochastic volatility models. *Journal of Business & Economic Statistics* **22** 107–120.

Bhatia, R. (2007). Positive Definite Matrices. Princeton University Press, *Princeton and Oxford*.

Bhattacharya, A. and Dunson, D. B. (2012). Strong consistency of nonparametric Bayes density estimation on compact metric spaces with applications to specific manifolds. *Annals of the Institute of Statistical Mathematics* **64** 687–714.

Bishop, C. M. (2006). *Pattern recognition and machine learning*. Springer.

Butler, R. W. and Wood, A. T. (2003). Laplace approximation for Bessel functions of matrix argument. *Journal of Computational and Applied Mathematics* **155** 359–382.

Casella, G. (1985). An introduction to empirical Bayes data analysis. *The American Statistician* **39** 83–87.

Casella, G. and Berger, R. L. (2002). *Statistical inference*. Duxbury Pacific Grove, CA.

Catani, M., Howard, R. J., Pajevic, S. and Jones, D. K. (2002). Virtual in vivo interactive dissection of white matter fasciculi in the human brain. *Neuroimage* **17** 77–94.

Chikuse, Y. (1991a). High dimensional limit theorems and matrix decompositions on the Stiefel manifold. *Journal of multivariate analysis* **36** 145–162.

Chikuse, Y. (1991b). Asymptotic expansions for distributions of the large sample matrix resultant and related statistics on the Stiefel manifold. *Journal of multivariate analysis* **39** 270–283.

Chikuse, Y. (1998). Density estimation on the Stiefel manifold. *Journal of multivariate analysis* **66** 188–206.

Chikuse, Y. (2012). *Statistics on special manifolds*. 174. Springer Science & Business Media.

Conway, J. (1990). A *Course in Functional Analysis*. Springer Verlag, New York.

Cowles, M. K. and Carlin, B. P. (1996). Markov chain Monte Carlo convergence diagnostics: a comparative review. *Journal of the American Statistical Association* **91** 883–904.

DeIorio, M. and Robert, C. P. (2002). Discussion of Bayesian measures of model complexity and fit. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* **64** 629–630.

Dempster, A. P., Laird, N. M. and Rubin, D. B. (1977). Maximum likelihood from incomplete data via the EM algorithm. *Journal of the royal statistical society. Series B (methodological)* **1**–38.

Diaconis, P. and Ylvisaker, D. (1979). Conjugate priors for exponential families. *The Annals of statistics* **7** 269–281.

Diebolt, J. and Robert, C. P. (1994). Estimation of Finite Mixture Distributions through Bayesian Sampling. *Journal of the Royal Statistical Society. Series B (Methodological)* **56** 363-375.
DONNISON, J. (2006). Some aspects of the statistics of Near-Earth Objects. *Proceedings of the International Astronomical Union* 2 69–76.

DOWNS, T. D. (1972). Orientation statistics. *Biometrika* 665–676.

EDELMAN, A., ARIAS, T. A. and SMITH, S. T. (1998). The geometry of algorithms with orthogonality constraints. *SIAM journal on Matrix Analysis and Applications* 20 303–353.

FRANÇOIS, O. and LAVAL, G. (2011). Deviance information criteria for model selection in approximate Bayesian computation. *arXiv preprint arXiv:1105.0269*.

GELMAN, A., CARLIN, J. B., STERN, H. S. and RUBIN, D. B. (2003). *Bayesian Data Analysis, Second Edition* (Chapman & Hall/CRC Texts in Statistical Science), 2 ed. Chapman and Hall/CRC.

GELMAN, A., CARLIN, J. B., STERN, H. S., DUNSON, D. B., VEHTARI, A. and RUBIN, D. B. (2014). *Bayesian data analysis* 2. CRC press Boca Raton, FL.

GROSS, K. I. and RICHARDS, D. S. P. (1987). Special functions of matrix argument. I. Algebraic induction, zonal polynomials, and hypergeometric functions. *Transactions of the American Mathematical Society* 301 781–811.

GROSS, K. I. and RICHARDS, D. S. P. (1989). Total positivity, spherical series, and hypergeometric functions of matrix argument. *Journal of Approximation theory* 59 224–246.

GUPTA, R. D. and RICHARDS, D. S. P. (1985). Hypergeometric functions of scalar matrix argument are expressible in terms of classical hypergeometric functions. *SIAM journal on mathematical analysis* 16 852–858.

GUY M MCKHANN, I. (2004). Non-invasive mapping of connections between human thalamus and cortex using diffusion imaging. *Neurosurgery* 54.

HARDY, G. H., LITTLEWOOD, J. E. and PÓLYA, G. (1952). *Inequalities*. Cambridge university press.

HERZ, C. S. (1955). Bessel functions of matrix argument. *Annals of Mathematics* 474–523.

HILL, R. D. and WATERS, S. R. (1987). On the cone of positive semidefinite matrices. *Linear Algebra and its Applications* 90 81–88.

HOFF, P. D. (2009). Simulation of the matrix Bingham–von Mises–Fisher distribution, with applications to multivariate and relational data. *Journal of Computational and Graphical Statistics* 18 438–456.

HOFMANN, T. and PUZICHA, J. (1998). Statistical models for co-occurrence data.

HORN, K. and GRÜN, B. (2013). On conjugate families and Jeffreys priors for von Mises-Fisher distributions. *J Stat Plan Inference* 143 992–999.

HORN, K. and GRÜN, B. (2014). movMF: An R package for fitting mixtures of von Mises-Fisher distributions. *Journal of Statistical Software* 58 1–31.

HUGHES, D. W. (1985). The position of earth at previous apparitions of Halley’s comet. *Quarterly Journal of the Royal Astronomical Society* 26 513–520.

JAMES, A. T. (1964). Distributions of matrix variates and latent roots derived from normal samples. *The Annals of Mathematical Statistics* 475–501.

JAMES, I. M. (1976). *The topology of Stiefel manifolds* 24. Cambridge Univer-
sity Press.

Jupp, P. E. and Mardia, K. V. (1979). Maximum likelihood estimators for the matrix von Mises-Fisher and Bingham distributions. The Annals of Statistics 599–606.

Jupp, P. and Mardia, K. (1980). A general correlation coefficient for directional data and related regression problems. Biometrika 163–173.

KaewTraKulPong, P. and Bowden, R. (2002). An improved adaptive background mixture model for real-time tracking with shadow detection. Video-based surveillance systems 1 135–144.

Khare, K., Pal, S. and Su, Z. (2017). A Bayesian approach for envelope models. The Annals of Statistics 45 196–222.

Khatri, C. and Mardia, K. (1977). The von Mises–Fisher matrix distribution in orientation statistics. Journal of the Royal Statistical Society. Series B (Methodological) 95–106.

Koev, P. and Edelman, A. (2006). The efficient evaluation of the hypergeometric function of a matrix argument. Mathematics of Computation 75 833–846.

Kristof, W. (1969). A theorem on the trace of certain matrix products and some applications. ETS Research Report Series 1969.

Lattin, J. M., Carroll, J. D. and Green, P. E. (2003). Analyzing multivariate data. Thomson Brooks/Cole Pacific Grove, CA.

Lazar, M. and Alexander, A. L. (2005). Bootstrap white matter tractography (BOOT-TRAC). NeuroImage 24 524–532.

Lewicki, M. S. (1998). A review of methods for spike sorting: the detection and classification of neural action potentials. Network: Computation in Neural Systems 9 R53–R78.

Lewis, J. S., Matthews, M. S. and Guerrieri, M. L. (1993). Resources of near-Earth space. Resources of near-earth space.

Lin, L., Rao, V. and Dunson, D. (2017). BAYESIAN NONPARAMETRIC INFERENCE ON THE STIEFEL MANIFOLD. Statistica Sinica 27 535–553.

Lui, Y. M. (2012). Advances in matrix manifolds for computer vision. Image and Vision Computing 30 380–388.

Lui, Y. and Beveridge, J. (2008). Grassmann registration manifolds for face recognition. Computer Vision–ECCV 2008 44–57.

Mardia, K. V. and Jupp, P. E. (2009). Directional statistics 494. John Wiley & Sons.

Mardia, K. and Khatri, C. (1977). Uniform distribution on a Stiefel manifold. Journal of Multivariate Analysis 7 468–473.

Mardia, K. V., Taylor, C. C. and Subramaniam, G. K. (2007). Protein bioinformatics and mixtures of bivariate von Mises distributions for angular data. Biometrics 63 505–512.

McGraw, T., Vemuri, B., Yezierski, R. and Mareci, T. (2006). Segmentation of high angular resolution diffusion MRI modeled as a field of von Mises-Fisher mixtures. In European Conference on Computer Vision 463–475. Springer.

McKenna, S. J., Raja, Y. and Gong, S. (1999). Tracking colour objects
using adaptive mixture models. Image and vision computing 17 225–231.
MCLACHLAN, G. and PEEL, D. (2004). Finite mixture models. John Wiley & Sons.
Mitra, R., Müller, P., Liang, S., Yue, L. and Ji, Y. (2013). A bayesian graphical model for chip-seq data on histone modifications. Journal of the American Statistical Association 108 69–80.
Mori, S. and Zhang, J. (2006). Principles of diffusion tensor imaging and its applications to basic neuroscience research. Neuron 51 527–539.
Muirhead, R. J. (1975). Expressions for some hypergeometric functions of matrix argument with applications. Journal of multivariate analysis 5 283–293.
Muirhead, R. J. (2009). Aspects of multivariate statistical theory 197. John Wiley & Sons.
Picard, F. (2007). An introduction to mixture models. Statistics for Systems Biology, Research Report 7.
Rand, W. M. (1971). Objective criteria for the evaluation of clustering methods. Journal of the American Statistical association 66 846–850.
Reisinger, J., Waters, A., Silverthorn, B. and Mooney, R. J. (2010). Spherical topic models. In Proceedings of the 27th international conference on machine learning (ICML-10) 903–910.
Robbins, H. (1985). An empirical Bayes approach to statistics. In Herbert Robbins Selected Papers 41–47. Springer.
Rokach, L. and Maimon, O. (2005). The Data Mining and Knowledge Discovery Handbook: A Complete Guide for Researchers and Practitioners.
Rudin, W. et al. (1964). Principles of mathematical analysis 3. McGraw-Hill New York.
Satterthwaite, T. D., Elliott, M. A., Ruparel, K., Loughead, J., Prabhakaran, K., Calkins, M. E., Hopson, R., Jackson, C., Keeffe, J., Riley, M. et al. (2014). Neuroimaging of the Philadelphia neurodevelopmental cohort. Neuroimage 86 544–553.
Schwartz, L. (1965). On bayes procedures. Probability Theory and Related Fields 4 10–26.
Schwartzman, A. (2006). Random ellipsoids and false discovery rates: Statistics for diffusion tensor imaging data PhD thesis, Stanford University.
Spiegelhalter, D. J., Best, N. G., Carlin, B. P. and Van Der Linde, A. (2002). Bayesian measures of model complexity and fit. Journal of the Royal Statistical Society: Series B (Statistical Methodology) 64 583–639.
Stauffer, C. and Grimson, W. E. L. (1999). Adaptive background mixture models for real-time tracking. In Computer Vision and Pattern Recognition, 1999. IEEE Computer Society Conference on. 2 246–252. IEEE.
Tang, H., Chu, S. M. and Huang, T. S. (2009). Generative model-based speaker clustering via mixture of von mises-fisher distributions. In Acoustics, Speech and Signal Processing, 2009. ICASSP 2009. IEEE International Conference on 4101–4104. IEEE.
Titterington, D. M., Robert, C. P., Forbes, F. and Celeux, G. (2006). Deviance information criteria for missing data models. Bayesian Analysis 1
651–673.

Turaga, P., Veeraraghavan, A. and Chellappa, R. (2008). Statistical analysis on Stiefel and Grassmann manifolds with applications in computer vision. In Computer Vision and Pattern Recognition, 2008. CVPR 2008. IEEE Conference on 1–8. IEEE.

Turaga, P., Veeraraghavan, A., Srivastava, A. and Chellappa, R. (2011). Statistical computations on Grassmann and Stiefel manifolds for image and video-based recognition. IEEE Transactions on Pattern Analysis and Machine Intelligence 33 2273–2286.

Vinh, N. X., Epps, J. and Bailey, J. (2010). Information theoretic measures for clusterings comparison: Variants, properties, normalization and correction for chance. Journal of Machine Learning Research 11 2837–2854.

Wood, E., Fellows, M., Donoghue, J. and Black, M. (2004). Automatic spike sorting for neural decoding. In Engineering in Medicine and Biology Society, 2004. IEMBS’04. 26th Annual International Conference of the IEEE 2 4009–4012. IEEE.

Woolrich, M. W., Jbabdi, S., Patenaude, B., Chappell, M., Makni, S., Behrens, T., Beckmann, C., Jenkinson, M. and Smith, S. M. (2009). Bayesian analysis of neuroimaging data in FSL. Neuroimage 45 S173–S186.

Wright, S. J. and Nocedal, J. (1999). Numerical optimization. Springer Science 35 7.

Yabushita, S., Hasegawa, I. and Kobayashi, K. (1979). The Distributions of Inclination and Perihelion Latitude of Long-Period Comets and Their Dynamical Implications. Publications of the Astronomical Society of Japan 31 801.

Zeng, X., Bian, W., Liu, W., Shen, J. and Tao, D. (2015). Dictionary pair learning on Grassmann manifolds for image denoising. IEEE Transactions on Image Processing 24 4556–4569.