Minimum message length estimation of mixtures of multivariate Gaussian and von Mises-Fisher distributions

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Abstract  Mixture modelling involves explaining some observed evidence using a combination of probability distributions. The crux of the problem is the inference of an optimal number of mixture components and their corresponding parameters. This paper discusses unsupervised learning of mixture models using the Bayesian Minimum Message Length (MML) criterion. To demonstrate the effectiveness of search and inference of mixture parameters using the proposed approach, we select two key probability distributions, each handling fundamentally different types of data: the multivariate Gaussian distribution to address mixture modelling of data distributed in Euclidean space, and the multivariate von Mises-Fisher (vMF) distribution to address mixture modelling of directional data distributed on a unit hypersphere. The key contributions of this paper, in addition to the general search and inference methodology, include the derivation of MML expressions for encoding the data using multivariate Gaussian and von Mises-Fisher distributions, and the analytical derivation of the MML estimates of the parameters of the two distributions. Our approach is tested on simulated and real world data sets. For instance, we infer vMF mixtures that concisely explain experimentally determined three-dimensional protein conformations, providing an effective null model description of protein structures that is central to many inference problems in structural bioinformatics. The experimental results demonstrate that the performance of our proposed search and inference method along with the encoding schemes improve on the state of the art mixture modelling techniques.

Keywords  mixture modelling · minimum message length · multivariate Gaussian · von Mises-Fisher · directional data

1 Introduction

Mixture models are common tools in statistical pattern recognition (McLachlan and Basford, 1988). They offer a mathematical basis to explain data in fields as diverse as astronomy, biology, ecology, engineering, and economics, amongst many others (McLachlan and Peel, 2000). A mixture model is composed of component probabilistic models; a component may variously correspond to a subtype, kind, species, or subpopulation of the observed data. These models aid in the identification of hidden patterns in the data through sound probabilistic formalisms. Mixture models have been extensively used in machine learning tasks such as classification and unsupervised learning (Titterington et al., 1985; McLachlan and Peel, 2000; Jain et al., 2000).

Formally, mixture modelling involves representing a distribution of data as a weighted sum of individual probability distributions. Specifically, the problem we consider here is to model the observed data using a mixture $\mathcal{M}$ of probability distributions of the form:

$$\Pr(x; \mathcal{M}) = \sum_{j=1}^{M} w_j f_j(x; \Theta_j)$$  (1)

where $x$ is a $d$-dimensional datum, $M$ is the number of mixture components, $w_j$ and $f_j(x; \Theta_j)$ are the weight and probability density of the $j^{th}$ component respectively; the weights are positive and sum to one.

The problem of modelling some observed data using a mixture distribution involves determining the number of components, $M$, and estimating the mixture parameters. Inferring the optimal number of mixture components involves the difficult

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problem of balancing the trade-off between two conflicting objectives: low hypothesis complexity as determined by the number of components and their respective parameters, versus good quality of fit to the observed data. Generally a hypothesis with more free parameters can fit observed data better than a hypothesis with fewer free parameters. A number of strategies have been used to control this balance as discussed in Section 7. These methods provide varied formulations to assess the mixture components and their ability to explain the data. Methods using the minimum message length criterion (Wallace and Boulton, 1968), a Bayesian method of inductive inference, have been proved to be effective in achieving a reliable balance between these conflicting aims (Wallace and Boulton, 1968; Oliver et al., 1996; Roberts et al., 1998; Figueiredo and Jain, 2002).

Although much of the literature concerns the theory and application of Gaussian mixtures (McLachlan and Peel, 2000; Jain and Dubes, 1988), mixture modelling using other probability distributions has been widely used. Some examples are: Poisson models (Wang et al., 1996; Wedel et al., 1993), exponential mixtures (Seidel et al., 2000), Laplace (Jones and McLachlan, 1990), t-distribution (Peel and McLachlan, 2000), Weibull (Patra and Dey, 1999), Kent (Peel et al., 2001), von Mises-Fisher (Banerjee et al., 2005), and many more. McLachlan and Peel (2000) provide a comprehensive summary of finite mixture models and their variations. The use of Gaussian mixtures in several research disciplines has been partly motivated by its computational tractability (McLachlan and Peel, 2000). For datasets where the direction of the constituent vectors is important, Gaussian mixtures are inappropriate and distributions such as the von Mises-Fisher may be used (Banerjee et al., 2005; Mardia et al., 1979). In any case, whatever the kind of distribution used for an individual component, one needs to estimate the parameters of the mixture, and provide a sound justification for selecting the appropriate number of mixture components.

Software for mixture modelling relies on the following elements:

1. An estimator of the parameters of each component of a mixture,
2. An objective function, that is a cost or score, that can be used to compare two hypothetical mixtures and decide which is better, and
3. A search strategy for the best number of components and their weights.

Traditionally, parameter estimation is done by strategies such as maximum likelihood (ML) or Bayesian maximum a posteriori probability (MAP) estimation. In this work, we use the Bayesian minimum message length (MML) principle. Unlike MAP, MML estimators are invariant under non-linear transformations of the data (Oliver and Baxter, 1994), and unlike ML, MML considers the number and precision of a model’s parameters. It has been used in the inference of several probability distributions (Wallace, 2005). MML-based inference operates by considering the problem as encoding first the parameter estimates and then the data given those estimates. The parameter values that result in the least overall message length to explain the whole data are taken as the MML estimates for an inference problem. The MML scheme thus incorporates the cost of stating parameters into model selection. It is self evident that a continuous parameter value can only be stated to some finite precision; the cost of encoding a parameter is determined by its prior and the precision. ML estimation ignores the cost of stating a parameter and MAP based estimation uses the probability density of a parameter instead of its probability measure. In contrast, the MML inference process calculates the optimal precision to which parameters should be stated and a probability value of the corresponding parameters is then computed. This is used in the computation of the message length corresponding to the parameter estimates. Thus, models with varying parameters are evaluated based on their resultant total message lengths. We use this characteristic property of MML to evaluate mixtures containing different numbers of components.

Although there have been several attempts to address the challenges of mixture modelling, the existing methods are shown to have some limitations in their formalisms (see Section 7). In particular, some methods based on MLE are incomplete in their formulation. We aim to rectify these drawbacks by proposing a comprehensive MML formulation and develop a search heuristic that selects the number of mixture components based on the proposed formulation. To demonstrate the effectiveness of the proposed search and parameter estimation, we first consider modelling problems using Gaussian mixtures and extend the work to include relevant discussion on mixture modelling of directional data using von Mises-Fisher distributions.

The importance of Gaussian mixtures in practical applications is well established. For a given number of components, the conventional method of estimating the parameters of a mixture relies on the expectation-maximization (EM) algorithm (Dempster et al., 1977). The standard EM is a local optimization method, is sensitive to initialization, and in certain cases may converge to the boundary of parameter space (Krishnan and McLachlan, 1997; Figueiredo and Jain, 2002). Previous attempts to infer Gaussian mixtures based on the MML framework have been undertaken using simplifying assumptions, such as the covariance matrices being diagonal (Oliver et al., 1996), or coarsely approximating the probabilities of mixture parameters (Roberts et al., 1998; Figueiredo and Jain, 2002). Further, the search heuristic adopted in some of these methods is to run the EM several times for different numbers of components, \( M \), and select the \( M \) with the best EM outcome (Oliver et al., 1996; Roberts et al., 1998; Biernacki et al., 2000). A search method based on iteratively deleting components has been proposed by Figueiredo and Jain (2002). It begins by assuming a very large number of components and selectively eliminates components deemed redundant; there is no provision for recovering from deleting a component in error.

In this work, we propose a search method which selectively splits, deletes, or merges components depending on improvement to the MML objective function. The operations, combined with EM steps, result in a sensible redistribution of
data between the mixture components. As an example, a component may be split into two children, and at a later stage, one of the children may be merged with another component. Unlike the method of Figueiredo and Jain (2002), our method starts with a one-component mixture and alters the number of components in subsequent iterations. This avoids the overhead of dealing with a large number of components unless required.

The proposed search heuristic can be used with probability distributions for which the MML expressions to calculate message lengths for estimates and for data given those estimates are known. As an instance of this, Section 8 discusses modelling directional data using the von Mises-Fisher distributions. Directional statistics have garnered support recently in real data mining problems where the direction, not magnitude, of vectors is significant. Examples of such scenarios are found in earth sciences, meteorology, physics, biology, and other fields (Mardia and Jupp, 2000). The statistical properties of directional data have been studied using several types of distributions (Fisher, 1953; Watson and Williams, 1956; Fisher, 1993; Mardia and Jupp, 2000), often described on surfaces of compact manifolds, such as the sphere, ellipsoid, torus etc. The most fundamental of these is the von Mises-Fisher (vMF) distribution which is analogous to a symmetric multivariate Gaussian distribution, wrapped around a unit hypersphere (Watson and Williams, 1956). The probability density function of a vMF distribution with parameters $\Theta = (\mu, \kappa) \equiv (\text{mean direction, concentration parameter})$ for a random unit vector $x \in \mathbb{R}^d$ on a $(d - 1)$-dimensional hypersphere $S^{d-1}$ is given by:

$$f(x; \mu, \kappa) = C_d(\kappa) e^{\mu^T x} \tag{2}$$

where $C_d(\kappa) = \frac{\kappa^{d/2 - 1}}{(2\pi)^{d/2} I_{d/2 - 1}(\kappa)}$ is the normalization constant and $I_v$ is a modified Bessel function of the first kind and order $v$.

The estimation of the parameters of the vMF distribution is often done using maximum likelihood. However, the complex nature of the mathematical form presents difficulty in estimating the concentration parameter $\kappa$. This has lead to researchers using many different approximations, as discussed in Section 3. Most of these methods perform well when the amount of data is large. At smaller sample sizes, they result in inaccurate estimates of $\kappa$, and are thus unreliable. We demonstrate this by the experiments conducted on a range of sample sizes. The problem is particularly evident when the dimensionality of the data is large, also affecting the application in which it is used, such as mixture modelling. We aim to rectify this issue by using MML estimates for $\kappa$. Our experiments section demonstrates that the MML estimate of $\kappa$ provides a more reliable answer and is an improvement on the current state of the art. These MML estimates are subsequently used in mixture modelling of vMF distributions (see Sections 8 and 11).

Previous studies have established the importance of von Mises circular (two-dimensional) and von Mises-Fisher (three-dimensional and higher) mixtures, and demonstrated applications to clustering of protein dihedral angles (Mardia et al., 2007; Dowe et al., 1996a), large-scale text clustering (Banerjee et al., 2003), and gene expression analyses (Banerjee et al., 2005). The merit of using cosine based similarity metrics, which are closely related to the vMF, for clustering high-dimensional text data has been investigated in Strehl et al. (2000). For text clustering, there is evidence that vMF mixture models have a superior performance compared to other statistical distributions such as normal, multinomial, and Bernoulli (Salton and Buckley, 1988; Salton and McGill, 1986; Zhong and Ghosh, 2003; Banerjee et al., 2005). movMF is a widely used package to perform clustering using vMF distributions (Hornik and Grün, 2013).

**Contributions:** The main contributions of this paper are as follows:

- We derive the analytical estimates of the parameters of a multivariate Gaussian distribution with full covariance matrix, using the MML principle (Wallace and Freeman, 1987).
- We derive the expression to infer the concentration parameter $\kappa$ of a generic $d$-dimensional vMF distribution using MML-based estimation. We demonstrate, through a series of experiments, that this estimate outperforms the previous ones, therefore making it a reliable candidate to be used in mixture modelling.
- A generalized MML-based search heuristic is proposed to infer the optimal number of mixture components that would best explain the observed data; it is based on the search used in various versions of the ‘Snob’ classification program (Wallace and Boulton, 1968; Wallace, 1986; Jorgensen and McLachlan, 2008). We compare it with the work of Figueiredo and Jain (2002) and demonstrate its effectiveness.
- The search implements a generic approach to mixture modelling and allows, in this instance, the use of $d$-dimensional Gaussian and vMF distributions under the MML framework. It infers the optimal number of mixture components, and their corresponding parameters.
- Further, we demonstrate the effectiveness of MML mixture modelling through its application to high dimensional text clustering and clustering of directional data that arises out of protein conformations.

The rest of the paper is organized as follows: Sections 2 and 3 describe the respective estimators of Gaussian and vMF distributions that are commonly used. Section 4 introduces the MML framework for parameter estimation. Section 5 outlines the derivation of the MML parameter estimates of multivariate Gaussian and vMF distributions. Section 6 describes the formulation of a mixture model using MML and the estimation of the mixture parameters under the framework. Section 7 reviews the existing methods for selecting the mixture components. Section 8 describes our proposed approach to determine
the number of mixture components. Section 9 depicts the competitive performance of the proposed MML-based search through experiments conducted with Gaussian mixtures. Section 10 presents the results for MML-based vMF parameter estimation and mixture modelling followed by results supporting its applications to text clustering and protein structural data in Section 11.

2 Existing methods of estimating the parameters of a Gaussian distribution

The probability density function $f$ of a $d$-variate Gaussian distribution is given as

$$f(x; \mu, C) = \frac{1}{(2\pi)^{d/2}|C|^{1/2}}e^{-\frac{1}{2}(x-\mu)^T C^{-1} (x-\mu)}$$  (3)

where $\mu$, $C$ are the respective mean, (symmetric) covariance matrix of the distribution, and $|C|$ is the determinant of the covariance matrix. The traditional method to estimate the parameters of a Gaussian distribution is by maximum likelihood. Given data $D = \{x_1, \ldots, x_N\}$, where $x_i \in \mathbb{R}^d$, the log-likelihood $\mathcal{L}$ is given by

$$\mathcal{L}(D; \mu, C) = -\frac{Nd}{2} \log(2\pi) - \frac{N}{2} \log|C| - \frac{1}{2} \sum_{i=1}^{N} (x_i - \mu)^T C^{-1} (x_i - \mu)$$  (4)

To compute the maximum likelihood estimates, Equation (4) needs to be maximized. This is achieved by computing the gradient of the log-likelihood function with respect to the parameters and solving the resultant equations. The gradient vector of $\mathcal{L}$ with respect to $\mu$ and the gradient matrix of $\mathcal{L}$ with respect to $C$ are given below.

$$\nabla_\mu \mathcal{L} = \frac{\partial \mathcal{L}}{\partial \mu} = \sum_{i=1}^{N} C^{-1} (x_i - \mu)$$  (5)

$$\nabla_C \mathcal{L} = \frac{\partial \mathcal{L}}{\partial C} = -\frac{N}{2} C^{-1} + \frac{1}{2} \sum_{i=1}^{N} C^{-1} (x_i - \mu)(x_i - \mu)^T C^{-1}$$  (6)

The maximum likelihood estimates are then computed by solving $\nabla_\mu \mathcal{L} = 0$ and $\nabla_C \mathcal{L} = 0$ and are given as:

$$\hat{\mu} = \frac{1}{N} \sum_{i=1}^{N} x_i$$  and  $$\hat{C}_{ML} = \frac{1}{N} \sum_{i=1}^{N} (x_i - \hat{\mu})(x_i - \hat{\mu})^T$$  (7)

$\hat{C}_{ML}$ is known to be a biased estimate of the covariance matrix (Barton, 1961; Basu, 1964; Eaton and Morris, 1970; White, 1982) and issues related with its use in mixture modelling have been documented in Gray (1994) and Lo (2011). An unbiased estimator of $C$ was proposed by Barton (1961) and is given below.

$\hat{C}_{\text{unbiased}} = \frac{1}{N-1} \sum_{i=1}^{N} (x_i - \hat{\mu})(x_i - \hat{\mu})^T$  (8)

In addition to the maximum likelihood estimates, Bayesian inference of Gaussian parameters involving conjugate priors over the parameters has also been dealt with in the literature (Bishop, 2006). However, the unbiased estimate of the covariance matrix, as determined by the sample covariance (Equation (8)), is typically used in the analysis of Gaussian distributions.

3 Existing methods of estimating the parameters of a von Mises-Fisher distribution

For a von Mises-Fisher (vMF) distribution $f$ characterized by Equation (2), and given data $D = \{x_1, \ldots, x_N\}$, such that $x_i \in S^{d-1}$, the log-likelihood $\mathcal{L}$ is given by

$$\mathcal{L}(D; \kappa) = N \log C_\kappa(\kappa) + \kappa^T R$$  (9)

where $N$ is the sample size and $R = \sum_{i=1}^{N} x_i$ (the vector sum). Let $R$ denote the magnitude of the resultant vector $R$ and let $\hat{\mu}$ and $\hat{\kappa}$ be the maximum likelihood estimators of $\mu$ and $\kappa$ respectively. Under the condition that $\hat{\mu}$ is a unit vector, the maximum likelihood estimates are obtained by maximizing $\mathcal{L}$ as follows:

$$\hat{\mu} = \frac{R}{\|R\|}, \quad \hat{\kappa} = A_d^{-1}(\hat{R}) \quad \text{where} \quad A_d(\hat{\kappa}) = -\frac{C'_d(\hat{\kappa})}{C_d(\hat{\kappa})} = \frac{R}{N} = \hat{R}$$  (10)
Solving the non-linear equation: $F(\kappa) \equiv A_d(\kappa) - \hat{R} = 0$ yields the corresponding maximum likelihood estimate where

$$A_d(\kappa) = \frac{I_{d/2}(\kappa)}{I_{d/2-1}(\kappa)}$$ (11)

represents the ratio of Bessel functions. Because of the difficulties in analytically solving Equation (10), there have been several approaches to approximating $\hat{\kappa}$ (Mardia and Jupp, 2000). Each of these methods is an improvement over their respective predecessors. Tanabe et al. (2007) is an improvement over the estimate proposed by Banerjee et al. (2005). Sra (2012) is an improvement over Tanabe et al. (2007) and Song et al. (2012) fares better when compared to Sra (2012). The methods are summarized below.

### 3.1 Banerjee et al. (2005)

The approximation given by Equation (12) is due to Banerjee et al. (2005) and provides an easy to use expression for $\hat{\kappa}$. The formula is very appealing as it eliminates the need to evaluate complex Bessel functions. Banerjee et al. (2005) demonstrated that this approximation yields better results compared to the ones suggested in Mardia and Jupp (2000). It is an empirical approximation which can be used as a starting point in estimating the root of Equation (10).

$$\kappa_B = \frac{\hat{R}(d - \hat{R}^2)}{1 - \hat{R}^2}$$ (12)

### 3.2 Tanabe et al. (2007)

The approximation given by Equation (13) is due to Tanabe et al. (2007). The method utilizes the properties of Bessel functions to determine the lower and upper bounds for $\hat{\kappa}$ and uses a fixed point iteration function in conjunction with linear interpolation to approximate $\hat{\kappa}$. The bounds for $\hat{\kappa}$ are given by

$$\kappa_l = \frac{\hat{R}(d - 2)}{1 - \hat{R}^2} \leq \hat{\kappa} \leq \frac{\hat{R}d}{1 - \hat{R}^2}$$

Tanabe et al. (2007) proposed to use a fixed point iteration function defined as $\phi_{2d}(\kappa) = \hat{\kappa}A_d(\kappa)^{-1}$ and used this to approximate $\hat{\kappa}$ as

$$\kappa_T = \frac{\kappa_0\phi_{2d}(\kappa_0) - \kappa_0\phi_{2d}(\kappa_1)}{\phi_{2d}(\kappa_0) - \phi_{2d}(\kappa_1)} - (\kappa_0 - \kappa_1)$$ (13)

### 3.3 Sra (2012) : Truncated Newton approximation

This a heuristic approximation provided by Sra (2012). It involves refining the approximation given by Banerjee et al. (2005) (Equation (12)) by performing two iterations of Newton’s method. Sra (2012) demonstrate that this approximation fares well when compared to the approximation proposed by Tanabe et al. (2007). The following two iterations result in $\kappa_N$, the approximation proposed by Sra (2012):

$$\kappa_1 = \kappa_0 - \frac{F(\kappa_0)}{F'(\kappa_0)} \quad \text{and} \quad \kappa_N = \kappa_1 - \frac{F(\kappa_1)}{F'(\kappa_1)}$$ (14)

where

$$F'(\kappa) = A_d'(\kappa) = 1 - A_d(\kappa)^2 - \frac{(d - 1)}{\kappa}A_d(\kappa)$$ (15)

### 3.4 Song et al. (2012) : Truncated Halley approximation

This approximation provided by Song et al. (2012) uses Halley’s method which is the second order expansion of Taylor’s series of a given function $F(\kappa)$. The higher order approximation results in a more accurate estimate as demonstrated by Song et al. (2012). The iterative Halley’s method is truncated after iterating through two steps of the root finding algorithm (similar to that done by Sra (2012)). The following two iterations result in $\kappa_H$, the approximation proposed by Song et al. (2012):

$$\kappa_1 = \kappa_0 - \frac{2F(\kappa_0)F'(\kappa_0)}{2F'(\kappa_0)^2 - F(\kappa_0)F''(\kappa_0)} \quad \text{and} \quad \kappa_H = \kappa_1 - \frac{2F(\kappa_1)F'(\kappa_1)}{2F'(\kappa_1)^2 - F(\kappa_1)F''(\kappa_1)}$$ (16)

where

$$F''(\kappa) = A_d''(\kappa) = 2A_d(\kappa)^3 + \frac{3(d - 1)}{\kappa}A_d(\kappa)^2 + \frac{(d^2 - 2d\kappa)}{\kappa^2}A_d(\kappa) - \frac{(d - 1)}{\kappa}$$ (17)
The common theme in all these methods is that they try to approximate the maximum likelihood estimate governed by Equation (10). It is to be noted that the maximum likelihood estimators (of concentration parameter $\kappa$) have considerable bias (Schou, 1978; Best and Fisher, 1981; Cordeiro and Vasconcellos, 1999). To counter this effect, we explore the minimum message length based estimation procedure. This Bayesian method of estimation not only results in an unbiased estimate but also provides a framework to choose from several competing models (Wallace and Freeman, 1987; Wallace, 1990). Through a series of empirical tests, we demonstrate that the MML estimate is more reliable than any of the contemporary methods. Dowe et al. (1996c) have demonstrated the superior performance of the MML estimate for a three-dimensional vMF distribution. We extend their work to derive the MML estimators for a generic $d$-dimensional vMF distribution and compare its performance with the existing methods.

4 Minimum Message Length (MML) Inference

4.1 Model selection using Minimum Message Length

Wallace and Boulton (1968) developed the first practical criterion for model selection to be based on information theory. The resulting framework provides a rigorous means to objectively compare two competing hypotheses and, hence, choose the best one. As per Bayes’s theorem,

$$
Pr(H \& D) = Pr(H) \times Pr(D|H) = Pr(D) \times Pr(H|D)
$$

where $D$ denotes some observed data, and $H$ some hypothesis about that data. Further, $Pr(H \& D)$ is the joint probability of data $D$ and hypothesis $H$, $Pr(H)$ is the prior probability of hypothesis $H$, $Pr(D)$ is the prior probability of data $D$, $Pr(H|D)$ is the posterior probability of $H$ given $D$, and $Pr(D|H)$ is the likelihood.

MML uses the following result from information theory (Shannon, 1948): given an event or outcome $E$ whose probability is $Pr(E)$, the length of the optimal lossless code $I(E)$ to represent that event requires $I(E) = -\log_2(Pr(E))$ bits. Applying Shannon’s insight to Bayes’s theorem, Wallace and Boulton (1968) got the following relationship between conditional probabilities in terms of optimal message lengths:

$$
I(H \& D) = I(H) + I(D|H) = I(D) + I(H|D)
$$

(18)

As a result, given two competing hypotheses $H$ and $H'$,

$$
\Delta I = I(H \& D) - I(H' \& D) = I(D|H) - I(D|H') = \log_2 \left( \frac{Pr(H'|D)}{Pr(H|D)} \right) \text{ bits.}
$$

(19)

gives the posterior log-odds ratio between the two competing hypotheses. Equation (18) can be interpreted as the total cost to encode a message comprising the hypothesis $H$ and data $D$. This message is composed over into two parts:

1. **First part**: the hypothesis $H$, which takes $I(H)$ bits,
2. **Second part**: the observed data $D$ using knowledge of $H$, which takes $I(D|H)$ bits.

Clearly, the message length can vary depending on the complexity of $H$ and how well it can explain $D$. A more complex $H$ may fit (i.e., explain) $D$ better but take more bits to be stated itself. The trade-off comes from the fact that (hypothetically) transmitting the message requires the encoding of both the hypothesis and the data given the hypothesis, that is, the model complexity $I(H)$ and the goodness of fit $I(D|H)$.

4.2 Minimum message length based parameter estimation

Our proposed method of parameter estimation uses the MML inference paradigm. It is a Bayesian method which has been applied to infer the parameters of several statistical distributions (Wallace, 2005). We apply it to infer the parameter estimates of multivariate Gaussian and vMF distributions. Wallace and Freeman (1987) introduced a generalized scheme to estimate a vector of parameters $\Theta$ of any distribution $f$ given data $D$. The method involves choosing a reasonable prior $h(\Theta)$ on the hypothesis and evaluating the determinant of the Fisher information matrix $|\mathcal{F}(\Theta)|$ of the expected second-order partial derivatives of the negative log-likelihood function, $-\mathcal{L}(D|\Theta)$. The parameter vector $\Theta$ that minimizes the message length expression (Equation (20)) is the MML estimate according to Wallace and Freeman (1987).

$$
I(\Theta, D) = \frac{p}{2} \log{q_\theta} - \log \left( \frac{h(\Theta)}{\sqrt{|\mathcal{F}(\Theta)|}} \right) - \mathcal{L}(D|\Theta) + \frac{p}{2}
$$

(20)

where $q_\theta$ is the prior density of the parameter vector $\Theta$. The MML estimate $\hat{\Theta}$ is defined as

$$
\hat{\Theta} = \arg \min_{\Theta} I(\Theta, D).
$$

This procedure uses Bayes’s theorem to update the prior $h(\Theta)$ to the posterior $Pr(\Theta|D)$. The MML estimate is thus obtained as $I(\hat{\Theta}, D) = \min_{\Theta} I(\Theta, D)$.
where \( p \) is the number of free parameters in the model, and \( q_p \) is the lattice quantization constant (Conway and Sloane, 1984) in \( p \)-dimensional space. The total message length \( I(\Theta, D) \) in MML framework is composed of two parts:

1. the statement cost of encoding the parameters, \( I(\Theta) \) and
2. the cost of encoding the data given the parameters, \( I(D|\Theta) \).

A concise description of the MML method is presented in Oliver and Baxter (1994).

We note here a few key differences between MML and ML/MAP based estimation methods. In maximum likelihood estimation, the statement cost of parameters is ignored, in effect considered constant, and minimizing the message length corresponds to minimizing the negative log-likelihood of the data (the second part). In MAP based estimation, a probability density rather than the probability measure is used. Continuous parameters can necessarily only be stated only to finite precision. MML incorporates this in the framework by determining the region of uncertainty in which the parameter is located. The value of \( \frac{q_p}{\sqrt{|F(\Theta)|}} \) gives a measure of the volume of the region of uncertainty in which the parameter \( \Theta \) is centered. This multiplied by the probability density \( h(\Theta) \) gives the probability of a particular \( \Theta \) and is proportional to \( \frac{h(\Theta)}{\sqrt{|F(\Theta)|}} \). This probability is used to compute the message length associated with encoding the continuous valued parameters (to a finite precision).

5 Derivation of the MML parameter estimates of Gaussian and von Mises-Fisher distributions

Based on the MML inference process discussed in Section 4, we now proceed to formulate the message length expressions and derive the parameter estimates of Gaussian and von Mises-Fisher distributions.

5.1 MML-based parameter estimation of a multivariate Gaussian distribution

The MML framework requires the statement of parameters to a finite precision. The optimal precision is related to the Fisher information and in conjunction with a reasonable prior, the probability of parameters is computed.

5.1.1 Prior probability of the parameters

A flat prior is usually chosen on each of the \( d \) dimensions of \( \mu \) (Roberts et al., 1998; Oliver et al., 1996) and a conjugate inverted Wishart prior is chosen for the covariance matrix \( \Sigma \) (Gauvain and Lee, 1994; Agusta and Dowe, 2003; Bishop, 2006). The joint prior density of the parameters is then given as

\[
h(\mu, \Sigma) \propto |\Sigma|^{-(d+1)/2}
\]

5.1.2 Fisher information of the parameters

The computation of the Fisher information requires the evaluation of the second order partial derivatives of \( -\mathcal{L}(D|\mu, \Sigma) \). Let \( |\mathcal{F}(\mu, \Sigma)| \) represent the determinant of the Fisher information matrix. This is approximated as the product of \( |\mathcal{F}(\mu)| \) and \( |\mathcal{F}(\Sigma)| \) (Oliver et al., 1996; Roberts et al., 1998), where \( |\mathcal{F}(\mu)| \) and \( |\mathcal{F}(\Sigma)| \) are the respective determinants of Fisher information matrices due to the parameters \( \mu \) and \( \Sigma \). Differentiating the gradient vector in Equation (5) with respect to \( \mu \), we have:

\[
-\nabla_\mu \mathcal{L} = NC^{-1}
\]

Hence,

\[
|\mathcal{F}(\mu)| = N^d |\Sigma|^{-1/2}
\]

To compute \( |\mathcal{F}(\Sigma)| \), Magnus and Neudecker (1988) derived an analytical expression using the theory of matrix derivatives based on matrix vectorization (Dwyer, 1967). Let \( \Sigma = [c_{ij}] \forall 1 \leq i, j \leq d \) where \( c_{ij} \) denotes the element corresponding to the \( i^{th} \) row and \( j^{th} \) column of the covariance matrix. Let \( v(\Sigma) = (c_{11}, \ldots, c_{1d}, c_{22}, \ldots, c_{2d}, \ldots, c_{dd}) \) be the vector containing the \( d(d+1)/2 \) free parameters that completely describe the symmetric matrix \( \Sigma \). Then, the Fisher information due to the vector of parameters \( v(\Sigma) \) is equal to \( |\mathcal{F}(\Sigma)| \) and is given by Equation (23) (Magnus and Neudecker, 1988; Bozdogan, 1990; Drton et al., 2009).

\[
|\mathcal{F}(\Sigma)| = N^{d(d+1)/2} 2^{-d} |\Sigma|^{-(d+1)/2}
\]

Multiplying Equations (22) and (23), we have

\[
|\mathcal{F}(\mu, \Sigma)| = N^{d^2+d} 2^{-d} |\mu|^{-(d+2)}
\]
5.1.3 Message length formulation

To derive the message length expression to encode data using a certain \( \boldsymbol{\mu}, \boldsymbol{C} \), substitute Equations (4), (21), and (24), in Equation (20) using the number of free parameters of the distribution as \( p = \frac{d(d + 3)}{2} \). Hence,

\[
I(\boldsymbol{\mu}, \boldsymbol{C}, D) = \frac{(N - 1)}{2} \log |\boldsymbol{C}| + \frac{1}{2} \sum_{i=1}^{N} (\boldsymbol{x}_i - \boldsymbol{\mu})^T \boldsymbol{C}^{-1} (\boldsymbol{x}_i - \boldsymbol{\mu}) + \text{constant} \tag{25}
\]

To obtain the MML estimates of \( \boldsymbol{\mu} \) and \( \boldsymbol{C} \), Equation (25) needs to be minimized. The MML estimate of \( \boldsymbol{\mu} \) is same as the maximum likelihood estimate (given in Equation (7)). To compute the MML estimate of \( \boldsymbol{C} \), we need to compute the gradient matrix of \( I(\boldsymbol{\mu}, \boldsymbol{C}, D) \) with respect to \( \boldsymbol{C} \) and is given by Equation (26)

\[
\nabla_C I = \frac{\partial I}{\partial C} = \frac{(N - 1)}{2} \boldsymbol{C}^{-1} - \frac{1}{2} \sum_{i=1}^{N} \boldsymbol{C}^{-1} (\boldsymbol{x}_i - \boldsymbol{\mu}) (\boldsymbol{x}_i - \boldsymbol{\mu})^T \boldsymbol{C}^{-1} \tag{26}
\]

The MML estimate of \( \boldsymbol{C} \) is obtained by solving \( \nabla_C I = 0 \) (given in Equation(27)).

\[
\nabla_C I = 0 \implies \hat{\boldsymbol{C}}_{\text{MML}} = \frac{1}{N-1} \sum_{i=1}^{N} (\boldsymbol{x}_i - \hat{\boldsymbol{\mu}})(\boldsymbol{x}_i - \hat{\boldsymbol{\mu}})^T \tag{27}
\]

We observe that the MML estimate \( \hat{\boldsymbol{C}}_{\text{MML}} \) is same as the unbiased estimate of the covariance matrix \( \boldsymbol{C} \), thus, lending credibility for its preference over the traditional ML estimate (Equation (7)).

5.2 MML-based parameter estimation of a von Mises-Fisher distribution

Parameter estimates for two and three-dimensional vMF have been explored previously (Wallace and Dow, 1994; Dowe et al., 1996b,c). MML estimators of three-dimensional vMF were explored in Dowe et al. (1996c), where they demonstrate that the MML-based inference compares favourably against the traditional ML and MAP based estimation methods. We use the Wallace and Freeman (1987) method to formulate the objective function (Equation (20)) corresponding to a generic vMF distribution.

5.2.1 Prior probability of the parameters

Regarding choosing a reasonable prior (in the absence of any supporting evidence) for the parameters \( \Theta = (\boldsymbol{\mu}, \kappa) \) of a vMF distribution, Wallace and Dow (1994) and Dowe et al. (1996c) suggest the use of the following “colourless prior that is uniform in direction, normalizable and locally uniform at the Cartesian origin in \( \kappa \)”: \( h(\boldsymbol{\mu}, \kappa) \propto \frac{\kappa^{d-1}}{(1 + \kappa^2)^{(d+1)/2}} \) \( \tag{28} \)

5.2.2 Fisher information of the parameters

Regarding evaluating the Fisher information, Dowe et al. (1996c) argue that in the general \( d \)-dimensional case,

\[
|\mathcal{F}(\boldsymbol{\mu}, \kappa)| = (N\kappa A_d(\kappa))^d \times \kappa A'_d(\kappa) \tag{29}
\]

where \( A_d(\kappa) \) and \( A'_d(\kappa) \) are described by Equations (11) and (15) respectively.

5.2.3 Message length formulation

Substituting Equations (9), (28) and (29) in Equation (20) with number of free parameters \( p = d \), we have the net message length expression:

\[
I(\boldsymbol{\mu}, \kappa, D) = \frac{(d - 1)}{2} \log \frac{A_d(\kappa)}{\kappa} + \frac{1}{2} \log A'_d(\kappa) + \frac{(d + 1)}{2} \log(1 + \kappa^2) - N \log C_d(\kappa) - \kappa \mu^T R + \text{constant} \tag{30}
\]

To obtain the MML estimates of \( \boldsymbol{\mu} \) and \( \kappa \), Equation (30) needs to be minimized. The estimate for \( \boldsymbol{\mu} \) is same as the maximum likelihood estimate (Equation (10)). The resultant equation in \( \kappa \) that needs to be minimized is then given by:

\[
I(\kappa) = \frac{(d - 1)}{2} \log \frac{A_d(\kappa)}{\kappa} + \frac{1}{2} \log A'_d(\kappa) + \frac{(d + 1)}{2} \log(1 + \kappa^2) - N \log C_d(\kappa) - \kappa R + \text{constant} \tag{31}
\]
To obtain the MML estimate of $\kappa$, we need to differentiate Equation (31) and set it to zero.

Let $G(\kappa) \equiv \frac{\partial I}{\partial \kappa} = - \frac{(d - 1)}{2\kappa} + \frac{(d + 1)\kappa}{1 + \kappa^2} + \frac{(d - 1)}{2} A'_d(\kappa) + \frac{1}{2} A''_d(\kappa) + NA_d(\kappa) - R$ (32)

The non-linear equation: $G(\kappa) = 0$ does not have a closed form solution. We try both the Newton and Halley’s method to find an approximate solution. We discuss both variants and comment on the effects of the two approximations in the experimental results. To be fair and consistent with Sra (2012) and Song et al. (2012), we use the initial guess of the root as $\kappa_0$ (Equation (12)) and iterate twice to obtain the MML estimate.

1. **Approximation using Newton’s method:**

   \[ k_1 = \kappa_0 - \frac{G(\kappa_0)}{G'(\kappa_0)} \] \[ \kappa_{MN} = k_1 - \frac{G(k_1)}{G'(k_1)} \] (33)

2. **Approximation using Halley’s method:**

   \[ k_1 = \kappa_0 - \frac{2G(\kappa_0)G'(\kappa_0)}{2G'(\kappa_0)^2 - G(\kappa_0)G''(\kappa_0)} \] \[ \kappa_{MH} = k_1 - \frac{2G(k_1)G'(k_1)}{2G'(k_1)^2 - G(k_1)G''(k_1)} \] (34)

The details of evaluating $G'(\kappa)$ and $G''(\kappa)$ are discussed in Appendix 13.1.

Equation (33) gives the MML estimate ($\kappa_{MN}$) using Newton’s method and Equation (34) gives the MML estimate ($\kappa_{MH}$) using Halley’s method. We used these values of MML estimates in mixture modelling using vMF distributions.

### 6 Minimum Message Length Approach to Mixture Modelling

Mixture modelling involves representing an observed distribution of data as a weighted sum of individual probability density functions. Specifically, the problem we consider here is to model the mixture distribution $\mathcal{M}$ as defined in Equation (1). For some observed data $D = \{x_1, \ldots, x_N\}$ ($N$ is the sample size), and a mixture $\mathcal{M}$, the log-likelihood using the mixture distribution is as follows:

\[ \mathcal{L}(D|\Phi) = \sum_{i=1}^{N} \log \sum_{j=1}^{M} w_j f_j(x_i;\Theta_j) \] (35)

where $\Phi = \{w_1, \ldots, w_M, \Theta_1, \ldots, \Theta_M\}$, $w_j$ and $f_j(x;\Theta_j)$ are the weight and probability density of the $j^{th}$ component respectively. For a fixed $M$, the mixture parameters $\Phi$ are traditionally estimated using a standard expectation-maximization (EM) algorithm (Dempster et al., 1977; Krishnan and McLachlan, 1997). This is briefly discussed below.

#### 6.1 Standard EM algorithm to estimate mixture parameters

The standard EM algorithm is based on maximizing the log-likelihood function of the data (Equation (35)). The maximum likelihood estimates are then given as $\Phi_{ML} = \arg \max \mathcal{L}(D|\Phi)$. Because of the absence of a closed form solution for $\Phi_{ML}$, a gradient descent method is employed where the parameter estimates are iteratively updated until convergence to some local optimum is achieved (Dempster et al., 1977; McLachlan and Basford, 1988; Xu and Jordan, 1996; Krishnan and McLachlan, 1997; McLachlan and Peel, 2000). The EM method consists of two steps:

- **E-step:** Each datum $x_i$ has fractional membership to each of the mixture components. These partial memberships of the data points to each of the components are defined using the responsibility matrix

   \[ r_{ij} = \frac{w_jf_j(x_i;\Theta_j)}{\sum_{k=1}^{M} w_kf_k(x_i;\Theta_k)}, \quad \forall 1 \leq i \leq N, 1 \leq j \leq M \] (36)

   where $r_{ij}$ denotes the conditional probability of a datum $x_i$ belonging to the $j^{th}$ component. The effective membership associated with each component is then given by

   \[ n_j = \sum_{i=1}^{N} r_{ij} \quad \text{and} \quad \sum_{j=1}^{M} n_j = N \] (37)

- **M-step:** Assuming $\Phi^{(t)}$ be the estimates at some iteration $t$, the expectation of the log-likelihood using $\Phi^{(t)}$ and the partial memberships is then maximized which is tantamount to computing $\Phi^{(t+1)}$, the updated maximum likelihood estimates for the next iteration ($t + 1$). The weights are updated as $w_j^{(t+1)} = \frac{n_j^{(t)}}{N}$. 


The above sequence of steps are repeated until a certain convergence criterion is satisfied. At some intermediate iteration $t$, the mixture parameters are updated using the corresponding ML estimates and are given below.

- **Gaussian:** The ML updates of the mean and covariance matrix are

\[
\hat{\mu}_j^{(t+1)} = \frac{1}{n_j^t} \sum_{i=1}^{N} r_{ij}^{(t)} x_i \quad \text{and} \quad \hat{\Sigma}_j^{(t+1)} = \frac{1}{n_j^t} \sum_{i=1}^{N} r_{ij}^{(t)} (x_i - \hat{\mu}_j^{(t+1)}) (x_i - \hat{\mu}_j^{(t+1)})^T
\]

- **von Mises-Fisher:** The resultant vector sum is updated as $R_j^{(t+1)} = \sum_{i=1}^{N} r_{ij}^{(t)} x_i$. If $R_j^{(t+1)}$ represents the magnitude of vector $R_j^{(t+1)}$, then the updated mean and concentration parameter are

\[
\hat{\mu}_j^{(t+1)} = \frac{R_j^{(t+1)}}{R_j^{(t+1)}}, \quad \hat{\kappa}_j^{(t+1)} = A_d^{-1} \left( \frac{R_j^{(t+1)}}{n_j^t} \right)
\]

6.2.1 Encoding a mixture model using MML

We refer to the discussion in Wallace (2005) to briefly describe the intuition behind mixture modelling using MML. Encoding of a message using MML requires the encoding of (1) the model parameters and then (2) the data using the parameters. The statement costs for encoding the mixture model and the data can be decomposed into:

1. Encoding the number of components $M$: In order to encode the message losslessly, it is required to initially state the number of components. In the absence of background knowledge, one would like to model the prior belief in such a way that the probability decreases for increasing number of components. If $h(M) \propto 2^{-M}$, then $I(M) = M \log 2 + \text{constant}$. The prior reflects that there is a difference of one bit in encoding the numbers $M$ and $M + 1$. Alternatively, one could assume a uniform prior over $M$ within some predefined range. The chosen prior has little effect as its contribution is minimal when compared to the magnitude of the total message length (Wallace, 2005).

2. Encoding the weights $w_1, \ldots, w_M$ which are treated as parameters of a multinomial distribution with sample size $n_j$, $\forall 1 \leq j \leq M$. The length of encoding all the weights is then given by the expression (Boulton and Wallace, 1969):

\[
I(w) = \frac{(M-1)}{2} \log N - \frac{1}{2} \sum_{j=1}^{M} \log w_j - (M-1)!
\]  

3. Encoding each of the component parameters $\Theta_j$, as given by $I(\Theta_j) = - \log \frac{h(\Theta_j)}{\sqrt{|\mathcal{F}(\Theta_j)|}}$ (discussed in Section 4.2).

4. Encoding the data: each datum $x_i$ can be stated to a finite precision which is dictated by the accuracy of measurement. If the precision to which each element of a $d$-dimensional vector can be stated is $\varepsilon$, then the probability of a datum $x_i \in \mathbb{R}^d$ is given as $\Pr(x_i) = \varepsilon^d \Pr(x_i | \mathcal{M})$ where $\Pr(x_i | \mathcal{M})$ is the probability density given by Equation (1). Hence, the total length of its encoding is given by

\[
I(x_i) = - \log \Pr(x_i) = -d \log \varepsilon - \log \sum_{j=1}^{M} w_j f_j(x_i | \Theta_j)
\]

The entire data $D$ can now be encoded as:

\[
I(D|\Phi) = -Nd \log \varepsilon - \sum_{i=1}^{N} \log \sum_{j=1}^{M} w_j f_j(x_i; \Theta_j)
\]

\footnote{We note that $\varepsilon$ is a constant value and has no effect on the overall inference process. It is used in order to maintain the theoretical validity when making the distinction between probability and probability density.}
Thus, the total message length of a $M$ component mixture is given by Equation (41).

$$I(\Phi, D) = I(M) + I(w) + \sum_{j=1}^{M} I(\Theta_j) + I(D|\Phi) + \text{constant}$$

$$= I(M) + I(w) + \left(-\sum_{j=1}^{M} \log h(\Theta_j) + \frac{1}{2} \sum_{j=1}^{M} \log |F(\Theta_j)|\right) + I(D|\Phi) + \text{constant} \quad (41)$$

Note that the constant term includes the lattice quantization constant (resulting from stating all the model parameters) in a $p$-dimensional space, where $p$ is equal to the number of free parameters in the mixture model.

6.2.2 Estimating the mixture parameters

The parameters of the mixture model are those that minimize Equation (41). To achieve this we use the standard EM algorithm (Section 6.1), where, iteratively, the parameters are updated using their respective MML estimates. The component weights are obtained by differentiating Equation (41) with respect to $w_j$ under the constraint $\sum_{j=1}^{M} w_j = 1$. The derivation of the MML updates of the weights is shown in Appendix 13.2 and are given as:

$$w_j^{(t+1)} = \frac{n_j^{(t)} + \frac{1}{2}}{N + \frac{1}{2}} \quad (42)$$

The parameters of the $j^{th}$ component are updated using $r_{ij}^{(t)}$ and $n_j^{(t)}$ (Equations (36), (37)), the partial memberships assigned to the $j^{th}$ component at some intermediate iteration $t$ and are given below.

- **Gaussian**: The MML updates of the mean and covariance matrix are

  $$\hat{\mu}_j^{(t+1)} = \frac{1}{n_j^{(t)}} \sum_{i=1}^{N} r_{ij}^{(t)} x_i \quad \text{and} \quad C_j^{(t+1)} = \frac{1}{n_j^{(t)}-1} \sum_{i=1}^{N} r_{ij}^{(t)} (x_i - \hat{\mu}_j^{(t+1)}) (x_i - \hat{\mu}_j^{(t+1)})^T \quad (43)$$

- **von Mises-Fisher**: The resultant vector sum is updated as $R_j^{(t+1)} = \sum_{i=1}^{N} r_{ij}^{(t)} x_i$. If $R_j^{(t+1)}$ represents the magnitude of vector $\mathbf{R}_j^{(t+1)}$, then the updated mean is given by Equation (44).

  $$\hat{\mu}_j^{(t+1)} = \frac{R_j^{(t+1)}}{R_j^{(t+1)}} \quad (44)$$

The MML update of the concentration parameter $\kappa_j^{(t+1)}$ is obtained by solving $G(\hat{\kappa}_j^{(t+1)}) = 0$ after substituting $N \rightarrow n_j^{(t)}$ and $R \rightarrow R_j^{(t+1)}$ in Equation (32).

The EM is terminated when the change in the total message length (improvement rate) between successive iterations is less than some predefined threshold. The difference between the two variants of standard EM discussed above is firstly the objective function that is being optimized. In Section 6.1, the log-likelihood function is maximized which corresponds to $I(D|\Phi)$ term in Section 6.2. Equation (41) includes additional terms that correspond to the cost associated with stating the mixture parameters. Secondly, in the M-step, in Section 6.1, the components are updated using their ML estimates whereas in Section 6.2, the components are updated using their MML estimates.

6.3 Issues arising from the use of EM algorithm

The standard EM algorithms outlined above can be used only when the number of mixture components $M$ is fixed or known a priori. Even when the number of components are fixed, EM has potential pitfalls. The method is sensitive to the initialization conditions. To overcome this, some reasonable start state for the EM may be determined by initially clustering the data (Krishnan and McLachlan, 1997; McLachlan and Peel, 2000). Another strategy is to run the EM a few times and choose the best amongst all the trials. Figueiredo and Jain (2002) point out that, in the case of Gaussian mixture modelling, EM can converge to the boundary of the parameter space when the corresponding covariance matrix is nearly singular or when there are few initial members assigned to that component.
7 Existing methods of inferring the number of mixture components

Inferring the “right” number of mixture components for unlabelled data has proven to be a thorny issue (McLachlan and Peel, 2000) and there have been numerous approaches proposed that attempt to tackle this problem (Akaike, 1974; Schwarz et al., 1978; Rissanen, 1978; Bozdogan, 1993; Oliver et al., 1996; Roberts et al., 1998; Biernacki et al., 2000; Figueiredo and Jain, 2002). Given some observed data, there are infinitely many mixtures that one can fit to the data. Any method that aims to selectively determine the optimal number of components should be able to factor the cost associated with the mixture parameters. To this end, several methods based on information theory have been proposed where there is some form of penalty associated with choosing a certain parameter value (Wallace and Boulton, 1968; Akaike, 1974; Schwarz et al., 1978; Wallace and Freeman, 1987; Rissanen, 1989). We briefly review some of these methods and discuss the state of the art and then proceed to explain our proposed method.

7.1 AIC (Akaike, 1974) & BIC (Schwarz et al., 1978)

AIC in the simplest form adds the number of free parameters \( p \) to the negative log-likelihood expression. There are some variants of AIC suggested (Bozdogan, 1983; Burnham and Anderson, 2002). However, these variants introduce the same penalty constants for each additional parameter:

\[
AIC(p) = p - \mathcal{L}(D|\Phi)
\]

BIC, similar to AIC, adds a constant multiple of \( \frac{1}{2} \log N \) (\( N \) being the sample size), for each free parameter in the model.

\[
BIC(p) = p \log N - \mathcal{L}(D|\Phi)
\]

Rissanen (1978) formulated minimum description length (MDL) which formally coincides with BIC (Oliver et al., 1996; Figueiredo and Jain, 2002).

7.1.1 Formulation of the scoring functions

AIC and BIC/MDL serve as scoring functions to evaluate a model and its corresponding fit to the data. The formulations suggest that the parameter cost associated with adopting a model is dependent only on the number of free parameters and not on the parameter values themselves. In other words, the criteria consider all models of a particular type (of probability distribution) to have the same statement cost associated with the parameters. For example, a generic \( d \)-dimensional Gaussian distribution has \( p = \frac{d(d+3)}{2} \) free parameters. All such distributions will have the same parameter costs regardless of their characterizing means and covariance matrices, which is an oversimplifying assumption which can hinder proper inference.

The criteria can be interpreted under the MML framework wherein the first part of the message is a constant multiplied by the number of free parameters. AIC and BIC formulations can be obtained as approximations to the two-part MML formulation governed by Equation (20) (Figueiredo and Jain, 2002). It has been argued that for tasks such as mixture modelling, where the number of free parameters potentially grows in proportion to the data, MML is known in theory to give consistent results as compared to AIC and BIC (Wallace, 1986; Wallace and Dowe, 1999).

7.1.2 Search method to determine the optimal number of mixture components

To determine the optimal number of mixture components \( M \), the AIC or BIC scores are computed for mixtures with varying values of \( M \). The mixture model with the least score is selected as per these criteria.

A \( d \)-variate Gaussian mixture with \( M \) number of components has \( p = \frac{Md(d+3)}{2} + (M-1) \) free parameters. All mixtures with a set number of components have the same cost associated with their parameters using these criteria. The mixture complexity is therefore treated as independent of the constituent mixture parameters. In contrast, the MML formulation incorporates the statement cost of losslessly encoding mixture parameters by calculating their relevant probabilities as discussed in Section 6.

7.2 MML Unsupervised (Oliver et al., 1996)

7.2.1 Formulation of the scoring function

A MML-based scoring function akin to the one shown in Equation (41) was used to model Gaussian mixtures. However, the authors only consider the specific case of Gaussians with diagonal covariance matrices, and fail to provide a general method dealing with full covariance matrices.
7.2.2 Search method to determine the optimal number of mixture components

A rigorous treatment on the selection of number of mixture components $M$ is lacking. Oliver et al. (1996) experiment with different values of $M$ and choose the one which results in the minimum message length. For each $M$, the standard EM algorithm (Section 6.1) was used to attain local convergence.

7.3 Approximate Bayesian (Roberts et al., 1998)

The method, also referred to as Laplace-empirical criterion (LEC) (McLachlan and Peel, 2000), uses a scoring function derived using Bayesian inference and serves to provide a tradeoff between model complexity and the quality of fit. The parameter estimates $\Phi$ are those that result in the minimum value of the following scoring function.

$$-\log P(D, \Phi) = -\mathcal{L}(D|\Phi) + Md \log(2\alpha\beta\sigma_p^2) - \log(M-1)! - \frac{Nd}{2} \log(2\pi) + \frac{1}{2} \log |H(\Phi)|$$  \hspace{1cm} (45)

where $D$ is the dataset, $-\mathcal{L}(D|\Phi)$ is the negative log-likelihood given the mixture parameters $\Phi$, $M$ is the number of mixture components, $d$ the dimensionality of the data, $\alpha, \beta$ are hyperparameters (which are set to 1 in their experiments), $\sigma_p$ is a pre-defined constant or is pre-computed using the entire data, $H(\Phi)$ is the Hessian matrix which is equivalent to the empirical Fisher matrix for the set of component parameters, and $p$ is the number of free parameters in the model.

7.3.1 Formulation of the scoring function

The formulation in Equation (45) can be obtained as an approximation to the message length expression in Equation (41) by identifying the following related terms in both equations.

1. $I(w) \rightarrow -\log(M-1)!$
2. For a $d$-variate Gaussian with mean $\mu$ and covariance matrix $C$, the joint prior $h(\mu, C)$ is calculated as follows:
   - Prior on $\mu$: Each of the $d$ parameters of the mean direction are assumed to be have uniform priors in the range $(-\alpha \sigma_p, \alpha \sigma_p)$, so that the prior density is $h(\mu) = \frac{1}{(2\alpha \sigma_p)^d}$.
   - Prior on $C$: It is assumed that the prior density is dependent only on the diagonal elements in $C$. Each diagonal covariance element is assumed to have a prior in the range $(0, \beta \sigma_p)$ so that the prior on $C$ is considered to be $h(C) = \frac{1}{(\beta \sigma_p)^d}$.

   The joint prior, is therefore, assumed to be $h(\mu, C) = \frac{1}{(2\alpha \beta \sigma_p^2)^d}$.

   Thus, $-\sum_{j=1}^M \log h(\Theta_j) \rightarrow Md \log(2\alpha \beta \sigma_p^2)$

3. $\frac{1}{2} \sum_{j=1}^M \log |\mathcal{F}(\Theta_j)| \rightarrow \frac{1}{2} \log |H|$

4. Constant $\rightarrow \frac{1}{2} \log(2\pi)$

Although the formulation is an improvement over the previously discussed methods, there are some limitations due to the assumptions made while proposing the scoring function:

- While computing the prior density of the covariance matrix, the off-diagonal elements are ignored.
- The computation of the determinant of the Fisher matrix is approximated by computing the Hessian $|H|$. It is to be noted that while the Hessian is the observed information (data dependent), the Fisher information is the expectation of the observed information. MML formulation requires the use of the expected value.
- Further, the approximated Hessian was derived for Gaussians with diagonal covariances. For Gaussians with full covariance matrices, the Hessian was approximated by replacing the diagonal elements with the corresponding eigen values in the Hessian expression. The empirical Fisher computed in this form does not guarantee the characteristic invariance property of the classic MML method (Oliver and Baxter, 1994).

7.3.2 Search method to determine the optimal number of mixture components

The search method used to select the optimal number of components is rudimentary. The optimal number of mixture components is chosen by running the EM 10 times for every value of $M$ within a given range. An optimal $M$ is selected as the one for which the best of the 10 trials results in the least value of the scoring function.
7.4 Integrated Complete Likelihood (ICL) (Biernacki et al., 2000)

The ICL criterion maximizes the complete log-likelihood (CL) given by

\[ CL(D, \Theta) = \mathcal{L}(D, \Phi) - \sum_{j=1}^{N} \log \left( \sum_{i=1}^{M} z_{ij} \right) \]

where \( \mathcal{L}(D, \Phi) \) is the log-likelihood (Equation (35)), \( r_{ij} \) is the responsibility term (Equation (36)), and \( z_{ij} = 1 \) if \( x_i \) arises from component \( j \) and zero otherwise. The term \( \sum_{i=1}^{N} \sum_{j=1}^{M} z_{ij} \log r_{ij} \) is explained as the estimated mean entropy.

7.4.1 Formulation of the scoring function

The ICL criterion is then defined as: \( ICL(\Phi, M) = CL(\Phi) - \frac{p}{2} \log N \), where \( p \) is the number of free parameters in the model. We observe that similar to BIC, the ICL scoring function penalizes each free parameter by a constant value and does not account for the model parameters.

7.4.2 Search method to determine the optimal number of mixture components

The search method adopted in this work is similar to the one used by (Roberts et al., 1998). The EM algorithm is initiated 20 times for each value of \( M \) with random starting points and the best amongst those is chosen.

7.5 Unsupervised Learning of Finite Mixtures (Figueiredo and Jain, 2002)

The method uses the MML criterion to formulate the scoring function given by Equation (46). The formulation can be interpreted as a two-part message for encoding the model parameters and the observed data.

\[ I(D, \Phi) = \frac{N_p}{2} \sum_{j=1}^{M} \log \left( \frac{N w_j}{12} \right) + \frac{M}{2} \log \frac{N}{12} + \frac{M(N_p + 1)}{2} - \mathcal{L}(D, \Phi) \]

where \( N_p \) is the number of free parameters per component and \( w_j \) is the component weight.

7.5.1 Formulation of the scoring function

The scoring function is derived from Equation (41) by assuming the prior density of the component parameters to be a Jeffreys prior. If \( \Theta_j \) is the vector of parameters describing the \( j \)th component, then the prior density \( h(\Theta_j) \propto \sqrt{\mathcal{J}(\Theta_j)} \) (Jeffreys, 1946). Similarly, a prior for weights would result in \( h(w_1, \ldots, w_M) \propto (w_1 \cdots w_M)^{-1/2} \). These assumptions are used in the encoding of the parameters which correspond to the first part of the message.

We note that the scoring function is consistent with the MML scheme of encoding parameters and the data using those parameters. However, the formulation can be improved by amending the assumptions as detailed in in Section 5. Further, the assumptions made in Figueiredo and Jain (2002) have the following side effects:

- The value of \( -\log \frac{h(\Theta_j)}{\sqrt{\mathcal{J}(\Theta_j)}} \) gives the cost of encoding the component parameters. By assuming \( h(\Theta_j) \propto \sqrt{\mathcal{J}(\Theta_j)} \), the message length associated with using any vector of parameters \( \Theta_j \) is essentially treated the same. To avoid this, the use of independent uniform priors over non-informative Jeffreys’s priors was advocated previously (Oliver et al., 1996; Lee, 1997; Roberts et al., 1998). The use of Jeffreys prior offers certain advantages, for example, not having to compute the Fisher information (Jeffreys, 1946). However, this is crucial and cannot be ignored as it dictates the precision of encoding the parameter vector. Wallace (2005) states that “Jeffreys, while noting the interesting properties of the prior formulation did not advocate its use as a genuine expression of prior knowledge.”

- By making this assumption, Figueiredo and Jain (2002) sidestep the difficulty associated with explicitly computing the Fisher information associated with the component parameters. Hence, for encoding the parameters of the entire mixture, only the cost associated with encoding the component weights is considered.

- The code length to state each \( \Theta_j \) is, therefore, greatly simplified as \( (N_p/2) \log(N w_j) \) (notice the sole dependence on weight \( w_j \)). Figueiredo and Jain (2002) interpret this as being similar to a MDL formulation because \( N w_j \) gives the expected number of data points generated by the \( j \)th component. This is equivalent to the BIC criterion discussed earlier. We note that MDL/BIC are highly simplified versions of MML formulation and therefore, Equation (46) does not capture the entire essence of complexity and goodness of fit accurately.
7.5.2 Search method to determine the optimal number of mixture components

The method begins by assuming a large number of components and updates the weights iteratively in the EM steps as

\[
w_j = \max \left\{ 0, n_j - \frac{N_p}{2} \right\} \sum_{j=1}^{M} \max \left\{ 0, n_j - \frac{N_p}{2} \right\}
\]

(47)

where \( n_j \) is the effective membership of data points in the \( j \)th component (Equation (37)). A component is annihilated when its weight becomes zero and consequently the number of mixture components decreases. We note that the search method proposed by Figueiredo and Jain (2002) using the MML criterion is an improvement over the methods they compare against. However, we make the following remarks about their search method.

- The method updates the weights as given by Equation (47). During any iteration, if the amount of data allocated to a component is less than \( N_p/2 \), its weight is updated as zero and this component is ignored in subsequent iterations. This imposes a lower bound on the amount of data that can be assigned to each component. As an example, for a Gaussian mixture in 10-dimensions, the number of free parameters per component is \( N_p = 65 \), and hence the lower bound is 33. Hence, in this example, if a component has \( \sim 30 \) data, the mixture size is reduced and these data are assigned to some other component(s). Consider a scenario where there are 50 observed 10 dimensional data points originally generated by a mixture with two components with equal mixing proportions. The method would always infer that there is only one component regardless of the separation between the two components. This is clearly a wrong inference! (see Section 9.4 for the relevant experiments).

- Once a component is discarded, the mixture size decreases by one, and it cannot be recovered. Because the memberships \( n_j \) are updated iteratively using an EM algorithm and because EM might not always lead to global optimum, it is conceivable that the updated values need not always be optimal. This might lead to situations where a component is deleted owing to its low prominence. There is no provision to increase the mixture size in the subsequent stages of the algorithm to account for such behaviour.

- The method assumes a large number of initial components in an attempt to be robust with respect to EM initialization. However, this places a significant overhead on the computation due to handling several components.

**Summary:** We observe that while all these methods (and many more) work well within their defined scope, they are incomplete in achieving the true objective that is to rigorously score models and their ability to fit the data. The methods discussed above can be seen as different approximations to the MML framework. They adopted various simplifying assumptions and approximations. To avoid such limitations, we developed a classic MML formulation, giving the complete message length formulations for Gaussian and von Mises-Fisher distributions in Section 5.

Secondly, in most of these methods, the search for the optimal number of mixture components is achieved by selecting the mixture that results in the best EM outcome out of many trials (Akaike, 1974; Schwarz et al., 1978; Oliver et al., 1996; Roberts et al., 1998; Biernacki et al., 2000). This is not an elegant solution and Figueiredo and Jain (2002) proposed a search heuristic which integrates estimation and model selection. A comparative study of these methods is presented in McLachlan and Peel (2000). Their analysis suggested the superior performance of ICL (Biernacki et al., 2000) and LEC (Roberts et al., 1998). Later, Figueiredo and Jain (2002) demonstrated that their proposed method outperforms the contemporary methods based on ICL and LEC and is regarded as the current state of the art. We, therefore, compare our method against that of Figueiredo and Jain (2002) and demonstrate its effectiveness.

With this background, we formulate an alternate search heuristic to infer the optimal number of mixture components which aims to address the above limitations.

**8 Proposed approach to infer an optimal mixture**

The space of candidate mixture models to explain the given data is infinitely large. As per the MML criterion (Equation (41)), the goal is to search for the mixture that has the smallest overall message length. We have seen in Section 6.2 that if the number of mixture components are fixed, then the EM algorithm can be used to estimate the mixture parameters, namely the component weights and the parameters of each component. However, here it is required to search for the optimal number of mixture components along with the corresponding mixture parameters.

Our proposed search heuristic extends the MML-based Snob program (Wallace and Boulton, 1968; Wallace, 1986; Jorgensen and McLachlan, 2008) for unsupervised learning. We define three operations, namely *split, delete,* and *merge* that can be applied to any component in the mixture.
### Algorithm 1: Achieve an optimal mixture model

```plaintext
1  current ← one-component-mixture
2  while true do
3      components ← current mixture components
4      M ← number of components
5      for i ← 1 to M do
6          /* exhaustively split all components */
7              splits[i] ← Split(current, components[i])
8              BestSplit ← best(splits)
9              /* remember the best split */
10             if M > 1 then
11                for i ← 1 to M do
12                    /* exhaustively delete all components */
13                       deletes[i] ← Delete(current, components[i])
14                       BestDelete ← best(deletes)
15                       /* remember the best deletion */
16                for i ← 1 to M do
17                    /* exhaustively merge all components */
18                       j ← closest-component(i)
19                       merges[i] ← Merge(current, i, j)
20                       BestMerge ← best(merges)
21                       /* remember the best merge */
22                BestPerturbation ← best(BestSplit, BestDelete, BestMerge)
23                /* select the best perturbation */
24                ΔM ← message_length(BestPerturbation) − message_length(current)
25                /* check for improvement */
26                if ΔM < 0 then
27                        current ← BestPerturbation
28                        continue
29                else
30                        break
31  return current
```

8.1 The complete algorithm

The pseudocode of our search method is presented in Algorithm 1. The basic idea behind the search strategy is to perturb a mixture from its current suboptimal state to obtain a new state (if the perturbed mixture results in a smaller message length). In general, if a (current) mixture has \( M \) components, it is perturbed using a series of Split, Delete, and Merge operations to check for improvement. Each component is split and the new \((M + 1)\)-component mixture is re-estimated. If there is an improvement (i.e., if there is a decrease in message length with respect to the current mixture), the new \((M + 1)\)-component mixture is retained. There are \( M \) splits possible and the one that results in the greatest improvement is recorded (lines 5 – 7 in Algorithm 1). A component is first split into two sub-components (children) which are locally optimized by the EM algorithm on the data that belongs to that sole component. The child components are then integrated with the others and the mixture is then optimized to generate a \( M + 1 \) component mixture. The reason for this is, rather than use random initial values for the EM, it is better if we start from some already optimized state to reach to a better state. Similarly, each of the components is then deleted, one after the other, and the \((M − 1)\)-component mixture is compared against the current mixture. There are \( M \) possible deletions and the best amongst these is recorded (lines 8 – 11 in Algorithm 1). Finally, the components in the current mixture are merged with their closest matches (determined by calculating the KL-divergence) and each of the resultant \((M − 1)\)-component mixtures are evaluated against the \( M \) component mixture. The best among these merged mixtures is then retained (lines 12 – 15 in Algorithm 1).

We initially start by assuming a one component mixture. This component is split into two children which are locally optimized. If the split results in a better model, it is retained. For any given \( M \)-component mixture, there might be improvement due to splitting, deleting and/or merging its components. We select the perturbation that best improves the current mixture. This process is repeated until there is no further improvement possible. and the algorithm is continued. The notion of best or improved mixture is based on the amount of reduction of message length that the perturbed mixture provides. In the current state, the observed data have partial memberships in each of the \( M \) components. Before the execution of each operation, these memberships need to be adjusted and an EM is subsequently carried out to achieve an optimum with a different number of components. We will now examine each operation in detail and see how the memberships are affected after each operation.

8.2 Strategic operations employed to determine an optimal mixture model

Let \( R = [r_{ij}] \) be the \( N \times M \) responsibility (membership) matrix and \( w_j \) be the weight of \( j^{th} \) component in mixture \( \mathcal{M} \).

1. Split (Line 6 in Algorithm 1): As an example, assume a component with index \( \alpha \in \{1, M\} \) and weight \( w_\alpha \) in the current mixture \( \mathcal{M} \) is split to generate two child components. The goal is to find two distinct clusters amongst the data associated with component \( \alpha \). It is to be noted that the data have fractional memberships to component \( \alpha \). The EM is therefore, carried out within the component \( \alpha \) assuming a two-component sub-mixture with the data weighted as per their current memberships \( r_{i\alpha} \). The remaining \( M − 1 \) components are untouched. An EM is carried out to optimize the two-component sub-mixture. The initial state and the subsequent updates in the Maximization-step are described below.
Parameter initialization of the two-component sub-mixture: The goal is to identify two distinct clusters within the component α. For Gaussian mixtures, to provide a reasonable starting point, we compute the direction of maximum variance of the parent component and locate two points which are one standard deviation away on either side of its mean (along this direction). These points serve as the initial means for the two children generated due to splitting the parent component. Selecting the initial means in this manner ensures they are reasonably apart from each other and serves as a good starting point for optimizing the two-component sub-mixture. The memberships are initialized by allocating the data points to the closest of the two means. Once the means and the memberships are initialized, the covariance matrices of the two child components are computed.

There are conceivably several variations to how the two-component sub-mixture can be initialized. These include random initialization, selecting two data points as the initial component means, and many others. However, the reason for selecting the direction of maximum variance is to utilize the available characteristic of data, i.e., the distribution within the component α. For von Mises-Fisher mixtures, the maximum variance strategy (as for Gaussian mixtures) cannot be easily adopted, as the data is distributed on the hypersphere. Hence, in this work, we randomly allocate data points

– The effective memberships are updated as given by Equation (48).

\[ r^{(k)}_{\alpha} = \sum_{i=1}^{N} r^{(k)}_{i\alpha} \quad \text{and} \quad n^{(1)}_{\alpha} + n^{(2)}_{\alpha} = N \]  

(48)

– As the sub-mixture comprises of two child components, substitute \( M = 2 \) in Equation (42) to obtain the updates for the weights. These are given by Equation (49).

\[ w^{(k)}_{\alpha} = \frac{n^{(k)}_{\alpha} + 1}{N + 1} \quad \text{and} \quad w^{(1)}_{\alpha} + w^{(2)}_{\alpha} = 1 \]  

(49)

– For Gaussian mixtures, the component parameters \( \Theta^{(k)}_{\alpha} = (\hat{\mu}^{(k)}_{\alpha}, C^{(k)}_{\alpha}) \) are updated as follows:

\[ \hat{\mu}^{(k)}_{a} = \frac{\sum_{i=1}^{N} r^{(k)}_{i\alpha} x_{i}}{\sum_{i=1}^{N} r^{(k)}_{i\alpha}} \quad \text{and} \quad C^{(k)}_{a} = \frac{\sum_{i=1}^{N} r^{(k)}_{i\alpha} (x_{i} - \hat{\mu}^{(k)}_{a}) (x_{i} - \hat{\mu}^{(k)}_{a})^{T}}{\sum_{i=1}^{N} r^{(k)}_{i\alpha} - 1} \]  

(50)

– For von Mises-Fisher mixtures, the component parameters \( \Theta^{(k)}_{\alpha} = (\hat{\mu}^{(k)}_{a}, \hat{\kappa}^{(k)}_{a}) \) are updated as follows:

\[ \hat{\mu}^{(k)}_{a} = \frac{R^{(k)}_{a}}{r^{(k)}_{a}} \quad \text{where} \quad R^{(k)}_{a} = \sum_{i=1}^{N} r^{(k)}_{i\alpha} x_{i} \]  

(51)

\( R^{(k)}_{a} \) represents the magnitude of vector \( R^{(k)}_{a} \). The update of the concentration parameter \( \hat{\kappa}^{(k)}_{a} \) is obtained by solving \( G(\hat{\kappa}^{(k)}_{a}) = 0 \) after substituting \( N \rightarrow \sum_{i=1}^{N} r^{(k)}_{i\alpha} \) and \( R \rightarrow R^{(k)}_{a} \) in Equation (32).

The difference between the EM updates in Equations (43), (44) and Equations (50), (51) is the presence of the coefficient \( r_{i\alpha} \) with each \( x_{i} \). Since we are considering the sub-mixture, the original responsibility \( r_{i\alpha} \) is multiplied by the responsibility within the sub-mixture \( r^{(k)}_{i\alpha} \) to quantify the influence of datum \( x_{i} \) to each of the child components.

After the sub-mixture is locally optimized, it is integrated with the untouched \( M - 1 \) components of \( \mathcal{M} \) to result in a \( M + 1 \) component mixture \( \mathcal{M}' \). An EM is finally carried out on the combined \( M + 1 \) components to estimate the parameters of \( \mathcal{M}' \) and result in an optimized \((M + 1)\)-component mixture as follows.

EM initialization for \( \mathcal{M}' \): Usually, the EM is started by a random initialization of the members. However, because the two-component sub-mixture is now optimal and the \( M - 1 \) components in \( \mathcal{M} \) are also in an optimal state, we exploit this situation to initialize the EM (for \( \mathcal{M}' \)) with a reasonable starting point. As mentioned above, the component with index α with component weight \( w_{\alpha} \) is split. Upon integration, the (child) components that replaced component α will now correspond to indices α and α + 1 in the new mixture \( \mathcal{M}' \). Let \( R' = [r'_{ij}] 1 \leq i \leq N, 1 \leq j \leq M + 1 \) be the responsibility matrix for the new mixture \( \mathcal{M}' \) and let \( w'_{j} \) be the component weights in \( \mathcal{M}' \).
2. **Delete (Line 10 in Algorithm 1):** The goal here is to remove a component from the current mixture and check whether it resulted in a better mixture model to explain the observed data. Assume the component with index \( \alpha \) and the corresponding weight \( w_{\alpha} \) is to be deleted from \( \mathcal{M} \) to generate a \( M - 1 \) component mixture \( \mathcal{M}' \). Once deleted, the data memberships of the component need to be redistributed between the remaining components. The redistribution of data results in a good starting point to employ the EM algorithm to estimate the parameters of \( \mathcal{M}' \) as follows.

**EM initialization for \( \mathcal{M}' \):** Let \( \mathcal{R}' = [r'_{ij}] \) be the \( N \times (M - 1) \) responsibility matrix for the new mixture \( \mathcal{M}' \) and let \( w'_j \) be the weight of \( j^{th} \) component in \( \mathcal{M}' \).

- **Component weights:** The weights are initialized as follows:
  \[
  w'_j = w_j \quad \text{if} \quad j < \alpha \\
  w'_\alpha = w_\alpha w_\alpha^{(1)} \quad \text{and} \quad w'_{\alpha + 1} = w_\alpha w_\alpha^{(2)} \\
  w'_{j-1} = w_j \quad \text{if} \quad j > \alpha + 1 \\
  \]
  (52)

- **Memberships:** The responsibility matrix \( \mathcal{R}' \) is initialized for all data \( x_i \), \( \forall 1 \leq i \leq N \) as follows:
  \[
  r'_{ij} = r_{ij} \quad \text{if} \quad j < \alpha \\
  r'_{i\alpha} = r_{i\alpha} r_{i1} \quad \text{and} \quad r'_{i\alpha + 1} = r_{i\alpha} r_{i2} \\
  r'_{ij} = r_{ij-1} \quad \text{if} \quad j > \alpha + 1 \\
  \text{and} \quad n'_j = \sum_{i=1}^{N} r'_{ij} \quad \forall 1 \leq j \leq M + 1 \\
  \]
  (53)

where \( n'_j \) are the effective memberships of the components in \( \mathcal{M}' \).

With these starting points, the parameters of \( \mathcal{M}' \) are estimated using the traditional EM algorithm with updates in the Maximization-step given by Equations (42), (43), and (44). The EM results in local convergence of the \( (M + 1) \)-component mixture. If the resultant message length of encoding data using \( \mathcal{M}' \) is lower than that due to \( \mathcal{M} \), that means the perturbation of \( \mathcal{M} \) because of splitting component \( \alpha \) resulted in a new mixture \( \mathcal{M}' \) that compresses the data better, and hence, is a better mixture model to explain the data.

2. **Delete (Line 10 in Algorithm 1):** The goal here is to remove a component from the current mixture and check whether it resulted in a better mixture model to explain the observed data. Assume the component with index \( \alpha \) and the corresponding weight \( w_{\alpha} \) is to be deleted from \( \mathcal{M} \) to generate a \( M - 1 \) component mixture \( \mathcal{M}' \). Once deleted, the data memberships of the component need to be redistributed between the remaining components. The redistribution of data results in a good starting point to employ the EM algorithm to estimate the parameters of \( \mathcal{M}' \) as follows.

**EM initialization for \( \mathcal{M}' \):** Let \( \mathcal{R}' = [r'_{ij}] \) be the \( N \times (M - 1) \) responsibility matrix for the new mixture \( \mathcal{M}' \) and let \( w'_j \) be the weight of \( j^{th} \) component in \( \mathcal{M}' \).

- **Component weights:** The weights are initialized as follows:
  \[
  w'_j = \frac{w_j}{1 - w_{\alpha}} \quad \text{if} \quad j < \alpha \\
  w'_j = \frac{w_{j+1}}{1 - w_{\alpha}} \quad \text{if} \quad j \geq \alpha \\
  \]
  (54)

It is to be noted that \( w_{\alpha} \neq 1 \) because the MML update expression in the M-step for the component weights always ensures non-zero weights during every iteration of the EM algorithm (see Equation (42)).

- **Memberships:** The responsibility matrix \( \mathcal{R}' \) is initialized for all data \( x_i \), \( \forall 1 \leq i \leq N \) as follows:
  \[
  r'_{ij} = \frac{r_{ij}}{1 - r_{i\alpha}} \quad \text{if} \quad j < \alpha \\
  r'_{ij} = \frac{r_{i(j+1)}}{1 - r_{i\alpha}} \quad \text{if} \quad j \geq \alpha \\
  \text{and} \quad n'_j = \sum_{i=1}^{N} r'_{ij} \forall 1 \leq j \leq M - 1 \\
  \]
  (55)

where \( n'_j \) are the effective memberships of the components in \( \mathcal{M}' \). It is possible for a datum \( x_i \) to have complete membership in component \( \alpha \) (i.e., \( r_{i\alpha} = 1 \)), in which case, its membership is equally distributed among the other \( M - 1 \) components (i.e., \( r'_{ij} = \frac{1}{M-1}, \forall j \in \{1, M - 1\} \)).

With these readjusted weights and memberships, and the constituent \( M - 1 \) components, the traditional EM algorithm is used to estimate the parameters of the new mixture \( \mathcal{M}' \). If the resultant message length of encoding data using \( \mathcal{M}' \) is lower than that due to \( \mathcal{M} \), that means the perturbation of \( \mathcal{M} \) because of deleting component \( \alpha \) resulted in a new mixture \( \mathcal{M}' \) with better explanatory power, which is an improvement over the current mixture.

3. **Merge (Line 14 in Algorithm 1):** The idea is to join a pair of components of \( \mathcal{M} \) and determine whether the resulting \( (M - 1) \)-component mixture \( \mathcal{M}' \) is any better than the current mixture \( \mathcal{M} \). One strategy to identify an improved mixture model would be to consider merging all possible pairs of components and choose the one which results in the greatest improvement. This would, however, lead to a runtime complexity of \( O(M^2) \), which could be significant for large values of \( M \). Another strategy is to consider merging components which are “close” to each other. For a given component, we identify its closest component by computing the Kullback-Leibler (KL) distance with all others and selecting the one
with the least value. This would result in a linear runtime complexity of \( O(M) \) as computation of KL-divergence is a constant time operation. For every component in \( \mathcal{M} \), its closest match is identified and they are merged to obtain a \( M - 1 \) component mixture \( \mathcal{M}' \). Merging the pair involves reassigning the component weights and the memberships. An EM algorithm is then employed to optimize \( \mathcal{M}' \).

Assume components with indices \( \alpha \) and \( \beta \) are merged. Let their weights be \( w_\alpha \) and \( w_\beta \); and their responsibility terms be \( r_{\alpha i} \) and \( r_{\beta i} \), \( 1 \leq i \leq N \) respectively. The component that is formed by merging the pair is determined first. It is then integrated with the \( M - 2 \) remaining components of \( \mathcal{M} \) to produce a \( (M - 1) \)-component mixture \( \mathcal{M}' \).

**EM initialization for \( \mathcal{M}' \):** Let \( w_i^{(m)} \) and \( r_i^{(m)} \) be the weight and responsibility vector of the merged component \( m \) respectively. They are given as follows:

\[
\begin{align*}
    w_i^{(m)} &= w_\alpha + w_\beta \\
    r_i^{(m)} &= r_{\alpha i} + r_{\beta i}, \quad 1 \leq i \leq N
\end{align*}
\]  

(56)

The parameters of this merged component are estimated as follows:

- **Gaussian:** The parameters \( \Theta^{(m)} = (\mathbf{\mu}^{(m)}, \mathbf{C}^{(m)}) \) are:

\[
\begin{align*}
    \mathbf{\mu}^{(m)} &= \frac{\sum_{i=1}^{N} r_i^{(m)} x_i}{\sum_{i=1}^{N} r_i^{(m)}} \quad \text{and} \quad \mathbf{C}^{(m)} = \frac{\sum_{i=1}^{N} r_i^{(m)} (x_i - \mathbf{\mu}^{(m)})(x_i - \mathbf{\mu}^{(m)})^T}{\sum_{i=1}^{N} r_i^{(m)} - 1}
\end{align*}
\]  

(57)

- **von Mises-Fisher:** The parameters \( \Theta^{(m)} = (\mathbf{\hat{\mu}}^{(m)}, \mathbf{\hat{\kappa}}^{(m)}) \) are:

\[
\mathbf{\hat{\mu}}^{(m)} = \frac{\mathbf{R}^{(m)}}{\mathbf{R}^{(m)}} \quad \text{where} \quad \mathbf{R}^{(m)} = \sum_{i=1}^{N} r_i^{(m)} x_i
\]  

(58)

The concentration parameter \( \mathbf{\hat{\kappa}}^{(m)} \) is obtained by solving \( G(\mathbf{\hat{\kappa}}^{(m)}) = 0 \) after substituting \( N \to \sum_{i=1}^{N} r_i^{(m)} \) and \( R \to \mathbf{R}^{(m)} \) in Equation (32).

The merged component \( m \) with weight \( w_i^{(m)} \), responsibility vector \( r_i^{(m)} \), and parameters \( \Theta^{(m)} \) is then integrated with the \( M - 2 \) components. The merged component and its associated memberships along with the \( M - 2 \) other components serve as the starting point for optimizing the new mixture \( \mathcal{M}' \). If \( \mathcal{M}' \) results in a lower message length compared to \( \mathcal{M} \) that means the perturbation of \( \mathcal{M} \) because of merging the pair of components resulted in an improvement to the current mixture.

### 8.3 Illustrative example of our search procedure

We explain the proposed inference of mixture components through the following example that was also considered by Figueiredo and Jain (2002). Consider a bivariate Gaussian mixture shown in Fig. 1. The mixture has three components with equal weights of 1/3 each and their means at (-2,0), (0,0), and (2,0). The covariance matrices of the three components are the same and are equal to \( \text{diag}(2,0.2) \). We simulate 900 data points from this mixture (as done by Figueiredo and Jain (2002)) and employ the proposed search strategy. The progression of the search method using various operations is detailed below.

**Search for the optimal mixture model:** The method begins by inferring a one-component mixture \( P_1 \) (see Fig. 2(a)). It then splits this component (as described in Split step of Section 8.2) and checks whether there is an improvement in explanation. The red ellipse in Fig 2(b) depicts the component being split. The direction of maximum variance (dotted black line) is first identified, and the means (shown by black dots at the end of the dotted line) are initialized. An EM algorithm is then used to optimize the two children and this results in a mixture \( P_2 \) shown in Fig 2(c). Since the new mixture has a lower message length, the current is updated as \( P_2 \).

In the second iteration, each component in \( P_2 \) is iteratively split, deleted, and merged. Fig. 3 shows the splitting (red) of the first component. On splitting, the new mixture \( P_3 \) results in a lower message length. Deletion of the first component is shown in Fig. 4. Before merging the first component, we identify its
Fig. 2 (a) $P_1$: the one-component mixture after the first iteration (message length $I = 22793$ bits) (b) Red colour denotes the component being split. The dotted line is the direction of maximum variance. The black dots represent the initial means of the two-component sub-mixture (c) $P_2$: optimized mixture post-EM phase ($I = 22673$ bits) results in an improvement.

Fig. 3 Second iteration: splitting the first component in $P_1$ ($I = 22673$ bits) (a) Initial means (shown by the black dots) (b) Optimized child mixture (denoted by red dashed lines) along with the second component of the parent (denoted by black dashes) ($I = 22691$ bits) (c) $P_3$: stabilized mixture post-EM phase ($I = 22460$ bits) results in a further improvement of message length.

closest component (the one with the least KL-divergence) (see Fig. 5). Deletion and merging operations, in this case, do not result in an improvement. These two operations have different intermediate EM initializations (Figures 4(b) and 5(b)) but result in the same optimized one-component mixture. The same set of operations are performed on the second component in $P_2$. In this particular case, splitting results in an improved mixture (same as $P_1$). $P_3$ is updated as the new parent and the series of split, delete, and merge operations are carried out on all components in $P_3$. Fig. 6 shows these operations on the first component. We see that splitting the first component in $P_3$ results in $P_4$ (see Fig. 6(c)). However, $P_4$ is not an improvement over $P_3$ as seen by the message lengths and is, therefore, discarded. Similarly, deletion and merging of the components do not yield improvements to $P_3$. The operations are carried out on the remaining two components in $P_3$ (not shown in the figure) too. These perturbations do not produce improved mixtures in terms of the total message length. Since the third iteration does not result in any further improvement, the search terminates and the parent $P_3$ is considered to be the best mixture.

In different stages of the search method, we have different intermediate mixtures. EM is a gradient descent technique and it can get trapped in a local optimum. By employing the suggested search, we are exhaustively considering the possible options, and aiming to reduce the possibility of the EM getting stuck in a local optimum. The proposed method infers a mixture by balancing the tradeoff due to model complexity and the fit to the data. This is particularly useful when there is no prior knowledge pertaining to the nature of the data. In such a case, this method provides an objective way to infer a mixture with suitable components that best explains the data through lossless compression. Another example is shown in Appendix 13.4, where the evolution of the inferred mixture is explored in the case of a mixture with overlapping components.

Variation of the two-part message length: The search method infers three components and terminates. In order to demonstrate that the inferred number of components is the optimum number, we infer mixtures with increasing number of components (until $M = 15$ as an example) and plot their resultant message lengths. For each $M > 3$, the standard EM algorithm (Section 6.2) is employed to infer the mixture parameters.
Fig. 4 Second iteration: deleting the first component in $P_2$ (a) Green ellipse denotes the component being deleted (b) EM initialization with the remaining component ($I = 25599$ bits) (c) Resultant mixture after deletion and post EM ($I = 22793$ bits) – no improvement.

Fig. 5 Second iteration: merging the two components in $P_2$ (a) Blue ellipses denote the components currently being merged (b) EM initialization with one merged component along with its parameters (c) Optimized mixture after merging ($I = 22793$ bits) – no improvement.

Fig. 7 shows the total message lengths to which the EM algorithm converges for varying number of components $M$. As expected, the total message length (green curve) drastically decreases initially until $M = 3$ components are inferred. Starting from $M = 4$, the total message length gradually increases, clearly suggesting that the inferred models are over-fitting the data with increasing statement cost to encode the additional parameters of these (more complex) models. We further elaborate on the reason for the initial decrease and subsequent increase in the total message length. As per MML evaluation criterion, the message length comprises of two parts – statement cost for the parameters and the cost for stating the data using those parameters. The model complexity (which corresponds to the mixture parameters) increases with increasing $M$. Therefore, the first part of the message to encode parameters increases with an increase in the number of parameters. This behaviour is illustrated by the red curve in Fig. 7. The first part message lengths are shown in red on the right side Y-axis in the figure. As the mixture model becomes increasingly more complex, the error of fitting the data decreases. This corresponds to the second part of the message in the MML encoding framework. This behaviour is consistent with what is observed in Fig. 7 (blue curve). There is a sharp fall until $M = 3$; then onwards increasing the model complexity does not lower the error significantly. The error saturates and there is minimal gain with
regards to encoding the data (the case of overfitting). However, the model complexity dominates after \( M = 3 \). The optimal balance is achieved when \( M = 3 \). In summary, the message length at \( M = 3 \) components was rightly observed to be the optimum for this example. We note that for a fixed number of mixture components, the EM algorithm for the MML metric is monotonically decreasing. However, while searching for the number of components, MML continues to decrease until some optimum is found and then steadily increases as illustrated through this example.

9 Experiments with Gaussian mixtures

We compare our proposed inference methodology against the widely cited method of Figueiredo and Jain (2002). The performance of their method is compared against that of Bayesian Information Criterion (BIC), Integrated Complete Likelihood (ICL), and approximate Bayesian (LEC) methods (discussed in Section 7). It was shown that the method of Figueiredo and Jain (2002) was far superior than BIC, ICL and LEC (using Gaussian mixtures). In the following sections, we demonstrate through a series of experiments that our proposed approach to infer mixtures fares better when compared to that of Figueiredo and Jain (2002). The experimental setup is as follows: we use a Gaussian mixture \( \mathcal{M} \) (true distribution), generate a random
sample from it, and infer the mixture using the data. This is repeated 50 times and we compare the performance of our method against that of Figueiredo and Jain (2002). As part of our analysis, we compare the number of inferred mixture components as well as the quality of mixtures.

9.1 Methodologies used to compare the mixtures inferred by our proposed approach and FJ’s method

Comparing message lengths: The MML framework allows us to objectively compare mixture models by computing the total message length used to encode the data. The difference in message length gives the log-odds posterior ratio of any two mixtures (Equation (19)). Given some observed data, and any two mixtures, one can determine which of the two best explains the data. Our search methodology uses the scoring function \( I_{\text{MML}} \) defined in Equation (41). As elaborated in Section 7.5, Figueiredo and Jain (2002) use an approximated MML-like scoring function \( I_{\text{FJ}} \) given by Equation (46).

We employ our search method and the method of Figueiredo and Jain (2002) to infer the mixtures using the same data; let the inferred mixtures be \( \mathcal{M}^* \) and \( \mathcal{M}_{\text{FJ}}^* \) respectively. We compute two quantities:

\[
\Delta I_{\text{MML}} = I_{\text{MML}}(\mathcal{M}_{\text{FJ}}^*) - I_{\text{MML}}(\mathcal{M}^*)
\]

and

\[
\Delta I_{\text{FJ}} = I_{\text{FJ}}(\mathcal{M}_{\text{FJ}}^*) - I_{\text{FJ}}(\mathcal{M}^*)
\]

We use the two different scoring functions to compute the differences in message lengths of the resulting mixtures \( \mathcal{M}_{\text{FJ}}^* \) and \( \mathcal{M}^* \). Since the search method used to obtain \( \mathcal{M}^* \) optimizes the scoring function \( I_{\text{MML}} \), it is expected that \( I_{\text{MML}}(\mathcal{M}^*) < I_{\text{MML}}(\mathcal{M}_{\text{FJ}}^*) \) and consequently \( \Delta I_{\text{MML}} > 0 \). This implies that our method is performing better using our defined objective function. However, if \( I_{\text{FJ}}(\mathcal{M}^*) < I_{\text{FJ}}(\mathcal{M}_{\text{FJ}}^*) \), this indicates that our inferred mixture \( \mathcal{M}^* \) results in a lower value of the scoring function that is defined by Figueiredo and Jain (2002). Such an evaluation not only demonstrates the superior performance of our search (leading to \( \mathcal{M}^* \)) using our defined scoring function but also proves it is better using the scoring function as defined by Figueiredo and Jain (2002).

Kullback Leibler (KL) divergence: In addition to using message length based evaluation criterion, we also compare the mixtures using KL-divergence (Kullback and Leibler, 1951). The metric gives a measure of the similarity between two distributions (the lower the value, the more similar the distributions). For a mixture probability distribution, there is no analytical form to compute the metric. However, one can calculate its empirical value (which asymptotically converges to the KL-divergence). In experiments relating to mixture simulations, we know the true mixture \( \mathcal{M}^* \) from which the data \( \{x_i\}, 1 \leq i \leq N \) is being sampled. The KL-divergence is given by the following expression:

\[
D_{\text{KL}}(\mathcal{M}^* || \mathcal{M}) = E_{\mathcal{M}^*} \left[ \log \frac{\Pr(x \mid \mathcal{M}^*)}{\Pr(x \mid \mathcal{M})} \right] \approx \frac{1}{N} \sum_{i=1}^{N} \log \frac{\Pr(x_i \mid \mathcal{M}^*)}{\Pr(x_i \mid \mathcal{M})}
\]

where \( \mathcal{M} \) is a mixture distribution (\( \mathcal{M}^* \) or \( \mathcal{M}_{\text{FJ}}^* \)) whose closeness to the true mixture \( \mathcal{M}^* \) is to be determined.

9.2 Bivariate mixture simulation

An experiment conducted by Figueiredo and Jain (2002) was to randomly generate \( N = 800 \) data points from a two-component (with equal mixing proportions) bivariate mixture \( \mathcal{M} \) whose means are at \( \mu_1 = (0, 0)^T \) and \( \mu_2 = (\delta, 0)^T \), and equal covariance matrices: \( C_1 = C_2 = I \) (the identity matrix), and compare the number of inferred components. We repeat the same experiment here and compare with the results of Figueiredo and Jain (2002). The separation \( \delta \) between the means is gradually increased and the percentage of the correct selections (over 50 simulations) as determined by the two search methods is plotted. Fig. 8(a) shows the results of this experiment. As the separation between the component means is increased, the number of correctly inferred components increases. We conducted another experiment where we fix the separation between the two components and increase the amount of data being sampled from the mixture. Fig. 8(b) illustrates the results for a separation of \( \delta = 2.0 \). As expected, increasing the sample size results in an increase in the number of correct selections. Both the search methods eventually infer the true number of components at sample size \( > 3500 \). We note that in both these cases, the differences in message lengths \( \Delta I_{\text{MML}} \) and \( \Delta I_{\text{FJ}} \) are close to zero. The KL-divergences for the mixtures inferred by the two search methods are also the same. Therefore, for this experimental setup, the performance of both the methods is roughly similar.

As the difference between the two search methods is not apparent from these experiments, we wanted to investigate the behaviour of the methods with smaller sample sizes. We repeated the experiment similar to that shown in Fig. 8(a) but with a sample size of \( N = 100 \). Our search method results in a mean value close to 1 for different values of \( \delta \) (see Table 1). The mean value of the number of inferred components using the search method of Figueiredo and Jain (2002) fluctuates between 2 and 3. However, there is significant variance in the number of inferred components (see Table 1). These results are also depicted through a boxplot (Fig. 9). There are many instances where the number of inferred components is more than 3. The results indicate that the search method (FJ) is overfitting the data.
Further, we evaluate the correctness of the mixtures inferred by the two search methods by comparisons using the message length formulations and KL-divergence. Fig. 10 shows the boxplot of the difference in message lengths of the mixtures $\mathcal{M}^*$ inferred using our proposed search method and the mixtures $\mathcal{M}^{FJ}$ inferred using that of Figueiredo and Jain (2002). $\Delta I_{\text{MML}} > 0$ across all values of $\delta$ for the 50 simulations. As per Equation (59), we have $I_{\text{MML}}(\mathcal{M}^*) < I_{\text{MML}}(\mathcal{M}^{FJ})$. This implies that $\mathcal{M}^*$ has a lower message length compared to $\mathcal{M}^{FJ}$ when evaluated using our scoring function. Similarly, we have $\Delta I_{\text{FJ}} < 0$, i.e., $I_{\text{FJ}}(\mathcal{M}^*) > I_{\text{FJ}}(\mathcal{M}^{FJ})$. This implies that $\mathcal{M}^{FJ}$ has a lower message length compared to $\mathcal{M}^*$ when evaluated using FJ’s scoring function. These results are not surprising as $\mathcal{M}^*$ and $\mathcal{M}^{FJ}$ are obtained using the search methods which optimize the respective MML and MML-like scoring functions.

We then analyzed the KL-divergence of $\mathcal{M}^*$ and $\mathcal{M}^{FJ}$ with respect to the true bivariate mixture $\mathcal{M}$ over all 50 simulations and across all values of $\delta$. Ideally, the KL-divergence should be close to zero. Fig. 11(a) shows the KL-divergence of the mixtures inferred using the two search

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**Table 1** The mean and variance of the number of inferred components for each $\delta$ value ($N = 100$ and over 50 simulations).

| Separation $\delta$ | Proposed Mean | Proposed Variance | FJ Mean | FJ Variance |
|---------------------|---------------|-------------------|---------|-------------|
| 1.8                 | 1.02          | 0.020             | 1.98    | 2.673       |
| 1.9                 | 1.00          | 0.000             | 2.26    | 2.482       |
| 2.0                 | 1.00          | 0.000             | 2.04    | 2.325       |
| 2.1                 | 1.02          | 0.020             | 2.20    | 3.510       |
| 2.2                 | 1.04          | 0.039             | 2.20    | 2.285       |
| 2.3                 | 1.06          | 0.057             | 2.44    | 3.639       |
| 2.4                 | 1.06          | 0.098             | 2.54    | 3.967       |
| 2.5                 | 1.04          | 0.039             | 2.98    | 3.203       |
| 2.6                 | 1.10          | 0.092             | 2.42    | 2.942       |

---

**Fig. 8** 2-dimensional mixture (a) Percentage of correct selections with varying separation for a fixed sample size of $N = 800$ (b) Average number of inferred mixture components with different sample sizes and a fixed separation of $\delta = 2.0$ between component means.

**Fig. 9** Box-whisker plot showing the variability in the number of inferred components ($N = 100$ and over 50 simulations).

**Fig. 10** Bivariate mixture ($N = 100$): difference in message lengths computed using the two different scoring functions (see Equation (59)).
methods with respect to \( \mathcal{M}^t \) when the separation is \( \delta = 2.0 \). The proposed search method infers mixtures whose KL-divergence (denoted by red lines) is close to zero, and more importantly less than the KL-divergence of mixtures inferred by the search method of Figueiredo and Jain (2002) (denoted by blue lines). The same type of behaviour is noticed with other values of \( \delta \). Fig. 11(b) compares the KL-divergence for varying values of \( \delta \). The median value of the KL-divergence due to the proposed search method is close to zero with not much variation. The search method of Figueiredo and Jain (2002) always result in KL-divergence higher than that of ours. The results suggest that, in this case, mixtures \( \mathcal{M}^{FJ} \) inferred by employing the search method of Figueiredo and Jain (2002) deviate significantly from the true mixture distribution \( \mathcal{M}^t \). This can also be explained by the fact that there is a wide spectrum of the number of inferred components (Fig. 9). This suggests that the MML-like scoring function is failing to control the tradeoff between complexity and quality of fit, and hence, is selecting overly complex mixture models.

**Fig. 11** Comparison of inferred mixtures using KL-divergence (bivariate example with \( N = 100 \) and 50 simulations) (a) Particular case of \( \delta = 2.0 \) (b) For all values of \( \delta \in \{1.8, \ldots, 2.6\} \).

### 9.3 Simulation of 10-dimensional mixtures

Along the lines of the previous experiment, Figueiredo and Jain (2002) conducted another experiment for a 10-variate two-component mixture \( \mathcal{M}^t \) with equal mixing proportions. The means are at \( \mathbf{\mu}_1 = (0, \ldots, 0)^T \) and \( \mathbf{\mu}_2 = (\delta, \ldots, \delta)^T \), so that the Euclidean distance between them is \( \delta \sqrt{10} \). The covariances of the two components are \( \mathbf{C}_1 = \mathbf{C}_2 = \mathbf{I} \) (the identity matrix). Random samples of size \( N = 800 \) were generated from the mixture and the number of inferred components are plotted. The experiment is repeated for different values of \( \delta \) and over 50 simulations. Fig. 12(a) shows the number of inferred components using the two search methods. At lower values of \( \delta \), the components are close to each other, and hence, it is relatively more difficult to correctly infer the true number of components. We observe that our proposed method performs clearly better than that of Figueiredo and Jain (2002) across all values of \( \delta \). We also compared the quality of these inferred mixtures by calculating the difference in message lengths using the two scoring functions and the KL-divergence with respect to \( \mathcal{M}^t \). For all values of \( \delta \), \( \Delta I_{MML} > 0 \), i.e., our inferred mixtures \( \mathcal{M}^* \) have a lower message length compared to \( \mathcal{M}^{FJ} \) when evaluated using our scoring function. More interestingly, we also note that \( \Delta I_{FJ} > 0 \) (see Fig. 13(a)). This reflects that \( \mathcal{M}^* \) have a lower message length compared to \( \mathcal{M}^{FJ} \) when evaluated using the scoring function of Figueiredo and Jain (2002). This suggests that their search method results in a sub-optimal mixture \( \mathcal{M}^{FJ} \) and fails to infer the better \( \mathcal{M}^* \).

In addition to the message lengths, we analyze the mixtures using KL-divergence. Similar to the bivariate example in Fig. 11(a), the KL-divergence of our inferred mixtures \( \mathcal{M}^* \) is lower than \( \mathcal{M}^{FJ} \), the mixtures inferred by Figueiredo and Jain (2002). Fig. 13(b) shows the boxplot of KL-divergence of the inferred mixtures \( \mathcal{M}^* \) and \( \mathcal{M}^{FJ} \). At higher values of \( \delta > 1.45 \), the median value of KL-divergence is close to zero, as the number of correctly inferred components (Fig. 12(a)) is more than 90%. However, our method always infers mixtures \( \mathcal{M}^* \) with lower KL-divergence compared to \( \mathcal{M}^{FJ} \). These experimental results demonstrate the superior performance of our proposed search method.

Another experiment was carried out where the \( \delta = 1.20 \) was held constant (extremely close components), gradually increased the sample size \( N \), and plotted the average number of inferred components by running 50 simulations for each \( N \). Fig. 12(b) shows the results for the average number of inferred components as the amount of data increases. Our search method, on average, infers the true mixture when the sample size is \( \sim 1000 \). However, the search method of Figueiredo and
Fig. 12 10-dimensional mixture: (a) Percentage of correct selections with varying $\delta$ for a fixed sample size of $N = 800$ (separation between the means is $\delta \sqrt{10}$) (b) Average number of inferred mixture components with different sample sizes and $\delta = 1.20$ between component means.

Fig. 13 Comparison of mixtures with respect to the 10-variate true mixture and $N = 800$ (a) Difference in message lengths computed using the two scoring functions (b) Box-whisker plot of KL-divergence

Jain (2002) requires larger amounts of data; even with a sample size of 2000, the average number of inferred components is $\sim 1.9$. In Fig. 12(b), the red curve reaches the true number of 2 and saturates more rapidly than the blue curve.

9.4 The impact of weight updates as formulated by Figueiredo and Jain (2002)

One of the drawbacks associated with the search method of Figueiredo and Jain (2002) is due to the form of the updating expression for the component weights (Equation (47)). As discussed in Section 7.5.2, a particular instance of wrong inference is bound to happen when the net membership of a (valid) component is less than $N_p/2$, where $N_p$ is the number of free parameters per component. In such a case, the component weight is updated as zero, and it is eliminated, effectively reducing the mixture size by one.

We conducted the following experiment to demonstrate this behaviour: we considered the two-component 10-variate mixture $M^t$ as before and randomly generate samples of size 50 from the mixture. Since the constituent components of $M^t$ have equal weights, on average, each component has a membership of 25. We used $\delta = \{10, 100, 1000\}$, so that the two components are well apart from each other. For each $\delta$, we run 50 simulations and analyze the number of inferred components. As expected, the search method of Figueiredo and Jain (2002) always infer a mixture with one component regardless of the separation $\delta$. Our method always infers the correct number of components. In order to test the validity of mixtures inferred by our proposed method, we analyze the resultant mixtures by comparing the message lengths as discussed.
in Section 9.1. Fig. 14(a) shows the difference in message lengths $\Delta I_{MML}$ given in Equation (59). We observe that $\Delta I_{MML} > 0$ for all $\delta$. This demonstrates that our search based mixtures $\mathcal{M}^*$ have lower message lengths compared to mixtures $\mathcal{M}^{FJ}$ using our scoring function. The same phenomenon is observed when using the MML-like scoring function of Figueiredo and Jain (2002). In Fig. 14(b), we observe that $\Delta I_{FJ} > 0$, which means our search based mixtures $\mathcal{M}^*$ have lower message lengths compared to mixtures $\mathcal{M}^{FJ}$ when evaluated using their scoring function.

This demonstrates that $\mathcal{M}^*$ is a better mixture as compared to $\mathcal{M}^{FJ}$ and their search method is unable to infer it. We also note that the differences in message lengths increases with increasing $\delta$. This is because for the one-component inferred mixture $\mathcal{M}^{FJ}$, the second part of the message (Equation (46)) which corresponds to the negative log-likelihood term increases because of poorer fit to the data. The two modes in the data become increasingly pronounced as the separation between constituent components of the true mixture increases, and hence, modelling such a distribution using a one-component mixture results in a poorer fit. This is clearly an incorrect inference.

We further strengthen our case by comparing the KL-divergence of the inferred mixtures $\mathcal{M}^*$ and $\mathcal{M}^{FJ}$ with respect to the true mixture. Fig. 15 illustrates the results. As $\delta$ increases, the blue coloured plots shift higher. These correspond to mixtures $\mathcal{M}^{FJ}$ inferred by Figueiredo and Jain (2002). Our search method, however, infers mixtures $\mathcal{M}^*$ which have lower KL-divergence. The figure indicates that the inferred mixtures $\mathcal{M}^*$ are more similar to the true distribution as compared to mixtures $\mathcal{M}^{FJ}$.

These experiments demonstrate the ability of our search method to perform better than the widely used method of Figueiredo and Jain (2002). We compared the resulting mixtures using our proposed MML formulation and the MML-like formulation of Figueiredo and Jain (2002), showing the advantages of the former over the latter. We also used a neutral metric, KL-divergence, to establish the closeness of our inferred mixtures to the true distributions. We will now illustrate the behaviour of our search method on two real world datasets.

9.5 Analysis of the computational cost

At any intermediate stage of the search procedure, a current mixture with $M$ components requires $M$ number of split, delete, and merge operations before it is updated. Each of the perturbations involve performing an EM to optimize the corresponding mixture parameters. To determine the convergence of EM, we used a threshold of $10^{-5}$ which was the same as used by
Figueiredo and Jain (2002). FJ’s method also requires to start from an initial large number of components. We used 25 as an initial number based on what was suggested in Figueiredo and Jain (2002). We investigate the number of times the EM routine is called and compare it with that of Figueiredo and Jain (2002). We examine with respect to the simulations that were carried out previously. For the bivariate mixture discussed in Section 9.2, the number of resulting EM iterations when the sample sizes are \(N = 800\) and \(N = 100\) are compared in Fig. 16(a), (b) respectively.

![Fig. 16](image)

Fig. 16 Number of EM iterations performed during the mixture simulations discussed in Sections 9.2 and 9.3.

As per the discussion in Section 9.2, at \(N = 800\), the average number of components inferred by the two methods are about the same (Fig. 8(a)). However, the number of EM iterations required by FJ’s method is greater than 200 across all values of \(\delta\) (Fig. 16(a)). In contrast, the proposed method, on average, requires fewer than 50 iterations. In this case, both methods produce a similar result with FJ’s method requiring more number of EM iterations. When the bivariate mixture simulation is carried out using \(N = 100\), the number of EM iterations required by FJ’s method, on average, is greater than 100, while the proposed method requires fewer than 40 iterations (Fig. 16(b)). In this case, the proposed method not only infers better mixtures (as discussed in Section 9.2) but is also conservative with respect to computational cost.

For the simulation results corresponding to the 10-variate mixtures in Section 9.3, the proposed method requires close to 50 iterations on average, while FJ’s method requires about 20 (Fig. 16(c)). However, the mixtures inferred by the proposed method fare better when compared to that of FJ (Figs. 12, 13). Furthermore, for the simulation results explained in Section 9.4, FJ’s method stops after 3 EM iterations. This is because their program does not accommodate components when the memberships are less than \(N_p/2\). The proposed method requires 18 EM iterations on average and infers the correct mixture components. In these two cases, our method infers better quality mixtures, with no significant overhead with regard to the computational cost.

9.6 Acidity data set (Richardson and Green, 1997; McLachlan and Peel, 1997)

The first example is the univariate acidity data set which contains 155 points. Our proposed search method infers a mixture \(M^*\) with 2 components whereas the search method of Figueiredo and Jain (2002) infers a mixture \(M^{FJ}\) with 3 components. The inferred mixtures are shown in Fig. 17 and their corresponding parameter estimates are given in Table 2. In order to compare the mixtures inferred by the two search methods, we compute the message lengths of the inferred mixtures using our complete MML and the approximated MML-like scoring functions.

When evaluated using our MML scoring function, our inferred mixture results in a gain of \(\sim 4\) bits (see Table 3). Based on the MML framework, our two-component mixture \(M^*\) is \(2^4\) times more likely than the three-component mixture \(M^{FJ}\) (as per Equation (19)). Furthermore, when the inferred mixtures are evaluated as per the MML-like scoring function, \(M^*\) is still considered better (\(\sim 298\) bits) than \(M^{FJ}\) (\(\sim 320\) bits). Thus, using both forms of scoring function, \(M^*\) is the better mixture model of this data set.
9.7 Iris data set (Anderson, 1935; Fisher, 1936)

The second example is the popular Iris data set. The data is 4-dimensional and comes from three Iris species namely, *Iris-setosa*, *Iris-versicolor*, and *Iris-virginica*. The data size is 150 with each class (species) comprising of 50 representative elements. Our search method infers a 4 component mixture \( \mathcal{M}^* \) and the search method of Figueiredo and Jain (2002) infers a 3 component mixture \( \mathcal{M}^{FJ} \) (see Fig. 18). Table 4 shows the memberships of the 150 elements in each of the components in the inferred mixtures. We notice an additional component M4 in \( \mathcal{M}^* \) which has a net membership of 9.51, that is \( \sim 6\% \) of the entire data set. It appears that the component M2 in \( \mathcal{M}^{FJ} \) (Table 4(b)) is split into two components M2 and M4 in \( \mathcal{M}^* \) (Table 4(a)). The quality of the inferred mixtures is determined by comparing their message lengths using the MML and MML-like scoring functions. Table 5 shows the values obtained using the two formulations. When evaluated using our complete MML formulation, our inferred mixture \( \mathcal{M}^* \) results in extra compression of \( \sim 1 \) bit, which makes it twice as likely as \( \mathcal{M}^{FJ} \) – it is a closely competing model compared to ours. When evaluated using the MML-like scoring function, our inferred mixture still has a lower message length compared to \( \mathcal{M}^{FJ} \). In both the cases, the mixture \( \mathcal{M}^* \) inferred by our search method is preferred.

### Table 2

The parameters of the inferred mixtures shown in Fig. 17

| Component index | Weight | Parameters \((\mu, \sigma^2)\) |
|-----------------|--------|----------------------------|
| 1               | 0.41   | 6.24, 0.28                 |
| 2               | 0.59   | 4.33, 0.14                 |

(a) Proposed

| Component index | Weight | Parameters \((\mu, \sigma^2)\) |
|-----------------|--------|----------------------------|
| 1               | 0.34   | 6.39, 0.17                 |
| 2               | 0.35   | 4.21, 0.05                 |
| 3               | 0.31   | 4.71, 0.36                 |

(b) FJ

### Table 3

Message lengths (measured in bits) of the mixtures (in Fig. 17) as evaluated using the MML and MML-like scoring functions.

| Scoring functions | Proposed \((\mathcal{M}^*)\) | FJ \((\mathcal{M}^{FJ})\) |
|-------------------|-----------------------------|---------------------------|
| MML               | 6373.01                     | 6374.27                   |
| MML-like          | 298.68                      | 320.02                    |

### Table 4

Memberships of Iris data as using the inferred mixtures in Fig. 18 (a) Distribution of data using \( \mathcal{M}^* \) (b) Distribution of data using \( \mathcal{M}^{FJ} \)

| Species          | M1  | M2  | M3  | M4  |
|------------------|-----|-----|-----|-----|
| setosa           | 50  | 0   | 0   | 0   |
| versicolor       | 0   | 5.64| 44.36| 0   |
| virginica        | 0   | 40.29| 0.20| 9.51|

(a) Data distribution using 4 components

| Species          | M1  | M2  | M3  |
|------------------|-----|-----|-----|
| setosa           | 50  | 0   | 0   |
| versicolor       | 0   | 5.55| 44.45|
| virginica        | 0   | 49.78| 0.22|

(b) Data distribution using 3 components

### Table 5

Message lengths (measured in bits) of the mixtures (in Fig. 18) as evaluated using the MML and MML-like scoring functions.

| Scoring functions | Proposed \((\mathcal{M}^*)\) | FJ \((\mathcal{M}^{FJ})\) |
|-------------------|-----------------------------|---------------------------|
| MML               | 6373.01                     | 6374.27                   |
| MML-like          | 323.31                      | 342.57                    |
Mixture
Principal component 2
-1.5
-1.5
-0.5
0.5
1.5
1.5
-2
-2
-1
-1
0
0
1
1
2
2
3
3
4
4
5
5

For different values of dimensionality \(d\) and concentration parameter \(\kappa\), data of sample size \(N\) are randomly generated from a vMF distribution using the algorithm proposed by Wood (1994). The parameters of a vMF distribution are estimated using the previously mentioned approximations. Let \(\hat{\kappa} = \{\kappa_T, \kappa_N, \kappa_H, \kappa_{MN}, \kappa_{MH}\}\) denote the estimate of \(\kappa\) due to the respective methods.

**Errors in \(\kappa\) estimation:** We first report the errors in \(\kappa\) estimation by calculating the absolute error \(|\hat{\kappa} - \kappa|\) and the squared error \((\hat{\kappa} - \kappa)^2\) averaged over 1000 simulations. The relative error \(\frac{|\hat{\kappa} - \kappa|}{\kappa}\) can be used to measure the percentage error in \(\kappa\) estimation. The following observations are made based on the results shown in Table 6.

- For \(N = 10, d = 10, \kappa = 10\), the average relative error of \(\kappa_T, \kappa_N, \kappa_H\) is \(~25\%\); for \(\kappa_{MN}, \kappa_{MH}\), it is \(~20\%\). When \(N\) is increased to 100, the average relative error of \(\kappa_T\) is 5.09\%, \(\kappa_N, \kappa_H\) is 5.05\%, and \(\kappa_{MN}, \kappa_{MH}\) is 4.9\%. We note that increasing \(N\) while holding \(d\) and \(\kappa\) reduces the error rate across all estimation methods and for all tested combinations of \(d\), \(\kappa\). This is expected because as more data becomes available, the inference becomes more accurate. The plots shown in Figure 19 reflect this behaviour. The mean error at lower values of \(N = 5, 10, 20, 30\) is noticeable. However, as \(N\) is increased to 1000, there is a drastic drop in the error. We note that this behaviour is consistent across all the different estimation methods.

- For fixed \(N\) and \(d\), increasing \(\kappa\) increases the mean absolute error. However, the average relative error decreases. As an example, for \(N = 100, d = 100, \kappa = 10\), the average relative error of \(\kappa_T, \kappa_N, \kappa_H\) is \(~42\%\); for \(\kappa_{MN}, \kappa_{MH}\), it is 36.7\% and 34\% respectively. When \(\kappa\) is increased to 100, the error rate for \(\kappa_T, \kappa_N, \kappa_H\) drops to 2.18\% and for \(\kappa_{MN}, \kappa_{MH}\), it drops to 1.68\%. Further increasing \(\kappa\) by an order of magnitude to 1000 results in average relative errors of 1.4\% for \(\kappa_T, \kappa_N, \kappa_H\) and 1.1\% for \(\kappa_{MN}, \kappa_{MH}\). This indicates that as the data becomes more concentrated, the errors in parameter estimation decrease.

- There does not appear to be a clear pattern of the variation in error rates when \(d\) is changed keeping \(N\) and \(\kappa\) fixed. However, in any case, MML-based approximations have the least mean absolute and mean squared error.

**KL-divergence and message lengths of the estimates:** The quality of parameter inference is further determined by computing the KL-divergence and the message lengths associated with the parameter estimates. The analytical expression to calculate

**Fig. 18** Mixtures inferred by the two search methods using the Iris data set. The data is projected onto the two principal components.
Table 6 Errors in $\kappa$ estimation. The averages are reported over 1000 simulations for each $(N, d, \kappa)$ triple.

| $(N, d, \kappa)$ | Mean absolute error | Mean squared error |
|------------------|---------------------|--------------------|
|                  | Tanabe $\kappa_T$  | Sra $\kappa_S$    | Song $\kappa_S$   | MML $\kappa_M$ | MML $\kappa_{MH}$ |
|                  | $k_T$               | $k_S$              | $k_S$             | $k_M$         | $k_{MH}$         |
| 10,10,10         | 2.501e+0            | 2.486e+0           | 2.486e+0          | 2.008e+0      | 2.012e+0         |
| 10,10,100        | 1.879e+1            | 1.877e+1           | 1.877e+1          | 1.316e+1      | 1.316e+1         |
| 10,100,10        | 1.838e+2            | 1.838e+2           | 1.838e+2          | 1.289e+2      | 1.289e+2         |
| 10,100,100       | 2.716e+1            | 2.716e+1           | 2.716e+1          | 2.708e+1      | 1.728e+1         |
| 10,1000,10       | 2.014e+1            | 2.014e+1           | 2.014e+1          | 1.274e+1      | 1.265e+1         |
| 10,1000,100      | 1.215e+2            | 1.215e+2           | 1.215e+2          | 3.873e+1      | 3.870e+1         |
| 10,10000,10      | 3.415e+2            | 3.415e+2           | 3.415e+2          | 1.129e+2      | 3.186e+2         |
| 10,10000,100     | 2.702e+2            | 2.702e+2           | 2.702e+2          | 1.652e+2      | 1.739e+2         |
| 10,100000,10     | 1.991e+2            | 1.991e+2           | 1.991e+2          | 4.014e+2      | 4.014e+2         |
|                  | 3.092e+1            | 3.097e+1           | 3.097e+1          | 4.906e+1      | 4.906e+1         |
|                  | 3.912e+0            | 3.915e+0           | 3.915e+0          | 3.813e+0      | 3.813e+0         |
|                  | 3.748e+1            | 3.747e+1           | 3.747e+1          | 3.669e+1      | 3.669e+1         |
|                  | 4.223e+0            | 4.223e+0           | 4.223e+0          | 3.674e+0      | 3.644e+0         |
|                  | 2.187e+0            | 2.186e+0           | 2.186e+0          | 1.685e+0      | 1.683e+0         |
|                  | 1.447e+1            | 1.447e+1           | 1.447e+1          | 1.129e+1      | 1.129e+1         |
|                  | 9.150e+1            | 9.150e+1           | 9.150e+1          | 9.146e+1      | 8.251e+1         |
|                  | 4.299e+1            | 4.299e+1           | 4.299e+1          | 4.882e+1      | 4.080e+1         |
|                  | 1.833e+1            | 1.833e+1           | 1.833e+1          | 8.821e+0      | 8.821e+0         |

Fig. 19 Box-whisker plots illustrating the $\kappa$ estimates as the sample size is gradually increased. True distribution is a 10-dimensional vMF with $\kappa = 10$. The plots are also indicative of the bias due to the estimates.

the KL-divergence of any two vMF distributions is derived in the Appendix. The KL-divergence is computed between the estimated parameters and the true vMF parameters. The minimum message length expression for encoding data using a vMF distribution is previously derived in Equation (31). Table 7 lists the average values of both the metrics. The MML estimates are the least. From Table 7, we notice that when $N = 10$, $k_{MH}$ result in extra compression of $\sim 1.5$ bits over $k_T$, $k_S$, $k_{MH}$, which makes the MML estimates 2.15 times more likely than the others (as per Equation (19)).

Bias of the parameter estimates: The maximum likelihood estimate of $\kappa$ is known to have significant bias (Schou, 1978; Best and Fisher, 1981; Cordeiro and Vasconcellos, 1999). Our goal here is to demonstrate that MML-based parameter approximations result in estimates with reduced bias. The mean squared error in Table 6 can be decomposed into the sum of
bias and variance terms as shown below (Taboga, 2012).

\[ \text{mean squared error} = \mathbb{E}[(\hat{\kappa} - \kappa)^2] = \mathbb{E}[(\hat{\kappa} - \mathbb{E}[\hat{\kappa}])^2] + \mathbb{E}[(\hat{\kappa} - \mathbb{E}[\hat{\kappa}])^2] \]

where \( \mathbb{E}[\cdot] \) denotes the expectation of the related quantity. Table 8 shows the bias-variance of the estimated concentration parameter \( \hat{\kappa} \) in the above simulations. The bias of \( \hat{\kappa}_{\text{MN}} \) and \( \hat{\kappa}_{\text{MML}} \) is lower compared to the other estimates. The variance of the MML estimates, however, is not always the least, as observed in Table 8. The combination of bias and variance, which is the mean squared error, is empirically demonstrated to be the least for the MML estimates.

### Table 7: Comparison of the \( \kappa \) estimates using KL-divergence and message length formulation (both metrics are measured in bits).

#### Table 8: Bias-variance decomposition of the squared error \((\hat{\kappa} - \kappa)^2\).

#### Statistical hypothesis testing: There have been several goodness-of-fit methods proposed in the literature to test the null hypothesis of a vMF distribution against some alternative hypothesis (Kent, 1982; Mardia et al., 1984; Mardia and Jupp, 2000). Recently, Figueroed (2012) suggested tests for the specific case of concentrated vMF distributions. Here, we examine the behavior of \( \kappa \) estimates for generic vMF distributions as proposed by Mardia et al. (1984). They derived a likelihood ratio test for the null hypothesis of a vMF distribution (\( H_0 \)) against the alternative of a Fisher-Bingham distribution (\( H_a \)). The asymptotically equivalent Rao’s score statistic (Rao, 1973) was used to test the hypothesis.
The score statistic $\mathcal{W}$, in this case, is a function of the concentration parameter. It has an asymptotic $\chi^2(p)$ distribution (with degrees of freedom $p = 2(d + 1) - 1$) under $H_0$ as the sample size $N \to \infty$. For $d = \{10, 100, 1000\}$, the critical values at 5% significance level are given in Table 9. If the computed test statistic exceeds the critical value, then the null hypothesis of a vMF distribution is rejected. We conduct a simulation study where we generate random samples of size $N = 1$ million from a vMF distribution with known mean and $\kappa = \{10, 100, 1000\}$. For each inferred estimate $\hat{\kappa}$, we compute the test statistic and compare it with the corresponding critical value. The results are shown in Table 9. For $d = 10$, the approximation $\kappa_T$ has a significant effect as its test statistic exceeds the critical value and consequently the p-value is close to zero. This implies that the null hypothesis of a vMF distribution is rejected by using the estimate $\kappa_T$. However, this is incorrect as the data was generated from a vMF distribution. The p-values due to the estimates $\kappa_{MN}$, $\kappa_{MH}$, $\kappa_{MN}$, $\kappa_{MH}$ are all greater than 0.05 (the significance level) which implies that the null hypothesis is accepted. For $d = \{100, 1000\}$, the p-values corresponding to the different estimates are greater than 0.05. In these cases, the use of all the estimates lead to the same conclusion of accepting the null hypothesis of a vMF distribution. As the amount of data increases, the error due to all the estimates decreases. This is further exemplified below.

### Table 9: Goodness-of-fit tests for the null hypothesis $H_0$: vMF distribution and the alternate hypothesis $H_1$: Fisher-Bingham distribution. Critical values of the test statistic correspond to a significance of 5%.

| $(d, \kappa)$ | Critical value $\chi^2(p)$ | Test statistic | $p$-value of the test |
|---------------|---------------------------|----------------|----------------------|
|               | $\kappa_T$                | $\kappa_S$    | $\kappa_H$          | $\kappa_M$ | $\kappa_M$ |
| 10, 10        | 7.215e+1                  | 5.353e+1      | 5.353e+1            | 5.353e+1 | 5.353e+1 | 0.000e+0 | 5.258e-1 | 5.258e-1 | 5.260e-1 | 5.260e-1 |
| 10, 100       | 7.216e+1                  | 4.949e+1      | 4.949e+1            | 4.949e+1 | 4.949e+1 | 0.000e+0 | 6.247e-1 | 6.247e-1 | 6.267e-1 | 6.267e-1 |
| 10, 1000      | 7.216e+1                  | 5.060e+1      | 5.060e+1            | 5.060e+1 | 5.060e+1 | 0.000e+0 | 5.671e-1 | 5.671e-1 | 5.724e-1 | 5.724e-1 |
| 100, 10       | 5.090e+3                  | 5.090e+3      | 5.090e+3            | 5.090e+3 | 5.090e+3 | 3.739e-1 | 3.739e-1 | 3.739e-1 | 3.741e-1 | 3.741e-1 |
| 100, 100      | 5.010e+3                  | 5.010e+3      | 5.010e+3            | 5.010e+3 | 5.010e+3 | 6.103e-1 | 6.127e-1 | 6.125e-1 | 6.125e-1 |
| 100, 1000     | 5.016e+3                  | 5.018e+3      | 5.018e+3            | 5.022e+3 | 5.022e+3 | 5.427e-1 | 5.597e-1 | 5.571e-1 | 5.571e-1 |
| 1000, 10      | 5.006e+5                  | 5.006e+5      | 5.006e+5            | 5.006e+5 | 5.006e+5 | 4.682e-1 | 4.682e-1 | 4.687e-1 | 4.687e-1 |
| 1000, 100     | 5.005e+5                  | 5.005e+5      | 5.005e+5            | 5.005e+5 | 5.005e+5 | 5.050e-1 | 5.050e-1 | 5.057e-1 | 5.057e-1 |
| 1000, 1000    | 5.007e+5                  | 5.007e+5      | 5.007e+5            | 5.007e+5 | 5.007e+5 | 4.283e-1 | 4.283e-1 | 4.196e-1 | 4.196e-1 |

**Asymptotic behaviour of MML estimates:** Based on the empirical tests, we have so far seen that MML estimates fare better when compared to the other approximations. We now discuss the behaviour of the MML estimates in the limiting case. For large sample sizes ($N \to \infty$), we plot the errors in $\kappa$ estimation. Song et al. (2012) demonstrated that their approximation $\kappa_{MH}$ results in the lowest error in the limiting case. We compute the variation in error in two scenarios with fixed $d = 1000$ and:

1. **increasing $\kappa$:** Fig. 20(a) illustrates the behaviour of the absolute error with increasing $\kappa$. The first observation is that irrespective of the estimation procedure, the error continues to increase with increasing $\kappa$ values (which corroborates our observations in the empirical tests) and then saturates. According to Song et al. (2012), their estimate $\kappa_T$ produces the lowest error which we also see in the figure. Further, our MML Newton approximation $\kappa_{MN}$ actually performs worse than Song’s approximation $\kappa_T$. However, we note that the errors due to MML Halley’s approximation $\kappa_{MH}$ are identical to those produced by $\kappa_T$. This suggests that asymptotically, the approximations achieved by $\kappa_T$ and $\kappa_{MH}$ are more accurate (note that the errors in the limiting case are extremely low).

2. **increasing $R$:** The maximum likelihood estimate of $\kappa$ aims to achieve $F(\kappa) \equiv A_d(\kappa) - \bar{R} = 0$ (Equation 10). Hence, $\log |A_d(\kappa) - \bar{R}|$ gives a measure of the error corresponding to an estimate of $\kappa$. Figure 20(b) depicts the variation of this error with increasing $\bar{R}$. We observe that $\kappa_{MN}$ and $\kappa_{MH}$ produce the least error. We also note that the error produced due to $\kappa_{MN}$ is greater than that produced by $\kappa_{MH}$. However, we highlight the fact that MML-based parameter inference aims to achieve $G(\kappa) \equiv 0$ (Equation 32), a fundamentally different objective function compared to the maximum likelihood based one.

The asymptotic results are shown here by assuming a value of $N = 10^{200}$ (note the corresponding extremely low error rates). In the limiting case, the MML estimate $\kappa_{MH}$ coincides with the ML estimate $\kappa_{ML}$. However, $\kappa_{ML}$’s performance is better compared to the MML Newton’s approximation $\kappa_{MN}$. The same behaviour is observed for when $\kappa$ is fixed and the dimensionality is increased. For enormous amount of data, the ML approximations converge to the MML ones.

### 10.2 MML-based inference of mixtures of vMF distributions

An empirical study is carried out where the proposed search method is employed to infer a mixture using data sampled from a known mixture distribution. The amount of data is gradually increased; for each sample size $N$, the simulation is repeated 50 times and the number of inferred components is plotted (we used MML Halley’s approximation in all the discussed results). The various case studies are discussed below.
1. The true components in the mixture have different mean directions (separated by an angle $\theta$).
2. The true components in the mixture have the same mean direction but different concentration parameters.

Case 1: The true mixture has two components with equal mixing proportions. We consider the case when $d = 3$. The mean of one of the vMF components is aligned with the Z-axis. The mean of the other component is chosen such that the angle between the two means is $\theta^\circ$. Fig. 21(a) illustrates the scenario when the concentration parameters of the constituent components are different. Fig. 21(b) shows the variation in the number of inferred components when the true vMF components have the same concentration parameter. In both scenarios, as the angular separation is increased, the components become more distinguishable and hence, less amount of data is required to correctly identify them.

When the concentration parameters of the constituent components are different, the inference of the mixture is relatively easier compared to the case when the concentration parameters are same. In Fig. 21(a), for all angular separations, the true number of components is correctly inferred at a sample size of $N = 200$. When $\theta = 20^\circ$, the search method converges faster at $N \sim 100$ as compared to $\theta = 5^\circ$, when the convergence is at $N \sim 180$. In Fig. 21(b), when $\theta = 5^\circ$, the search method infers only one-component as the true mixture components are hardly distinguishable. When $\theta = 10^\circ$, even at $N \sim 1000$, the average number of inferred components is $\sim 1.8$. When $\theta = 15^\circ$, the search method converges at $N \sim 300$ as compared to $N \sim 120$ in Fig. 21(a). Clearly, when the component means are different, it is easier to correctly infer mixtures whose components have different concentration parameters.

![Figure 21](image-url)

**Fig. 21** Case 1: Average number of components inferred for the two-component mixture whose means are separated by $\theta^\circ$. 
Case 2: In this case, multivariate \( (d = \{2, 3, 10\}) \) vMF mixtures with equal mixing proportions and same component means are considered. The simulation results of true mixtures with two and three components are presented here.

Fig. 22(a) shows the average number of components inferred for a two-component mixture whose concentration parameters are \( \kappa_1 = 10 \) and \( \kappa_2 = 100 \). For each value of \( d \), as the sample size increases, the average number of inferred components gradually increases until it saturates and reaches the true value (2 in this case). Increasing the sample size beyond this does not impact the number of inferred mixture components. The results for a 3-component mixture with identical means and concentration parameters \( \kappa_1 = 10, \kappa_2 = 100, \) and \( \kappa_3 = 1000 \) are shown in Fig. 22(b). As expected, the average number of inferred components increases in light of greater evidence. However, we note that it requires greater amount of data to correctly infer the three mixture components as compared to the two-component case. In the two-component case (Fig. 22(a)), at around \( N = 450 \), all the three curves converge to the right number of components. For the three-component mixture in Fig. 22(b), up until \( N = 500 \), there is no convergence for \( d = 2, 3 \). For \( d = 10 \), the average number of inferred components converges quickly (at \( N \sim 25 \)) for the 2-component mixture when compared with \( N \sim 100 \) for the 3-component mixture. This is expected as correctly distinguishing three components (with same means) requires far more data.

![Fig. 22](image.png)

**Fig. 22** Case 2: Average number of components inferred when the true mixture has components with the same mean directions but different concentration parameters. (a) 2-component mixture \((\kappa_1 = 10, \kappa_2 = 100)\) (b) 3-component mixture \((\kappa_1 = 10, \kappa_2 = 100, \kappa_3 = 1000)\)

It is also interesting to note that for \( d = 2 \) in Fig. 22(b), the average number of inferred components saturates at 2, while the actual number of mixture components is 3. However, as the amount of available data increases, the (almost) horizontal line shows signs of gradual increase in its slope. Fig. 23 shows the increase in the average number for \( d = 2, 3 \) as the data is increased beyond \( N = 500 \). The blue curve representing \( d = 3 \) stabilizes at \( N \sim 2500 \). However, the red curve \((d = 2)\) slowly starts to move up but the average is still well below the true number. This demonstrates the relative difficulty in estimating the true mixture when the means coincide especially at lower dimensions.

One can imagine that when the means coincide, it would require greater amount of data to accurately infer the true mixture components. However, the amount of data required also depends on the dimensionality in consideration. It appears that as the dimensionality increases, we need smaller amounts of data (as can be seen for the \( d = 10 \) case). In \( d \)-dimensional space, each datum comprises of \( d \) real values with the constraint that it should lie on the unit hypersphere. So the estimation of the mean direction requires the estimation of \((d - 1)\) values and one value for \( \kappa \). When there is \( N \) data, we actually have \( n_d = N \times (d - 1) \) values available for estimating the \( d \) free parameters. For instance, given a sample of size \( N \), for \( d = 2, n_2 = N \) and for \( d = 10, n_{10} = 9N \). We conjecture that this could be a possible reason for faster convergence in high dimensional space. Through these experiments, we have demonstrated the ability of our search method to infer appropriate mixtures in situations with varying difficulty levels.

![Fig. 23](image.png)

**Fig. 23** Gradual increase in the average inferred components for the 3-component mixture in Fig. 22(b).
11 Applications of vMF mixtures

11.1 Application to text clustering

The use of vMF mixtures in modelling high dimensional text data has been investigated by Banerjee et al. (2005). To compute the similarity between text documents requires their representation in some vector form. The elements of the vectors are typically a function of the word and document frequencies in a given collection. These vector representations are commonly used in clustering textual data with cosine based similarity metrics being central to such analyses (Strehl et al., 2000). There is a strong argument for transforming the vectors into points on a unit hypersphere (Salton and McGill, 1986; Salton and Buckley, 1988). Such a normalized representation of text data (which compensates for different document lengths) motivates their modelling using vMF mixture distributions.

Banerjee et al. (2005) used their proposed approximation (Equation (12)) to estimate the parameters of a mixture with known number of components. They did not, however, propose a method to search for the optimal number of mixture components. We not only derived MML estimates which fare better compared to the previous approximations but also apply them to devise a search method to infer the optimal mixtures. Ideally, the search is continued until there is no further improvement in the message length (Algorithm 1). For practical purposes, the search is terminated when the improvement due to the intermediate split, delete and merge operations during the search process is less than 0.01%. Our proposed method to infer mixtures was employed on the datasets that were used in the analysis by Banerjee et al. (2005). The parameters of the intermediate mixtures are estimated using the MML Halley’s estimates (Equation (34)) for the component vMF distributions. Banerjee et al. (2005) use mutual information (MI) to assess the quality of clustering. For given cluster assignments \(X\) and the (known) class labels \(Y\), MI is defined as: 

\[
E \left[ \log \frac{\Pr(X,Y)}{\Pr(X)\Pr(Y)} \right].
\]

Along with the message lengths, we use MI as one other evaluation criterion in our analysis. We also compute the average F-measure when the number of clusters is same as the number of actual classes.

For each of the datasets, in the preprocessing step, we generate feature vectors using the most frequently occurring words and generating a TF-IDF score for each feature (word) based on Okapi BM25 score (Robertson and Zaragoza, 2009). These feature vectors are then normalized to generate unit vectors in some \(d\)-dimensional space. Using this as directional data on a hypersphere, a suitable mixture model was inferred using the greedy search proposed in Section 8.

11.1.1 Classic3 dataset

The dataset\(^2\) contains documents from three distinct categories: 1398 Cranfield (aeronautical related), 1033 Medline (medical journals) and 1460 Cisi (information retrieval related) documents. The processed data has \(d = 4358\) features.

**Optimal number of clusters:** In this example, it is known that there are three distinct categories. However, this information is not usually known in real world setting (and we do not know if they are from three vMF distributions). Assuming no knowledge of the nature of the data, the search method infers a mixture with 16 components. The corresponding assignments are shown in Table 10. A closer look at the generated assignments illustrate that each category of documents is represented by more than one component. The three categories are split to possibly represent specialized sub-categories. The Cisi category is distributed among 6 main components (M4 – M9). The Cranfield documents are distributed among M6, M10 – M15 components and the Medline category is split into M0 – M3, and M6 components. We observe that all but three components are non-overlapping; only M6 has representative documents from all three categories.

|       | M0 | M1 | M2 | M3 | M4 | M5 | M6 | M7 | M8 | M9 | M10 | M11 | M12 | M13 | M14 | M15 |
|-------|----|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|
| cisi  | 0  | 0  | 0  | 0  | 288| 133| 28 | 555| 197| 255| 0   | 0   | 0   | 0   | 0   |
| cran  | 0  | 0  | 0  | 0  | 2  | 0  | 362| 1  | 0  | 0  | 58  | 144 | 135 | 175 | 223 |
| med   | 9  | 249| 376| 138| 2  | 0  | 9  | 0  | 0  | 0  | 0   | 0   | 0   | 0   | 0   |

Table 10 Confusion matrix for 16-component assignment (MML Halley).

The 16-component mixture inferred by the search method is a finer segregation of the data when compared to modelling using a 3-component mixture. The parameters of the 3-component mixture are estimated using an EM algorithm (Section 6.2). Table 11 shows the confusion matrices obtained for the cluster assignments using the various estimation methods. We see that all the estimates perform comparably with each other; there is not much difference in the assignments of data to the individual mixture components.

The collection is comprised of documents that belong to dissimilar categories and hence, the clusters obtained are wide apart. This can be seen from the extremely high F-measure scores (Table 12). For the 3-component mixture, all the five different estimates result in high F-measure values with Song being the best with an average F-measure of 0.978 and a MI

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\(^2\) http://www.dataminingresearch.com/index.php/2010/09/classic3-classic4-datasets/
of 0.982. MML (Halley’s) estimate are close with an average F-measure of 0.976 and a MI of 0.976. However, based on the message length criterion, the MML estimate results in the least message length (∼ 190 bits less than Song’s). The mutual information score using MML estimate is 1.04 (for 16 components) compared to 0.976 for 3 components. Also, the message length is lower for the 16 component case. However, Song’s estimator results in a MI score of 1.043, very close to the score of 1.040 obtained using MML estimates.

### Table 11 Confusion matrices for 3-cluster assignment.

|     | cisi | cran | med |
|-----|------|------|-----|
| cisi | 1441 | 0    | 19  |
| cran | 22   | 1293 | 83  |
| med  | 8    | 0    | 1025|

(a) Banerjee

|     | cisi | cran | med |
|-----|------|------|-----|
| cisi | 1449 | 0    | 11  |
| cran | 24   | 1331 | 43  |
| med  | 8    | 0    | 1025|

(b) Tanabe

|     | cisi | cran | med |
|-----|------|------|-----|
| cisi | 1450 | 0    | 10  |
| cran | 24   | 1339 | 35  |
| med  | 13   | 0    | 1020|

(c) Song

|     | cisi | cran | med |
|-----|------|------|-----|
| cisi | 1450 | 0    | 10  |
| cran | 24   | 1339 | 35  |
| med  | 13   | 0    | 1020|

(d) MML (Halley)

For the Classic3 dataset, Banerjee et al. (2005) analyzed mixtures with greater numbers of components than the “natural” number of clusters. They report that a 3-component mixture is not necessarily a good model and more number of clusters may be preferred for this example. As part of their observations, they suggest to “generate greater number of clusters and combine them appropriately”. However, this is subjective and requires some background information about the likely number of clusters. Our search method in conjunction with the inference framework is able to resolve this dilemma and determine the optimal number of mixture components in a completely unsupervised setting.

### Table 12 Clustering performance on Classic3 dataset.

| Number of clusters | Evaluation metric | Banerjee | Tanabe | Sra | Song | MML (Halley) |
|--------------------|-------------------|----------|--------|-----|------|--------------|
| 3                  | Message length    | 100678069 | 100677085 | 100677087 | 100677080 | 100676891 |
|                    | Avg. F-measure    | 0.9644   | 0.9758   | 0.9758   | 0.9780   | 0.9761   |
|                    | Mutual Information| 0.944    | 0.975    | 0.975    | 0.982    | 0.976    |
| 16                 | Message length    | 100458153 | 100452893 | 100439983 | 100444649 | 100427178 |
|                    | Mutual Information| 1.029    | 1.036    | 0.978    | 1.043    | 1.040    |

### Table 13 Clustering performance on CMU Newsgroup dataset.

| Number of clusters | Evaluation metric | Banerjee | Tanabe | Sra | Song | MML (Halley) |
|--------------------|-------------------|----------|--------|-----|------|--------------|
| 20                 | Message length    | 728666702 | 728545471 | 728585441 | 728536451 | 728523254 |
|                    | Avg. F-measure    | 0.502    | 0.470    | 0.487    | 0.435    | 0.509    |
|                    | Mutual Information| 1.391    | 1.383    | 1.417    | 1.244    | 1.379    |
| 21                 | Message length    | 728497453 | 728498076 | 728432625 | 728374429 | 728275820 |
|                    | Mutual Information| 1.313    | 1.229    | 1.396    | 1.377    | 1.375    |

### 11.1.2 CMU Newsgroup

The dataset contains documents from 20 different news categories each containing 1000 documents. Preprocessing of the data, as discussed above, resulted in feature vectors of dimensionality \( d = 6448 \). The data is first modelled using a mixture containing 20 components. The evaluation metrics are shown in Table 13. The average F-measure is 0.509 for MML-based estimation, slightly better than Banerjee’s score of 0.502. The low F-measure values are indicative of the difficulty in accurately distinguishing the news categories. The mutual information score for MML case is 1.375 which is lower than that of Sra’s. However, the total message length is lower for MML mixture compared to that of others.

**Optimal number of clusters:** The proposed search method when applied to this dataset infers a mixture with 21 components. This is close to the “true” number of 20 (although there is no strong reason to believe that each category corresponds to a vMF component). The mutual information for the 21-cluster assignment is highest for Sra’s mixture with a score of 1.396 and for MML mixture, it is 1.375 (Table 13). However, the total message length is the least for the MML-based mixture.

The analysis of vMF mixtures by Banerjee et al. (2005) for both the datasets considered here shows a continued increase in the MI scores even beyond the true number of clusters. As such, using the MI evaluation metric for different number of mixture components does not aid in the inference of an optimal mixture model. Our search method balances the tradeoff.

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3 http://archive.ics.uci.edu/ml/datasets/Twenty+Newsgroups
between using a certain mixture and its ability to explain the observed data, and thus, objectively aids in inferring mixtures to model the normalized vector representations of a given collection of text documents.

A mixture modelling problem of this kind where there is some information available regarding the nature of the data can be studied by altering the proposed search method. We provide some alternate strategies where the mixture modelling can be done in a semi-supervised setting.

- The priors on the number of components and their parameters can be modelled based on the background knowledge.
- If the true number of clusters are known, only splits may be carried out until we near the true number (each split being the best one given the current mixture). As the mixture size approaches the true number, all the three operations (split, delete, and merge) can be resumed until convergence. This increases the chance that the inferred mixture would have about the same number of components as the true model.
- Another variant could be to start from a number close to the true number and prefer delete/merge operations over the splits. We cannot ignore splits completely because a component after splitting may be merged at a later iteration if there would be an improvement to the message length.
- Another strategy could be to employ the EM algorithm and infer a mixture with the true number of components. This mixture can then be perturbed using split, delete, and merge operations until convergence.

11.2 Mixture modelling of protein coordinate data

The following application concerns the vMF mixture modelling of directional data arising from the orientation of main chain carbon atoms in protein structures. The structures that proteins adopt are largely dictated by the interactions between the constituent atoms. These chemical interactions impose constraints on the orientation of atoms with respect to one another. The directional nature of the protein data and the (almost constant) bond length between the main chain carbon atoms motivate the modelling using vMF mixtures. Further, structural modelling tasks such as generating random protein chain conformations, three-dimensional protein structure alignment, secondary structure assignment, and representing protein folding patterns using concise protein fragments require efficient encoding of protein data (Konagurthu et al., 2012, 2013; Collier et al., 2014). As part of our results, we demonstrate that vMF mixtures offer a better means of encoding and can potentially serve as strong candidate models to be used in such varied tasks.

The dataset considered here is a collection of 8453 non-redundant experimentally determined protein structures from the publicly available ASTRAL SCOP-40 (version 1.75) database (Murzin et al., 1995). For each protein structure, the coordinates of the central carbon, $C_\alpha$, of successive residues (amino acids) are considered. Protein coordinate data is transformed into directional data and each direction vector is characterized by $(\theta, \phi) = (\text{co-latitude}, \text{longitude})$, where $\theta \in [0, 180^\circ]$ and $\phi \in [0, 360^\circ]$. Note that these $(\theta, \phi)$ values have to be measured in a consistent, canonical manner.

To compute $(\theta, \phi)$ corresponding to the point $P_{i+1}$ associated to residue $i + 1$, we consider this point in the context of 3 preceding points, forming a 4-mer comprising of the points $P_{i-2}, P_{i-1}, P_i$ and $P_{i+1}$. This 4-mer is orthogonally transformed into a canonical orientation (Fig. 24) in the following steps:

- translate the 4-mer such that $P_i$ is at the origin.
- rotate the resultant 4-mer so that $P_{i-1}$ lies on the negative X-axis.
- rotate further so that $P_{i-2}$ lies in the XY plane such that the angle between the vector $P_{i-2} - P_{i-1}$ and the positive Y-axis is acute.

The transformation yields a canonical orientation for $P_{i+1}$ with respect to its previous 3 coordinates. Using the transformed coordinates of $P_{i+1}$, the direction $(\theta, \phi)$ of $P_{i+1}$ is computed. We repeat this transformation for every successive set of 4-mers in the protein chain, over all possible source structures in our collection. The data collected in this way resulted in a total of $\sim 1.3$ million $(\theta, \phi)$ pairs for all the 8453 structures in the database.

Protein data is an example where the number of mixture components are not known a priori. Hence, we use the method outlined in Section 8 to infer suitable mixture models. The original dataset comprises of 7 different categories of proteins. The proposed search method using MML (Halley’s) estimates infers a mixture containing 13 vMF components. Further, each protein category can be individually modelled using a mixture. As an example, for the “$\beta$ class” proteins which contains 1802 protein structures and 251,346 corresponding $(\theta, \phi)$ pairs, our search method terminates after inferring 11 vMF components. We compare the MML-based mixtures with those inferred by the standalone EM algorithm (Section 6.2) using
other estimates. These values are presented in Table 14. We observe that the mixtures inferred using the MML estimates result in a message length lower than that obtained using the other estimates.

Fig. 25(a) shows the empirical distribution of directional data of \( C_\alpha \) coordinates belonging to \( \beta \) class. The \((\theta, \phi)\) values with their corresponding frequencies are plotted in Fig. 25(a). Fig. 25(b) is a plot illustrating the 11-component vMF mixture density as inferred for this class of proteins. Notice that the two major modes in the figure correspond to commonly observed local secondary structural bias of residues towards, helices and strands of sheet. Also notice the empty region in the middle which corresponds to physically unrealizable directions in the local chain, excluded in the observed samples due to steric hindrance of the atoms in proteins. If we were to model such data using truncated distributions, the regions of zero probability will be modelled using an infinite code length. As an example, at \((\theta, \phi) = (100^\circ, 200^\circ)\), the truncated distribution would have zero probability and consequently an infinite code length. However, when the same point is explained using the 11-component mixture, it would have a probability of \( \Pr = 3.36 \times 10^{-12} \) and a corresponding code length of \(-\log_2 \Pr = 38.11\) bits. For protein data, it is possible to have such (rare exceptional) observations, due to reasons such as experimental error, noise, or the conformation of the protein itself. Hence, although the empirical distribution has distinct modes, it is better off modelled as a vMF mixture distribution, rather than by truncated distributions.

![Fig. 25](image.png)

**Fig. 25** Distribution of directional data of \( \beta \) class \( C_\alpha \) atoms (a) Empirical distribution (b) Mixture density corresponding to the 11 inferred vMF components

**Compressibility of protein structures:** The explanatory framework of MML allows for testing competing hypotheses. Recently, Konagurthu et al. (2012) developed a null model description of protein coordinate data as part of the statistical inference of protein secondary structure. A null model gives a baseline for transmitting the raw coordinate data. Each \( C_\alpha \) atom is described using the distance and orientation with respect to the preceding \( C_\alpha \) atoms. Because the distance between successive \( C_\alpha \) atoms is highly constrained, compression can only be gained in describing the orientation of a \( C_\alpha \) atom with respect to its previous one.

Konagurthu et al. (2012) describe their null hypothesis by discretizing the surface of a 3D-sphere into chunks of equal areas (of \( \varepsilon^2 \), where \( \varepsilon \) is the accuracy of measurement of coordinate data). This results in \( 4\pi r^2 / \varepsilon^2 \) cells distributed uniformly on the surface of the sphere of radius \( r \) (the distance between successive \( C_\alpha \) coordinates). The cells are uniquely numbered. To encode \( C_\alpha^{i+1} \) with respect to \( C_\alpha^i \), the location of \( C_\alpha^{i+1} \) on the surface is identified and the corresponding cell index is encoded. Using this description, the stated null model results in a message length expression Konagurthu et al. (2012) given by

\[
\text{Uniform Null} = - \log_2 \left( \frac{\varepsilon^2}{4\pi r^2} \right) = \log_2 (4\pi) - 2\log_2 \left( \frac{\varepsilon}{r} \right) \text{ bits.} \tag{61}
\]

The null model of Konagurthu et al. (2012) assumes a uniform distribution of orientation angles on the surface of the sphere. However, this is a crude assumption and one can leverage the directional properties of protein coordinates to build an efficient null model. To this effect, we explore the use of vMF mixtures as null model descriptors for protein structures. Using vMF mixtures, we encode the co-latitude \((\theta)\) and longitude \((\phi)\) angles (described in Section 11.2). The message length expression to encode the orientation angles (using Equation 1) is then given by

\[
\text{vMF Null} = - \log_2 \left( \sum_{j=1}^{M} w_j f_j(x; \Theta_j) \right) - 2\log_2 \left( \frac{\varepsilon}{r} \right) \text{ bits.} \tag{62}
\]
where \( \mathbf{x} \) corresponds to a unit vector described by \((\theta, \phi)\) on the surface of the sphere. Equations (61) and (62) are two competing null models. These are used to encode the directional data corresponding to the 8453 protein structures in the ASTRAL SCOP-40 database. The results are shown in Table 15.

| Category | Tanabe | Sra | Song | MML (Halley) |
|----------|--------|-----|------|--------------|
| \( \beta \) | 5514800 | 5518679 | 5520073 | 5513507 |
| All      | 27818524 | 27833704 | 27839802 | 27803427 |

Table 14 Message lengths (in bits) computed for the inferred protein mixtures using various methods (‘All’ refers to all the 7 protein categories).

| Null model | Total message length (in bits) | Bits per residue |
|------------|--------------------------------|------------------|
| Uniform    | 36119900                        | 27.437           |
| vMF        | 32869700                        | 24.968           |

Table 15 Comparison of the uniform and vMF null model encoding schemes.

The per residue statistic is calculated by dividing the total message length by the sample size (the number of \((\theta, \phi)\) pairs).

This statistic shows that close to 2.5 bits can be saved (on average) if the protein data is encoded using the vMF null model. The vMF null model thus supercedes the naive model of encoding. This can potentially improve the accuracy of statistical inference that is central to the various protein modelling tasks briefly introduced above.

12 Conclusion

We presented a statistically robust approach for inferring mixtures of (i) multivariate Gaussian distributions, and (ii) von Mises-Fisher distributions for \(d\)-dimensional directional data. It is based on the general information-theoretic framework of minimum message length inference. This provides an objective tradeoff between the hypothesis complexity and the quality of fit to the data. An associated search procedure for an optimal mixture model of given data chooses the number of component distributions, \( M \), by minimizing the total message length. We established the better performance of the proposed search algorithm by comparing with a popularly used search method (Figueiredo and Jain, 2002). We demonstrated the effectiveness of our approach through extensive experimentation and validation of our results. We also applied our method to real-world high dimensional text data and to directional data that arises from protein chain conformations. The experimental results demonstrate that our proposed method fares better when compared with the current state of the art techniques.

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13 Appendix

13.1 Supporting derivations required for evaluating $\kappa_{MN}$ and $\kappa_{MH}$

For brevity, we represent $A_0(\kappa)$, $A_0'(\kappa)$, $A_0''(\kappa)$, and $A_0'''(\kappa)$ as $A, A', A''$, and $A'''$ respectively. Expressions to evaluate $A, A'$, and $A''$ are given in Equations (11), (15), and (17) respectively. We require $A'''$ for its use in the remainder of the derivation and we provide its expression below:

$$
A''' = -2AA'' - (d - 1)\frac{A''}{\kappa} - 2(d - 1)\frac{A}{\kappa^2} + 2(d - 1)\frac{1}{\kappa^2}.
$$

Now we discuss the derivation of $G'(\kappa)$ and $G''(\kappa)$ that are required for computing the MML estimate $\kappa_M$ (Equations (33) and (34)). Differentiating Equation 32, we have

$$
G'(\kappa) = \frac{(d - 1)}{2\kappa} + (d + 1)\left(\frac{1}{1 + \kappa^2}\right)^2 + \frac{(d - 1)}{2}\frac{\partial}{\partial \kappa}\left(\frac{A'}{A}\right) + \frac{1}{2}\frac{\partial}{\partial \kappa}\left(\frac{A''}{A'}\right) + nA'\tag{64}
$$

and

$$
G''(\kappa) = \frac{-(d - 1)}{\kappa^3} + (d + 1)\left(\frac{2\kappa^2 - 3}{1 + \kappa^2}\right)^2 + \frac{(d - 1)}{2}\frac{\partial^2}{\partial \kappa^2}\left(\frac{A'}{A}\right) + \frac{1}{2}\frac{\partial^2}{\partial \kappa^2}\left(\frac{A''}{A'}\right) + nA''\tag{65}
$$

Using Equations (11) and (15), we have

$$
\frac{A'}{A} = 1 - A - \frac{(d - 1)}{\kappa}.
$$

$$
\frac{\partial}{\partial \kappa}\left(\frac{A'}{A}\right) = \frac{A'}{A^2} - A' + \frac{(d - 1)}{\kappa^2}.
$$

$$
\frac{\partial^2}{\partial \kappa^2}\left(\frac{A'}{A}\right) = \frac{2}{A^3} - \frac{A''}{A^2} - A'' - \frac{2(d - 1)}{\kappa^3}.
$$

Using Equations (11), (15), (17), and (63) we have

$$
\frac{A''}{A'} = -2A - \frac{(d - 1)}{\kappa} + \frac{(d - 1)A}{\kappa^2}.
$$

$$
\frac{\partial}{\partial \kappa}\left(\frac{A''}{A'}\right) = -2A'' + 2\frac{(d - 1)}{\kappa^2} - \frac{(d - 1)A}{\kappa^3}\left(\frac{\kappa A''}{A'} + 2\right).
$$

$$
\frac{\partial^2}{\partial \kappa^2}\left(\frac{A''}{A'}\right) = -2A''' - \frac{4(d - 1)}{\kappa^3} - (d - 1)\frac{\partial}{\partial \kappa}\left(\frac{AA''}{\kappa^2 A'^2}\right) - 2(d - 1)\frac{\partial}{\partial \kappa}\left(\frac{A}{\kappa^3 A'}\right) + \frac{1}{\kappa^3} - \frac{A}{\kappa^3 A'}(\kappa A'' + 3A')\tag{67}
$$

where

$$
\frac{\partial}{\partial \kappa}\left(\frac{AA''}{\kappa^2 A'^2}\right) = \kappa A A'' + \kappa A^2 A'' - 2\kappa A A'' - 2A A A''
$$

and

$$
\frac{\partial}{\partial \kappa}\left(\frac{A}{\kappa^3 A'}\right) = \kappa^3 A
$$

Equations (66) and (67) can be used to evaluate $G'(\kappa)$ and $G''(\kappa)$ which can then be used to approximate the MML estimates $\kappa_{MN}$ and $\kappa_{MH}$ (Equations (33) and (34)) respectively.
13.2 Derivation of the weight estimates in MML mixture modelling

As per Equation (41), we have

\[ I(\Phi, D) = -\frac{1}{2} \sum_{j=1}^{M} w_j - \sum_{i=1}^{N} \log \sum_{j=1}^{M} w_j f_j(x_i; \Theta_j) + \text{terms independent of } w_j \]

To obtain the optimal weights under the constraint \( \sum_{j=1}^{M} w_j = 1 \), the above equation is optimized using the Lagrangian objective function defined below using some Lagrangian multiplier \( \lambda \).

\[ L(\Phi, D, \lambda) = I(\Phi, D) + \lambda \left( \sum_{j=1}^{M} w_j - 1 \right) \]

For some \( k \in \{1, M\} \), the equation resulting from computing the partial derivative of \( L \) with respect to \( w_k \) and equating it to zero gives the optimal weight \( w_k \).

\[ \frac{\partial L}{\partial w_k} = 0 \implies \lambda = \frac{1}{2w_k} + \sum_{i=1}^{N} w_i f_i(x_i; \Theta_k) \]

We have

\[ \sum_{i=1}^{N} w_i f_i(x_i; \Theta_k) = \frac{1}{w_k} \sum_{i=1}^{N} w_i f_i(x_i; \Theta_k) = \frac{1}{w_k} \sum_{i=1}^{N} r_{ik} = n_k \]

where \( r_{ik} \) and \( n_k \) are the responsibility and effective membership terms given as per Equations (36) and (37) respectively. Substituting the above value in Equation (68), we have

\[ \lambda = \frac{1}{2w_k} + \frac{n_k}{w_k} \implies \lambda w_k = n_k + \frac{1}{2} \]  \quad (69)

There are \( M \) equations similar to Equation (69) for values of \( k \in \{1, M\} \). Adding all these equations together, we get

\[ \lambda \sum_{j=1}^{M} w_j = \sum_{j=1}^{M} n_j + \frac{M}{2} \implies \lambda = N + \frac{M}{2} \]

Substituting the above value of \( \lambda \) in Equation (69), we get \( w_k = \frac{n_k + \frac{1}{2}}{N + \frac{M}{2}} \)

13.3 Derivation of the Kullback-Leibler (KL) distance between two von Mises-Fisher distributions

The closed form expression to calculate the KL divergence between two vMF distributions is presented below. Let \( f(x) = C_d(\kappa_1)e^{\kappa_1 \mu_1^T x} \) and \( g(x) = C_d(\kappa_2)e^{\kappa_2 \mu_2^T x} \) be two von Mises-Fisher distributions with mean directions \( \mu_1, \mu_2 \) and concentration parameters \( \kappa_1, \kappa_2 \). The KL distance between any two distributions is given by

\[ D_{KL}(f\|g) = \int f(x) \log \frac{f(x)}{g(x)} d\mathbf{x} = E_f \left[ \log \frac{f(x)}{g(x)} \right] \]  \quad (70)

where \( E_f[\cdot] \) is the expectation of the quantity \([\cdot]\) using the probability density function \( f \).

\[ \log \frac{f(x)}{g(x)} = \log \frac{C_d(\kappa_1)}{C_d(\kappa_2)} + (\kappa_1 \mu_1 - \kappa_2 \mu_2)^T \mathbf{x} \]

Using the fact that \( E_f[\mathbf{x}] = A_d(\kappa_1) \mu_1 \) (Mardia et al., 1984; Fisher, 1993), we have the following expression:

\[ E_f \left[ \log \frac{f(x)}{g(x)} \right] = \log \frac{C_d(\kappa_1)}{C_d(\kappa_2)} + (\kappa_1 \mu_1 - \kappa_2 \mu_2)^T A_d(\kappa_1) \mu_1 \]

\[ D_{KL}(f\|g) = \log \frac{C_d(\kappa_1)}{C_d(\kappa_2)} + A_d(\kappa_1)(\kappa_1 - \kappa_2 \mu_1^T \mu_2) \]

\[ D_{KL}(f\|g) = \log \frac{C_d(\kappa_1)}{C_d(\kappa_2)} + A_d(\kappa_1)(\kappa_1 - \kappa_2 \mu_1^T \mu_2) \]  \quad (71)
13.4 An example showing the evolution of the mixture model

We consider an example of a mixture with overlapping components and employ the proposed search method to determine the number of mixture components. Figueiredo and Jain (2002) considered the mixture shown in Fig. 26 which is described as follows: let $w_i, \mu_i, \Sigma_i, i \in \{1, 4\}$ be the weight, mean, and covariance matrix of the $i$th component respectively. Then, the mixture parameters are given as

\[
\begin{align*}
    w_1 &= w_2 = w_3 = 0.3, w_4 = 0.1 \\
    \mu_1 &= \mu_2 = (-4, -4)^T, \quad \mu_3 = (2, 2)^T, \quad \mu_4 = (-1, -6)^T \\
    \Sigma_1 &= \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}, \Sigma_2 = \begin{bmatrix} 6 & -2 \\ -2 & 6 \end{bmatrix}, \Sigma_3 = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}, \Sigma_4 = \begin{bmatrix} 0.125 & 0 \\ 0 & 0.125 \end{bmatrix}
\end{align*}
\]

We generate a random sample of size 1000 (similar to Figueiredo and Jain (2002)) and infer mixtures using the proposed heuristic. Below are diagrams which portray the splitting of the individual components. We show a selection of operations which result in improved mixtures.

![Fig. 26 Original mixture consisting of overlapping components.](image)

Fig. 27 First iteration (a) $P_1$: the one-component mixture ($l = 27199$ bits) (b) Red colour denotes the component being split. The dotted line is the direction of maximum variance. The black dots represent the initial means of the two-component sub-mixture (c) $P_2$: optimized mixture post-EM ($l = 26479$ bits) results in an improvement.

![Fig. 28 Second iteration: splitting the (red) component in parent $P_2$ ($l = 26479$ bits) results in an improvement (a) Initial means of the child components (b) Optimized child mixture (denoted by red dashed lines) along with the second component of $P_2$ (denoted by black dashes) ($l = 26467$ bits) (c) $P_3$: stabilized mixture post-EM ($l = 26448$ bits) results in an improvement.](image)
Fig. 29 Third iteration: splitting the (red) components in parent \( P_3 \) \((I = 26418\) bits). We see that there are two splits which result in improved mixtures \( P'_4 \) and \( P_4 \). We select \( P_4 \) as the new parent as it has a lower message length compared to \( P'_4 \).

Fig. 30 Fourth iteration: mixtures resulting from splitting each of the components in parent \( P_4 \) \((I = 26266\) bits). We see that none of the 5-component mixtures result in further reduction of the message length. The search terminated and \( P_4 \) is considered the best mixture.