Robust M-Estimation Based Bayesian Cluster Enumeration for Real Elliptically Symmetric Distributions

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Abstract

Robustly determining the optimal number of clusters in a data set is an essential factor in a wide range of applications. Cluster enumeration becomes challenging when the true underlying structure in the observed data is corrupted by heavy-tailed noise and outliers. Recently, Bayesian cluster enumeration criteria have been derived by formulating cluster enumeration as maximization of the posterior probability of candidate models. This article generalizes robust Bayesian cluster enumeration so that it can be used with any arbitrary Real Elliptically Symmetric (RES) distributed mixture model. Our framework also covers the case of M-estimators that allow for mixture models, which are decoupled from a specific probability distribution. Examples of Huber’s and Tukey’s M-estimators are discussed. We derive a robust criterion for data sets with finite sample size, and also provide an asymptotic approximation to reduce the computational cost at large sample sizes. The algorithms are applied to simulated and real-world data sets, including radar-based person identification, and show a significant robustness improvement in comparison to existing methods.

Index Terms

robust, outlier, cluster enumeration, Bayesian information criterion (BIC), cluster analysis, M-estimation, unsupervised learning, multivariate RES distributions, Huber distribution, Tukey’s loss function, EM algorithm

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I. INTRODUCTION

Cluster enumeration refers to the task of answering the question: How many subgroups of similar points are there in a given data set? Robustly determining the optimal number of clusters, $K$, is an essential factor in a wide range of applications. Providing a universal and objective answer, however, is challenging. It depends on the users’ understanding of what constitutes a cluster and how to deal with outliers and uncertainty about the data. Popular clustering algorithms [1]–[5] rely on small distances (or other measures of similarity) between cluster members, dense areas of the data space, or mixture models of particular statistical distributions.

The focus of this work lies on robust statistical model-based cluster analysis. The algorithms should provide reliable results, even if the cluster distribution is heavy-tailed or if the data set contains outliers. These are untypical data points that may not belong to any of the clusters. The methods should also work for the case when the data size is not huge, such that, clusters may have a relatively small number of associated data samples. Compared to purely data driven unsupervised approaches, model-based methods allow for incorporating prior knowledge and assumptions. Statistically robust methods [6]–[8], such as M-estimators [6] can deal with uncertainty: They account for the fact that the prior knowledge is inexact and the assumptions are only approximately fulfilled.

M-estimators are a generalization of Maximum-Likelihood-Estimators (MLE) where the negative log-likelihood function may be replaced by a robustness inducing objective function. For example, M-estimators may be designed based on the likelihood function of a Real Elliptically Symmetric (RES) distribution. This wide family of distributions is useful in statistically modeling the non-Gaussian behavior of noisy data in many practical applications [9]–[12]. RES distributions include, for example, Gaussian, the Generalized Gaussian [13], the t-distribution, the Compound Gaussian [14], and Huber’s distribution, as special cases. Some M-estimators are not an MLE. For example, Tukey’s estimator is designed to completely reject outlying observations by giving them zero-weight. This behavior is beneficial when outliers are generated by a contaminating distribution that strongly differs from the assumed distribution (often the Gaussian).

A popular strategy in robust cluster enumeration is to use model selection criteria, such as the Bayesian Information Criterion (BIC) derived by Schwarz [15], [16] in combination with robust clustering algorithms. For example, after either outlier detection and removal [17]–[20],
modeling noise or outliers using an additional component in a mixture model [21], [22], or by modeling the data as a mixture of heavy tailed distributions [23], [24]. A “robustified likelihood” is complemented by a general penalty term to establish a trade-off between robust data-fit and model complexity. However, Schwarz’ BIC is generic and it does not take the specific clustering problem into account. The penalty term only depends on the number of model parameters and on the number of data points. Therefore, it penalizes two structurally different models the same way if they have the same number of unknown parameters [25], [26].

Recently, a BIC for cluster analysis has been derived by formulating cluster enumeration as maximization of the posterior probability of candidate models [27], [28]. For these approaches, the penalty term incorporates more information about the clustering problem. It depends on the number of model parameters, the assumed data distribution, the number of data points per cluster, and the estimated parameters. A first attempt at robust Bayesian cluster enumeration has been recently derived by formulating the cluster enumeration problem as maximization of the posterior probability of multivariate t-distributed candidate models [29]. Although this heavy-tailed model provided a significant increase in robustness compared to using Gaussian candidate models, it still relied on a specific distributional model. Our main contribution is to generalize robust Bayesian cluster enumeration so that it can be used with any arbitrary RES distributed mixture model, and even M-estimators that allow for mixture models that are decoupled from a specific probability distribution.

The paper is organized as follows. Section II gives a brief introduction to RES distributions and its loss functions, including a more detailed discussion of the Huber distribution and Tukey’s loss function. Section III introduces the BIC for general distributions, followed by Section IV with the proposed cluster enumeration criterion. Section V details the proposed robust cluster enumeration algorithm. Simulations and a real-world example of radar-based human gait analysis are provided in Section VI. Finally, conclusions are drawn in Section VII. The appendices include derivatives for the Fisher Information Matrix (FIM) as well as ML estimators for RES distributions. Further details on the derivation of the FIM can be found in the online supplementary material.

**Notation:** Normal-font letter \((n, N)\) denote a scalar, bold lowercase \(\mathbf{a}\) a vector and bold uppercase \(\mathbf{A}\) a matrix; calligraphic letters \(\mathcal{X}\) denote a set, with the exception of \(\mathcal{L}\), which denotes the likelihood function; \(\mathbb{R}\) denotes the set of real numbers and \(\mathbb{R}^{r \times 1}, \mathbb{R}^{r \times r}\) the set of column vectors of size \(r \times 1\), matrices of size \(r \times r\), respectively; \(\mathbf{A}^{-1}\) is the matrix inverse; \(\mathbf{A}^\top\) is the matrix transpose; \(|a|\) is the absolute value of a scalar; \(|\mathbf{A}|\) is the determinate of a matrix;
⊗ represents the Kronecker product; \( \text{vec}(\cdot) \) is the vectorization operator, \( D \) is the duplication matrix and \( \text{vech}(\cdot) \) is the vector half operator as defined in [30], [31].

II. RES DISTRIBUTIONS & LOSS FUNCTIONS

This section briefly revisits RES distributions and introduces the used loss functions.

A. RES Distributions

Assuming that the observed data \( x \in \mathbb{R}^{r \times 1} \) follows a RES distribution, let \( \mu \in \mathbb{R}^{r \times 1} \) be the centroid and let \( S \in \mathbb{R}^{r \times r} \) be the positive definite symmetric scatter matrix of a distribution with a pdf, see [7, p. 109] and [32]:

\[
f(x|\mu, S, g) = |S|^{-\frac{r}{2}} g \left( (x - \mu)^\top S^{-1} (x - \mu) \right),
\]

where the squared Mahalanobis distance is denoted by \( t = (x - \mu)^\top S^{-1} (x - \mu) \). The function \( g \), often referred to as the density generator, is a function defined by

\[
g(t) = \frac{\Gamma \left( \frac{r}{2} \right)}{\pi^{r/2}} \left( \int_0^\infty u^{r/2-1} h(u; r) du \right)^{-1} h(t; r),
\]

where \( h(t; r) \) is a function such that

\[
\int_0^\infty u^{r/2-1} h(u; r) du < \infty
\]

holds. Note, that \( h(t; r) \) can be a function of multiple parameters, not only of \( r \).

B. Loss Functions

Assuming an observation of \( N \) iid samples \( x_1, \ldots, x_N \), the likelihood function is given by

\[
\mathcal{L}(\mu, S|x) = \prod_{n=1}^N |S^{-1}|^{-\frac{1}{2}} g \left( (x_n - \mu)^\top S^{-1} (x_n - \mu) \right)
\]

and the ML estimator minimizes the log-likelihood function

\[
-\ln (\mathcal{L}(\mu, S|x)) = -\ln \left( \prod_{n=1}^N |S^{-1}|^{-\frac{1}{2}} g \left( (x_n - \mu)^\top S^{-1} (x_n - \mu) \right) \right)
\]

\[
= \sum_{n=1}^N -\ln (g(t_n)) - \frac{N}{2} \ln (|S^{-1}|)
\]

\[
= \sum_{n=1}^N \rho_{\text{ML}}(t_n) + \frac{N}{2} \ln (|S|)
\]

(5)
with the associated ML loss function \[7, \text{p. 109}\]

\[
\rho_{\text{ML}}(t_n) = -\ln(g(t_n)). \tag{6}
\]

The corresponding first and second derivatives are denoted, respectively, by

\[
\psi_{\text{ML}}(t_n) = \frac{\partial \rho_{\text{ML}}(t_n)}{\partial t_n}, \quad \eta_{\text{ML}}(t_n) = \frac{\partial \psi_{\text{ML}}(t_n)}{\partial t_n}. \tag{7}
\]

The basic idea of M-estimation \[6\] is to replace the ML loss function \(\rho_{\text{ML}}(t_n)\) in Eq. (6) with a more general loss function \(\rho(t_n)\) that may not correspond to an ML estimator. A Non-ML loss function is not based on a specific distribution, but is designed to downweight outlying data points according to desired characteristics.

C. Examples for RES Distributions and Loss Functions

An overview of some exemplary loss functions and their derivatives can be found in Tables I and II. Since the Gaussian and t distribution are well-known they will not be further discussed, but for the Huber distribution and Tukey’s loss function a brief discussion is provided.

1) Huber Distribution: As \[7, \text{p. 115}\] and \[33, \text{p. 8}\] point out, Huber’s M-estimator can be viewed as a ML estimator for a RES distribution, which we will call Huber distribution. It is defined by

\[
h(t; r, c) = \exp\left(-\frac{1}{2} \rho_H(t; c)\right) \tag{8}
\]

with

\[
\rho_H(t; c) = \begin{cases} 
\frac{t}{b} & , \; t \leq c^2 \\
\frac{c^2}{b} \left(\ln\left( \frac{t}{c^2} \right) + 1 \right) & , \; t > c^2
\end{cases} \tag{9}
\]

and to obtain Fisher consistency

\[
b = F_{\chi^2_{r+2}} \left(c^2\right) + \frac{c^2}{r} \left(1 - F_{\chi^2_{r}} \left(c^2\right)\right), \tag{10}
\]

where \(F_{\chi^2_{r}} (\cdot)\) is the Chi-square cumulative distribution function with degree of freedom \(r\). To obtain a valid pdf the normalization factor, according to \[32\], has to be calculated as

\[
\int_0^{\infty} u^{r/2-1} h(u; r, c) du = \int_0^{c^2} u^{r/2-1} \exp \left(-\frac{u}{2b}\right) du + \int_{c^2}^{\infty} u^{r/2-1} \left(\frac{u}{c^2}\right)^{-\frac{c^2}{2b}} \exp \left(-\frac{c^2}{2b}\right) du \\
= (2b)^{r/2} \left(\Gamma \left(\frac{r}{2}\right) - \Gamma \left(\frac{r}{2}, \frac{c^2}{2b}\right)\right) + \frac{2bc^r \exp \left(-\frac{c^2}{2b}\right)}{c^2 - br}, \tag{11}
\]
with the gamma function $\Gamma(\cdot)$ and the upper incomplete gamma function $\Gamma(\cdot, \cdot)$. We can now write the density generator of a Huber distribution as

$$
g(t) = \begin{cases} 
A_H \exp \left( -\frac{t}{2b} \right), & t \leq c^2 \\
A_H \left( \frac{t}{c^2} \right)^{c^2/2} \exp \left( -\frac{c^2}{2b} \right), & t > c^2 
\end{cases}, 
$$

(12)

with

$$A_H = \frac{\Gamma \left( \frac{r}{2} \right)}{\pi^{r/2}} \left( (2b)^{r/2} \left( \Gamma \left( \frac{r}{2} \right) - \Gamma \left( \frac{r}{2}, \frac{c^2}{2b} \right) \right) + \frac{2bc^r \exp \left( -\frac{c^2}{2b} \right)}{c^2 - br} \right)^{-1}. 
$$

(13)

2) Tukey’s Loss Function: One of the most commonly used Non-ML loss functions is Tukey’s loss function. It is a redescending loss function because it redescends to zero, i.e., it gives values larger than $c$ zero weight. In [7, p. 11], Tukey’s loss function, for the univariate case, is given as

$$
\rho(x) = \begin{cases} 
\frac{x^6}{6c^4} - \frac{x^4}{2c^2} + \frac{x^2}{2}, & |x| \leq c \\
\frac{c^2}{6}, & |x| > c 
\end{cases}, 
$$

(14)

which can be generalized to the multivariate case with $x^2 = t_n$ and $|x| = \sqrt{t_n}$. We are also adding the constant $\frac{c}{2} \ln (2\pi)$ so that for $c \to \infty$, Tukey’s loss function is equal to the Gaussian loss function. The resulting expression for Tukey’s $\rho(t_n)$ is given in Table I, while $\psi(t_n)$ and $\eta(t_n)$ can be found in Table III.

III. BAYESIAN CLUSTER ENUMERATION FOR A GENERAL DISTRIBUTION

This section briefly revisits the BIC for cluster analysis that formulations cluster enumeration as maximization of the posterior probability of candidate models [27]. The general definition forms the basis of the specific robust criteria that we derive in Section IV. Following the definition and notation in [27], [34], $\mathcal{X} = \{x_1, \ldots, x_N\}$ is the observed data set of length $N$. It can be partitioned into $K$ mutually exclusive subsets (clusters) $\{\mathcal{X}_1, \ldots, \mathcal{X}_K\}$, each cluster $\mathcal{X}_k \subseteq \mathcal{X}$, $k \in \mathcal{K} = \{1, \ldots, K\}$ containing $N_k > 0$ observations of iid random variables $x_k \in \mathbb{R}^{r \times 1}$. The set of candidate models is defined as $\mathcal{M} = \{M_{L_{\min}}, \ldots, M_{L_{\max}}\}$, each $\mathcal{M}_l$ represents the partitioning of $\mathcal{X}$ into $l \in \{L_{\min}, \ldots, L_{\max}\}$, $l \in \mathbb{Z}^+$ subsets $\mathcal{X}_m$, $m = 1, \ldots, l$. The true number of subsets $K$ is assumed to lie within $L_{\min} \leq K \leq L_{\max}$. For each $\mathcal{M}_l$ the parameters are stored...
TABLE I
OVERVIEW OF $g(t_n)$ AND $\rho(t_n)$ FUNCTIONS

|        | $g(t_n)$                                      | $\rho(t_n)$                                      |
|--------|----------------------------------------------|-------------------------------------------------|
| Gaussian | $(2\pi)^{-\frac{n}{2}} \exp\left(-\frac{1}{2} \Theta\right)$ | $\frac{1}{2} l_n + \frac{1}{2} \ln(2\pi)$    |
| $t$     | $\frac{\Gamma((\nu+2)/2)}{\Gamma(\nu/2)} (1 + \frac{t_n}{\nu})^{-\frac{\nu+2}{2}}$ | $-\ln\left(\frac{\Gamma((\nu+2)/2)}{\Gamma(\nu/2)}(\nu/\nu)^{\nu/2}\pi\right) + \frac{\nu+2}{2} \ln(1 + \frac{t_n}{\nu})$ |
| Huber   | $A_n \exp\left(-\frac{t_n}{2b}\right)$, $t_n \leq c^2$ | $-\ln(A_n) + \frac{t_n}{2b}$, $t_n \leq c^2$ |
|         | $A_n \left(\frac{t_n}{c}\right)^{-\frac{2}{\nu}} \exp\left(-\frac{2}{\nu} \left|\frac{t_n}{c}\right|^\nu\right)$, $t_n > c^2$ | $-\ln(A_n) + \frac{c}{2} \ln\left(\frac{t_n}{c}\right) + 1$, $t_n > c^2$ |
| Tukey   | n.a.                                      | $\frac{t_n^2}{6c^2} - \frac{t_n^2}{2c^2} + \frac{t_n}{2} + \frac{r}{2} \ln(2\pi)$, $t_n \leq c^2$ |
|         |                                           | $\frac{c^2}{6} + \frac{r}{2} \ln(2\pi)$, $t_n > c^2$ |

TABLE II
OVERVIEW OF $\psi(t_n)$ AND $\eta(t_n)$ FUNCTIONS

|        | $\psi(t_n)$                                      | $\eta(t_n)$                                      |
|--------|----------------------------------------------|-------------------------------------------------|
| Gaussian | $\frac{1}{2}$                                      | 0                                              |
| $t$     | $\frac{1}{2} \cdot \frac{\nu+2}{\nu+t_n} = \frac{1}{2} \psi_n$ | $-\frac{1}{2} \cdot \frac{\nu+2}{(\nu+t_n)^2} = -\frac{1}{2} \cdot \frac{2}{\nu+t_n^2}$ |
| Huber   | $\begin{cases} 
\frac{1}{2b} \quad & t_n \leq c^2 \\
\frac{c^2}{2b_n} \quad & t_n > c^2 \end{cases}$ | $\begin{cases} 
0 \quad & t_n \leq c^2 \\
-\frac{c^2}{2b'_n} \quad & t_n > c^2 \end{cases}$ |
| Tukey   | $\begin{cases} 
\frac{t_n^2}{2c^2} - \frac{t_n}{c} + \frac{1}{2} \quad & t_n \leq c^2 \\
0 \quad & t_n > c^2 \end{cases}$ | $\begin{cases} 
\frac{t_n}{c} - \frac{1}{c^2} \quad & t_n \leq c^2 \\
0 \quad & t_n > c^2 \end{cases}$ |

in $\Theta_t = [\theta_1, \ldots, \theta_t] \in \mathbb{R}^{q \times l}$, with $q$ being the number of parameters per cluster. Now, [34, p. 18] derives a Bayesian criterion specifically for the cluster enumeration problem as

\[
\text{BIC}_G(M_t) \triangleq \ln(p(M_t | X)) \approx \ln(p(M_t)) + \ln\left(f\left(\hat{\Theta}_t | M_t\right)\right) + \ln\left(\mathcal{L}\left(\hat{\Theta}_t | X\right)\right)
\]

\[
+ \frac{1}{2} l_q \ln(2\pi) - \frac{1}{2} \sum_{m=1}^t \ln\left(|J_m|\right) - \ln(f(X))
\]

(15)
where \( p(M_l) \) is the discrete prior on the model \( M_l \in \mathcal{M} \),

\[
f \left( \hat{\Theta}_l | M_l \right) = \prod_{m=1}^{l} f \left( \hat{\theta}_m | M_l \right)
\]

(16)
is a prior on the parameter vectors in \( \hat{\Theta}_l \) given \( M_l \),

\[
\mathcal{L} \left( \hat{\Theta}_l | \mathcal{X} \right) = \prod_{m=1}^{l} \mathcal{L} \left( \hat{\theta}_m | \mathcal{x}_m \right)
\]

(17)
is the likelihood function, and

\[
\hat{J}_m = -\frac{d^2 \ln \left( \mathcal{L} \left( \hat{\theta}_m | \mathcal{x}_m \right) \right)}{d\hat{\theta}_m d\hat{\theta}_m^\top} \in \mathbb{R}^{q \times q}
\]

(18)
is the FIM and \( f(\mathcal{X}) \) is the pdf of \( \mathcal{X} \). We can further simplify the BIC\(_G\) by assuming an equal prior and noting that \( f(\mathcal{X}) \) is model independent, hence we can remove both terms. Lastly we can assume that each parameter vector is equally probable as follows

\[
f \left( \hat{\Theta}_l | M_l \right) = \prod_{m=1}^{l} f \left( \hat{\theta}_m | M_l \right) = \prod_{m=1}^{l} \frac{1}{l} = l^{-l}
\]

(19)

and finally

\[
\text{BIC\(_G\)}(M_l) \approx \sum_{m=1}^{l} \ln \left( \mathcal{L} \left( \hat{\theta}_m | \mathcal{x}_m \right) \right) - l \ln (l) + \frac{ql}{2} \ln (2\pi) - \frac{1}{2} \sum_{m=1}^{l} \ln \left( |\hat{J}_m| \right).
\]

(20)
The number of clusters can be estimated by evaluating

\[
\hat{K} = \arg \max_{l=L_{\min}, \ldots, L_{\max}} \text{BIC\(_G\)}(M_l).
\]

(21)

IV. Proposed Bayesian Cluster Enumeration for RES Distributions and M-Estimation

A. Proposed Finite Sample Criterion

Our first main result is stated in Theorem 1. Based on Eq. (20), we derive a BIC which can be used for any RES distribution and even for Non-ML loss functions, such as, Tukey’s M-estimator. Firstly, the parameter vector is defined as \( \hat{\theta}_m = \begin{bmatrix} \hat{\mu}_m^\top, \vech(\hat{S}_m)^\top \end{bmatrix}^\top \in \mathbb{R}^{q \times 1} \), \( q = \frac{r}{2}(r + 3) \). Because \( \hat{S}_m \) is symmetric, it has only \( \frac{r}{2}(r + 1) \) unique elements, therefore \( \vech(\hat{S}_m) \) has to be used [31, p. 367]. The \( \vech \) (vector half) operator takes a symmetric \( r \times r \) matrix and stacks the lower triangular half into a single vector of length \( \frac{r}{2}(r + 1) \).

**Theorem 1.** The posterior probability of \( M_l \) given \( \mathcal{X} \), based on any ML or Non-ML loss function \( \rho(t) \), can be calculated by
BIC$_F(M_l) \approx - \sum_{m=1}^{l} \left( \sum_{x_n \in \mathcal{X}_m} \rho(\hat{t}_{nm}) \right) + \sum_{m=1}^{l} N_m \ln(N_m) - \sum_{m=1}^{l} \frac{N_m}{2} \ln \left( |S_m| \right) + \left( l \ln(l) + \frac{q}{2} \ln(2\pi) - \frac{1}{2} \sum_{m=1}^{l} \ln \left( |\hat{J}_m| \right) \right) - \frac{N_m}{2} \ln(N) - \frac{N_m}{2} \sum_{m=1}^{l} \ln \left( |\hat{S}_m| \right), \quad (22)

with $|\hat{J}_m|$ given in Eq. (28), using Eqs. (24)- (26).

Theorem I is derived from Eq. (20) by ignoring model independent terms in the log-likelihood function for an arbitrary RES distribution

\[ \ln \left( L(\hat{\theta}_m | \mathcal{X}_m) \right) = \ln \left( \prod_{x_n \in \mathcal{X}_m} p(x_n \in \mathcal{X}_m) \right) \]

\[ = \sum_{x_n \in \mathcal{X}_m} \ln \left( \frac{N_m}{N} |S_m^{-1}|^{\frac{1}{2}} g(\hat{t}_{nm}) \right) \]

\[ = - \sum_{x_n \in \mathcal{X}_m} \rho(\hat{t}_{nm}) + \sum_{m=1}^{l} N_m \ln(N_m) - N \ln(N) - \frac{N_m}{2} \ln \left( |S_m| \right), \quad (23) \]

and computing the FIM

\[ \hat{J}_m = \begin{bmatrix} -\hat{F}_{\mu\mu} & -\hat{F}_{\mu S} \\ -\hat{F}_{S\mu} & -\hat{F}_{SS} \end{bmatrix} \in \mathbb{R}^{q \times q}. \quad (24) \]

All derivatives are evaluated with the ML estimates of $S_m$ and $\mu_m$, respectively, $\hat{S}_m$ and $\hat{\mu}_m$. M-estimation based cluster enumeration, decouples the loss-function $\rho(t)$ in Eq. (23) from a specific distribution. This extends the applicability to non-ML loss functions, such as, for example, Tukey’s. The proof of Theorem I is provided in Appendix A. Due to limited space, some detailed explanations are left out. A complete and comprehensive step-by-step derivation for all elements of the FIM in Eq. (24) is given in the online supplementary material. The final resulting expressions are as follows:

\[ \hat{F}_{\mu\mu} = -4 \hat{S}_m^{-1} \left( \sum_{x_n \in \mathcal{X}_m} \eta(\hat{t}_{nm}) \tilde{x}_n \tilde{x}_n^\top \right) \hat{S}_m^{-1} - 2 \hat{S}_m^{-1} \sum_{x_n \in \mathcal{X}_m} \psi(\hat{t}_{nm}) \in \mathbb{R}^{r \times r}, \quad (25) \]

\[ \hat{F}_{\mu S} = \hat{F}_{S\mu} = -2 \sum_{x_n \in \mathcal{X}_m} \eta(\hat{t}_{nm}) \left( \hat{S}_m^{-1} \tilde{x}_n \tilde{x}_n^\top \hat{S}_m^{-1} \otimes \tilde{x}_n \hat{S}_m^{-1} \right) D_v \in \mathbb{R}^{r \times L^{(r+1)}}, \quad (26) \]
and
\[
\hat{F}_{ss} = - D_r^\top \left( \hat{S}_m^{-1} \otimes \hat{S}_m^{-1} \right) \left( \sum_{x_n \in X_m} \eta(\hat{t}_{nm}) \left( \hat{x}_n \hat{x}_n^\top \otimes \hat{x}_n \hat{x}_n^\top \right) \right) \left( \hat{S}_m^{-1} \otimes \hat{S}_m^{-1} \right) D_r
\]
\[
- \frac{N_m}{2} D_r^\top \left( \hat{S}_m^{-1} \otimes \hat{S}_m^{-1} \right) D_r \in \mathbb{R}^{r(r+1) \times r(r+1)}.
\]
Here, \( D_r \in \mathbb{R}^{r^2 \times \frac{r(r+1)}{2}} \) is the duplication matrix, and \( \hat{x}_n \triangleq x_n - \hat{\mu}_m \). The FIM is a partitioned matrix [31, p. 114] and the determinant follows as
\[
\left| \hat{J}_m \right| = \left| - \hat{F}_{\mu\mu} \right| \cdot \left| - \hat{F}_{ss} + \hat{F}_{s\mu} \hat{F}^{-1}_{\mu\mu} \hat{F}_{\mu s} \right|.
\]
Based on (22), the number of clusters can be estimated by evaluating
\[
\hat{K} = \arg \max_{l=L_{\min}^\ldots L_{\max}} \text{BIC}_F(M_l).
\]

**B. Asymptotic Sample Penalty Term**

Our second main result is stated in Theorem 2. Because it can be numerically expensive to calculate the FIM, especially for large sample sizes, it can be advantageous to asymptotically approximate the FIM.

**Theorem 2.** Ignoring terms in Eq. (28) that do not grow as \( N \to \infty \), the posterior probability of \( M_l \) given \( X \) becomes
\[
\text{BIC}_A(M_l) \approx - \sum_{m=1}^l \left( \sum_{x_n \in X_m} \rho(\hat{t}_{nm}) \right) + \sum_{m=1}^l N_m \ln (N_m) - \sum_{m=1}^l \frac{N_m}{2} \ln \left( |\hat{S}_m| \right) - \frac{q}{2} \sum_{m=1}^l \ln (\varepsilon_m)
\]
with \( \varepsilon_m \) given in Eq. (32).

The scalar variable \( \varepsilon_m \) is computed, such that
\[
\left| \frac{1}{\varepsilon_m} \hat{J}_m \right| = \text{const},
\]
leads to a term that does not grow as \( N \to \infty \). From Eqs. (25), (26) and (27) we can extract three normalization factors to fulfill Eq. (31) the maximum must be taken, which yields
\[
\varepsilon_m = \max \left( \left| \sum_{x_n \in X_m} \psi(\hat{t}_{nm}) \right|, \left| \sum_{x_n \in X_m} \eta(\hat{t}_{nm}) \right|, N_m \right).
\]
Based on (30), the number of clusters can be estimated by evaluating
\[
\hat{K} = \arg \max_{l=L_{\min}^\ldots L_{\max}} \text{BIC}_A(M_l).
\]
V. PROPOSED ROBUST CLUSTER ENUMERATION ALGORITHM

To evaluate the BIC, our approach requires a robust clustering algorithm to partition the data according to the number of clusters specified by each candidate model and to compute the associated parameter estimates. Accordingly, we will derive an expectation maximization (EM) algorithm for RES distributions in Section V-A. The resulting two-step approach is summarized in Algorithm 1, where we provide a unified framework for the robust estimation of the number of clusters and cluster memberships.

**Algorithm 1:** Proposed robust cluster enumeration algorithm.

**Input:** $X$, $L_{\text{min}}$, $L_{\text{max}}$

**Output:** $\hat{K}$

for $l = L_{\text{min}}, \ldots, L_{\text{max}}$ do

Compute Parameter Estimates using Algorithm 2

Hard Clustering:

for $m = 1, \ldots, l$ do

for $n = 1, \ldots, N$ do

\[
\gamma_{nm} = \begin{cases} 
1 & , m = \text{arg max}_{j=1,\ldots,l} \hat{v}_{nj}^{(i)} \\
0 & , \text{else}
\end{cases}
\]

for $m = 1, \ldots, l$ do

\[
N_m = \sum_{n=1}^{N} \gamma_{nm}
\]

calculate BIC($M_l$) according to (22) or (30)

Estimate the number of clusters $\hat{K}$ with Eq. (29) or (33)

A. Expectation Maximization (EM) Algorithm for a Mixture of RES Distributions

This section describes the EM algorithm that is used to find ML estimates of the RES mixture model parameters [1], [34], [35], and the cluster memberships of the data vectors $x_n$, which are latent variables. For a mixture of $l$ RES distributions, the log-likelihood function is given by

\[
\ln (\mathcal{L}(\Phi_l|X)) = \sum_{n=1}^{N} \ln \left( \sum_{m=1}^{l} \gamma_m |S_m|^{-\frac{1}{2}} g(t_{nm}) \right)
\]

with $\gamma_m$ being the mixing coefficient, $S_m$ the scatter matrix, $g(t_{nm})$ the density generator and $\Phi_l = [\gamma_l, \Theta_l^\top]$ with $\gamma_l = [\gamma_1, \ldots, \gamma_l]^\top$. Using the matrix calculus rules from [30], [31], [36], we
define $F$ as a $1 \times 1$ scalar function of the $r \times 1$ vector $\mu_m$. Hence, the resulting Jacobian matrix is of size $1 \times r$. Setting $F$ equal to (34)

$$F(\mu_m) = \ln (L(\Phi_t|X)) = \sum_{n=1}^{N} \ln \left( \sum_{m=1}^{l} \gamma_{m} |S_{m}|^{-\frac{1}{2}} g(t_{nm}) \right)$$

and applying the differential

$$dF(\mu_m) = \sum_{n=1}^{N} d \ln \left( \sum_{m=1}^{l} \gamma_{m} |S_{m}|^{-\frac{1}{2}} g(t_{nm}) \right)$$

$$= - \sum_{n=1}^{N} \frac{\gamma_{m} |S_{m}|^{-\frac{1}{2}} g'(t_{nm})}{\sum_{j=1}^{l} \gamma_{j} |S_{j}|^{-\frac{1}{2}} g(t_{nj})} 2 (x_n - \mu_m)^\top S_{m}^{-1} d\mu_m$$

the Jacobian matrix follows as

$$DF(\mu_m) = \sum_{n=1}^{N} v_{nm} \psi(t_{nm}) 2 (x_n - \mu_m)^\top S_{m}^{-1}$$

with

$$g'(t_{nm}) = -\psi(t_{nm}) g(t_{nm})$$

and

$$v_{nm} = \frac{\gamma_{m} |S_{m}|^{-\frac{1}{2}} g(t_{nm})}{\sum_{j=1}^{l} \gamma_{j} |S_{j}|^{-\frac{1}{2}} g(t_{nj})}.$$
The ML estimate can be calculated by setting (43) equal to zero with \( \hat{\mathbf{x}}_n = \mathbf{x}_n - \mu_m \), followed by the vectorization

\[
d\vec{\mathbf{F}}(\mathbf{S}_m) = \sum_{n=1}^{N} \left[ -\frac{v_{nm}}{2} \text{Tr} \left( \mathbf{S}_m^{-1} \mathbf{dS}_m \right) + v_{nm} \psi(t_{nm}) \vec{\left( \mathbf{x}_n^\top \mathbf{S}_m^{-1} \mathbf{dS}_m \mathbf{S}_m^{-1} \mathbf{x}_n \right)} \right]
\]

\[
= \sum_{n=1}^{N} \left[ -\frac{v_{nm}}{2} \vec{\mathbf{v}}(\mathbf{S}_m^{-1})^\top + v_{nm} \psi(t_{nm}) \left( \mathbf{x}_n^\top \mathbf{S}_m^{-1} \otimes \mathbf{x}_n^\top \mathbf{S}_m^{-1} \right) \right] \vec{\mathbf{v}}(\mathbf{S}_m) \tag{42}
\]

leads to the Jacobian matrix

\[
\mathbf{D}\mathbf{F}(\mathbf{S}_m) = \sum_{n=1}^{N} \left[ v_{nm} \psi(t_{nm}) \left( \mathbf{x}_n^\top \mathbf{S}_m^{-1} \otimes \mathbf{x}_n^\top \mathbf{S}_m^{-1} \right) - \frac{v_{nm}}{2} \vec{\mathbf{v}}(\mathbf{S}_m^{-1})^\top \right]
\]

The ML estimate can be calculated by setting (43) equal to zero

\[
\Rightarrow \sum_{n=1}^{N} v_{nm} \psi(t_{nm}) \left( \mathbf{x}_n^\top \otimes \mathbf{x}_n^\top \right) \left( \mathbf{S}_m^{-1} \otimes \mathbf{S}_m^{-1} \right) = \sum_{n=1}^{N} \frac{v_{nm}}{2} \vec{\mathbf{v}}(\mathbf{S}_m^{-1})^\top
\]

\[
\Rightarrow \sum_{n=1}^{N} \frac{v_{nm}}{2} \vec{\mathbf{v}}(\mathbf{S}_m^{-1})^\top \left( \mathbf{S}_m \otimes \mathbf{S}_m \right) = \sum_{n=1}^{N} v_{nm} \psi(t_{nm}) \left( \mathbf{x}_n^\top \otimes \mathbf{x}_n^\top \right)
\]

\[
\Rightarrow \vec{\mathbf{v}}(\mathbf{S}_m) = \frac{2 \sum_{n=1}^{N} v_{nm} \psi(t_{nm}) \left( \mathbf{x}_n^\top \otimes \mathbf{x}_n^\top \right)}{\sum_{n=1}^{N} v_{nm}}
\]

\[
\Rightarrow \hat{\mathbf{S}}_m = \frac{2 \sum_{n=1}^{N} v_{nm} \psi(t_{nm}) \left( \mathbf{x}_n - \hat{\mu}_m \right) \left( \mathbf{x}_n - \hat{\mu}_m \right)^\top}{\sum_{n=1}^{N} v_{nm}} \tag{44}
\]

Finally, we have to maximize with regard to the mixing coefficients \( \gamma_m \). Since they have the constraint

\[
\sum_{m=1}^{l} \gamma_m = 1 \tag{45}
\]

a Lagrange multiplier is used

\[
d\mathbf{F}(\gamma_m) = \sum_{n=1}^{N} d\ln \left( \sum_{m=1}^{l} \gamma_m \left| \mathbf{S}_m^{-1} \right|^\frac{1}{2} g(t_{nm}) \right) + \lambda \left( \sum_{m=1}^{l} \gamma_m - 1 \right)
\]

\[
= \sum_{n=1}^{N} \frac{\left| \mathbf{S}_m^{-1} \right|^\frac{1}{2} g(t_{nm})}{\sum_{j=1}^{l} \gamma_j \left| \mathbf{S}_j^{-1} \right|^\frac{1}{2} g(t_{nj})} + \lambda. \tag{46}
\]

First we solve for \( \lambda \), which leads to

\[
\Rightarrow 0 = \sum_{n=1}^{N} \sum_{m=1}^{l} \frac{\gamma_m \left| \mathbf{S}_m^{-1} \right|^\frac{1}{2} g(t_{nm})}{\sum_{j=1}^{l} \gamma_j \left| \mathbf{S}_j^{-1} \right|^\frac{1}{2} g(t_{nj})} + \lambda \sum_{m=1}^{l} \gamma_m
\]

\[
\Rightarrow \lambda = -N \tag{47}
\]

and after the elimination of \( \lambda \) we find

\[
\hat{\gamma}_m = \frac{1}{N} \sum_{n=1}^{N} v_{nm}. \tag{48}
\]

The resulting iterative EM algorithm to compute these parameters is summarized in Algorithm 2.
VI. EXPERIMENTAL RESULTS

The proposed cluster enumeration framework allows for a variety of possible algorithms which include the recently proposed cluster enumeration criteria for the Gaussian distribution [27], [28] and for the t-distribution [29], as special cases. Further, as a benchmark comparison, Schwarz penalty can be combined with the robust data fit, as provided by the EM algorithm. Figure 1 summarizes all implemented cluster enumeration algorithms. The code that implements our proposed two-step algorithm for robust Bayesian cluster enumeration is available at: https://github.com/schrchr/Robust-Cluster-Enumeration

We use the same simulated data as in [27]–[29], to be able to compare the results. Results can therefore be compared to the Robust Trimmed BIC [18] and the Robust Gravitational Clustering Method [37]. The simulated data set is defined by \( x_k \sim \mathcal{N}(\mu_k, \Sigma_k) \), \( k = 1, 2, 3 \), the cluster centroids \( \mu_1 = [0, 5]^{\top}, \mu_2 = [5, 0]^{\top} \) and \( \mu_3 = [-5, 0]^{\top} \) and the covariance matrices

\[
\Sigma_1 = \begin{bmatrix} 2 & 0.5 \\ 0.5 & 0.5 \end{bmatrix}, \quad \Sigma_2 = \begin{bmatrix} 1 & 0 \\ 0 & 0.1 \end{bmatrix}, \quad \Sigma_3 = \begin{bmatrix} 2 & -0.5 \\ -0.5 & 0.5 \end{bmatrix}.
\]

Every cluster has \( N_k \) data points and the outliers are replacement outliers where \( \epsilon \) is the percentage of replaced data points. These replacements are uniformly distributed in the range of \([-20, 20]\) in each dimension. Two exemplary realizations with different values of \( \epsilon \) are shown in Figure 2. For the Huber distribution, [7, p. 116] suggest to choose \( c^2 \) as the \( q_{H}^{th} \) upper quantile of a \( \chi^2_r \) distribution

\[
c^2 = F_{\chi^2_r}^{-1}(q_{H}), \quad 0 < q_{H} < 1.
\]

In [7, p. 121], a value of \( q_{H} = 0.8 \) is used, which leads to \( c = 1.282 \). From [7, p. 23], we have the value \( c = 1.345 \), which will achieve an asymptotic relative efficiency (ARE) of 95%. Since both values are quite similar, there should not be a large performance difference and we choose to use \( q_{H} = 0.8 \) in all simulations. For Tukey’s loss function we will use \( c = 4.685 \), according to [7, p. 23].

To evaluate the sensitivity of the proposed cluster enumeration algorithm to the position of a single replacement outlier, we simulated the sensitivity curves over 500 Monte Carlo iterations with \( N_k = 50 \). Here, we replaced a randomly selected data point with an outlier that takes values over the range \([-20; 20]\) on each variate at each iteration. In Figure 3 six exemplary results for the resulting empirical probability of correctly deciding for \( K = 3 \) clusters are shown as a function of the outlier position. The first row is based on the BIC\(_F\) and the second row on the
BIC_A. Due to the relatively small sample size, BIC_F clearly performs better than BIC_A for all shown loss functions. As expected the Gaussian loss function is not robust against outliers and only has a very small area with a high probability of detection. A Huber and Tukey based loss function increases the probability of detection significantly. The difference between those two loss function is less prominent, but when comparing Figures 3b and 3e with Figures 3c and 3f one can observe a higher probability of detection for the Tukey based loss function, because it completely rejects large outliers.

Figure 4 shows the robustness against a fraction of replacement outliers, where the contaminating distribution is a uniform distribution in the interval [20, 20] for each outlier variate in each Monte Carlo iteration. The uniform distribution is chosen so that the outliers do not form a cluster, which would lead to an ambiguity in the cluster enumeration results for larger amounts of outliers. The first row of plots in Figure 4 represents the results for a cluster size of $N_k = 10$ and the second row a cluster size of $N_k = 250$. We can observe two different behaviors based on the number of samples. Firstly, for $N_k = 10$, the results are similar for the same penalty term. So in Figure 4a the finite based BIC is able to perform quite well for all applied distributions. In contrast, Figure 4b shows that the asymptotic based BIC is not able to detect anything and the Schwarz based BIC in Figure 4c also does not perform well. In the second row, the opposite effect can be observed. In Figures 4d, 4e and 4f the best performing combination is always observed for a similar loss function combination. The EM with a Huber distribution and Tukey BIC, followed by an EM with t distribution and Tukey BIC always has the best performance.
This effect can be explained by the actual values of the likelihood and the penalty term of the BIC. For $N_k = 10$ the values of the likelihood and penalty term are in the same magnitude, whereas for $N_k = 250$ the values of the likelihood and penalty term are one to two magnitudes apart. Hence, for low sample sizes, the penalty term has a large influence and for large sample sizes, the penalty term has almost no influence.

A. Real Data Simulations

The data set is composed of four walking persons. Their walks, measured by a 24GHz radar system, were processed to calculate the spectrogram and afterwards a feature extraction was performed [38]. To reduce the dimensionality from $r = 12800$, a PCA was applied and the first five components were extracted to form the final data set with $N = 187$ and $r = 5$. A subset of the first three components is shown in Figure 5a. The correct number of different persons is estimated by a BIC$_F$ with EM: Gaussian, BIC: Gaussian (also used by [38]), EM: t, BIC: Tukey and EM: Huber, BIC: Tukey as shown in Figure 5b. In comparison to the method used by [38] one can note, that the peaks in the newly proposed methods are more prominent, hence, they lead to a more stable result. Additionally in Figure 5c we show the results based on a Schwarz penalty term. It is clearly overestimating the number of clusters, properly due to the small sample size.
VII. Conclusion

We have presented a general Robust Bayesian cluster enumeration framework. This was done by deriving an EM algorithm for arbitrary RES distributions and adapting the generic BIC from [27] to the class of RES distributions and to the class of M-estimators. Robust M-estimators may correspond to ML estimators for a specific RES distribution, such as Huber’s estimator. Our framework, however, also allows for non-ML loss functions, such as Tukey’s loss function. The performance was evaluated on simulated and real world examples, which show a superior robustness against outliers, compared to existing work. Further research may be done to derive alternatives for the EM algorithm or to include skewed data distributions or high-dimensionality [39]–[41].

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Fig. 4. Breakdown point simulation for two different samples per cluster $N_k$.

(a) $N_k = 10$, BIC: Finite
(b) $N_k = 10$, BIC: Asymptotic
(c) $N_k = 10$, BIC: Schwarz

(d) $N_k = 250$, BIC: Finite
(e) $N_k = 250$, BIC: Asymptotic
(f) $N_k = 250$, BIC: Schwarz

Fig. 5. Results of the cluster enumeration of the radar-based human gait data.

(a) Exemplary first three PCA features.
(b) Proposed cluster enumeration criteria.
(c) BIC based on Schwarz criterion.
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APPENDIX A

DERIVATIVES FOR THE FIM OF THE RES DISTRIBUTION

A. First derivative with respect to the mean

First, we define \( F \) as a \( 1 \times 1 \) scalar function of the \( r \times 1 \) vector \( \mu_m \). Hence, the resulting Jacobian matrix is of size \( 1 \times r \). Setting \( F(\mu_m) \) equal to the log-likelihood function we get

\[
F(\mu_m) = \ln (\mathcal{L}(\theta_m | x_m)) = - \sum_{x_n \in X_m} \rho(t_{nm}) \ln \left( \frac{N_m}{N} \right) + \frac{N_m}{2} \ln \left( |S_m^{-1}| \right)
\]  

and afterwards apply the differential

\[
dF(\mu_m) = - \sum_{x_n \in X_m} d\rho(t_{nm})
\]

\[
= - \sum_{x_n \in X_m} \psi(t_{nm}) d \left( (x_n - \mu_m)^\top S_m^{-1} (x_n - \mu_m) \right)
\]

\[
= - \sum_{x_n \in X_m} \psi(t_{nm}) \left( (-d\mu_m)^\top S_m^{-1} (x_n - \mu_m) + (x_n - \mu_m)^\top S_m^{-1} (-d\mu_m) \right)
\]

\[
= \sum_{x_n \in X_m} 2\psi(t_{nm}) (x_n - \mu_m)^\top S_m^{-1} d\mu_m.
\]

Finally, the Jacobian matrix of \( F(\mu_m) \), which we will denote as \( F_\mu \), becomes

\[
DF(\mu_m) = F_\mu = 2 \sum_{x_n \in X_m} \psi(t_{nm}) (x_n - \mu_m)^\top S_m^{-1}.
\]  

For the second derivative, \( F_\mu \) is a \( 1 \times r \) vector function of the \( r \times 1 \) vector \( \mu_m \), hence the resulting Jacobian matrix is of size \( r \times r \). Starting with the differential of (52)

\[
dF_\mu(\mu_m) = 2 \sum_{x_n \in X_m} \left[ \frac{d\psi(t_{nm}) (x_n - \mu_m)^\top S_m^{-1} + \psi(t_{nm}) d \left( (x_n - \mu_m)^\top S_m^{-1} \right) }{d\mu_m} \right]
\]

\[
= - 2 \sum_{x_n \in X_m} 2\eta(t_{nm}) (x_n - \mu_m)^\top S_m^{-1} d\mu_m (x_n - \mu_m)^\top S_m^{-1} + \psi(t_{nm}) (d\mu_m)^\top S_m^{-1}
\]

and applying the vec operator

\[
dvec(F_\mu(\mu_m)) = - \sum_{x_n \in X_m} \left[ 4\eta(t_{nm}) \text{vec} \left( (x_n - \mu_m)^\top S_m^{-1} d\mu_m (x_n - \mu_m)^\top S_m^{-1} \right) + 2\psi(t_{nm}) \text{vec} \left( (d\mu_m)^\top S_m^{-1} \right) \right]
\]

\[
= - \sum_{x_n \in X_m} \left[ 4\eta(t_{nm}) \left( S_m^{-1} (x_n - \mu_m) (x_n - \mu_m)^\top S_m^{-1} \right) + 2\psi(t_{nm}) S_m^{-1} \right] d\mu_m
\]
yields the Jacobian matrix $F_{\mu \mu}$ as
\[
DF_{\mu}(\mu_m) = F_{\mu \mu} = - \sum_{x_n \in X_m} \left[ 4\eta(t_{nm}) S_{m}^{-1} (x_n - \mu_m)(x_n - \mu_m)^\top S_{m}^{-1} + 2\psi(t_{nm}) S_{m}^{-1} \right].
\]

(53)

Evaluating $F_{\mu \mu}$ at $\hat{S}_m$ and $\hat{\mu}_m$ from Appendix [B] leads to
\[
\hat{F}_{\mu \mu} = -4\hat{S}_m^{-1} \left( \sum_{x_n \in X_m} \eta(\hat{t}_{nm}) (x_n - \hat{\mu}_m)(x_n - \hat{\mu}_m)^\top \right) \hat{S}_m^{-1} - 2\hat{S}_m^{-1} \sum_{x_n \in X_m} \psi(\hat{t}_{nm}).
\]

(54)

For the other second derivative, $F_{\mu}$ is a $1 \times r$ vector function of the $r \times r$ matrix $S_m$, hence the resulting Jacobian matrix should be of size $r \times r^2$, but because $S_m$ is a symmetric matrix and only the unique elements are needed, we use the duplication matrix $D_r$ to only keep the unique elements of $S_m$. Therefore the resulting matrix only has the size $r \times \frac{1}{2}r(r+1)$. Starting with the differential of (52) and introducing $\hat{x}_n \triangleq x_n - \mu_m$
\[
dF_{\mu}(S_m) = 2 \sum_{x_n \in X_m} \left[ d\psi(t_{nm}) \bar{x}_n^\top S_m^{-1} + \psi(t_{nm}) d\left( \bar{x}_n^\top S_m^{-1} \right) \right]
\]
\[
= -2 \sum_{x_n \in X_m} \left[ \eta(t_{nm}) \bar{x}_n^\top S_m^{-1} dS_m S_m^{-1} \bar{x}_n \bar{x}_n^\top S_m^{-1} + \psi(t_{nm}) \bar{x}_n^\top S_m^{-1} dS_m S_m^{-1} \right].
\]

(55)

Application of the vec operator leads to
\[
dvec(F_{\mu}(S_m)) = -2 \sum_{x_n \in X_m} \left[ \eta(t_{nm}) \left( \left( S_m^{-1} \bar{x}_n \bar{x}_n^\top S_m^{-1} \right)^\top \otimes \bar{x}_n S_m^{-1} \right) D_r \ dvec(S_m)
\]
\[
+ \psi(t_{nm}) \left( S_m^{-1} \otimes \bar{x}_n S_m^{-1} \right) D_r \ dvec(S_m) \]
so that
\[
DF_{\mu}(S_m) = F_{\mu S} = -2 \sum_{x_n \in X_m} \left[ \eta(t_{nm}) \left( S_m^{-1} \bar{x}_n \bar{x}_n^\top S_m^{-1} \otimes \bar{x}_n S_m^{-1} \right) + \psi(t_{nm}) \left( S_m^{-1} \otimes \bar{x}_n S_m^{-1} \right) \right] D_r.
\]

Evaluating $F_{\mu S}$ at $\hat{S}_m$ and $\hat{\mu}_m$ with $\hat{x}_n \triangleq x_n - \mu_m$ from Appendix [B] leads to
\[
\hat{F}_{\mu S} = -2 \sum_{x_n \in X_m} \left[ \eta(\hat{t}_{nm}) \left( \hat{S}_m^{-1} \bar{x}_n \bar{x}_n^\top \hat{S}_m^{-1} \otimes \bar{x}_n \hat{S}_m^{-1} \right) D_r + \psi(\hat{t}_{nm}) \left( \hat{S}_m^{-1} \otimes \bar{x}_n \hat{S}_m^{-1} \right) D_r \right]
\]
\[
= -2 \sum_{x_n \in X_m} \eta(\hat{t}_{nm}) \left( \hat{S}_m^{-1} \bar{x}_n \bar{x}_n^\top \hat{S}_m^{-1} \otimes \bar{x}_n \hat{S}_m^{-1} \right) D_r - 2 \left( \hat{S}_m^{-1} \otimes \left( \sum_{x_n \in X_m} \psi(\hat{t}_{nm}) \bar{x}_n \right) \hat{S}_m^{-1} \right) D_r
\]
\[
= -2 \sum_{x_n \in X_m} \eta(\hat{t}_{nm}) \left( \hat{S}_m^{-1} \bar{x}_n \bar{x}_n^\top \hat{S}_m^{-1} \otimes \bar{x}_n \hat{S}_m^{-1} \right) D_r.
\]

(56)

Here, we used that
\[
\sum_{x_n \in X_m} \psi(\hat{t}_{nm}) \bar{x}_n = \sum_{x_n \in X_m} \psi(\hat{t}_{nm}) \bar{x}_n - \left( \sum_{x_n \in X_m} \psi(\hat{t}_{nm}) \right) \frac{\sum_{x_n \in X_m} \psi(\hat{t}_{nm}) \bar{x}_n}{\sum_{x_n \in X_m} \psi(\hat{t}_{nm})} = 0
\]

(57)
B. First derivative with respect to the variance

We define $F$ as a $1 \times 1$ scalar function of the $r \times r$ matrix $S_m$. Hence, the resulting Jacobian matrix should be of size $1 \times r^2$. Again, we only keep the unique elements, such that, $F_S$ is of size $r \times \frac{1}{2}r(r + 1)$. Setting $F(S_m)$ equal to the log-likelihood function we get

$$F(S_m) = \ln (L(\theta_m | X_m)) = - \sum_{x_n \in X_m} \rho(t_{nm}) + N_m \ln \left( \frac{N_m}{N} \right) + \frac{N_m}{2} \ln \left( |S_m^{-1}| \right)$$

(58)

and taking the differential yields

$$dF(S_m) = - \sum_{x_n \in X_m} d\rho(t_{nm}) - \frac{N_m}{2} d\ln \left( |S_m| \right)$$

$$= \sum_{x_n \in X_m} \psi(t_{nm}) (x_n - \mu_m)^\top S_m^{-1} dS_m S_m^{-1} (x_n - \mu_m) - \frac{N_m}{2} \text{Tr} \left( S_m^{-1} dS_m \right)$$

(59)

and vectorization results in

$$d\text{vec}(F(S_m)) = \sum_{x_n \in X_m} \psi(t_{nm}) \left( (S_m^{-1} (x_n - \mu_m))^\top \otimes (x_n - \mu_m)^\top S_m^{-1} \right) d\text{vec}(S_m)$$

$$- \frac{N_m}{2} \text{Tr} \left( S_m^{-1} dS_m \right)$$

$$= \sum_{x_n \in X_m} \psi(t_{nm}) \left( (x_n - \mu_m)^\top S_m^{-1} \otimes (x_n - \mu_m)^\top S_m^{-1} \right) D_r \ d\text{vec}(S_m)$$

$$- \frac{N_m}{2} \text{vec}(S_m^{-1})^\top D_r \ d\text{vec}(S_m)$$

(60)

and the Jacobian matrix becomes

$$DF(S_m) = F'_S = \sum_{x_n \in X_m} \psi(t_{nm}) \left( \tilde{x}^\top S_m^{-1} \otimes \tilde{x}^\top S_m^{-1} \right) D_r - \frac{N_m}{2} \text{vec}(S_m^{-1})^\top D_r.$$ 

(61)

Defining $F_S$ as a $1 \times \frac{1}{2}r(r + 1)$ scalar function of the $r \times 1$ vector $\mu_m$, the resulting Jacobian matrix is of size $\frac{1}{2}r(r + 1) \times r$. Starting with the differential of (61)

$$dF_S(\mu_m)$$

$$= \sum_{x_n \in X_m} \left[ d\psi(t_{nm}) \left( (x_n - \mu_m)^\top S_m^{-1} \otimes (x_n - \mu_m)^\top S_m^{-1} \right) D_r \right.$$

$$+ \psi(t_{nm}) d \left( (x_n - \mu_m)^\top S_m^{-1} \otimes (x_n - \mu_m)^\top S_m^{-1} \right) D_r \left. \right]$$

$$= \sum_{x_n \in X_m} \left[ -2\eta(t_{nm}) (x_n - \mu_m)^\top S_m^{-1} d\mu_m \left( (x_n - \mu_m)^\top S_m^{-1} \otimes (x_n - \mu_m)^\top S_m^{-1} \right) D_r \right.$$

$$+ \psi(t_{nm}) \left( -d\mu_m^\top S_m^{-1} \otimes (x_n - \mu_m)^\top S_m^{-1} + (x_n - \mu_m)^\top S_m^{-1} \otimes (-d\mu_m)^\top S_m^{-1} \right) D_r \left. \right]$$
and applying the vectorization yields

\[
dvec(F_S(\mu_m)) = \sum_{x_n \in X_m} \left[ -2\eta(t_{nm}) \left( (\hat{x}_n^T S_m^{-1} \otimes \hat{x}_n S_m^{-1}) \vec{D}_r \otimes \hat{x}_n^T S_m^{-1} \right) \right. \]
\[
\left. + \psi(t_{nm}) \left( (D_r^T \otimes I_1) \vec{(-d\mu_m)} \otimes \hat{x}_n S_m^{-1} \right) \right. \]
\[
\left. + \left( D_r^T \otimes I_1 \right) \vec{((-d\mu_m)} \otimes \hat{x}_n S_m^{-1} \right) \right] \] 
= \sum_{x_n \in X_m} \left[ -2\eta(t_{nm}) \left( D_r^T \left( S_m^{-1} \hat{x}_n \otimes S_m^{-1} \hat{x}_n \right) \hat{x}_n^T S_m^{-1} \right) \right. \]
\[
\left. dvec(\mu_m) \right] 
- \psi(t_{nm}) D_r^T \left( (I_r \otimes I_r) \left( (S_m^{-1} \otimes I_1) \vec{(d\mu_m)} \otimes (S_m^{-1} \otimes I_1) \vec{(\hat{x}_n)} \right) \right. \]
\[
\left. \left( S_m^{-1} \otimes I_1 \right) \vec{(\hat{x}_n)} \otimes \left( (d\mu_m)^T \right) \right) \right] 
= -2 \sum_{x_n \in X_m} \left[ \eta(t_{nm}) \left( D_r^T \left( S_m^{-1} \hat{x}_n \otimes S_m^{-1} \hat{x}_n \right) \hat{x}_n^T S_m^{-1} \right) \right. \[
\left. + \psi(t_{nm}) D_r^T \left( S_m^{-1} \otimes S_m^{-1} \hat{x}_n \right) \right] \right] \]

(62)

and the final Jacobian matrix

\[
DF_S(\mu_m) = F_{S\mu} 
= -2 \sum_{x_n \in X_m} \left[ \eta(t_{nm}) \left( D_r^T \left( S_m^{-1} \hat{x}_n \otimes S_m^{-1} \hat{x}_n \right) \hat{x}_n^T S_m^{-1} \right) + \psi(t_{nm}) D_r^T \left( S_m^{-1} \otimes S_m^{-1} \hat{x}_n \right) \right] \]

(63)

Comparing (56) with (63) it is evident that

\[
F_{\mu S} = (F_{S\mu})^T. 
\]

(64)

Evaluating \( F_{S\mu} \) at \( \hat{S}_m \) and \( \hat{\mu}_m \) from Appendix B leads to

\[
\hat{F}_{S\mu} = -2 \sum_{x_n \in X_m} \left[ \eta(\hat{t}_{nm}) D_r^T \left( \hat{S}_m^{-1} \hat{x}_n \otimes \hat{S}_m^{-1} \hat{x}_n \hat{x}_n^T \hat{S}_m^{-1} \right) + \psi(\hat{t}_{nm}) D_r^T \left( \hat{S}_m^{-1} \otimes \hat{S}_m^{-1} \hat{x}_n \right) \right] 
\]
\[
= -2 \sum_{x_n \in X_m} \eta(\hat{t}_{nm}) D_r^T \left( \hat{S}_m^{-1} \hat{x}_n \otimes \hat{S}_m^{-1} \hat{x}_n \hat{x}_n^T \hat{S}_m^{-1} \right) - 2D_r^T \left( \hat{S}_m^{-1} \otimes \hat{S}_m^{-1} \sum_{x_n \in X_m} \psi(\hat{t}_{nm}) \hat{x}_n \right) 
\]
\[
= -2 \sum_{x_n \in X_m} \eta(\hat{t}_{nm}) D_r^T \left( \hat{S}_m^{-1} \hat{x}_n \otimes \hat{S}_m^{-1} \hat{x}_n \hat{x}_n^T \hat{S}_m^{-1} \right) \]

(65)
Finally, equivalently to (64),

\[
\hat{F}_\mu = \left( \hat{F}_s^\mu \right)^\top.
\] (66)

Defining \( F_s \) as a \( 1 \times \frac{1}{2} r (r+1) \) scalar function of the \( r \times r \) matrix \( S_m \), the resulting Jacobian matrix should be of size \( \frac{1}{2} r (r+1) \times r^2 \). As before, only the unique elements are of interest. Hence, the final size is \( \frac{1}{2} r (r+1) \times \frac{1}{2} r (r+1) \). Starting with the differential of (61) yields

\[
d(F_s(S_m)) = \sum_{x_n \in X_m} \left[ \psi(t_{nm}) \left( \tilde{x}_n S_m^{-1} \otimes \tilde{x}_n S_m^{-1} \right) D_r + \psi(t_{nm}) \right. \\
- \frac{N_m}{2} \text{vec} \left( dS_m^{-1} \right)^\top D_r \\
- \sum_{x_n \in X_m} \left[ \eta(t_{nm}) \left( \bar{S}^{-1} \bar{x}_n S_m^{-1} \otimes \bar{x}_n S_m^{-1} \right) \bar{D}_r \right] \\
- \psi(t_{nm}) \left( \text{vec} \left( \tilde{x}_n S_m^{-1} \right) \otimes \tilde{x}_n S_m^{-1} \right) \text{dvec} (S_m) \\

\]

and applying the vec operator leads to

\[
dvec(F_s(S_m)) = \sum_{x_n \in X_m} \left[ \eta(t_{nm}) \text{vec} \left( \tilde{x}_n S_m^{-1} dS_m S_m^{-1} \tilde{x}_n \left( \tilde{x}_n S_m^{-1} \otimes \tilde{x}_n S_m^{-1} \right) D_r \right) \\
- \psi(t_{nm}) \text{vec} \left( \tilde{x}_n S_m^{-1} \otimes \tilde{x}_n S_m^{-1} \right) D_r \right] + \frac{N_m}{2} \text{vec} \left( S_m^{-1} dS_m S_m^{-1} \right)^\top D_r
\]

with the commutation matrix \( K_{r,1} = I_r \).
Now, the Jacobian matrix is obtained as
\[
DF_S(S_m) = F_{SS} = - \sum_{x_n \in \mathcal{X}_m} \left[ \eta(t_{nm}) D_r^T \left( S_{m}^{-1} \hat{x}_n \hat{x}_n^T S_{m}^{-1} \otimes S_{m}^{-1} \hat{x}_n \hat{x}_n^T S_{m}^{-1} \right) D_r 
+ \psi(t_{nm}) D_r^T \left( S_{m}^{-1} \otimes S_{m}^{-1} \hat{x}_n \hat{x}_n^T S_{m}^{-1} \right) D_r 
+ \psi(t_{nm}) D_r^T \left( S_{m}^{-1} \hat{x}_n \hat{x}_n^T S_{m}^{-1} \otimes S_{m}^{-1} \right) D_r \right] + \frac{N_m}{2} D_r^T \left( S_{m}^{-1} \otimes S_{m}^{-1} \right) D_r.
\]

(68)

Evaluating \( F_{SS} \) at \( \hat{S}_m \) and \( \hat{\mu}_m \) from Appendix B leads to
\[
\hat{F}_{SS} = - \sum_{x_n \in \mathcal{X}_m} \eta(t_{nm}) D_r^T \left( \hat{S}_{m}^{-1} \hat{x}_n \hat{x}_n^T \hat{S}_{m}^{-1} \otimes \hat{S}_{m}^{-1} \hat{x}_n \hat{x}_n^T \hat{S}_{m}^{-1} \right) D_r 
- \sum_{x_n \in \mathcal{X}_m} \psi(t_{nm}) D_r^T \left( \hat{S}_{m}^{-1} \otimes \hat{S}_{m}^{-1} \hat{x}_n \hat{x}_n^T \hat{S}_{m}^{-1} \right) D_r 
- \sum_{x_n \in \mathcal{X}_m} \psi(t_{nm}) D_r^T \left( \hat{S}_{m}^{-1} \hat{x}_n \hat{x}_n^T \hat{S}_{m}^{-1} \otimes \hat{S}_{m}^{-1} \right) D_r 
+ \frac{N_m}{2} D_r^T \left( \hat{S}_{m}^{-1} \otimes \hat{S}_{m}^{-1} \right) D_r 
= - \sum_{x_n \in \mathcal{X}_m} \eta(t_{nm}) D_r^T \left( \hat{S}_{m}^{-1} \hat{x}_n \hat{x}_n^T \hat{S}_{m}^{-1} \otimes \hat{S}_{m}^{-1} \hat{x}_n \hat{x}_n^T \hat{S}_{m}^{-1} \right) D_r 
- D_r^T \left( \hat{S}_{m}^{-1} \otimes \hat{S}_{m}^{-1} \left( \sum_{x_n \in \mathcal{X}_m} \psi(t_{nm}) \hat{x}_n \hat{x}_n^T \right) \hat{S}_{m}^{-1} \right) D_r 
- D_r^T \left( \hat{S}_{m}^{-1} \left( \sum_{x_n \in \mathcal{X}_m} \psi(t_{nm}) \hat{x}_n \hat{x}_n^T \right) \hat{S}_{m}^{-1} \otimes \hat{S}_{m}^{-1} \right) D_r 
+ \frac{N_m}{2} D_r^T \left( \hat{S}_{m}^{-1} \otimes \hat{S}_{m}^{-1} \right) D_r.
\]

(69)
APPENDIX B

MAXIMUM LIKELIHOOD ESTIMATORS FOR RES DISTRIBUTIONS

A. Maximum Likelihood Estimator for the mean

Setting (52) equal to zero and solving for $\hat{\mu}_m$ leads to the ML estimator of $\mu_m$ as

$$\hat{\mu}_m = \frac{\sum_{x_n \in \mathcal{X}_m} \psi(t_{nm})x_n}{\sum_{x_n \in \mathcal{X}_m} \psi(t_{nm})}$$  \hspace{1cm} (70)

with

$$t_{nm} = (x_n - \hat{\mu}_m)^\top \bar{S}_m^{-1} (x_n - \hat{\mu}_m).$$  \hspace{1cm} (71)

B. Maximum Likelihood Estimator for the variance

Setting the first derivative (61) equal to zero yields

$$\sum_{x_n \in \mathcal{X}_m} \psi(t_{nm}) (\bar{x}_n^\top S_m^{-1} \otimes \bar{x}_n S_m^{-1}) D_r D_r^+ = \frac{N_m}{2} \operatorname{vec} \left( S_m^{-1} \right)^\top D_r D_r^+$$

$$\Rightarrow \sum_{x_n \in \mathcal{X}_m} \psi(t_{nm}) (\bar{x}_n \otimes \bar{x}_n) \left( S_m^{-1} \otimes S_m^{-1} \right) = \frac{N_m}{2} \operatorname{vec} \left( S_m^{-1} \right)^\top \left( S_m \otimes S_m \right)$$

$$\Rightarrow \sum_{x_n \in \mathcal{X}_m} \psi(t_{nm}) (\bar{x}_n \otimes \bar{x}_n) = \frac{N_m}{2} \operatorname{vec} \left( S_m S_m^{-1} S_m \right)$$

$$\Rightarrow \operatorname{vec} \left( \hat{S}_m \right) = \frac{2}{N_m} \sum_{x_n \in \mathcal{X}_m} \psi(t_{nm}) (\hat{x}_n \otimes \hat{x}_n)$$  \hspace{1cm} (72)

leads to a vectorized form of the ML estimator with $\hat{x}_n = x_n - \hat{\mu}_m$. To obtain the matrix form, we apply the inverse vec operator

$$\hat{S}_m = \frac{2}{N_m} \sum_{x_n \in \mathcal{X}_m} \left( \operatorname{vec} (I_r)^\top \otimes I_r \right) \left( I_r \otimes \hat{x}_n \otimes \psi(t_{nm}) \hat{x}_n \right)$$

$$= \frac{2}{N_m} \sum_{x_n \in \mathcal{X}_m} \left( \operatorname{vec} (I_r)^\top (I_r \otimes \hat{x}_n) \right) \otimes \psi(t_{nm}) I_r \hat{x}_n$$

$$= \frac{2}{N_m} \sum_{x_n \in \mathcal{X}_m} \left( \operatorname{vec} \left( \bar{x}_n^\top I_r I_r \right) \right)^\top \otimes \psi(t_{nm}) \hat{x}_n$$

$$= \frac{2}{N_m} \sum_{x_n \in \mathcal{X}_m} \bar{x}_n^\top \otimes \psi(t_{nm}) \hat{x}_n$$

$$= \frac{2}{N_m} \sum_{x_n \in \mathcal{X}_m} \psi(t_{nm}) \hat{x}_n \hat{x}_n^\top$$  \hspace{1cm} (73)
Algorithm 2: EM algorithm for RES distributions

Input: $X$, $i_{\text{max}}$, $l$, $g(t)$, $\psi(t)$

Output: $\hat{\mu}_m$, $\hat{S}_m$, $\hat{\gamma}_m$

for $m = 1, \ldots, l$ do

Initialize $\hat{\mu}_m^{(0)}$ with K-medoids

\[
\hat{S}_m^{(0)} = \frac{1}{N_m} \sum_{x_n \in X_m} (x_n - \hat{\mu}_m^{(0)}) (x_n - \hat{\mu}_m^{(0)})^\top
\]

\[
\hat{\gamma}_m^{(0)} = N_m / N
\]

for $i = 1, \ldots, i_{\text{max}}$ do

E-step:

for $m = 1, \ldots, l$ do

for $n = 1, \ldots, N$ do

\[
\hat{v}_{nm}^{(i)} = \frac{\hat{\gamma}_m^{(i-1)} |\hat{S}_m^{(i-1)}|^{-\frac{1}{2}} g \left(\hat{t}_{nm}^{(i-1)}\right)}{\sum_{j=1}^l \hat{\gamma}_j^{(i-1)} |\hat{S}_j^{(i-1)}|^{-\frac{1}{2}} g \left(\hat{t}_{nj}^{(i-1)}\right)}
\]

\[
\hat{v}_{nm}^{(i)} = \hat{v}_{nm}^{(i)} \psi \left(\hat{t}_{nm}^{(i-1)}\right)
\]

M-Step:

for $m = 1, \ldots, l$ do

\[
\hat{\mu}_m^{(i)} = \frac{\sum_{n=1}^N \hat{v}_{nm}^{(i)} x_n^{(i)}}{\sum_{n=1}^N \hat{v}_{nm}^{(i)}}
\]

\[
\hat{S}_m^{(i)} = \left[ 2 \sum_{n=1}^N \hat{v}_{nm}^{(i)} (x_n^{(i)} - \hat{\mu}_m^{(i)}) (x_n^{(i)} - \hat{\mu}_m^{(i)})^\top \right] / \sum_{n=1}^N \hat{v}_{nm}^{(i)}
\]

\[
\hat{\gamma}_m^{(i)} = \frac{1}{N} \sum_{n=1}^N \hat{v}_{nm}^{(i)}
\]

Calculate log-likelihood:

\[
\ln \left( \mathcal{L} \left( \hat{\Phi}_t^{(i)} | \mathcal{X} \right) \right) = \sum_{n=1}^N \ln \left( \sum_{m=1}^l \hat{\gamma}_m^{(i)} |\hat{S}_m^{(i)}|^{-\frac{1}{2}} g \left(\hat{t}_{nm}^{(i)}\right) \right)
\]

if $\left| \ln \left( \mathcal{L} \left( \hat{\Phi}_t^{(i)} | \mathcal{X} \right) \right) - \ln \left( \mathcal{L} \left( \hat{\Phi}_t^{(i-1)} | \mathcal{X} \right) \right) \right| < \delta$ then

break loop
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Supplementary Information: Robust M-Estimation Based Bayesian Cluster Enumeration for Real Elliptically Symmetric Distributions

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I. STRUCTURE

This Supplementary Information for the paper 'Robust M-Estimation Based Bayesian Cluster Enumeration for Real Elliptically Symmetric Distributions' is organized as follows: In Appendix A, a detailed step by step solution of the second derivatives of the log-likelihood function for the FIM is given. Afterwards the ML estimates for $\hat{S}_m$ and $\hat{\mu}_m$ based on the first derivatives are calculated and some used identities are shown. Finally we provide a comprehensive summary of the used matrix calculus in Appendix C.

APPENDIX A

DERIVATIVES FOR THE FIM OF THE RES DISTRIBUTION

The FIM requires the calculation of the second derivative of the log-likelihood function. In this appendix this is done for the set of RES distributions. Since the differentiation of matrices is not straightforward, the derivation is shown in detail. A short introduction on matrix calculus can be found in [1], a more detailed explanation is provided in [2] and a large number of examples are discussed in [3]. Most of the used matrix calculus rules can be found in these references and are also noted in Appendix C.

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A. First derivative with respect to the mean

First, we define \( F \) as a \( 1 \times 1 \) scalar function of the \( r \times 1 \) vector \( \mu_m \). Hence, the resulting Jacobian matrix is of size \( 1 \times r \). Setting \( F(\mu_m) \) equal to the log-likelihood function we get

\[
F(\mu_m) = \ln \left( \mathcal{L}(\theta_m | \mathcal{X}_m) \right) = - \sum_{x_n \in \mathcal{X}_m} \rho(t_{nm}) + N_m \ln \left( \frac{N_m}{N} \right) + \frac{N_m}{2} \ln \left( |S_m^{-1}| \right)
\]  

(1)

and afterwards apply the differential

\[
dF(\mu_m) = - \sum_{x_n \in \mathcal{X}_m} d\rho(t_{nm})
\]

with \( \psi(t_{nm}) = \frac{\partial \rho(t_{nm})}{\partial t_{nm}} \)

\[
= - \sum_{x_n \in \mathcal{X}_m} \psi(t_{nm}) d \left( (x_n - \mu_m)^\top S_m^{-1} (x_n - \mu_m) \right)
\]

\[
= - \sum_{x_n \in \mathcal{X}_m} \psi(t_{nm}) \left( (-d\mu_m)^\top S_m^{-1} (x_n - \mu_m) + (x_n - \mu_m)^\top S_m^{-1} (-d\mu_m) \right)
\]

with \( \alpha = \alpha^\top, \alpha \) being a scalar

\[
= \sum_{x_n \in \mathcal{X}_m} \psi(t_{nm}) \left( \left( (d\mu_m)^\top S_m^{-1} (x_n - \mu_m) \right)^\top + (x_n - \mu_m)^\top S_m^{-1} (d\mu_m) \right)
\]

with \( (AB)^\top = B^\top A^\top \)

\[
= \sum_{x_n \in \mathcal{X}_m} \psi(t_{nm}) \left( (x_n - \mu_m)^\top S_m^{-1} (d\mu_m) + (x_n - \mu_m)^\top S_m^{-1} S_m (d\mu_m) \right)
\]

\[
= \sum_{x_n \in \mathcal{X}_m} 2\psi(t_{nm}) (x_n - \mu_m)^\top S_m^{-1} d\mu_m.
\]

(2)

Finally, the Jacobian matrix of \( F(\mu_m) \), which we will denote as \( F_\mu \), becomes

\[
DF(\mu_m) = F_\mu = 2 \sum_{x_n \in \mathcal{X}_m} \psi(t_{nm}) (x_n - \mu_m)^\top S_m^{-1}.
\]

(3)

For the second derivative, \( F_\mu \) is a \( 1 \times r \) vector function of the \( r \times 1 \) vector \( \mu_m \), hence the resulting Jacobian matrix is of size \( r \times r \). Starting with the differential of (3)

\[
dF_\mu(\mu_m) = 2 \sum_{x_n \in \mathcal{X}_m} \left[ d\psi(t_{nm}) (x_n - \mu_m)^\top S_m^{-1} + \psi(t_{nm}) d \left( (x_n - \mu_m)^\top S_m^{-1} \right) \right]
\]

with \( \eta(t_{nm}) = \frac{\partial \psi(t_{nm})}{\partial t_{nm}} \)

\[
= - 2 \sum_{x_n \in \mathcal{X}_m} \left[ 2\eta(t_{nm}) (x_n - \mu_m)^\top S_m^{-1} d\mu_m (x_n - \mu_m)^\top S_m^{-1} + \psi(t_{nm}) (d\mu_m)^\top S_m^{-1} \right]
\]

(4)
and applying the vec operator
\[
dvec(F_\mu(\mu_m)) = - \sum_{x_n \in \mathcal{X}_m} 4\eta(t_{nm}) \text{vec} \left( (x_n - \mu_m)^\top S_m^{-1} \mu_m (x_n - \mu_m)^\top S_m^{-1} \right) + 2\psi(t_{nm}) \text{vec} \left( (\mu_m)^\top S_m^{-1} \right)
\]
with (38) and (39)
\[
= - \sum_{x_n \in \mathcal{X}_m} 4\eta(t_{nm}) \left( S_m^{-1} (x_n - \mu_m) \otimes (x_n - \mu_m)^\top S_m^{-1} \right) \text{dvec}(\mu_m) + 2\psi(t_{nm}) S_m^{-1} \text{d}\mu_m.
\]

Hence, we obtain the Jacobian matrix \( F_{\mu\mu} \) as
\[
DF_{\mu}(\mu_m) = F_{\mu\mu} = - \sum_{x_n \in \mathcal{X}_m} 4\eta(t_{nm}) S_m^{-1} (x_n - \mu_m) (x_n - \mu_m)^\top S_m^{-1} + 2\psi(t_{nm}) S_m^{-1} \]
(5)

Evaluating \( F_{\mu\mu} \) at \( \hat{S}_m \) and \( \hat{\mu}_m \) from Appendix B leads to
\[
\hat{F}_{\mu\mu} = -4\hat{S}_m^{-1} \left( \sum_{x_n \in \mathcal{X}_m} \eta(\hat{t}_{nm}) (x_n - \mu_m) (x_n - \hat{\mu}_m)^\top \right) \hat{S}_m^{-1} - 2\hat{S}_m^{-1} \sum_{x_n \in \mathcal{X}_m} \psi(\hat{t}_{nm})
\]
(7)

For the other second derivative, \( F_\mu \) is a \( 1 \times r \) vector function of the \( r \times r \) matrix \( S_m \), hence the resulting Jacobian matrix should be of size \( r \times r^2 \), but because \( S_m \) is a symmetric matrix and only the unique elements are needed, we use the duplication matrix (76) to only keep the unique elements of \( S_m \). Therefore the resulting matrix only has the size \( r \times \frac{1}{2}r(r+1) \). Starting with the differential of (3)
\[
dF_\mu(S_m) = -2 \sum_{x_n \in \mathcal{X}_m} \left[ d\psi(t_{nm}) (x_n - \mu_m)^\top S_m^{-1} + \psi(t_{nm}) \text{d} \left( (x_n - \mu_m)^\top S_m^{-1} \right) \right]
\]
with (58)
\[
= -2 \sum_{x_n \in \mathcal{X}_m} \left[ \eta(t_{nm}) (x_n - \mu_m)^\top S_m^{-1} \text{d} S_m S_m^{-1} (x_n - \mu_m) (x_n - \mu_m)^\top S_m^{-1} + \psi(t_{nm}) (x_n - \mu_m)^\top S_m^{-1} \text{d} S_m S_m^{-1} \right]
\]
(8)
For ease of notation, we introduce
\[ \tilde{x}_n \triangleq x_n - \mu_m \] (9)
and continue with the application of the vec operator
\[
dvec(F_\mu(S_m)) = -2 \sum_{x_n \in \mathcal{X}_m} \left[ \eta(t_{nm}) \text{vec} \left( \tilde{x}_n S_m^{-1} dS_m S_m^{-1} \tilde{x}_n \tilde{x}_n^T S_m^{-1} \right) \right.
\]
\[ + \psi(t_{nm}) \text{vec} \left( \tilde{x}_n S_m^{-1} dS_m S_m^{-1} \right) \]
with (76)
\[
= -2 \sum_{x_n \in \mathcal{X}_m} \left[ \eta(t_{nm}) \left( \left( S_m^{-1} \tilde{x}_n \tilde{x}_n^T S_m^{-1} \right) \otimes \tilde{x}_n S_m^{-1} \right) D_r \text{dvec}(S_m) \right.
\]
\[ + \psi(t_{nm}) \left( S_m^{-1} \otimes \tilde{x}_n S_m^{-1} \right) D_r \text{dvec}(S_m) \]
so that
\[
DF_\mu(S_m) = F_{\mu S} = -2 \sum_{x_n \in \mathcal{X}_m} \left[ \eta(t_{nm}) \left( S_m^{-1} \tilde{x}_n \tilde{x}_n^T S_m^{-1} \otimes \tilde{x}_n S_m^{-1} \right) D_r + \psi(t_{nm}) \left( S_m^{-1} \otimes \tilde{x}_n S_m^{-1} \right) D_r \right]. \tag{10}
\]
Evaluating \( F_{\mu S} \) at \( \hat{S}_m \) and \( \hat{\mu}_m \) with \( \tilde{x}_n \triangleq x_n - \mu_m \) from Appendix B leads to
\[
\hat{F}_{\mu S} = -2 \sum_{x_n \in \mathcal{X}_m} \left[ \eta(t_{nm}) \left( \hat{S}_m^{-1} \tilde{x}_n \tilde{x}_n^T \hat{S}_m^{-1} \otimes \tilde{x}_n \hat{S}_m^{-1} \right) D_r + \psi(t_{nm}) \left( \hat{S}_m^{-1} \otimes \tilde{x}_n \hat{S}_m^{-1} \right) D_r \right.
\]
\[ = -2 \sum_{x_n \in \mathcal{X}_m} \eta(t_{nm}) \left( \hat{S}_m^{-1} \tilde{x}_n \tilde{x}_n^T \hat{S}_m^{-1} \otimes \tilde{x}_n \hat{S}_m^{-1} \right) D_r - 2 \sum_{x_n \in \mathcal{X}_m} \psi(t_{nm}) \left( \hat{S}_m^{-1} \otimes \tilde{x}_n \hat{S}_m^{-1} \right) D_r \]
\[ = -2 \sum_{x_n \in \mathcal{X}_m} \eta(t_{nm}) \left( \hat{S}_m^{-1} \tilde{x}_n \tilde{x}_n^T \hat{S}_m^{-1} \otimes \tilde{x}_n \hat{S}_m^{-1} \right) D_r - 2 \left( \hat{S}_m^{-1} \otimes \left( \sum_{x_n \in \mathcal{X}_m} \psi(t_{nm}) \tilde{x}_n \right) \hat{S}_m^{-1} \right) D_r \]
with (32)
\[
= -2 \sum_{x_n \in \mathcal{X}_m} \eta(t_{nm}) \left( \hat{S}_m^{-1} \tilde{x}_n \tilde{x}_n^T \hat{S}_m^{-1} \otimes \tilde{x}_n \hat{S}_m^{-1} \right) D_r \tag{12}
\]

B. First derivative with respect to the variance

We define \( F \) as a \( 1 \times 1 \) scalar function of the \( r \times r \) matrix \( S_m \). Hence, the resulting Jacobian matrix should be of size \( 1 \times r^2 \). Again, we only keep the unique elements, such that, \( F_S \) is of size \( r \times \frac{1}{2} r(r + 1) \). Setting \( F(S_m) \) equal to the log-likelihood function we get
\[
F(S_m) = \ln(\mathcal{L}(\theta_m|\mathcal{X}_m)) = - \sum_{x_n \in \mathcal{X}_m} \rho(t_{nm}) + N_m \ln \left( \frac{N_m}{N} \right) + \frac{N_m}{2} \ln \left( |S_m^{-1}| \right) \tag{13}
\]
and taking the differential yields
\[
dF(S_m) = - \sum_{x_n \in X_m} d\rho(t_{nm}) - \frac{N_m}{2} d \ln (|S_m|)
\]
with (58) and (60)
\[
= \sum_{x_n \in X_m} \psi(t_{nm}) (x_n - \mu_m)^T S_m^{-1} dS_m S_m^{-1} (x_n - \mu_m) - \frac{N_m}{2} \text{Tr} (S_m^{-1} dS_m)
\]
\[
= \sum_{x_n \in X_m} \psi(t_{nm}) (x_n - \mu_m)^T S_m^{-1} dS_m S_m^{-1} (x_n - \mu_m) - \frac{N_m}{2} \text{Tr} (S_m^{-1} dS_m)
\]
(14)
with vectorization
\[
dvec(F(S_m)) = \sum_{x_n \in X_m} \psi(t_{nm}) \text{vec} \left((x_n - \mu_m)^T S_m^{-1} dS_m S_m^{-1} (x_n - \mu_m)\right)
\]
\[
- \frac{N_m}{2} \text{vec} \left(\text{Tr} (S_m^{-1} dS_m)\right)
\]
\[
= \sum_{x_n \in X_m} \psi(t_{nm}) \left((S_m^{-1} (x_n - \mu_m))^T \otimes (x_n - \mu_m)^T S_m^{-1}\right) dvec(S_m)
\]
\[
- \frac{N_m}{2} \text{Tr} (S_m^{-1} dS_m)
\]
with (41)
\[
= \sum_{x_n \in X_m} \psi(t_{nm}) \left((x_n - \mu_m)^T S_m^{-1} \otimes (x_n - \mu_m)^T S_m^{-1}\right) dvec(S_m)
\]
\[
- \frac{N_m}{2} \text{vec} \left(S_m^{-1}\right)^T dvec(S_m)
\]
\[
= \sum_{x_n \in X_m} \psi(t_{nm}) \left((x_n - \mu_m)^T S_m^{-1} \otimes (x_n - \mu_m)^T S_m^{-1}\right) D_r \text{ dvec}(S_m)
\]
\[
- \frac{N_m}{2} \text{vec} \left(S_m^{-1}\right)^T D_r \text{ dvec}(S_m)
\]
(15)
and the Jacobian matrix
\[
DF(S_m) = F_S
\]
\[
= \sum_{x_n \in X_m} \psi(t_{nm}) \left((x_n - \mu_m)^T S_m^{-1} \otimes (x_n - \mu_m)^T S_m^{-1}\right) D_r - \frac{N_m}{2} \text{vec} \left(S_m^{-1}\right)^T D_r.
\]
(16)

Defining \(F_S\) as a \(1 \times \frac{1}{2} r(r + 1)\) scalar function of the \(r \times 1\) vector \(\mu_m\), the resulting Jacobian matrix is of size \(\frac{1}{2} r(r + 1) \times r\). Starting with the differential of (16)
\[
dF_S(\mu_m)
\]
\[
= \sum_{x_n \in X_m} d \left(\psi(t_{nm}) \left((x_n - \mu_m)^T S_m^{-1} \otimes (x_n - \mu_m)^T S_m^{-1}\right) D_r\right)
\]
\[
= \sum_{x_n \in \mathcal{X}_m} \left[ \psi(t_{nm}) \left( (x_n - \mu_m)^\top S_m^{-1} \otimes (x_n - \mu_m)^\top S_m^{-1} \right) D_r 
+ \psi(t_{nm}) d \left( (x_n - \mu_m)^\top S_m^{-1} \otimes (x_n - \mu_m)^\top S_m^{-1} \right) D_r \right]
\]

with \[(61)\]

\[
= \sum_{x_n \in \mathcal{X}_m} \left[ -2\eta(t_{nm}) (x_n - \mu_m)^\top S_m^{-1} d \mu_m \left( (x_n - \mu_m)^\top S_m^{-1} \otimes (x_n - \mu_m)^\top S_m^{-1} \right) D_r 
+ \psi(t_{nm}) \left[ \text{vec} \left( (x_n - \mu_m)^\top S_m^{-1} \otimes \tilde{x}_n S_m^{-1} \right) D_r \right] 
+ \text{vec} \left( (x_n S_m^{-1} \otimes (-d \mu_m)^\top S_m^{-1}) D_r \right) \right]
\]

and the vectorization
\[
d \text{vec}(F_S(\mu_m))
\]

\[
= \sum_{x_n \in \mathcal{X}_m} \left[ -2\eta(t_{nm}) \text{vec} \left( \tilde{x}_n S_m^{-1} d \mu_m \left( \tilde{x}_n S_m^{-1} \otimes \tilde{x}_n S_m^{-1} \right) D_r \right) 
+ \psi(t_{nm}) \left[ \text{vec} \left( (x_n - \mu_m)^\top S_m^{-1} \otimes \tilde{x}_n S_m^{-1} \right) D_r \right] 
+ \text{vec} \left( (x_n S_m^{-1} \otimes (-d \mu_m)^\top S_m^{-1}) D_r \right) \right]
\]

\[
= \sum_{x_n \in \mathcal{X}_m} \left[ -2\eta(t_{nm}) \left[ \left( (\tilde{x}_n S_m^{-1} \otimes \tilde{x}_n S_m^{-1}) D_r \right)^\top \otimes \tilde{x}_n S_m^{-1} \right] \text{dvec} \left( \mu_m \right) 
+ \psi(t_{nm}) \left[ \left( D_r^\top \otimes I_1 \right) \text{vec} \left( (x_n S_m^{-1} \otimes (-d \mu_m)^\top S_m^{-1}) \right) \right] 
+ \left( D_r^\top \otimes I_1 \right) \text{vec} \left( \tilde{x}_n S_m^{-1} \otimes (-d \mu_m)^\top S_m^{-1} \right) \right]
\]

with \[(40)\]

\[
= \sum_{x_n \in \mathcal{X}_m} \left[ -2\eta(t_{nm}) \left[ \left( D_r^\top (S_m^{-1} \otimes S_m^{-1}) \right) \otimes \tilde{x}_n S_m^{-1} \right] \text{dvec} \left( \mu_m \right) 
+ \psi(t_{nm}) D_r^\top \left[ (I_r \otimes K_{r1} \otimes I_1) \left( \text{vec} \left( (x_n S_m^{-1}) \otimes \tilde{x}_n S_m^{-1} \right) \right) \right] 
+ \left( I_r \otimes K_{r1} \otimes I_1 \right) \text{vec} \left( \tilde{x}_n S_m^{-1} \otimes \text{vec} \left( (-d \mu_m)^\top S_m^{-1} \right) \right) \right]
\]

with \[(44)\] and \[(69)\]
\[ \begin{align*}
&= \sum_{x_n \in \mathcal{X}_m} \left[ -2\eta(t_{nm}) \left[ D_r^T \left( S_m^{-1} \bar{x}_n \otimes S_m^{-1} \bar{x}_n \right) \bar{x}_n S_m^{-1} \right] \text{dvec} (\mu_m) \\
&\quad - \psi(t_{nm}) D_r^T \left[ (I_r \otimes I_r) \left( (S_m^{-1} \otimes I_1) \text{vec} \left( (d\mu_m)^T \right) \otimes (S_m^{-1} \otimes I_1) \text{vec} \left( \bar{x}_n^T \right) \right) \right] \\
&\quad + (I_r \otimes I_r) \left( (S_m^{-1} \otimes I_1) \text{vec} \left( \bar{x}_n^T \right) \otimes (S_m^{-1} \otimes I_1) \text{vec} \left( (d\mu_m)^T \right) \right) \right] \\
\end{align*} \]

with (33)

\[ \begin{align*}
&= \sum_{x_n \in \mathcal{X}_m} \left[ -2\eta(t_{nm}) \left[ D_r^T \left( S_m^{-1} \bar{x}_n \otimes S_m^{-1} \bar{x}_n \right) \bar{x}_n S_m^{-1} \right] \text{dvec} (\mu_m) \\
&\quad - \psi(t_{nm}) D_r^T \left[ I_r^2 \left( S_m^{-1} \text{dvec} (\mu_m) \otimes S_m^{-1} \bar{x}_n \right) \right. \\
&\left. \quad + I_r^2 \left( S_m^{-1} \bar{x}_n \otimes S_m^{-1} \text{dvec} (\mu_m) \right) \right] \\
\end{align*} \]

\[ \begin{align*}
&= \sum_{x_n \in \mathcal{X}_m} \left[ -2\eta(t_{nm}) D_r^T \left( S_m^{-1} \bar{x}_n \otimes S_m^{-1} \bar{x}_n \right) \bar{x}_n S_m^{-1} \text{dvec} (\mu_m) \\
&\quad - \psi(t_{nm}) D_r^T \left( (S_m^{-1} \otimes S_m^{-1}) \bar{x}_n \right) \text{dvec} (\mu_m) \right] \\
\end{align*} \]

with (75) and (77)

\[ \begin{align*}
&= -2 \sum_{x_n \in \mathcal{X}_m} \left[ \eta(t_{nm}) D_r^T \left( S_m^{-1} \bar{x}_n \otimes S_m^{-1} \bar{x}_n \right) \bar{x}_n S_m^{-1} \text{dvec} (\mu_m) \\
&\quad + \psi(t_{nm}) D_r^T \left( S_m^{-1} \otimes S_m^{-1} \bar{x}_n \right) \text{dvec} (\mu_m) \right] \\
&\quad + \psi(t_{nm}) D_r^T \left( S_m^{-1} \otimes S_m^{-1} \bar{x}_n \right) \text{dvec} (\mu_m) \right] \right] \\
&\quad + \psi(t_{nm}) D_r^T \left( S_m^{-1} \otimes S_m^{-1} \bar{x}_n \right) \text{dvec} (\mu_m) \right] \\
\end{align*} \]

and the final Jacobian matrix

\[ DF_S(\mu_m) = F_{S\mu} \]

\[ \begin{align*}
&= -2 \sum_{x_n \in \mathcal{X}_m} \left[ \eta(t_{nm}) D_r^T \left( S_m^{-1} \bar{x}_n \otimes S_m^{-1} \bar{x}_n \bar{x}_n S_m^{-1} \right) + \psi(t_{nm}) D_r^T \left( S_m^{-1} \otimes S_m^{-1} \bar{x}_n \right) \right]. \\
\end{align*} \]

(18)

Comparing (11) with (19) it is evident that

\[ F_{\mu S} = (F_{S\mu})^T. \]

Evaluating \( F_{S\mu} \) at \( \hat{S}_m \) and \( \hat{\mu}_m \) from Appendix B leads to

\[ \begin{align*}
\hat{F}_{S\mu} &= -2 \sum_{x_n \in \mathcal{X}_m} \left[ \eta(t_{nm}) D_r^T \left( \hat{S}_m^{-1} \hat{x}_n \otimes \hat{S}_m^{-1} \hat{x}_n \hat{x}_n \hat{S}_m^{-1} \right) + \psi(t_{nm}) D_r^T \left( \hat{S}_m^{-1} \otimes \hat{S}_m^{-1} \hat{x}_n \right) \right] \\
&= -2 \sum_{x_n \in \mathcal{X}_m} \eta(t_{nm}) D_r^T \left( \hat{S}_m^{-1} \hat{x}_n \otimes \hat{S}_m^{-1} \hat{x}_n \hat{x}_n \hat{S}_m^{-1} \right) - 2 \sum_{x_n \in \mathcal{X}_m} \psi(t_{nm}) D_r^T \left( \hat{S}_m^{-1} \otimes \hat{S}_m^{-1} \hat{x}_n \right) \\
\end{align*} \]
\[
\begin{align*}
&= -2 \sum_{x_n \in X_m} \eta(t_{nm}) D_r^T \left( \bar{S}_{m}^{-1} \bar{x}_n \otimes \bar{S}_{m}^{-1} \bar{x}_n \bar{S}_{m}^{-1} \right) - 2D_r^T \left( \bar{S}_{m}^{-1} \otimes \bar{S}_{m}^{-1} \sum_{x_n \in X_m} \psi(t_{nm}) \bar{x}_n \right) \\
&\quad \text{with (32)} \\
&= -2 \sum_{x_n \in X_m} \eta(t_{nm}) D_r^T \left( \bar{S}_{m}^{-1} \bar{x}_n \otimes \bar{S}_{m}^{-1} \bar{x}_n \bar{S}_{m}^{-1} \right)
\end{align*}
\]

and equivalently to (20)
\[
\hat{F}_{\mu}S = \left( \hat{F}_{S\mu} \right)^T.
\]

Defining \( F_S \) as a \( 1 \times \frac{1}{2} r(r+1) \) scalar function of the \( r \times r \) matrix \( S_m \), the resulting Jacobian matrix should be of size \( \frac{1}{2} r(r+1) \times r^2 \). As before, only the unique elements are of interest. Hence, the final size is \( \frac{1}{2} r(r+1) \times \frac{1}{2} r(r+1) \). Starting with the differential of (16)
\[
d(F_S(S_m)) = \sum_{x_n \in X_m} d \left( \psi(t_{nm}) \left( \bar{x}_n^T S_m^{-1} \otimes \bar{x}_n^T S_m^{-1} \right) \right) D_r - \frac{N_m}{2} \text{vec} \left( dS_m^{-1} \right)^T D_r
\]

\[
= \sum_{x_n \in X_m} \left[ d\psi(t_{nm}) \left( \bar{x}_n^T S_m^{-1} \otimes \bar{x}_n^T S_m^{-1} \right) D_r + \psi(t_{nm}) \right. \left. d \left( \bar{x}_n^T S_m^{-1} \otimes \bar{x}_n^T S_m^{-1} \right) D_r \right]
\]

\[
- \frac{N_m}{2} \text{vec} \left( dS_m^{-1} \right)^T D_r
\]

\[
= - \sum_{x_n \in X_m} \left[ \eta(t_{nm}) \bar{x}_n^T S_m^{-1} dS_m S_m^{-1} \bar{x}_n \left( \bar{x}_n^T S_m^{-1} \otimes \bar{x}_n^T S_m^{-1} \right) D_r \right]
\]

\[
- \frac{N_m}{2} \text{vec} \left( S_m^{-1} dS_m S_m^{-1} \right)^T D_r
\]

and applying the vec operator

\[
dvec(F_S(S_m))
\]

\[
= - \sum_{x_n \in X_m} \left[ \eta(t_{nm}) \text{vec} \left( \bar{x}_n^T S_m^{-1} dS_m S_m^{-1} \bar{x}_n \left( \bar{x}_n^T S_m^{-1} \otimes \bar{x}_n^T S_m^{-1} \right) D_r \right) \right.
\]

\[
- \frac{N_m}{2} \text{vec} \left( S_m^{-1} dS_m S_m^{-1} \right)^T D_r \]

with Equations (39) and (64)

\[
= - \sum_{x_n \in X_m} \left[ \eta(t_{nm}) \left( S_m^{-1} \bar{x}_n \left( \bar{x}_n^T S_m^{-1} \otimes \bar{x}_n^T S_m^{-1} \right) D_r \right)^T \otimes \bar{x}_n^T S_m^{-1} \right] \text{dvec} \left( S_m \right)
\]

\[
- \psi(t_{nm}) D_r^T \left( I_r \otimes K_{r1} \otimes I_1 \right) \left[ \left( I_r \otimes \text{vec} \left( \bar{x}_n^T S_m^{-1} \right) \right) \right]
\]

\[
+ \left( \text{vec} \left( \bar{x}_n^T S_m^{-1} \right) \otimes I_r \right) \text{dvec} \left( \bar{x}_n^T S_m^{-1} \right) \right] + \frac{N_m}{2} D_r^T \text{vec} \left( S_m^{-1} dS_m S_m^{-1} \right)
\]
we finally obtain the Jacobian matrix

\[
\mathbf{F}_{\mu} = \mathbf{F}_{\mu}\end{array}
\]

Evaluating \( \mathbf{F}_{\mu} \) at \( \hat{S}_m \) and \( \hat{\mu}_m \) from Appendix B leads to

\[
\hat{\mathbf{F}}_{\mu} = - \sum_{x_n \in \mathcal{X}_m} \eta(t_{nm}) \mathbf{D}_r^T \left( \hat{S}_m^{-1} \hat{x}_n \otimes \hat{S}_m^{-1} \hat{x}_n \right) \mathbf{D}_r\]

\[
- \sum_{x_n \in \mathcal{X}_m} \psi(t_{mn}) \mathbf{D}_r^T \left( \hat{S}_m^{-1} \hat{\mu}_n \otimes \hat{S}_m^{-1} \hat{\mu}_n \right) \mathbf{D}_r + \frac{N_m}{2} \mathbf{D}_r^T \left( \hat{S}_m^{-1} \otimes \hat{S}_m^{-1} \right) \mathbf{D}_r.
\]
A. Maximum Likelihood Estimator for the mean

Setting (3) equal to zero leads to the ML estimator $\hat{\mu}_m$ of $\mu_m$, which results in

$$2 \sum_{x_n \in X_m} \psi(t_{nm}) (x_n - \mu_m)^\top S_m^{-1} = 0$$

$$\Rightarrow \sum_{x_n \in X_m} \psi(t_{nm}) (x_n - \mu_m)^\top = 0$$

$$\Rightarrow \hat{\mu}_m = \frac{\sum_{x_n \in X_m} \psi(t_{nm}) x_n}{\sum_{x_n \in X_m} \psi(t_{nm})}$$

with

$$i_{nm} = (x_n - \hat{\mu}_m)^\top \hat{S}_m^{-1} (x_n - \hat{\mu}_m).$$

B. Maximum Likelihood Estimator for the variance

Again setting the first derivative (16) equal to zero

$$\sum_{x_n \in X_m} \psi(t_{nm}) (\hat{x}_n S_m^{-1} \otimes \hat{x}_n S_m^{-1}) D_r - \frac{N_m}{2} \text{vec} (S_m^{-1})^\top D_r = 0$$
leads to a vectorized form of the ML estimator with \( \hat{x}_n \triangleq x_n - \hat{\mu}_m \). To obtain the matrix form, we apply (37)

\[
\hat{S}_m = \frac{2}{N_m} \sum_{x_n \in X_m} \psi(\hat{t}_{nm}) (\hat{x}_n \otimes \hat{x}_n) = \frac{2}{N_m} \sum_{x_n \in X_m} \psi(\hat{t}_{nm}) \hat{x}_n
\]

C. Interesting Identities

Using the ML estimators, some interesting identities can be shown, which can be used to further simplify the final results. Firstly in [4] we find

\[
\hat{S}_m = \frac{2}{N_m} \sum_{x_n \in X_m} \psi(\hat{t}_{nm}) \hat{x}_n \hat{x}_n^T
\]
\[ I_r = \frac{2}{N_m} \sum_{x_n \in \mathcal{X}_m} \psi(\hat{t}_{nm})\hat{x}_n \hat{x}_n^\top \hat{S}_m^{-1} \]

\[ \Rightarrow \text{Tr} (I_r) = \frac{2}{N_m} \sum_{x_n \in \mathcal{X}_m} \psi(\hat{t}_{nm}) \text{Tr} \left( \hat{x}_n \hat{x}_n^\top \hat{S}_m^{-1} \right) \]

\[ \Rightarrow r = \frac{2}{N_m} \sum_{x_n \in \mathcal{X}_m} \psi(\hat{t}_{nm}) \text{Tr} \left( \hat{x}_n^\top \hat{S}_m^{-1} \hat{x}_n \right) \]

\[ \Rightarrow r = \frac{2}{N_m} \sum_{x_n \in \mathcal{X}_m} \psi(\hat{t}_{nm})\hat{t}_{nm}. \quad (31) \]

Also, one can find

\[ \sum_{x_n \in \mathcal{X}_m} \psi(\hat{t}_{nm})\hat{x}_n = \sum_{x_n \in \mathcal{X}_m} \psi(\hat{t}_{nm})(x_n - \hat{\mu}_m) \]

\[ = \sum_{x_n \in \mathcal{X}_m} \psi(\hat{t}_{nm})x_n - \left( \sum_{x_n \in \mathcal{X}_m} \psi(\hat{t}_{nm}) \right) \hat{\mu}_m \]

\[ = \sum_{x_n \in \mathcal{X}_m} \psi(\hat{t}_{nm})x_n - \left( \sum_{x_n \in \mathcal{X}_m} \psi(\hat{t}_{nm}) \right) \frac{\sum_{x_n \in \mathcal{X}_m} \psi(\hat{t}_{nm})x_n}{\sum_{x_n \in \mathcal{X}_m} \psi(\hat{t}_{nm})} \]

\[ = 0 \quad (32) \]

**APPENDIX C**

**MATRIX CALCULUS**

In this Appendix, a brief overview of the used matrix calculus is given. Most of the formulae can be found in [1]–[3] with some additions from [5]–[7].

**A. vec-Operator and inverse vec-Operator**

\[ a \text{ is a } m \times 1 \text{ column vector} \]

\[ \text{vec}(a) = \text{vec} \left( a^\top \right) = a \quad (33) \]

\[ \text{vec} \left( ab^\top \right) = b \otimes a \quad (34) \]

\[ A = [a_1 \cdots a_n] \text{ is a } m \times n \text{ matrix} \]

\[ \text{vec} (A) = \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix} , \quad mn \times 1 \text{ column vector} \quad (35) \]
\[ \text{vec}_{m \times n}^{-1}(\text{vec}(A)) = A \] (36)
\[ \text{vec}_{m \times n}^{-1}(a) = \left( \text{vec}(I_n)^\top \otimes I_m \right) (I_n \otimes a) \] (37)
\[ \text{vec}(ABC) = \left( C^\top \otimes A \right) \text{vec}(B) \] (38)

\( B \) is a \( n \times q \) matrix

\[ \text{vec}(AB) = \left( B^\top \otimes I_m \right) \text{vec}(A) \]
\[ = (I_q \otimes A) \text{vec}(B) \] (39)

\( X \) is a \( n \times q \) and \( Y \) is a \( p \times r \) matrix

\[ \text{vec} (X \otimes Y) = (I_q \otimes K_{r,n} \otimes I_p) (\text{vec}(X) \otimes \text{vec}(Y)) \] (40)

**B. Trace**

\[ \text{Tr} \left( A^\top B \right) = \text{vec} (A)^\top \text{vec} (B) \] (41)
\[ \text{Tr} (A + B) = \text{Tr} (A) + \text{Tr} (B) \] (42)
\[ \text{Tr} (\alpha A) = \alpha \text{Tr} (A) \] (43)

**C. Kronecker Product**

\[ a^\top \otimes b = b \otimes a^\top = ba^\top \] (44)
\[ A \otimes B \otimes C = (A \otimes B) \otimes C = A \otimes (B \otimes C) \] (45)
\[ (A + B) \otimes (C + D) = A \otimes C + A \otimes D + B \otimes C + B \otimes D \] (46)
\[ \sum_{n=1}^{N} (A \otimes B_n) = (A \otimes B_1) + \cdots + (A \otimes B_N) = A \otimes \sum_{n=1}^{N} B_n \] (47)
\[ (A \otimes B)(C \otimes D) = AC \otimes BD \] (48)
\[ \alpha \otimes A = \alpha A = A \alpha = A \otimes \alpha \] (49)
\[ \alpha(A \otimes B) = (\alpha A) \otimes B = A \otimes (\alpha B) \] (50)
\[ (A \otimes B)^\top = A^\top \otimes B^\top \] (51)
\[ (A \otimes B)^{-1} = A^{-1} \otimes B^{-1} \] (52)
D. Definition of the Matrix Derivative

$F$ is a differentiable $m \times p$ matrix function of a $n \times q$ matrix $X$. Then, the Jacobian matrix of $F$ at $X$ is a $mp \times nq$ matrix

$$DF(X) = \frac{\partial \text{vec}(F(X))}{\partial (\text{vec}(X))^{\top}}.$$  (53)

E. Differentials

$$d \left( X^{\top} \right) = (dX)^{\top}$$  (54)
$$d\text{vec} \left( X \right) = \text{vec} \left( dX \right)$$  (55)
$$d \text{Tr} \left( X \right) = \text{Tr} \left( dX \right)$$  (56)

$\phi$ is a scalar function

$$d \left( \phi^\alpha \right) = \alpha \phi^{\alpha-1} d\phi$$  (57)
$$dX^{-1} = -X^{-1} dXX^{-1}$$  (58)
$$d |X| = |X| \text{Tr} \left( X^{-1}dX \right)$$  (59)
$$d \ln(|X|) = \text{Tr} \left( X^{-1}dX \right)$$  (60)
$$d \left( X \otimes Y \right) = dX \otimes Y + X \otimes dY$$  (61)

$x$ is a $n \times 1$ vector

$$d\text{vec} \left( xx^{\top} \right) = \left( (x \otimes I_{n}) + (I_{n} \otimes x) \right) \text{dvec} \left( x \right)$$  (62)

$A$ is symmetric

$$d\text{vec} \left( x^{\top}Ax \right) = 2x^{\top}A \text{dvec} \left( x \right)$$  (63)

$X$ is a $n \times q$ and $Y$ is a $p \times r$ matrix

$$d\text{vec} \left( X \otimes Y \right) = \left( I_{q} \otimes K_{r,n} \otimes I_{p} \right) \left[ (I_{nq} \otimes \text{vec}(Y)) \text{dvec} \left( X \right) + (\text{vec}(X) \otimes I_{pr}) \text{dvec} \left( Y \right) \right]$$  (64)
F. Commutation Matrix

$A$ is a $m \times n$ matrix, $K_{m,n}$ is a $mn \times mn$ matrix such that

$$K_{m,n} \text{vec}(A) = \text{vec} \left(A^\top\right)$$

with the properties

$$K_{m,n}^\top = K_{m,n}^{-1} = K_{n,m}$$

(66)

$$K_{n,n} = K_n$$

(67)

$$K_{n,m} K_{m,n} = I_n$$

(68)

$$K_{n,1} = K_{1,n} = I_n$$

(69)

$B$ is a $p \times q$ matrix, $b$ is a $p \times 1$ vector

$$K_{p,m}(A \otimes B) = (B \otimes A)K_{q,n}$$

(70)

$$K_{p,m}(A \otimes B)K_{n,q} = (B \otimes A)$$

(71)

$$K_{p,m}(A \otimes b) = (b \otimes A)$$

(72)

$$K_{m,p}(b \otimes A) = (A \otimes b)$$

(73)

$$(A \otimes b^\top)K_{n,p} = (b^\top \otimes A)$$

(74)

$$(b^\top \otimes A)K_{p,n} = (A \otimes b^\top)$$

(75)

G. Duplication Matrix

$A$ is a symmetric $n \times n$ matrix with $\frac{1}{2}n(n+1)$ unique elements, $D_n$ is a $n^2 \times \frac{1}{2}n(n+1)$ matrix, such that

$$\text{vec}(A) = D_n \text{vech}(A), \quad A = A^\top$$

(76)

$$K_n D_n = D_n$$

(77)

$$D_n^+ = \left(D_n^\top D_n\right)^{-1} D_n^\top$$

(78)

$$D_n^+ D_n = I_{\frac{1}{2}n(n+1)}$$

(79)

$$D_n D_n^+ = \frac{1}{2} \left(I_{\frac{1}{2}n^2} + K_n\right)$$

(80)
\( b \) is a \( n \times 1 \) vector

\[
D_n D_n^+ (b \otimes A) = \frac{1}{2} (b \otimes A + A \otimes b)
\]  

(81)

Why are we using the duplication matrix for derivatives with respect to symmetric matrices?

**Remark 1.** Since \( A \) is symmetric, say of order \( n \), its \( n^2 \) elements cannot move independently. The symmetry imposes \( n(n-1)/2 \) restrictions. The free elements are precisely the \( n(n+1)/2 \) elements in \( \text{vech}(A) \), and the derivative is therefore defined by considering \( F \) as a function of \( \text{vech}(A) \) and not as a function of \( \text{vec}(A) \). ([3, p. 367])

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