Swiss Federal Institute of Technology Zurich

Seminar for Statistics

Department of Mathematics

Bachelor Thesis Winter 2019

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Comparing the EM-algorithm and Maximum Likelihood Estimation Using the Cholesky Decomposition

Submission Date: November 1st 2019

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Abstract

The intent of this work is to compare The EM algorithm to an MLE approach in the case of multivariate normal mixture models. The EM algorithm is widely used in statistics and is proven to converge, however in pathological cases convergence slows down considerably.

Our proposed alternative consists of a clustering algorithm as initialization step, followed by a parametrization step, that is then fed into a general optimizer.

We compare two implementations of each algorithm with two different initialization strategies by judging their performance in model selection. Model selection is decided by the Bayesian Information Criterion (BIC).

The results are promising. In many cases MLE is equal or better than EM. It is certainly a competitive model selection strategy. This could yield improvements in the field of model selection. The algorithm design is also versatile and translates easily to other problems.

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Chapter 1

Introduction to normal mixture models

1.1 Definitions

A good and thorough introductory book is the work of McLachlan and Peel (2000) and the reader is encouraged to study it to learn in depth about normal mixtures and clustering. We will here give a short overview of normal mixtures to fix notation and nomenclature. The motivating idea behind mixture models is, that in real world examples a sample might be suspected to arise from more than one population or be more simply modelled by several overlaid distributions. The example of this, that is generally considered to be the first of this kind, is the one by Karl Pearson, who fitted two normal distributions with different means and variances to a dataset. In his book, Pearson and Henrici (1896)[Section 4.d.; page 266], Pearson analyzed measurements of forehead to body length of crabs sampled from the bay of Naples. His mixture model-based approach suggested, that the crabs were evolving into two new subspecies. This is a historically important example, because it presents statistical evidence of evolution in process.

While the theory of mixture models holds for a much broader class of distributions, we restrict ourselves here to the case of normal mixture models, because normal distributions allow for a parsimonious parametrization, that is of interest to study.

This parametrization is the $\boldsymbol{LDL}\top$ decomposition, a variation of the Cholesky decomposition, which allows for a very simple parametrization and a straightforward connection between degrees of freedom and necessarily generated numerical values. This will be explained further in section 1.4.

But before we delve deeper into the topic of this research, we first need to define the concept of a normal mixture model:

Let $\mu \in \mathbb{R}^p, \quad \Sigma \in \mathbb{R}^{p \times p}$ be symmetric positive definite and $\phi(-;\mu,\Sigma)$ be the normal distribution with mean μ and covariance matrix Σ with density function:

$$\phi(\boldsymbol{x};\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{\exp(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})\boldsymbol{\Sigma}^{-\frac{1}{2}}(\boldsymbol{x}-\boldsymbol{\mu})^\top)}{\sqrt{(2\pi)^k \det \boldsymbol{\Sigma}}} \tag{1.1.0.1}$$

for $\boldsymbol{x} \in \mathbb{R}^p$.

Since we are studying mixture models, we will need several overlapping of normal distributions, of differing means and covariance. Therefore, we choose notation allowing us to refer to the components in shorthand. Let us assume we have $K \in \mathbb{N}$ normal distributions with means and covariance $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \quad k \in \{1, \ldots, K\}$, then we fix:

$$\phi_k(\boldsymbol{x}) := \phi(\boldsymbol{x}; \boldsymbol{\mu_k}, \boldsymbol{\Sigma_k}) \tag{1.1.0.2}$$

And going forward, we will refer to components by the subscript k.
Definition 1.1.0.1. *Suppose we have a random sample $\boldsymbol{Y}_1, \ldots, \boldsymbol{Y}_n$, where $\boldsymbol{Y}_i$ is a p-dimensional random vector with probability density function $\boldsymbol{Y}_i \sim f(\boldsymbol{y}_i)$ on $\mathbb{R}^p$.*

We assume that the density $f(\boldsymbol{y}_i)$ of $\boldsymbol{Y}_i$ can be written in the form:

$$f(\boldsymbol{y}_i) = \sum_{k=1}^{K} \pi_k \phi_k(\boldsymbol{y}_i) \tag{1.1.0.3}$$

The ϕ_k are normal distributions and are called the mixture components with parameters $\boldsymbol{\mu}_k$ and $\boldsymbol{\Sigma}_k$ as described above (1.1.0.2). The π_k are called the component densities of the mixture and are constrained by the rules $\pi_k > 0$ and $\sum_k \pi_k = 1$.

For 'large' datasets there are applicable constraints to the $\boldsymbol{\Sigma}_k$, that reduce the number of necessary parameters. These, for example, assume that all components have the same covariance, or have certain restrictions placed on them. We will give a detailed description of the models assumed in this thesis in section 1.4.

1.2 The EM-algorithm in Sketch

With this definition, we immediately face the problem of how to fit these mixture components to given data. A popular algorithm to solve this problem is the **E**xpectation-**M**aximization algorithm, abbreviated as EM-algorithm.

We give here a sketch of the EM-algorithm in the case of normal mixtures. This roughly follows the content in McLachlan and Peel (2000). For a more thorough treatment of the matter see chapter 3.

Suppose we have a $p-$dimensional dataset of n samples $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n$, onto which we would like to fit a K component normal mixture with mixture components $\phi_k, \ k \in 1, \ldots, n$.

For the EM-algorithm further parameters are introduced. These are denoted $\tau_j(\boldsymbol{y}_i)$ and they represent the posterior probabilities that observation i is a member of component j.

The EM-algorithm is a two step, iterative process consisting of an 'e'-step and an 'm'-step. In the e-step the expectation of component membership is updated.

$$\tau_j(\boldsymbol{y}_i; \Psi) = \phi_j(\boldsymbol{y}_i) / \sum_{k=1}^{K} \phi_k(\boldsymbol{y}_i) \tag{1.2.0.1}$$

and in the m-step given the component membership information we update the component means and covariances by weighted versions of the usual estimators.

$$\boldsymbol{\mu}_j = \sum_{i=1}^{n} \tau_j(\boldsymbol{y}_i)\boldsymbol{y}_i / \sum_{j=1}^{n} \tau_j(\boldsymbol{y}_i) \tag{1.2.0.2}$$

$$\boldsymbol{\Sigma}_j = \sum_{i=1}^{n} \tau_j(\boldsymbol{y}_i)(\boldsymbol{y}_i - \boldsymbol{\mu}_j)(\boldsymbol{y}_i - \boldsymbol{\mu}_j)^\top / \sum_{i=1}^{n} \tau_j(\boldsymbol{y}_i) \tag{1.2.0.3}$$

There remains to be stated how to start the algorithm. Since both steps of the algorithm depend on data from the other, the EM-algorithm needs some form of initialization step. Most popular implementations use some form of pre clustering and use the EM-algorithm as subsequent tools to fit the data. The R-package `mclust` for example uses hierarchical agglomerative clustering Scrucca, Fop, Murphy, and Raftery (2016).

1.3 Choice of Notation

The classification of models in this paper relies heavily on the work of Celeux and Govaert (1995), however, out of necessity for clarity, we break with their notation. So as to not confuse the reader we describe here in depth the differences between Celeux and Govaert (1995) and this work.

The basis of classification in Celeux and Govaert (1995) is the decomposition of a symmetric matrix into an orthogonal and a diagonal component. A symmetric positive definite matrix Σ can be decomposed as

$$\Sigma = \lambda \boldsymbol{D}\boldsymbol{A}\boldsymbol{D}^\top \tag{1.3.0.1}$$

with $\boldsymbol{D}$ an orthogonal matrix and $\boldsymbol{A}$ a diagonal matrix and $\lambda = \sqrt[p]{det(\Sigma)}$ the p-th root of the determinant of Σ.

This decomposition has an appealing geometric interpretation, with $\boldsymbol{D}$ as the *orientation* of the distribution, $\boldsymbol{A}$ the *shape*, and λ the *volume*. The problem of notation comes from standard conventions in linear algebra, where the letters A and D are usually occupied by arbitrary and diagonal matrices respectively. Furthermore, we intend to apply a variant of the Cholesky decomposition to Σ, the $\alpha\boldsymbol{L}\boldsymbol{D}\boldsymbol{L}^\top$ decomposition. This obviously raises some conflicts in notation.

Therefore we, from here on, when referring to the decomposition as described by Celeux and Govaert (1995), will use the following modification of notation:

$$\boldsymbol{D} \longmapsto \boldsymbol{Q} \tag{1.3.0.2}$$

$$\boldsymbol{A} \longmapsto \boldsymbol{\Lambda} \tag{1.3.0.3}$$

$$\lambda \longmapsto \alpha \tag{1.3.0.4}$$

$$\Sigma = \lambda \boldsymbol{D}\boldsymbol{A}\boldsymbol{D}^\top \longmapsto \alpha \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^\top \tag{1.3.0.5}$$

These were chosen according to general conventions of linear algebra. $\boldsymbol{Q}$ is usually chosen for orthonormal matrices; $\boldsymbol{\Lambda}$ is often a choice for diagonal matrices of eigenvectors and α was chosen arbitrarily.

1.4 Models of Covariance Matrices

As mentioned in the introduction, there are ways to constrain the covariance matrices. There are instances where the resulting loss of information is seen as acceptable, for example if, through consideration of the data, that a simplified model is acceptable. Another is if the sheer size of the data makes application of full generality impossible.

With the above mentioned decomposition, we have the following options to constrain the covariance model:

- We restrict the complexity of the decomposition, substituting it with a simpler component.
- We restrict the variability of the mixture components, fixing a part of the decomposition to be equal.

Let us look at the first case. We take the decomposition of a covariance matrix as $\Sigma = \alpha\boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^\top$. Of these, we can simplify the structure of $\boldsymbol{Q}$ and $\boldsymbol{\Lambda}$, by replacing them with the identity. If we set $\boldsymbol{Q} = \mathrm{Id}$, we lose the freedom of orientation and if we set $\boldsymbol{\Lambda} = \mathrm{Id}$ we restrict ourselves to spherical distributions. Of course, we cannot restrict $\boldsymbol{\lambda}$ while letting $\boldsymbol{q}$ free, since

$$\boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^\top = \boldsymbol{Q}\mathrm{Id}\boldsymbol{Q}^\top = \mathrm{Id} \tag{1.4.0.1}$$

The second restriction simply means we hold the decomposition fixed throughout all covariance matrices.

There is however an issue with the Cholesky decomposition. For ten out of fourteen cases defined by Celeux and Govaert (1995), there exists a canonical translation of decompositions, but for four of them no translation is possible.

The six diagonal cases need no translation; the eigen- and Cholesky decomposition are equal to the non decomposed form. For the non diagonal cases note that for a given symmetric positive definite matrix Σ we have decompositions:

$$\Sigma = \alpha\boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^\top \quad \Sigma = \alpha\boldsymbol{L}\boldsymbol{D}\boldsymbol{L}^\top \tag{1.4.0.2}$$

Since in both cases the enclosing matrices $\boldsymbol{Q}$ and $\boldsymbol{L}$ have determinant 1 the determinant of Σ falls entirely on α. Therefore α, in these particular decompositions, is equal for both. Celeux and Govaert (1995) vary σ by either varying or holding fixed the volume (α/α_k), shape ($\boldsymbol{\Lambda}/\boldsymbol{\Lambda_k}$) and orientation ($\boldsymbol{Q}/\boldsymbol{Q}_k$).

These three times two cases would yield the eight out of fourteen cases of non diagonal cases. However there is no canonical transform for either variable orientation and fixed shape or fixed orientation and variable shape. The reason for this is that in the $\boldsymbol{L}\boldsymbol{D}\boldsymbol{L}^\top$ decomposition the lower diagonal matrix $\boldsymbol{L}$ holds some of the shape of the matrix, which in the eigendecomposition is in the $\boldsymbol{\Lambda}$ matrix. In fact, $\boldsymbol{L}$ is orthogonal if and only if $\boldsymbol{L} = \mathrm{Id}_{n\times n}$. Therefore we can only decompose matrices where either both or neither shape and orientation vary. See table 1.1.

While we could in theory construct the cases $\boldsymbol{L}\boldsymbol{D}_k\boldsymbol{L}^\top$ and $\boldsymbol{L}_k\boldsymbol{D}\boldsymbol{L}_k^\top$, however they do not correspond to the desired geometric intent behind the differentiation of models and are therefore not included.

Model	$\boldsymbol{\Sigma}_k$ C&G	volume	shape	orientation	parameters	$\boldsymbol{LDL}^\top$	parameters	count
EII	$\alpha\boldsymbol{I}$	equal	equal	-	α	as in C&G		1
VII	$\alpha_k\boldsymbol{I}$	var.	equal	-	α_k			K
EEI	$\alpha\boldsymbol{\Lambda}$	equal	equal	coord. axes	α, λ_i			$1 + (p-1)$
VEI	$\alpha_k\boldsymbol{\Lambda}$	var.	equal	coord. axes	α_k, λ_i			$K + (p-1)$
EVI	$\alpha\boldsymbol{\Lambda}_k$	equal	var.	coord. axes	$\alpha, \lambda_{i,k}$			$1 + K(p-1)$
VVI	$\alpha_k\boldsymbol{\Lambda}_k$	var.	var.	coord. axes	$\alpha_k, \lambda_{i,k}$			$K + K(p-1)$
EEE	$\alpha\boldsymbol{Q\Lambda Q}^\top$	equal	equal	equal	$\alpha, \lambda_i, q_{i,j}$	$\alpha\boldsymbol{LDL}^\top$	$\lambda, d_i, l_{i,j}$	$1 + (p-1) + \frac{p(p-1)}{2}$
EVE	$\alpha\boldsymbol{Q\Lambda}_k\boldsymbol{Q}^\top$	equal	var.	equal	$\alpha, \lambda_{i,k}, q_{i,j}$	doesn't exist		$1 + K(p-1) + \frac{p(p-1)}{2}$
VEE	$\alpha_k\boldsymbol{Q\Lambda Q}^\top$	var.	equal	equal	$\alpha_k, \lambda_i, q_{i,j}$	$\alpha_k\boldsymbol{LDL}^\top$	$\lambda_k, d_i, l_{i,j}$	$K + (p-1) + \frac{p(p-1)}{2}$
VVE	$\alpha_k\boldsymbol{Q\Lambda}_k\boldsymbol{Q}^\top$	var.	var.	equal	$\alpha_k, \lambda_{i,k}, q_{i,j}$	don't exist		$K + K(p-1) + \frac{p(p-1)}{2}$
EEV	$\alpha\boldsymbol{Q}_k\boldsymbol{\Lambda Q}_k^\top$	equal	equal	var.	$\alpha, \lambda_i, q_{i,j,k}$			$1 + (p-1) + K\frac{p(p-1)}{2}$
VEV	$\alpha_k\boldsymbol{Q}_k\boldsymbol{\Lambda Q}_k^\top$	var.	equal	var.	$\alpha_k, \lambda_i, q_{i,j,k}$			$K + (p-1) + K\frac{p(p-1)}{2}$
EVV	$\alpha\boldsymbol{Q}_k\boldsymbol{\Lambda}_k\boldsymbol{Q}_k^\top$	equal	var.	var.	$\alpha, \lambda_i, q_{i,j,k}$	$\alpha\boldsymbol{L}_k\boldsymbol{D}_k\boldsymbol{L}_k^\top$	$\lambda, d_{i,k}, l_{i,j,k}\ j > i$	$1 + K(p-1) + K\frac{p(p-1)}{2}$
VVV	$\alpha_k\boldsymbol{Q}_k\boldsymbol{\Lambda}_k\boldsymbol{Q}_k^\top$	var.	var.	var.	$\alpha_k, \lambda_i, q_{i,j,k}$	$\alpha_k\boldsymbol{L}_k\boldsymbol{D}_k\boldsymbol{L}_k^\top$	$\lambda_k, d_{i,k}, l_{i,j,k}\ j > i$	$K + K(p-1) + K\frac{p(p-1)}{2}$

Table 1.1: Table of Parameters of the Covariance Matrices

Σ model	μ, π	Σ	total #{par}	$\mathcal{O}()$
EII	$K-1+pK$	1	$Kp+K$	Kp
VII	$K-1+pK$	K	$Kp+2K-1$	Kp
EEI	$K-1+pK$	$1+(p-1)$	$Kp+p+K-1$	Kp
VEI	$K-1+pK$	$K+(p-1)$	$Kp+p+2K-2$	Kp
EVI	$K-1+pK$	$1+K(p-1)$	$2Kp$	Kp
VVI	$K-1+pK$	$K+K(p-1)$	$2Kp+K-1$	Kp
EEE	$K-1+pK$	$1+(p-1)+\frac{p(p-1)}{2}$	$\frac{(p+2)(p-1)}{2}+Kp+K$	p^2+Kp
VEE	$K-1+pK$	$K+(p-1)+\frac{p(p-1)}{2}$	$\frac{(p+2)(p-1)}{2}+Kp+2K-2$	p^2+Kp
EVV	$K-1+pK$	$1+K(p-1)+K\frac{p(p-1)}{2}$	$K\frac{(p+2)(p-1)}{2}+Kp+K$	Kp^2
VVV	$K-1+pK$	$K+K(p-1)+K\frac{p(p-1)}{2}$	$K\frac{(p+2)(p-1)}{2}+Kp+2K-1$	Kp^2

Table 1.2: Full Table of Parameters

There is an attractive advantage in using the $\boldsymbol{LDL}^\top$ decomposition. Since both the $\boldsymbol{LDL}^\top$ and eigendecomposition derive from the same covariance matrix, the necessary parameters are the same in cardinality. In the case of the $\boldsymbol{Q}$ and $\boldsymbol{L}$ matrices, there need to be $\frac{p(p-1)}{2}$ parameters that uniquely define these matrices. In the case of the $\boldsymbol{L}$ matrix these are straightforward the entries of the lower diagonal matrix, whereas $\boldsymbol{Q}$ needs a nontrivial amount of work to determine a minimal generating set of parameters, which makes computation of the decomposition as in Celeux and Govaert (1995) a lot more difficult.

1.5 Problems of the EM-algorithm

In their seminal work, Dempster, Laird, and Rubin (1977), have proven that the EM-algorithm converges under mild regularity conditions. However, convergence does not guarantee fast convergence. In fact, a lot of the work, that has gone into the research around the EM-algorithm has been concerned with speeding up convergence, see McLachlan and Peel (2000)[section 2.17]. The concern here is that a slowing in convergence might be mistaken for actual convergence.

This phenomenon is not infrequent and in difficult mixtures quite visible. To illustrate let us look at a particular mixture taken from Marron and Wand (1992) and the `nor1mix` package Maechler (2019a). `nor1mix` is a package designed and developed for educational purposes to teach about univariate normal mixtures. It is also the spiritual predecessor of this thesis' R code.

The mixture is a trimodal mixture of uneven weight, as shown in figure 1.1. While not the most difficult mixture studied by Marron and Wand (1992), it is certainly not trivial either. In the figures below, 1.5 and 1.5, we demonstrate, that even after 200 iterations of the EM-algorithm the convergence is poor. In this instance, the initialization is done using R 's CLARA implementation from the cluster package ??.

```
>     library("nor1mix")
>     MW.nm9 ## Trimodal mixture
```

```
'Normal Mixture' object         ``#9 Trimodal''
       mu sigma    w
[1,] -1.2  0.60 0.45
```

```
[2,]  1.2  0.60 0.45
[3,]  0.0  0.25 0.10
```

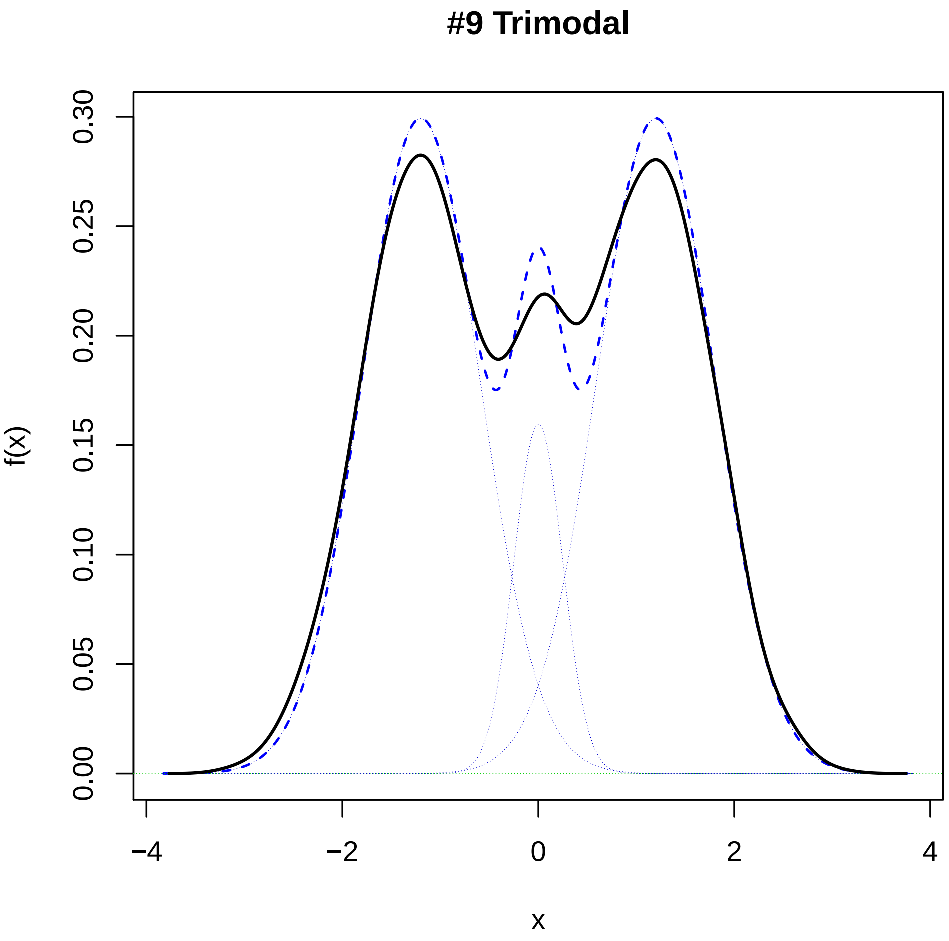


Figure 1.1: True and estimated density of `MW.nm9`

We can see in 1.5, that the EM-algorithm seems to converge to an intermediary solution, where the smaller middle solution is weighted lower, until it manages to correct back and find the correct components.

We see how change in log-likelihood seems to stagnate. However, this does not stay that way. If we let EM run a bit further we see in figure 1.5, the log-likelihood hits a flatspot, after which convergence accelerates again.

In fact, it seems that the previous solution is a saddle point in the likelihood function, where EM has chronic problems continuing improvements.

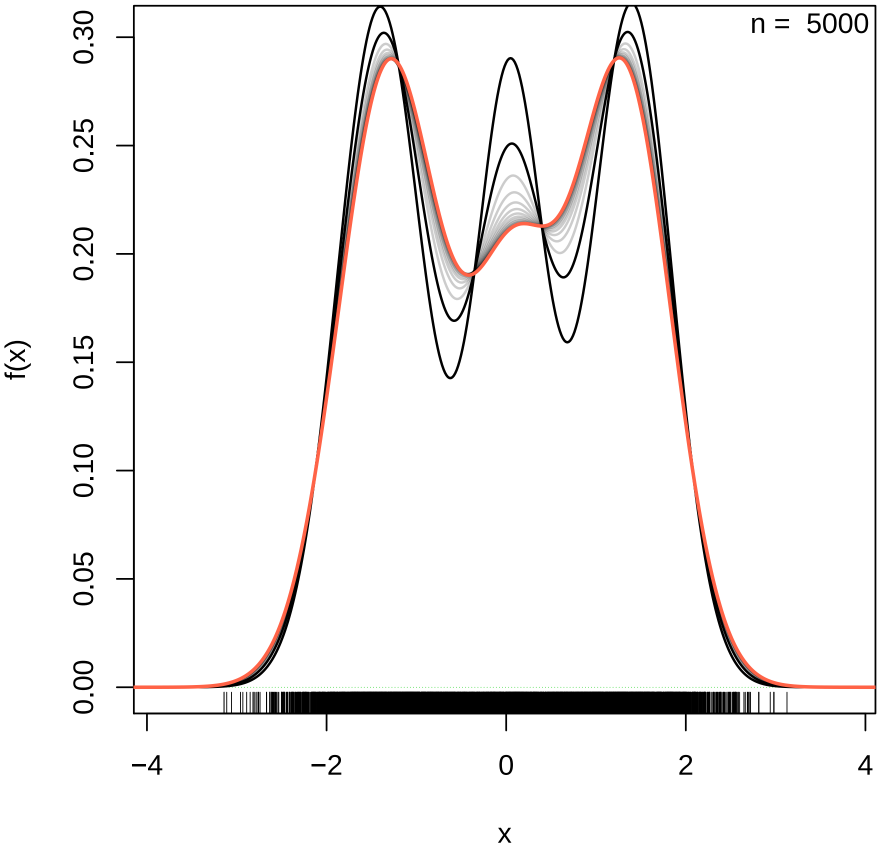


Figure 1.2: 20 EM steps

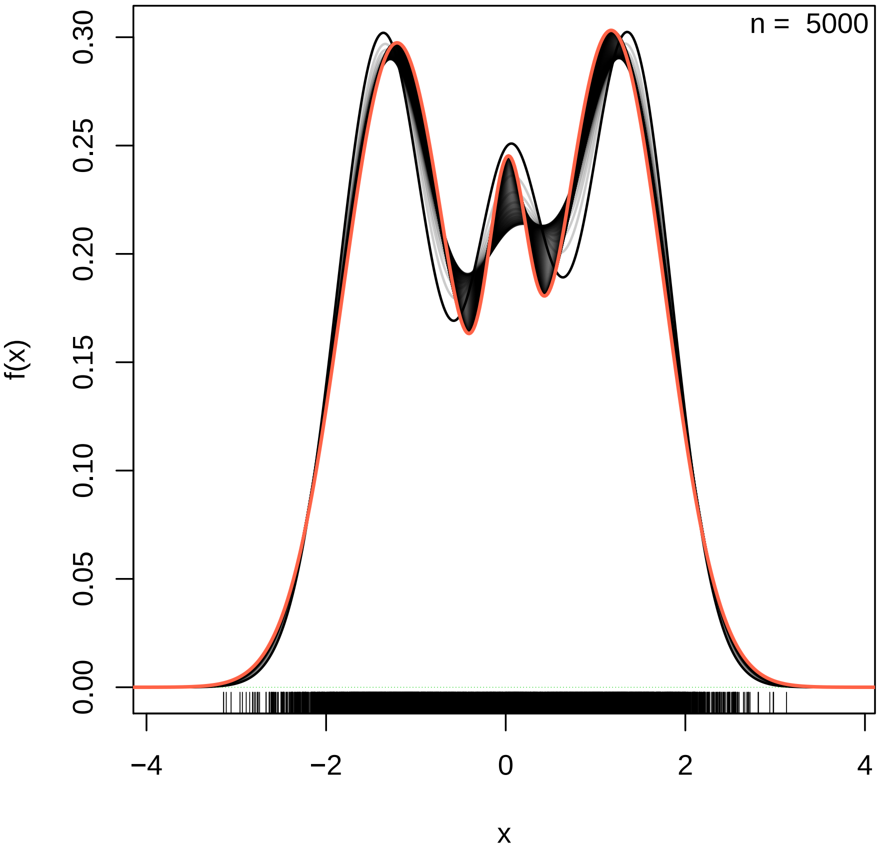


Figure 1.3: 200 EM steps

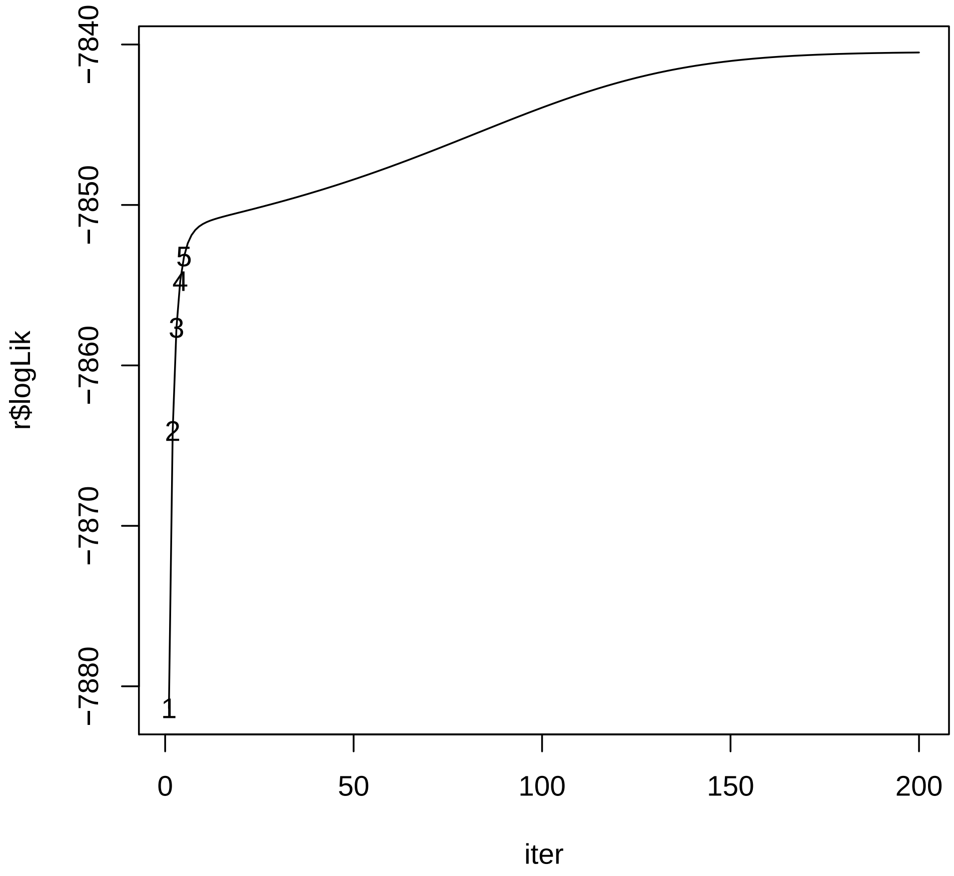


Figure 1.4: Log-likelihood plotted against iteration count for the example in 1.5

Chapter 2

The norMmix Package

2.1 Introduction to the norMmix Package

For this thesis, an R package was developed that implements an algorithm that fits multivariate normal mixtures to given data. [1]

The algorithm is reasonably straightforward:

i.) Initialize using a common clustering algorithm.

ii.) Perform one m-step, to transform clustering results into the form of a normal mixture.

iii.) Apply a general optimizer, using the mixture's log-likelihood function.

The `norMmix` package is constructed around the `norMmix` object that codifies a `nor`mal `M`ultivariate `mix`ture model, and the `llnorMmix()` function, that calculates the log-likelihood given a model and data.

In the table 2.1 the notation used in code is listed along with a translation to the previously used mathematical notation. Additionally, functions with ambiguous names are listed here.

The package contains the following functionality:

[1] The package was written with R version 3.6.1 (2019-07-05) last updated on 2019-10-22.

In Notation	In Code
π_i	`w, weights`
Σ	`Sigma`
μ	`mu`
K	`k`
dimension	`p, dim, dims`
components	`cl, components`
$\boldsymbol{\Sigma}$ model	`model`
`cluster`'s CLARA	`clara`
`mclust`'s hierarchical clustering	`mclVVV`
`mclust`'s `Mclust` function	`mclust`

Table 2.1: Translation Table: Mathematical Notation to R Code

norMmix `norMmix()` is the 'init-method' for `norMmix` objects. There exist `is.norMmix` `rnorMmix` and `dnorMmix` functions.

parametrization The main functions that handle reparametrization of models from and to the $\boldsymbol{LDL}^\top$ decomposition are `nMm2par` and `par2nMm`, which are inverse to each other.

MLE The function `norMmixMLE` marries the main components of this package. It initializes a model and parametrizes it for use with `optim`

model choice Using `norMmixMLE`, the function fitnMm allows fitting of multiple models and components. Functions analyzing the output of this are also provided, e.g. `BIC` and `print` methods.

example objects Following the paper of Marron and Wand (1992) various example objects are provided and used for study. They follow the naming convention: MW + dimension + number. For example `MW213` for the 13th model of dimension 2.

simulations A good portion of the package is designed with the study of simulations in mind. Therefore there are functions provided to study large collections of evaluated data. e.g `compplot`

misc There are also various methods of generics, like `logLik, print, BIC, AIC` and `nobs` as well as various `print` methods.

The package relies on `optim` from the `stats` package R Core Team (2019) for general optimization. We use the standard method implemented in `optim` which is `BFGS`, which is a quasi-Newton method (also known as a variable metric algorithm) as described in Broyden (1970) among others.

The workflow when using the package is as follows. The function `rnorMmix` can be used to generate data from a `norMmix` object. The `MW` objects provide ready made examples and objects of study and the `norMmix` function can be used to define normal mixtures from scratch. Of course, other data sets can be used for analysis. The following functions rely, however, on the `matrix` data structure. So data frames must be converted beforehand and non numerical data is not accepted.

The functions that accept it for analysis are mainly `norMmixMLE` and `fitnMm`. The former performs model fit on data, and the latter performs model selection, by calling `norMmixMLE` for specified `k` and `model` vectors.

2.1.1 norMmixMLE

The core of `norMmixMLE` is the application of `optim` in conjunction with `llnorMmix` as function to be optimized. `llnorMmix` can be accessed directly, however, it needs a transposed dataset. The `norMmixMLE` function implicitly performs initialization.

There are two options for this initialization step. One is the CLARA clustering algoritm, with non-standard arguments. The standard arguments are somewhat historic in origin and were, at the time, chosen because of hardware limitations. The arguments used in this work are defined by a function, due to this thesis' advisor Martin Mächler, which was designed to be a 'sensible' alternative, but should be subject to further scrutiny. It is reproduced here.

```
>     norMmix:::ssClaraL
```

```
function (n, k, p)
pmin(n, pmax(40, round(10 * log(n))) + round(2 * k * pmax(1,
    log(n * p))))
<bytecode: 0x45358d8>
<environment: namespace:norMmix>
```

It is dependent on the size and dimension of the dataset, as well as the demanded number of clusters.

The alternative to CLARA is `mclust`'s hierarchical agglomerative clustering, which follows the work of Fraley (1998). The intention behind using `mclust`'s initialization function is to directly compare how much difference the initialization process makes.

The initialization stage does not yield a normal mixture. This requires a way to transform a clustering into a mixture. The method chosen in this package is to use an m-step from the EM-algorithm. Unlike the EM-algorithm, clustering algorithms like CLARA produce binary cluster membership results, whereas the component membership of EM is determined as a probability value between 0 and 1. This is resolved by interpreting the results as probability values which are either 0 or 1. These are then used as the τ_j as described in section 1.2. This m-step is also taken from the `mclust` package for reasons better explained in section 2.2. It has the advantage of being able to generate a mixture object with the correct covariance model.

This mixture object is still in human readable form and not the necessary parameter vector demanded by `optim`. So an application of the function `nMm2par` is carried out, resulting in a starting value for `optim`.

The returned results from `norMmixMLE` are more than abundant. Not only is the fitted model returned but also everything produced by `optim` and the entire dataset. Here the return values are listed:

```
>      data(fSMI.12, package="norMmix")
>      str(fSMI.12$nMm[3,3][[1]], max=2)
```

```
List of 6
 $ norMmix:List of 6
  ..$ mu    : num [1:20, 1:3] 15.9 30.7 36.2 21.8 753 ...
  ..$ Sigma : num [1:20, 1:20, 1:3] 0.358 0 0 0 0 ...
  ..$ weight: num [1:3] 0.219 0.419 0.362
  ..$ k     : int 3
  ..$ dim   : int 20
  ..$ model : chr "EEI"
  ..- attr(*, "name")= chr "model = EEI , clusters = 3"
  ..- attr(*, "class")= chr "norMmix"
 $ optr   :List of 5
  ..$ par        : num [1:82] 0.264 0.118 15.903 30.67 36.155 ...
  ..$ value      : num 7370
  ..$ counts     : Named int [1:2] 232 88
  .. ..- attr(*, "names")= chr [1:2] "function" "gradient"
  ..$ convergence: int 0
  ..$ message    : NULL
 $ npar   : int 82
 $ n      : int 141
 $ x      : num [1:141, 1:20] 16.1 15.7 15.7 16.1 16.6 ...
  ..- attr(*, "dimnames")=List of 2
 $ cond   : num 1.72
 - attr(*, "class")= chr "norMmixMLE"
```

Besides mclust and cluster, the package also relies on a number of other packages for various tasks. Listed in no particular order: MASS Venables and Ripley (2002), mvtnorm Genz, Bretz, Miwa, Mi, Leisch, Scheipl, and Hothorn (2019), mixtools Benaglia, Chauveau, Hunter, and Young (2009) and sfsmisc Maechler (2019b).

2.2 On The Development of norMmix

During the development of the norMmix package several mistakes were made and dead-ends were reached. In the interest of documentation, we discuss some of them in this section.

One dead-end was the parametrization of the weights of a mixture using the logit function.

```
> logit <- function(e) {
+     stopifnot(is.numeric(e) ,all(e >= 0), all.equal(sum(e),1))
+     qlogis(e[-1L])
+ }
> logitinv <- function(e) {
+     if (length(e)==0) {return(c(1))}
+     stopifnot(is.numeric(e))
+     e<- plogis(e)
+     sp. <- sum(e)
+     w <- c((1-sp.), e)
+ }
```

This uses the logistical function logis to transform to reduce the number of weights from K to $K-1$. Much like clr1, given a list of weights logit will transform them and logitinv will correctly reverse the transformation. However, unlike clr1, it will not transform an arbitrary list of length $K-1$ into a valid weight parameter. For example:

```
> w <- runif(7); ret <- logitinv(w)
> ret
```

```
[1] -3.1906158  0.6511258  0.5136217  0.5337424  0.5794803  0.6053432  0.5846750
[8]  0.7226274
```

The issue here is that the last line of logitinv, which is necessary to sum to one, but results in a negative value in ret[1] which is not a valid weight. The underlying issue is that not every tuple in $\mathbb{R}^{K-1}$ is a result of logit.

The option to use logit is still an argument to norMmixMLE by specifying trafo="logit", but it shouldn't be used.

Another issue during development cropped up during fitting of high dimensional data. We studied the dataset SMI.12 from the package copula, Hofert, Kojadinovic, Maechler, and Yan (2018):

```
>     plot(MW215)
```

Figure 2.1: Demonstration of the MW object `MW215`. Correct model: `model="VEE", k=3`.

```
> data(SMI.12, package="copula")
> str(SMI.12)
```

```
 num [1:141, 1:20] 16.1 15.7 15.7 16.1 16.6 ...
 - attr(*, "dimnames")=List of 2
  ..$ : chr [1:141] "2011-09-09" "2011-09-12" "2011-09-13" "2011-09-14" ...
  ..$ : chr [1:20] "ABBN" "ATLN" "ADEN" "CSGN" ...
```

A consequence of high dimensions is that matrix multiplication is no longer very stable. As a result, the covariance matrices produced by our own implementation of the EM-algorithms m-step (`mstep.nMm`) were not positive definite. In the case of `SMI.12`, several covariance matrices are degenerate, which results in cancellation error with near-zero entries. We attempted to correct this with the function `forcePositive`, which simply tries to set $\boldsymbol{D}$ in $\boldsymbol{LDL}^\top$ greater than zero. This didn't resolve the issue, since a non-negligible part of the numerical error was in the $\boldsymbol{L}$ matrix and the resultant covariance matrix was still not positive definite.

We eventually resolved this issue by abandoning our own implementation and using the functions from the `Mclust` package. Not only were these numerically stable they were also able to differentiate between models, whereas ours would assume VVV for every fit.

2.3 Demonstration

To end this chapter, here a small demonstration of the capabilities of `norMmix`. First a small plot to show an MW mixture.

It is a trimodal mixture along the diagonal.

The results of a run of `norMmixMLE` are shown along with a plot of the fitted mixture overlaid over the correct mixture in figure 2.2.

```
>     set.seed(2019); x <- rnorMmix(500, MW215)
>     system.time(mleResult <- norMmixMLE(x, 3, "VEE"))
```

```
initial  value 2206.907425
iter  10 value 2147.633703
iter  20 value 2125.658743
final  value 2125.658364
converged
   user  system elapsed
  0.256   0.012   0.266
```

```
>     mleResult
```

```
object of class 'norMmixMLE'
norMmix object:
multivariate normal mixture model with the following attributes:
name:                  model = VEE , components = 3
 model:                  VEE
 dimension:         2
 components:         3
weight of components 0.365 0.325 0.31

returned from optim:
function gradient
      75       22

log-likelihood: -2125.658

 nobs        npar        nobs/npar
 500          13          38.46154
```

```
>    op <- par(mfrow=c(1,2), mar=c(1,2,3,1))
>    plot(MW215, asp=1, ylab='', xlab='')
>    points(x, col=adjustcolor("black", 0.5))
>    plot(MW215, asp=1, ylab='', xlab='')
>    plot(mleResult, fillcolor=norMmix::nMmcols[2], newWindow=FALSE, points=FALSE)
>    legend("bottomright", legend=c("correct", "fitted"),
+           fill=norMmix::nMmcols[1:2])
>    par(op)
```

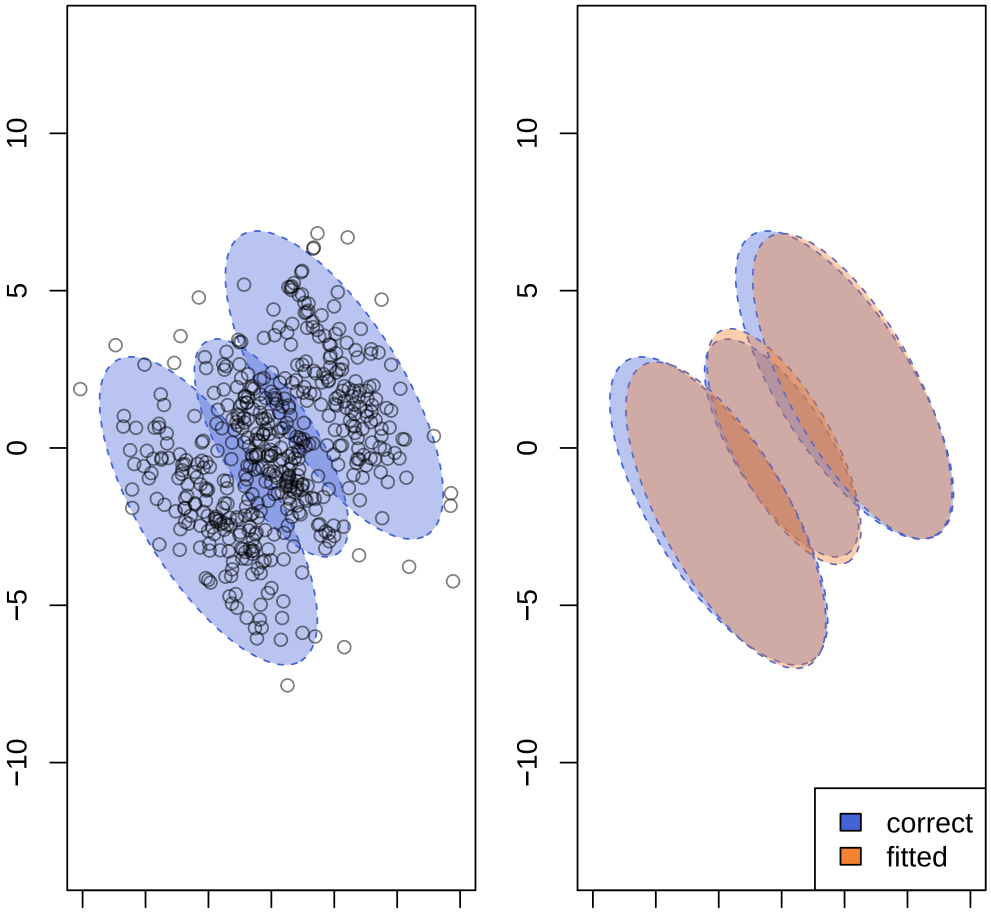


Figure 2.2: Correct Mixture (left) and Fitted overlayed in orange (right)

Chapter 3

Comparing Algorithms

With the `norMmix` package explained, we can turn to comparing it to existing methods. As previously stated, the implementation representing the EM-algorithm is the `mclust` package. It will be used with very little deviation from out-of-the-box settings, safe for restriction of the covariance models. This is done, so we can compare like with like. The specific command that performs the EM-algorithm is:

```
>     mclust::Mclust(x, G=cl, modelNames=mo)$BIC
```

Where `cl` is a vector of integers of however many components we are trying to fit and `mo` are the model names:

```
 [1] "EII" "VII" "EEI" "VEI" "EVI" "VVI" "EEE" "VEE" "EVV" "VVV"
```

The `$BIC` element of the results is taken as the main tool for model selection, as it is advertised in the package authors paper Scrucca et al. (2016).

There is however a small but crucial change applied to these results. The `mclust` package authors have flipped the definition of the BIC to mean:

$$2ln(\hat{L}) - ln(n)\#\{par\} \tag{3.0.0.1}$$

instead of the more common

$$ln(n)\#\{par\} - 2ln(\hat{L}) \tag{3.0.0.2}$$

Where n is the number of observations, $\#\{\text{par}\}$ is the cardinality of the parameter vector and $\hat{L}$ is the estimated log-likelihood.

So, even if not explicitly mentioned, we use the negative of the values returned by `mclust`.

Another thing that should be stated before all else is the difference in initialization between mclust's pre-clustering and CLARA. CLARA is dependent on random number generators. As such, unless a fixed seed is chosen, every iteration of CLARA will return a different result. Unlike `mclust`, which will, for given data, always return the same results. The effect on the following findings is that results will spread out for data obtained from CLARA results.

First, we illustrate the structure of the graphical results we will be presenting hereafter. The basic shape of the plots will be the BIC value plotted against the number of components. This is in line with `mclust`'s manner of visualizing data, however since our method is to some extent RNG dependent, we are forced to display multiple runs of the algorithm on the same graph. Therefore we split the plot according to covariance model, putting 10 models in 10 graphs in a plot. Here an example:

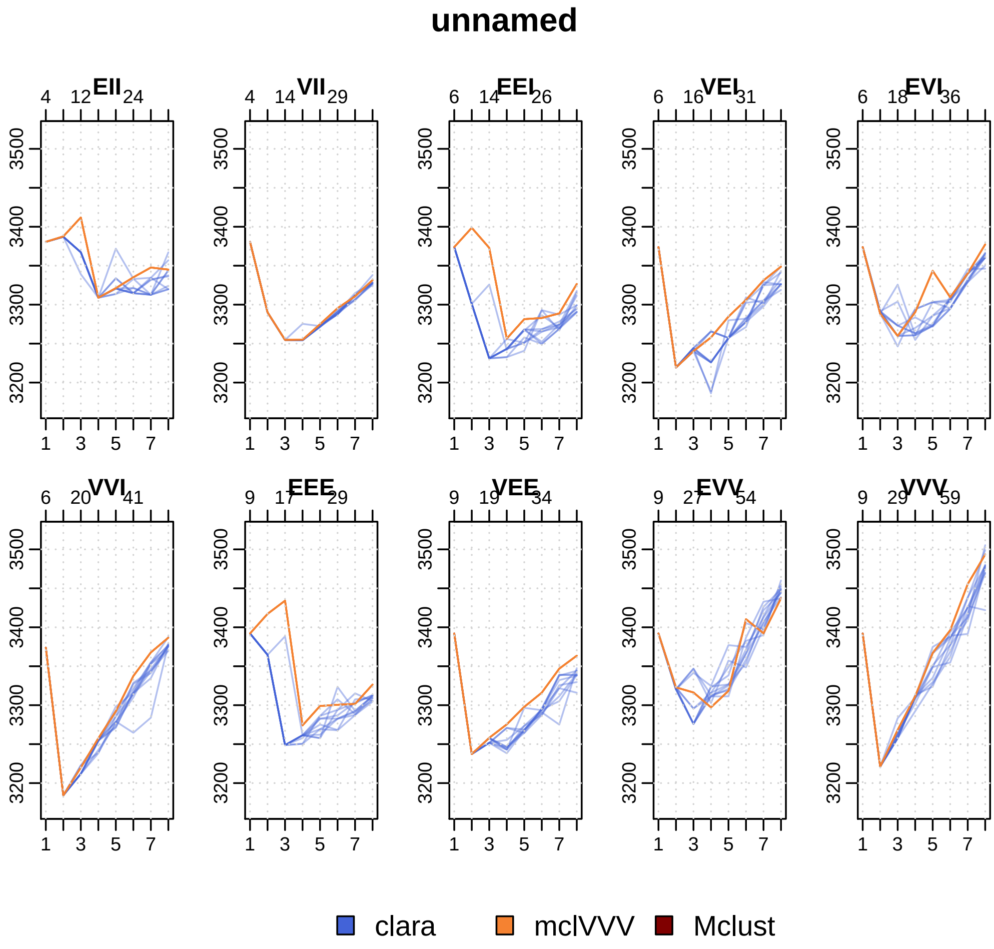


Figure 3.1: Example of comparison plot

As can be seen from the formula of the BIC value 3.0.0.2, lower is better. When selecting a model based on BIC, we take the model and component with the lowest value to be the best fitting model. Although this may not necessarily the 'correct' model, that is, the model from which the data arises.

There are many ways in which this type of model selection might miss the correct model, for example by 'gluing together' multiple components into one, or covering the dataset in a 'patchwork' of smaller components, to name a few. We will discuss them as they arise in the following analysis of simulations.

The simulations were set up very simply. An R script was written and in each the `norMmix` package is loaded, the datasets are defined and `fitnMm` was applied a number of times. An example script can be found in the appendix A.2.

A few things of interest are what happens:

- To time needed for the simulation

- When we vary the sample size of the data sets.
- When the generating mixture is 'difficult'.
- When the data does not arise from a normal mixture.

The data used here should have been provided along with this thesis in digital form in a folder called `/simulations`, with individual simulations in their own subfolder.

3.1 Time Analysis

The data used here is taken from the subfolder `/simulations/2time`. In this simulation we take several example mixtures and generate $n = \{500, 1000, 2000\}$. We apply `fitnMm` with `clara` using ten different seeds and `mclVVV` initializations, and `Mclust`. From these, the system time was extracted and analyzed as can be gleaned from the following code. In it, we apply R 's `lm` function for fitting linear models to the times returned by the function call:

```
>     system.time(norMmixMLE(x, ...))[[1]]
```

We make here a choice that does not preserve any generality, as `system.time` produces more results, that could hold important information. However, since there is quite some measurement error to be expected as time approaches zero, we will content ourselves with lower expectations to the accuracy of the following results.

```
>     library(norMmix, lib.loc="~/ethz/BA/norMmix.Rcheck/")
>     # change this dir to whereever the simulations are saved
>     mainsav <- normalizePath("~/ethz/BA/Rscripts/")
>     savdir <- file.path(mainsav, "2time")
>     filelist <- list.files(savdir, pattern=".rds")
>     filelist <- grep("mcl.rds", filelist, invert=TRUE, value=TRUE)
>     f <- lapply(file.path(savdir,filelist), function(j) readRDS(j)$fit)
>     times <- unlist(lapply(f, function(j) extracttimes(j)[,,1]))
>     dims <- unlist(lapply(f, function(j) attr(extracttimes(j), "p")))
>     size <- unlist(lapply(f, function(j) attr(extracttimes(j), "n")))
>     ddims <- rep(dims, each=80)
>     ssize <- rep(size, each=80)
>     pars <- unlist(lapply(f, npar))
>     r <- lm(times ~ pars + ddims + ssize)
>     summary(r)
```

```
Call:
lm(formula = times ~ pars + ddims + ssize)

Residuals:
   Min     1Q Median     3Q    Max
-86.89  -7.45  -1.55   6.30 556.32

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept) -1.727e+01  8.274e-01  -20.87   <2e-16 ***
```

```
pars         9.729e-01  1.056e-02   92.16   <2e-16 ***
ddims       -3.749e+00  2.216e-01  -16.92   <2e-16 ***
ssize        9.258e-03  3.887e-04   23.82   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 21.57 on 7916 degrees of freedom
Multiple R-squared:  0.559,        Adjusted R-squared:  0.5588
F-statistic:  3344 on 3 and 7916 DF,  p-value: < 2.2e-16
```

The necessary time appears to be well explained by the parameter count. The purpose of this thesis is not to conduct complexity analysis, so we will leave it at this, satisfying our curiosity with a cursory look in figure 3.2, where we plot system time against parameter length.

We can see that time is almost one to one proportional to parameter length. It should be noted, that MW51 is a very simple mixture. It is therefore sensible, that MLE should find an optimum faster.

```
>     plot(times~pars, log="xy", yaxt="n", xaxt="n", type="n")
>     legend("bottomright", legend=c("MW214", "MW34","MW51"),
+            fill=nMmcols[c(3,4,2)])
>     points(times[1:(80*30)]~pars[1:(80*30)],
+            log="xy", yaxt="n", xaxt="n", col=nMmcols[3], pch=1)
>     points(times[(80*30+1):(80*60)]~pars[(80*30+1):(80*60)]
+            , log="xy", yaxt="n", xaxt="n", col=nMmcols[4], pch=9)
>     points(times[(60*80+1):(80*90)]~pars[(60*80+1):(80*90)],
+            log="xy", yaxt="n", xaxt="n", col=nMmcols[2], pch=8)
>     grid()
>     sfsmisc::eaxis(1)
>     sfsmisc::eaxis(2)
```

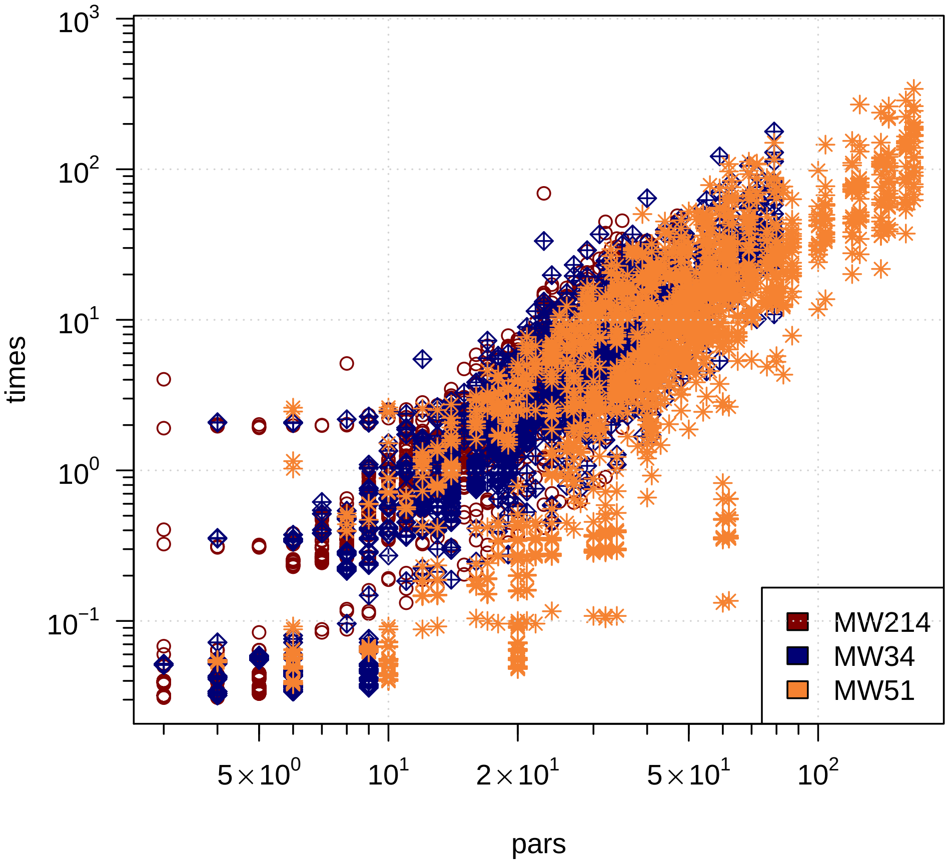


Figure 3.2: Log-log plot of system time against parameter length

3.2 Behaviour in n

What we would expect and like to see as we increase sample size, is a decrease in scattering of BIC values. To that end we again use simulation data `/simulations/2time`. In particular we show here the results of fitting to mixture model `MW34`, shown in figure 3.3. The graphs B.3 and B.4 show three columns of BIC plots, each representing different sample sizes, with $n = \{500, 1000, 2000\}$ respectively. Furthermore, the BIC values were divided by the samplesize, to normalize the values to an equal scale.

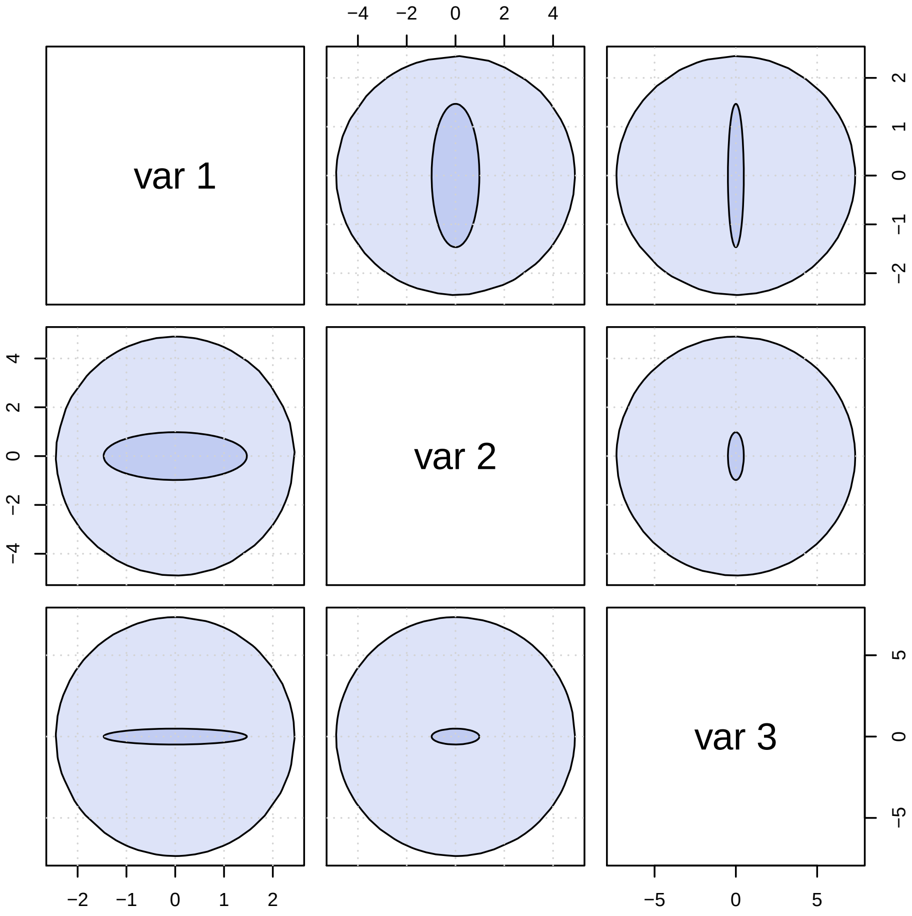


Figure 3.3: The mixture model `MW34`, a three dimensional, two component mixture with one smaller, lesser weighted component inside a smaller one.

As can be seen the desired effect is achieved. Of note are the behaviour of the model `VEI`, where the increase in observation corrects a selection error appearing at $n = 500$. Furthermore, the correct model `VVI` exhibits a very tight grouping. The instances where `mclust` is better than `norMmix` are quite infrequent.

This type of analysis was also conducted with mixture objects `MW214` and `MW51`, but were omitted due to the lack of clear results. They are provided in the appendix B.1, with brief discussions.

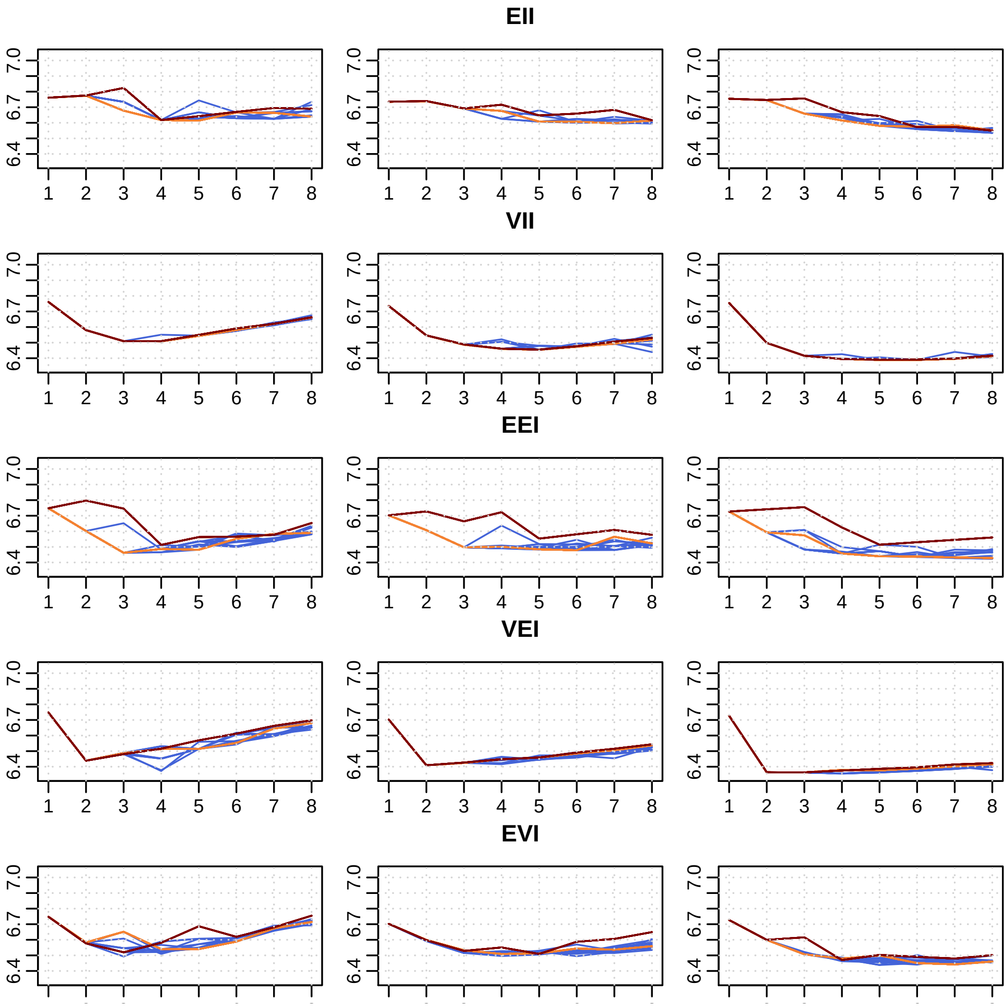


Figure 3.4: BIC values of MW34 with $n = \{500, 1000, 2000\}$. Clara was applied with 10 seeds.

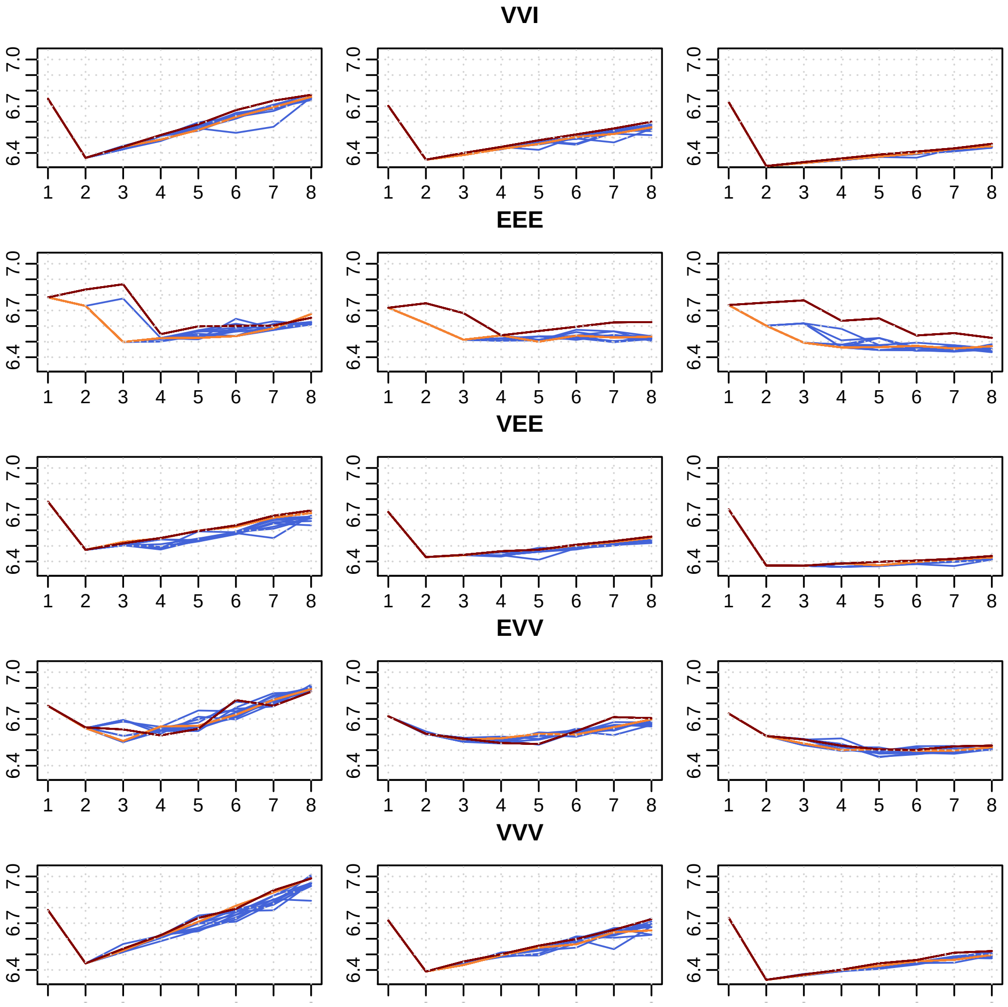


Figure 3.5: BIC values of MW34 with $n = \{500, 1000, 2000\}$. CLARA was applied with 10 seeds.

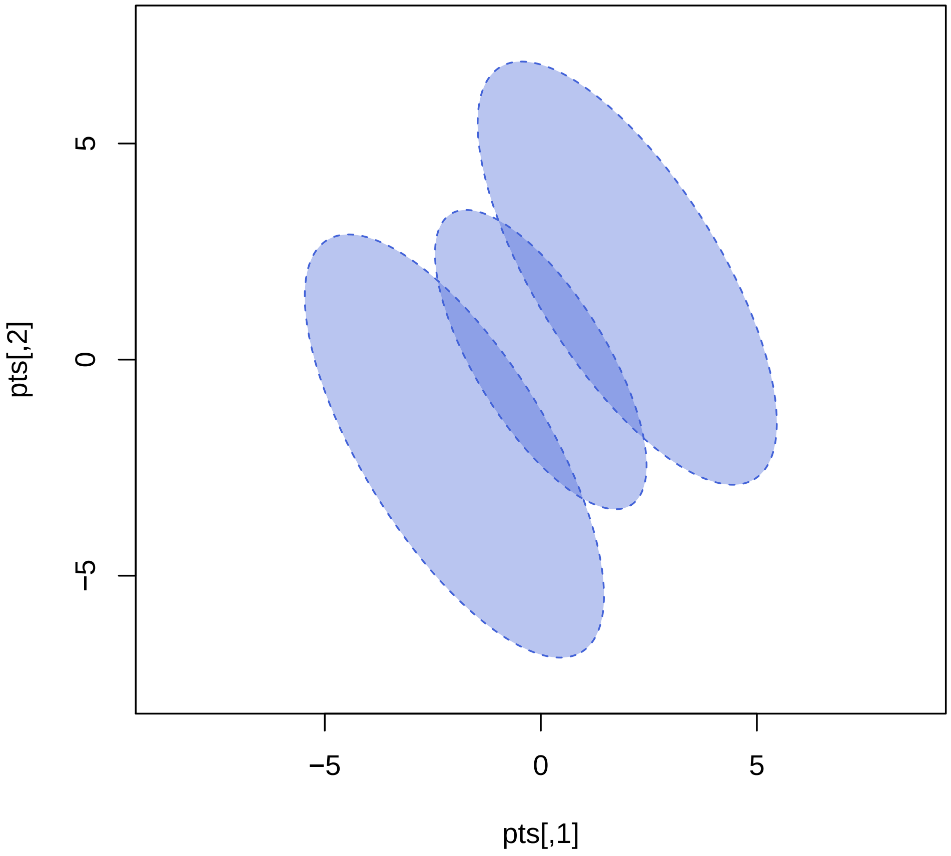


Figure 3.6: Trimodal mixture `MW215`. Three equally weighted, oriented, and shaped components of different volumes along the diagonal

3.3 Difficult Mixtures

In this section we analyze the two mixtures given by `MW215` and `MW214`. These were generated with $n = 500$ and CLARA was applied 50 times. These are a trimodal and a claw-like distribution. These types of mixtures were also discussed in Marron and Wand (1992), in the univariate case, where they proved to be difficult to fit.

First the trimodal mixture shown in figure 3.6. The difficulty lies in the components of various sizes lying close together.

We can see, that in many cases both initialization methods `clara` and `mclVVV` manage to achieve a lower BIC value than `mclust`. Although in the case of the correct model and cluster, `k=3, model="VEE"` the three algorithms coincide.

A search for best values reveals, that the best models selected are in almost all cases the correct model.

```
     model   count
[1,] "2 VVI" "49"
```

```
>     compplot(clarabic, mclbic, mclustbic, main="Fit of MW34")
```

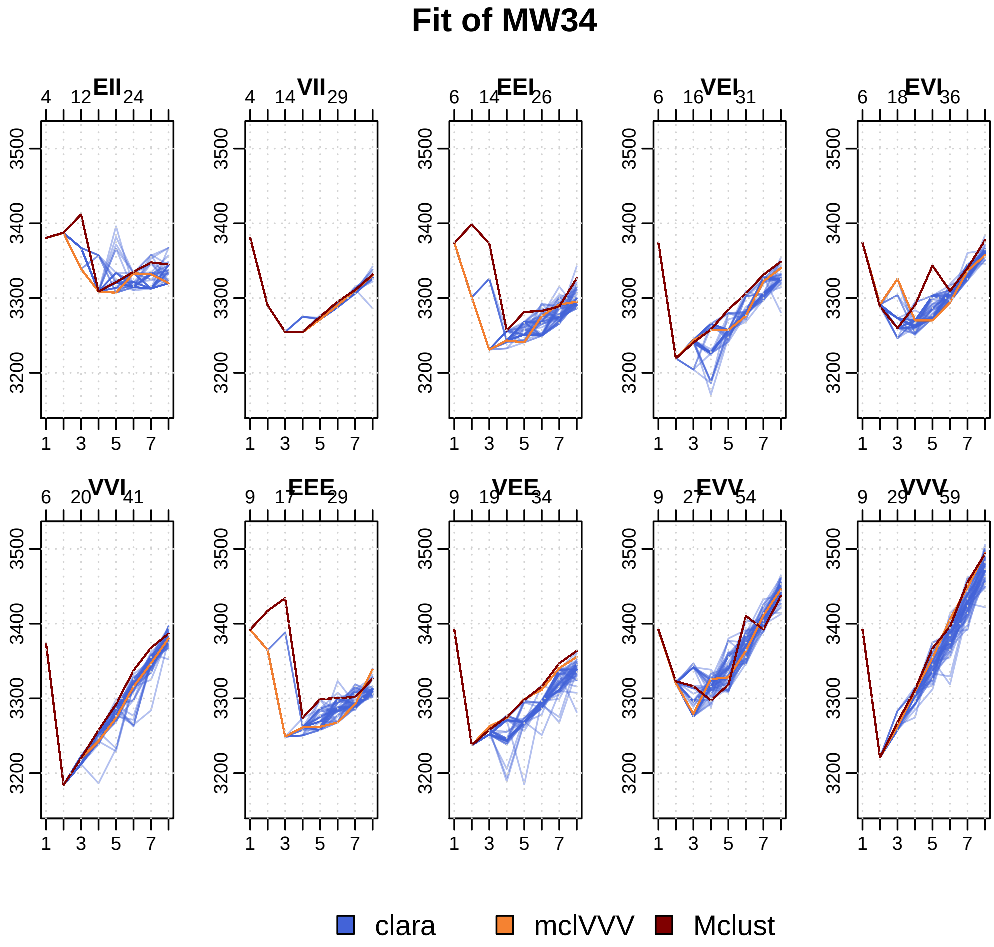
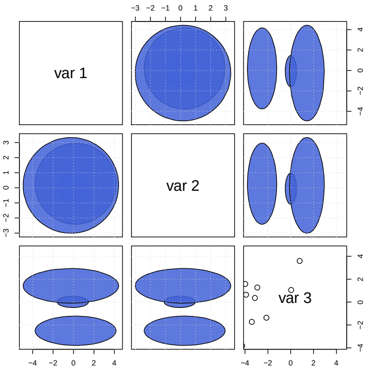
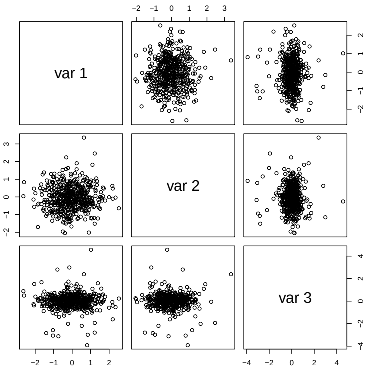


Figure 3.7: BIC values of MW34, correct: `model="VVI", k=2`. $n = 500$, CLARA was applied 50 times.

```
[2,] "4 VEI" "1"
```

The one incorrect model looks like this:





and has the weights: 0.942, 0.0321, 0.0244, 0.002. This is an issue of spurious clusters.

These are clusters formed by a low number of data points conjoined into a component with small determinant of its covariance matrix. It is a flaw in the `norMmix` package, that is not addressed.

Now for the claw-like mixture, `MW214`. It is a mixture of six components and a very simple `"VII"` covariance model. A large encompassing component and five smaller, lightly weighted components closely together along the diagonal. The inherent difficulty lies in the fact that the components overlap and are close together as well. It is shown in figure 3.8.

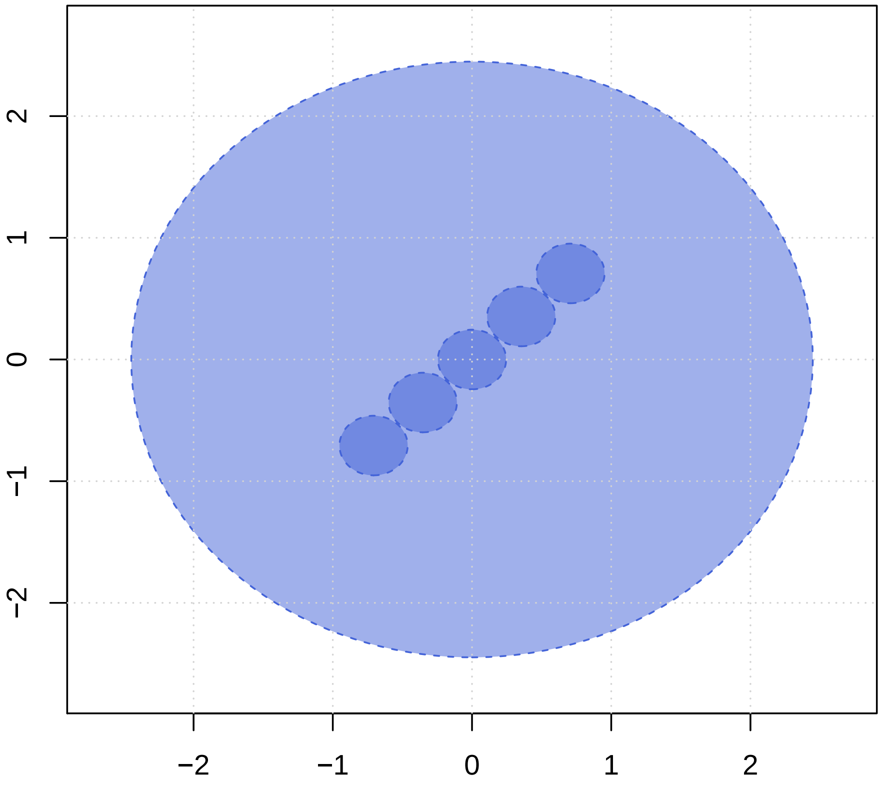


Figure 3.8: Claw-like mixture `MW214`

We take a look at the best results per simulation again:

```
     model   count
[1,] "8 VII" "27"
[2,] "7 VEE" "8"
[3,] "7 VEI" "8"
[4,] "7 VII" "4"
[5,] "8 VEE" "3"
```

And here are the ten best values:

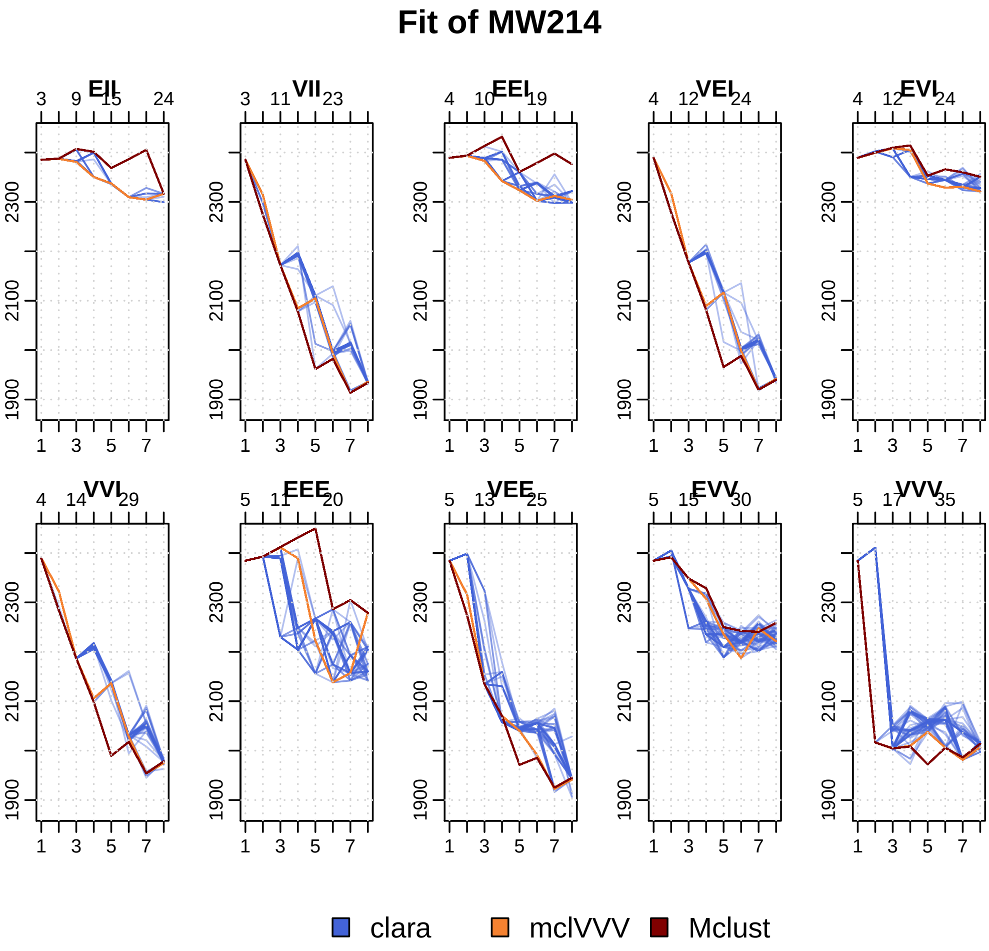


Figure 3.9: BIC values of claw-like mixture. Best fit: `model="VEE", k=8`, correct: model="VII", k=6. $n = 500$, CLARA was applied 50 times.

```
      comp model BIC
 [1,] "8"  "VEE" "1905.61014581771"
 [2,] "8"  "VEE" "1907.24944742008"
 [3,] "8"  "VEE" "1913.57109788463"
 [4,] "7"  "VII" "1913.68061849043"
 [5,] "7"  "VII" "1913.68062199219"
 [6,] "7"  "VEE" "1916.40190209225"
 [7,] "7"  "VEE" "1916.40195605402"
 [8,] "7"  "VEI" "1918.15484419568"
 [9,] "7"  "VII" "1918.35924550811"
[10,] "7"  "VII" "1918.4864952664"
```

Here some examples of fitted mixtures:

We can see, that, subtracting the obvious hiccups of the small erroneous components, `norMmix` has correctly found the 'intended' distribution. This is remarkable, given the small sample size and difficulty of distribution. As can be seen in figure 3.11, there are mistakes in the near best clusters, where the data is overlaid with a 'patchwork' of

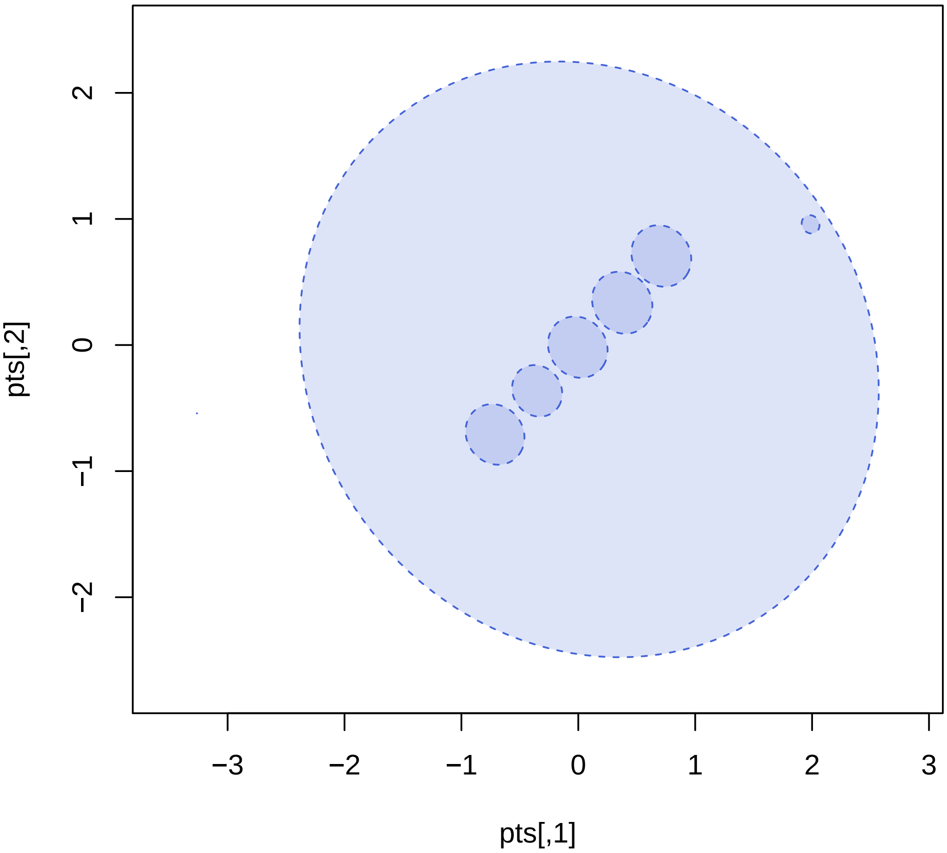


Figure 3.10: `model="VEE", k=8`, correct model: `model="VII", k=6`. Of Note Here are the Spurious Clusters Appearing.

components.

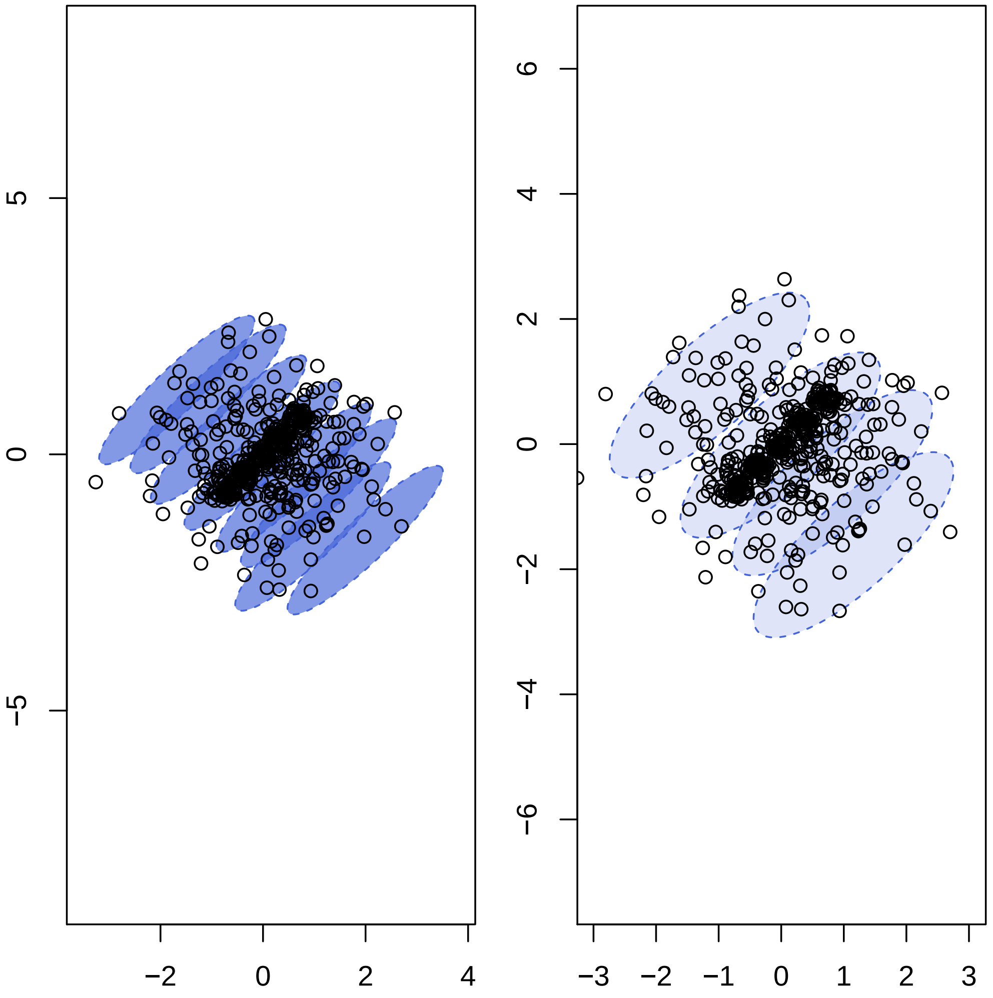


Figure 3.11: Two of the better clusters. They both follow the 'patchwork' covering strategy, laying patches of components over the data.

3.4 Nonnormal Mixtures

Using only datasets generated from the intended model can hide important structural errors in an algorithm. To that end we also applied `norMmix` to nonnormal data to see if any erratic behaviour appears.

The data used are the `SMI.12` and `loss` from the package `copula` Hofert et al. (2018), as well as the `iris` data included in base R .

We begin with the `SMI.12` dataset, described as ”SMI.12 contains the close prices of all 20 constituents of the Swiss Market Index (SMI) from 2011-09-09 to 2012-03-28.” This also doubles as high-dimensional analysis, as it is 20 dimensional.

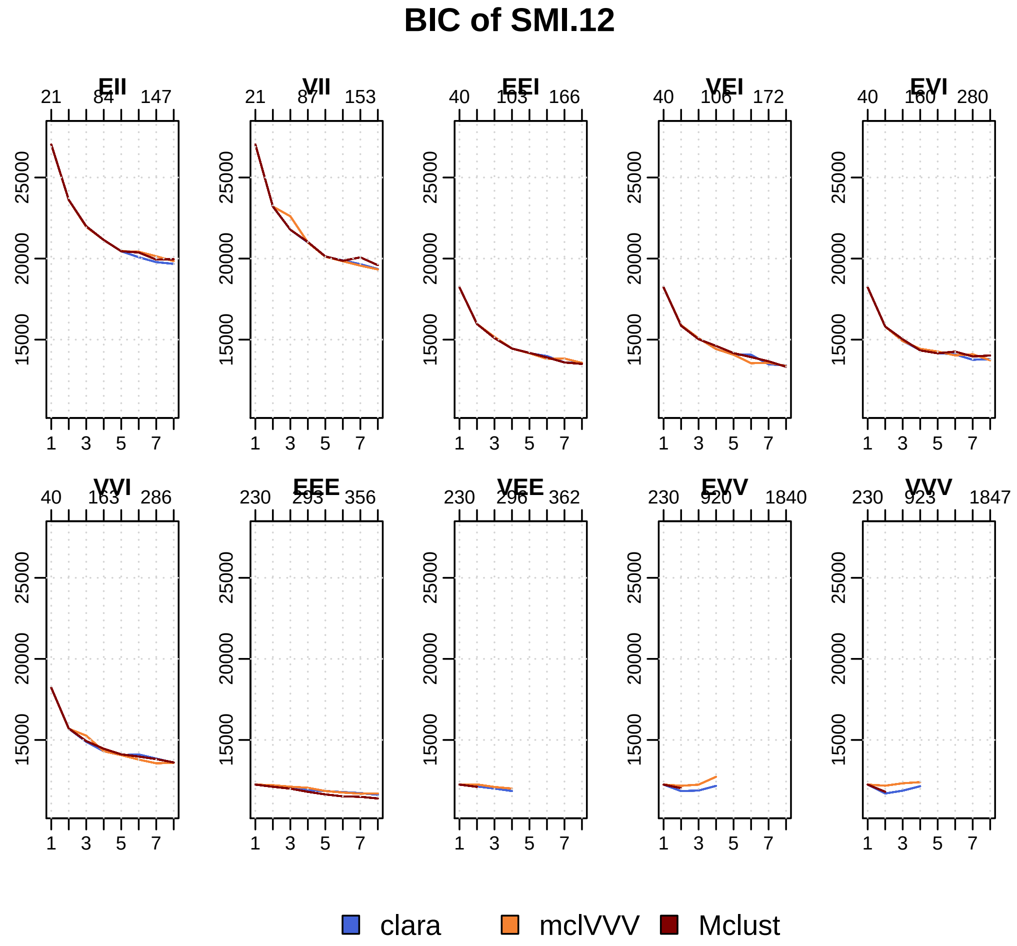


Figure 3.12: The BIC values of the `SMI.12` data. The blue line representing the `clara` values is covered by the other lines. The last three models are not plotted for all component sizes, as the algorithm returns an error if the fitting problem is ill defined.

While not very spectacular, the graphs show that even at large parameter counts our algorithm closes in on the same values as `mclust`. At these dimensions it is difficult to compare if these are actually equal, or even similar fits, but going by BIC values, it is at the very least equally viable as a working model. The last three models are not fully plotted for all components. The reason for this is that `norMmix` relies on `mclust` in its m-step. The mclust package halts computation when the clustering problem is badly posed. In this instance the problem is that the parameter count is much larger than the number of observations.

To illustrate, here are the parameter sizes for this simulation:

```
  EII VII EEI VEI EVI VVI EEE VEE  EVV  VVV
1  21  21  40  40  40  40 230 230  230  230
2  42  43  61  62  80  81 251 252  460  461
3  63  65  82  84 120 122 272 274  690  692
4  84  87 103 106 160 163 293 296  920  923
5 105 109 124 128 200 204 314 318 1150 1154
6 126 131 145 150 240 245 335 340 1380 1385
7 147 153 166 172 280 286 356 362 1610 1616
8 168 175 187 194 320 327 377 384 1840 1847
```

SMI.12 has 141 observations, which is exceeded by the parameter count by all component sizes and covariance models. With a ratio of observations to parameters this low, it is desirable for clustering algorithms to break off and return an error, so conclusions are not drawn from ill posed problems.

For curiosity's sake we include here the system times taken for the simulations

```
   models
k     EII    VII    EEI    VEI     EVI    VVI     EEE     VEE      EVV      VVV
  1 0.059  0.051  0.058  0.059   0.070  0.070   0.201   0.202    0.273    0.275
  2 0.273  0.331  1.719  1.763   4.545  3.805  61.951  59.924  224.436  232.331
  3 0.435  1.950  4.816  5.248  12.660 12.860  96.099 125.053  660.375  638.954
  4 1.384  2.456  8.715  9.145  22.173 23.065 136.370 151.448 1438.264 1556.838
  5 1.869  3.289 13.293 14.703  26.584 28.580 218.786   0.683    0.690    0.682
  6 2.703  4.125 20.578 20.490  45.355 41.667 256.036   0.010    0.011    0.022
  7 2.235  4.337 31.705 34.893  89.809 83.015 353.466   0.012    0.014    0.025
  8 3.079 13.737 63.725 44.501 110.690 98.954 396.502   0.011    0.014    0.026
```

The longest, model="VVV", k=4, took 25.9473 minutes.

Next, we take a look at the iris dataset with 150 observations of 4 variables. The fitnMm was run with 25 different seeds. In this instance the mclVVV initialization was not applied, so we only compare to mclust.

The iris data originates from three types of plant species, which is not correctly identified by either norMmix or mclust. The best models chosen are:

```
     model   count
[1,] "6 VVV" "18"
[2,] "7 VVV" "7"
```

Both far from three components. Furthermore mclust does not return values for some combinations of k and model. It is not clear what causes this, as a call to Mclust simply returns NULL.

Lastly, the data loss, from the copula package Hofert et al. (2018). This data is described as ”Indemnity payment and allocated loss adjustment expense from an insurance company.” It consists of 1500 observations with 4 variables. The BIC values are shown in 3.14

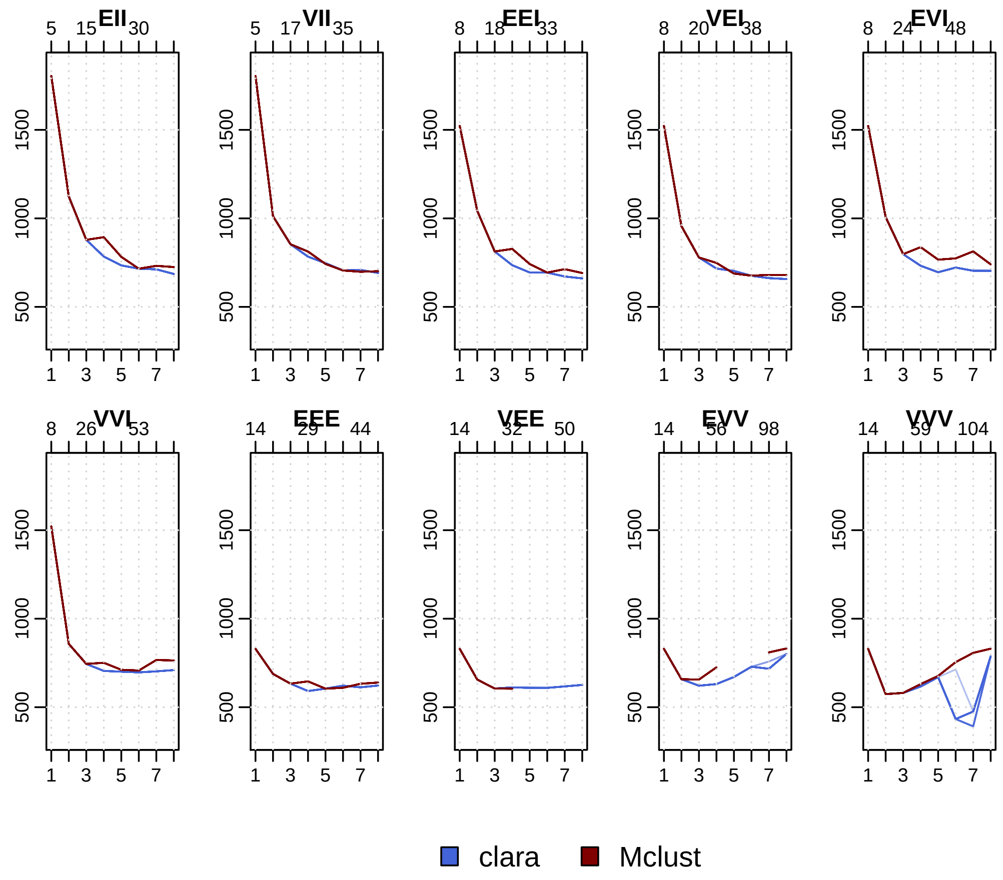


Figure 3.13: The BIC values of the `iris` data

The data resists any attempt at fitting. `mclust` returns `NULL`, as with `iris`. In `norMmix`, the `optim` function encounters an error.

```
>     data(loss, package="copula")
>     to <- try(norMmixMLE(loss, k=3, model="EEI"))
```

```
initial  value 58082.835867
iter  10 value 56418.201189
iter  20 value 53014.372756
iter  30 value 49490.970255
iter  40 value 46802.853871
```

```
>     print(to)
```

```
[1] "Error in optim(initpar., neglogl, method = method, control = control) : \n  non-finite
attr(,"class")
[1] "try-error"
attr(,"condition")
<simpleError in optim(initpar., neglogl, method = method, control = control): non-finite fi
```

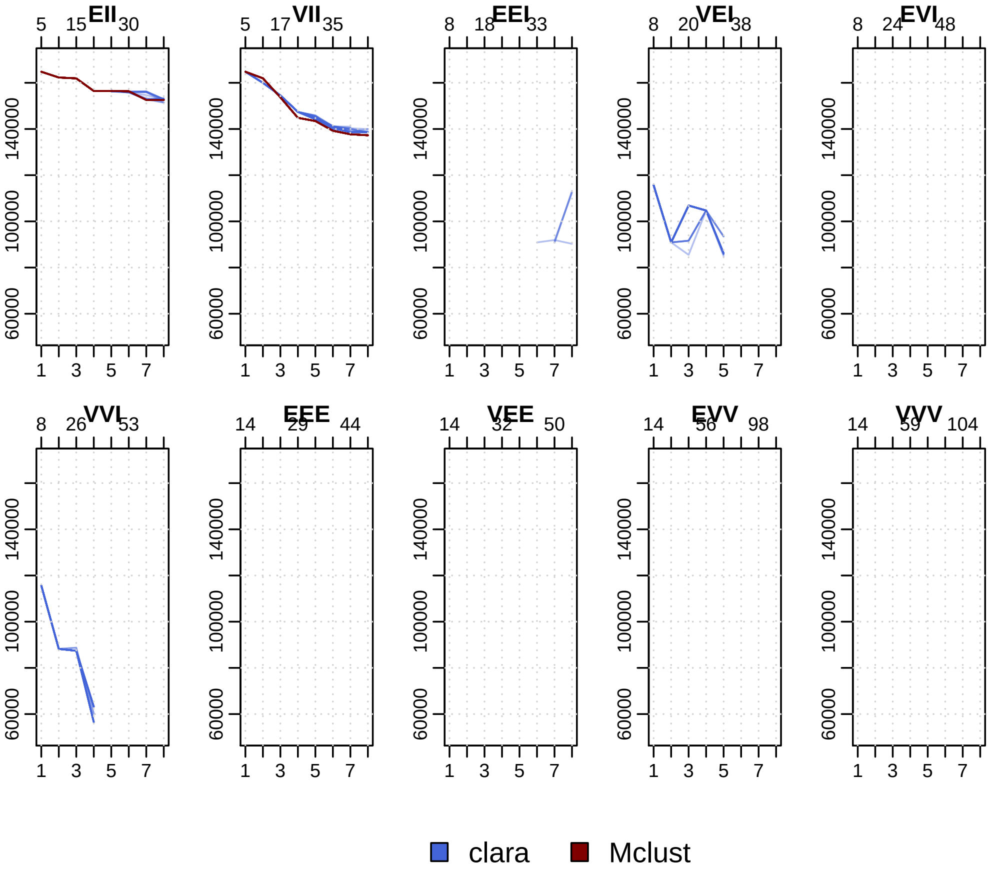


Figure 3.14: The BIC values of the `loss`data

Chapter 4

Discussion

As we have seen, the algorithm works and is in many cases equal if not better to existing clustering methods. The approach is also very generalizable, with the biggest hurdle being an efficient implementation of a log-likelihood function and a parametrization strategy. Should this approach be improved upon, it may provide a valuable tool in the arsenal of mixture model analysis.

There are many directions further research in this area may be conducted. For instance, the initialization methods may prove to be an essential factor in correct model selection. Furthermore, in the case of CLARA, the parameters chosen are somewhat arbitrary. It could yield useful results how CLARA behaves with different sampling parameters.

The investigation conducted in this thesis also falls short in the study of high-dimensional datasets. While we have looked into it with the analysis of the `SMI.12` data, the behaviour in these cases might also hold its own difficulties, that have not cropped up in the study of one dataset.

Further research could also go in the direction of model selection theory. The Bayesian Information Criterion was chosen in this work for its reliable results and usefulness, but other methods might yield more appropriate results.

There are also implementation related improvements, that could prove useful. For example, as seen in figure 3.10, spurious clusters are not accounted for at all in our implementation, which could strongly impact the strength of this tool. This is most likely the most pressing issue with the implementation in this package, that no measures against spurious clusters have been developed.

4.1 Acknowledgements

The Author would like to thank the 'Seminar für Statistik' and ETH Zurich for providing the computing resources needed for the simulations used in this thesis.

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Appendix A

R Code

A.1 llnorMmix

```
#### the llnorMmix function, calculating log likelihood for a given
#### parameter vector

## Author: Nicolas Trutmann 2019-07-06

## Log-likelihood of parameter vector given data
#
# par:   parameter vector
# tx:    transposed sample matrix
# k:     number of components
# model: assumed distribution model of normal mixture
# trafo: either centered log ratio or logit
llnorMmix ← function(par, tx, k,
                      trafo=c("clr1", "logit"),
                      model=c("EII","VII","EEI","VEI","EVI",
                              "VVI","EEE","VEE","EVV","VVV")
                      ) {
    stopifnot(is.matrix(tx),
              length(k ← as.integer(k)) == 1, k >= 1)
    p ← nrow(tx)
#     x ← t(x) ## then only needed in   (x-mu[,i])^2  i=1..k

    # 2. transform

    model ← match.arg(model)
    trafo ← match.arg(trafo)

    l2pi ← log(2*pi)

    # 3. calc log-lik

    # get w

    w ← if (k==1) 1
         else switch(trafo,
                     "clr1" = clr1inv (par[1:(k-1)]),
                     "logit"= logitinv(par[1:(k-1)]),
                     stop("invalid ’trafo’: ", trafo)
         )

    # start of relevant parameters:

    f ← k + p*k # weights -1 + means +1 => start of alpha
    # get mu
    mu ← matrix(par[k:(f-1L)], p,k)

    f1 ← f       # end of alpha if uniform
    f2 ← f+k-1L # end of alpha if var

    f1.1 ← f1 +1L # start of D. if alpha unif.
    f2.1 ← f1 + k # start of D. if alpha variable

    f11 ← f1 + p-1     # end of D. if D. uniform and alpha uniform
    f12 ← f1 +(p-1)*k # end    D. if D.   var   and alpha unif.
    f21 ← f2 + p-1     # end of D. if D. uniform and alpha variable
    f22 ← f2 +(p-1)*k # end of D. if D.   var   and alpha var.

    f11.1 ← f11 +1L # start of L if alpha unif  D unif
    f21.1 ← f21 +1L # start of L if alpha var   D unif
    f12.1 ← f12 +1L # start of L if alpha unif  D var
    f22.1 ← f22 +1L # start of L if alpha var   D var

    f111 ← f11 +   p*(p-1)/2 # end of L if alpha unif  D unif
    f211 ← f21 +   p*(p-1)/2 # end of L if alpha var   D unif
    f121 ← f12 + k*p*(p-1)/2 # end of L if alpha unif  D var
    f221 ← f22 + k*p*(p-1)/2 # end of L if alpha var   D var


    # initialize f(tx_i) i=1..n  vector of density values
    invl ← 0

    # calculate log-lik, see first case for explanation
    switch(model,
    "EII" = {
        alpha ← par[f]
        invalpha ← exp(-alpha)# = 1/exp(alpha)
        for (i in 1:k) {
            rss ← colSums(invalpha*(tx-mu[,i])^2)
            # this is vector of length n=sample size
            # calculates (tx-mu)t * Sigma^-1 * (tx-mu) for diagonal
            # cases.
            invl ← invl+w[i]*exp(-0.5*(p*(alpha+l2pi)+rss))
            # adds likelihood of one component to invl
            # the formula in exp() is the log of likelihood
            # still of length n
        }
    },
    # hereafter differences are difference in dimension in alpha and D.
    # alpha / alpha[i] and D. / D.[,i]

    "VII" = {
        alpha ← par[f:f2]
        for (i in 1:k) {
            rss ← colSums((tx-mu[,i])^2/exp(alpha[i]))
            invl ← invl+w[i]*exp(-0.5*(p*(alpha[i]+l2pi)+rss))
        }
    },

    "EEI" = {
        alpha ← par[f]
        D. ← par[f1.1:f11]
        D. ← c(-sum(D.),D.)
        D. ← D.-sum(D.)/p
        invD ← exp(alpha+D.)
        for (i in 1:k) {
            rss ← colSums((tx-mu[,i])^2/invD)
            invl ← invl+w[i]*exp(-0.5*(p*(alpha+l2pi)+rss))
        }
    },

    "VEI" = {
        alpha ← par[f:f2]
        D. ← par[f2.1:f21]
        D. ← c(-sum(D.), D.)
        D. ← D.-sum(D.)/p
        for (i in 1:k) {
            rss ← colSums((tx-mu[,i])^2/exp(alpha[i]+D.))
            invl ← invl+w[i]*exp(-0.5*(p*(alpha[i]+l2pi)+rss))
        }
    },

    "EVI" = {
        alpha ← par[f]
        D. ← matrix(par[f1.1:f12],p-1,k)
        D. ← apply(D.,2, function(j) c(-sum(j), j))
        D. ← apply(D.,2, function(j) j-sum(j)/p)
        for (i in 1:k) {
            rss ← colSums((tx-mu[,i])^2/exp(alpha+D.[,i]))
            invl ← invl+w[i]*exp(-0.5*(p*(alpha+l2pi)+rss))
        }
    },

    "VVI" = {
        alpha ← par[f:f2]
        D. ← matrix(par[f2.1:f22],p-1,k)
        D. ← apply(D.,2, function(j) c(-sum(j), j))
        D. ← apply(D.,2, function(j) j-sum(j)/p)
        for (i in 1:k) {
            rss ← colSums((tx-mu[,i])^2/exp(alpha[i]+D.[,i]))
            invl ← invl+w[i]*exp(-0.5*(p*(alpha[i]+l2pi)+rss))
        }
    },

    # here start the non-diagonal cases. main difference is the use
    # of backsolve() to calculate tx^t Sigma^-1 tx, works as follows:
    # assume Sigma = L D L^t, then Sigma^-1 = (L^t)^-1 D^-1 L^-1
    # y = L^-1 tx  => tx^t Sigma^-1 tx = y^t D^-1 y
    # y = backsolve(L., tx)

    "EEE" = {
        alpha ← par[f]
        D. ← par[f1.1:f11]
        D. ← c(-sum(D.), D.)
        D. ← D.-sum(D./p)
        invD ← exp(alpha+D.)
        L. ← diag(1,p)
        L.[lower.tri(L., diag=FALSE)] ← par[f11.1:f111]
        for (i in 1:k) {
            rss ← colSums(backsolve(L.,(tx-mu[,i]), upper.tri=FALSE)^2/invD)
            invl ← invl+w[i]*exp(-0.5*(p*(alpha+l2pi)+rss))
        }
    },

    "VEE" = {
        alpha ← par[f:f2]
        D. ← par[f2.1:f21]
        D. ← c(-sum(D.), D.)
        D. ← D.-sum(D./p)
        L. ← diag(1,p)
        L.[lower.tri(L., diag=FALSE)] ← par[f21.1:f211]
        for (i in 1:k) {
            rss ← colSums(backsolve(L., (tx-mu[,i]), upper.tri=FALSE)^2/exp(alpha
                [i]+D.))
            invl ← invl+w[i]*exp(-0.5*(p*(alpha[i]+l2pi)+rss))
        }
    },

    "EVV" = {
        alpha ← par[f]
        D. ← matrix(par[f1.1:f12],p-1,k)
        D. ← apply(D.,2, function(j) c(-sum(j), j))
        D. ← apply(D.,2, function(j) j-sum(j)/p)
        L.temp ← matrix(par[f12.1:f121],p*(p-1)/2,k)
        for (i in 1:k) {
            L. ← diag(1,p)
            L.[lower.tri(L., diag=FALSE)] ← L.temp[,i]
            rss ← colSums(backsolve(L., (tx-mu[,i]), upper.tri=FALSE)^2/exp(alpha+D.[,i]))
            invl ← invl+w[i]*exp(-0.5*(p*(alpha+l2pi)+rss))
        }
    },

    "VVV" = {
        alpha ← par[f:f2]
        D. ← matrix(par[f2.1:f22],p-1,k)
        D. ← apply(D.,2, function(j) c(-sum(j), j))
        D. ← apply(D.,2, function(j) j-sum(j)/p)
        invalpha ← exp(rep(alpha, each=p)+D.)
        L.temp ← matrix(par[f22.1:f221],p*(p-1)/2,k)
        L. ← diag(1,p)
        for (i in 1:k) {
            L.[lower.tri(L., diag=FALSE)] ← L.temp[,i]
            rss ← colSums(backsolve(L., (tx-mu[,i]), upper.tri=FALSE)^2/invalpha[,i])
            invl ← invl+w[i]*exp(-0.5*(p*(alpha[i]+l2pi)+rss))
        }
    },
    ## otherwise
    stop("invalid model:", model)
    )

    ## return  sum_{i=1}^n log( f(tx_i) ) :
    sum(log(invl))
}
```

A.2 Example Simulation Script

```
## Intent: analyse time as function of p,k,n

nmmdir ← normalizePath("~/BachelorArbeit/norMmix.Rcheck/")
savdir ← normalizePath("~/BachelorArbeit/Rscripts/2time")
stopifnot(dir.exists(nmmdir), dir.exists(savdir))
library(norMmix, lib.loc=nmmdir)
library(mclust)

## at n=500,p=2 can do about 250xfitnMm(x,1:10) in 24h
seeds ← 1:10
sizes ← c(500, 1000, 2000)
nmm ← list(MW214, MW34, MW51)
## => about 100 cases

# for naming purposes
nmnames ← c("MW214", "MW34", "MW51")
sizenames ← c("500", "1000", "2000")
files ← vector(mode="character")

for (nm in 1:3) {
    for (size in sizes) {
    set.seed(2019); x ← rnorMmix(size, nmm[[nm]])
        for (seed in seeds) {
            set.seed(2019+seed)
            r ← tryCatch(fitnMm(x, k=1:8,
                                 optREPORT=1e4, maxit=1e4),
                          error = identity)
            filename ← sprintf("%s_size=%0.4d_seed=%0.2d.rds",
                                nmnames[nm], size, seed)
            files ← append(files, filename)
            cat("===> saving to file:", filename, "\n")
            saveRDS(list(fit=r), file=file.path(savdir, filename))
        }
    }
}

fillis ← list()
for (i in seq_along(sizes)) {
    for (j in seq_along(nmnames)) {
        # for lack of AND matching, OR match everything else and invert
        ret ← grep(paste(sizenames[-i], nmnames[-j], sep="|"),
                    files, value=TRUE, invert=TRUE)
        fillis[[paste0(sizenames[i], nmnames[j])]] ← ret
    }
}

epfl(fillis, savdir)
```

Appendix B

Further Plots

```
>     library(norMmix, lib.loc="~/ethz/BA/norMmix.Rcheck/")
>     mainsav <- normalizePath("~/ethz/BA/Rscripts/")
```

B.1 Behaviour in n

Here are the further plots ommited in section 3.2. First is a very difficult mixture, ommited because it is studied in greater detail in section 1.1. Second is a very easy mixture, because all fitting lines overlap, making meaningful analysis futile.

B.1.1 MW214

```
>     MW214
```

```
norMmix object:
multivariate normal mixture model with the following attributes:
name:                  #14 Smooth Comb
 model:                  VII
 dimension:         2
 components:         6
weight of components 0.5 0.1 0.1 0.1 0.1 0.1
```

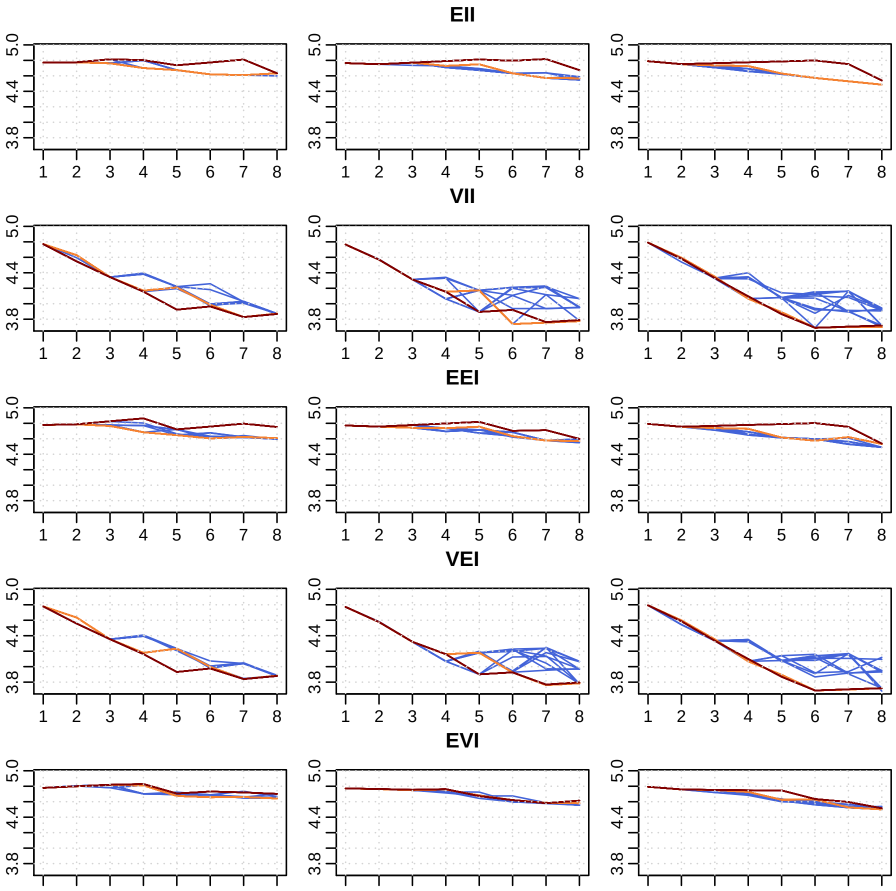


Figure B.1: BIC values of MW214 with $n = \{500, 1000, 2000\}$, first five models

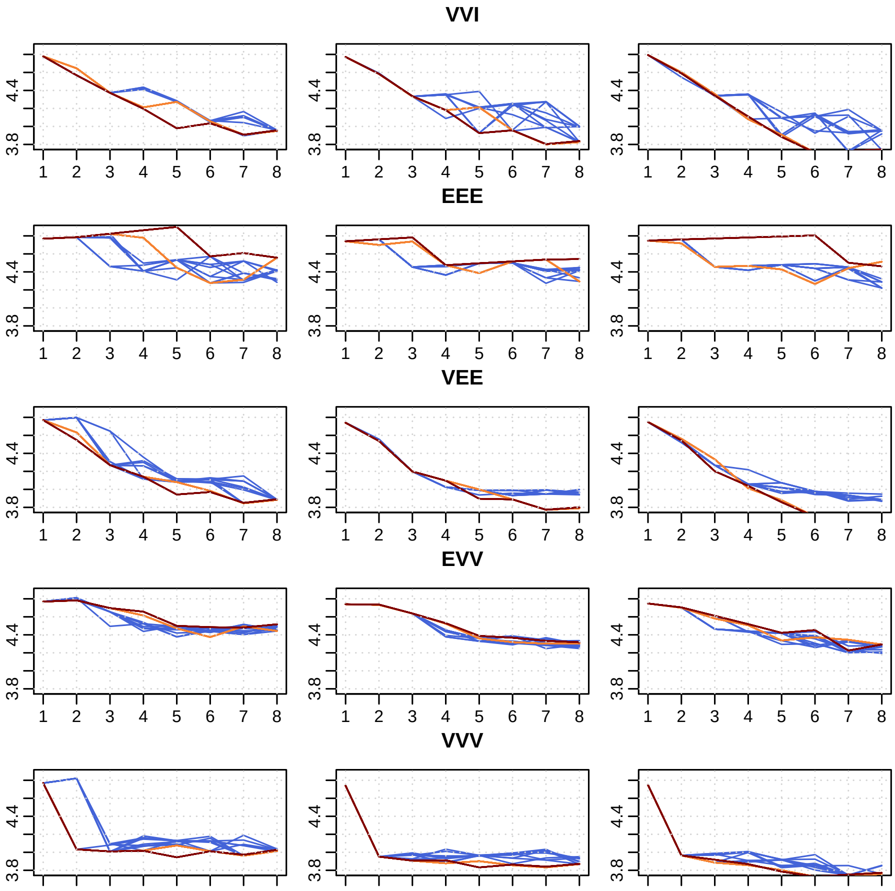


Figure B.2: BIC values of MW214 with $n = \{500, 1000, 2000\}$, last five models.

B.1.2 MW51

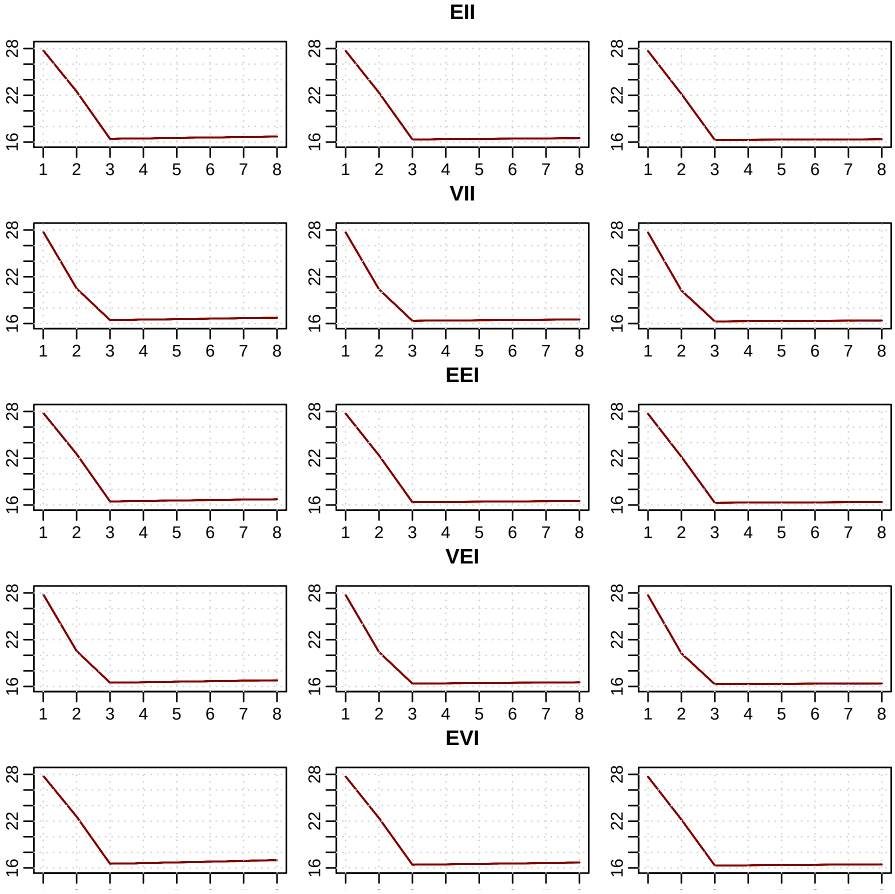


Figure B.3: BIC values of MW51 with $n = \{500, 1000, 2000\}$

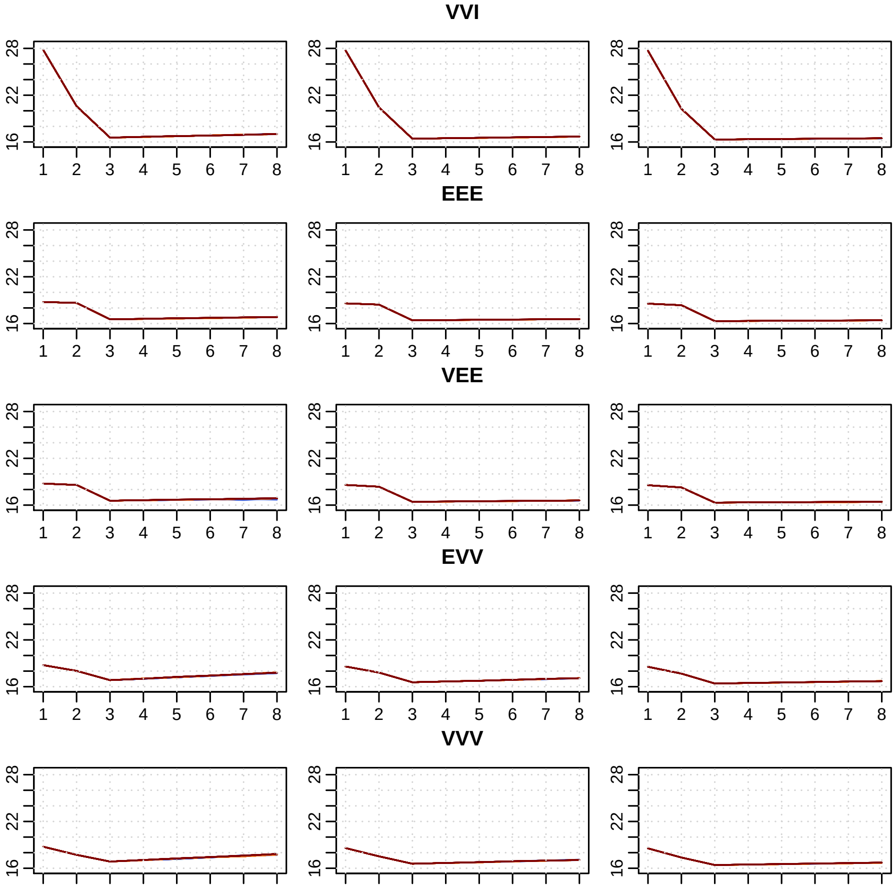
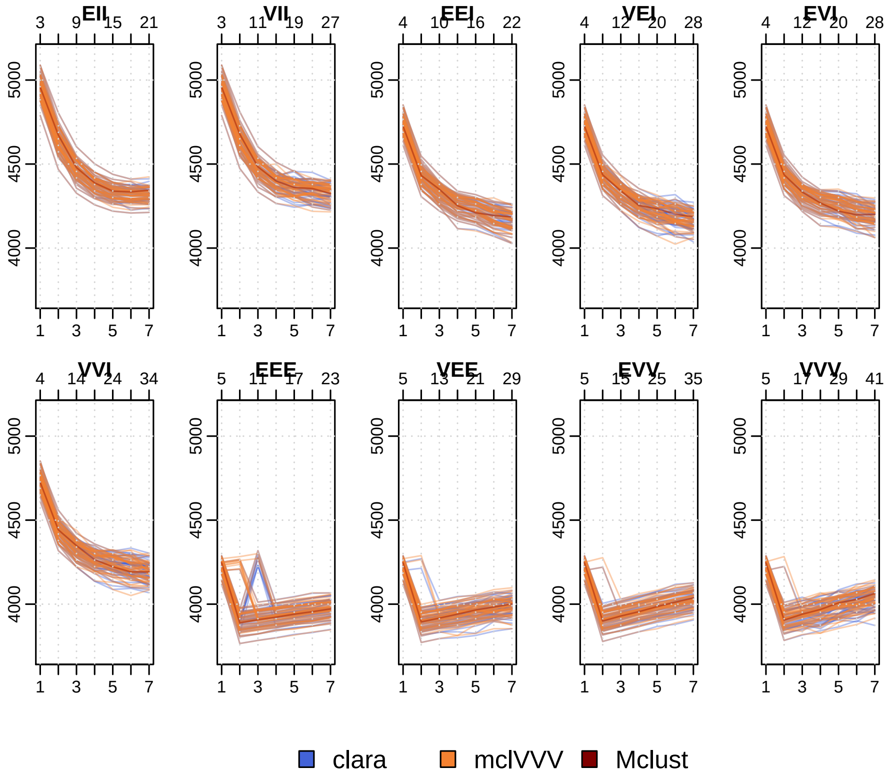


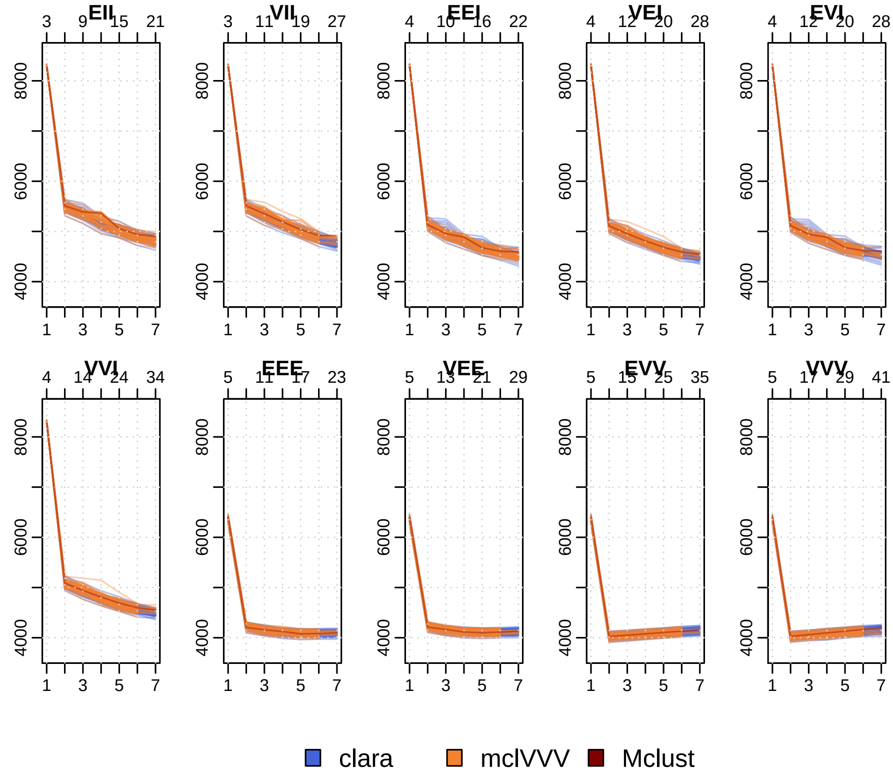
Figure B.4: BIC values of `MW51` with $n = \{500, 1000, 2000\}$

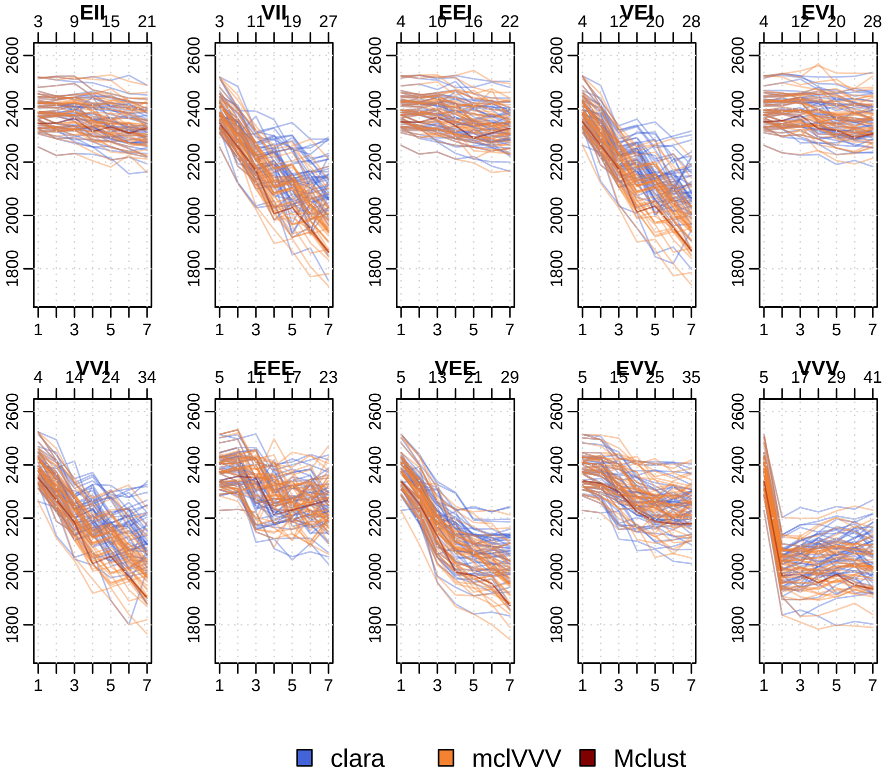


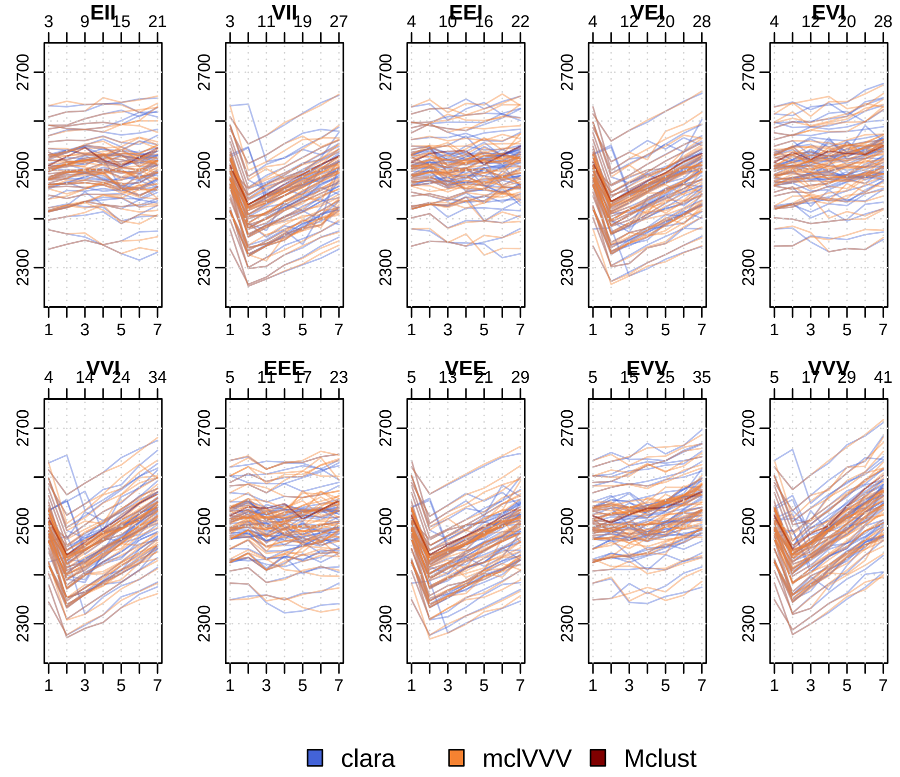
B.2 Other Data

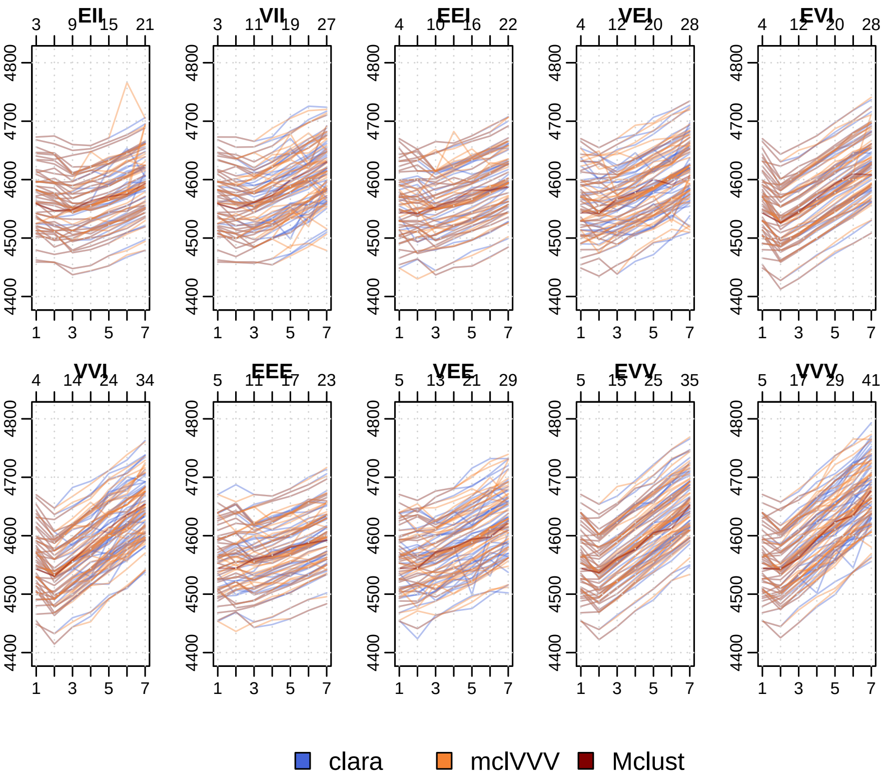
Unfortunately not all simulations were as useful to show in the main body of this work. In part, because they were done for exploratory purposes. However, they show some other properties that are of interest.

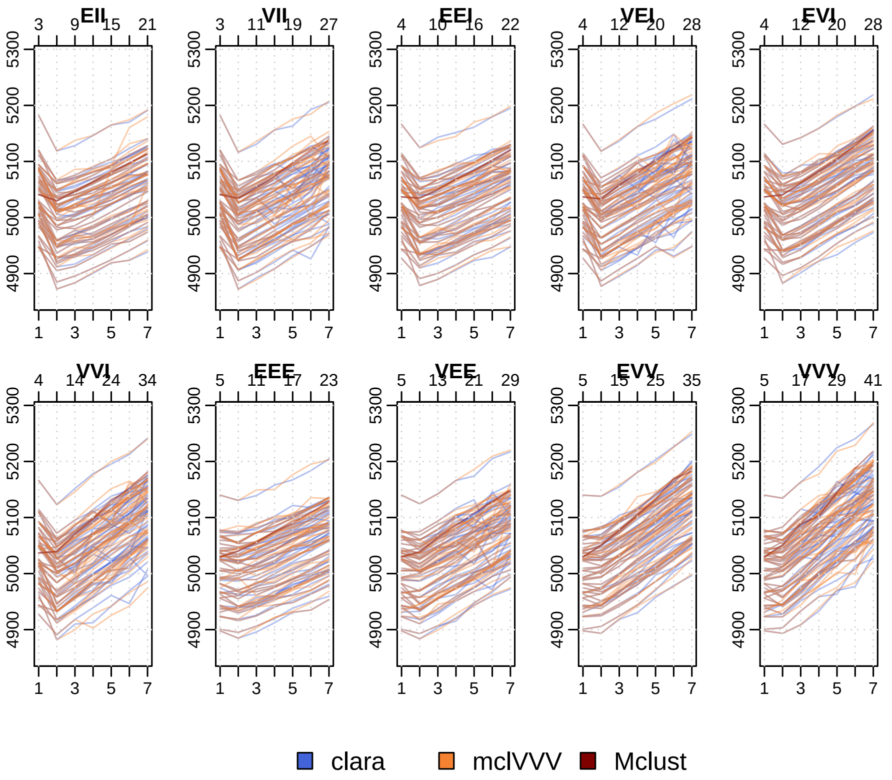
The data in `/simulations/smallinit` varied the dataset with a set seed. The values for every individual dataset are not as interesting as `/simulations/2time`, but they show that `norMmix` is consistent in its results for similar datasets.

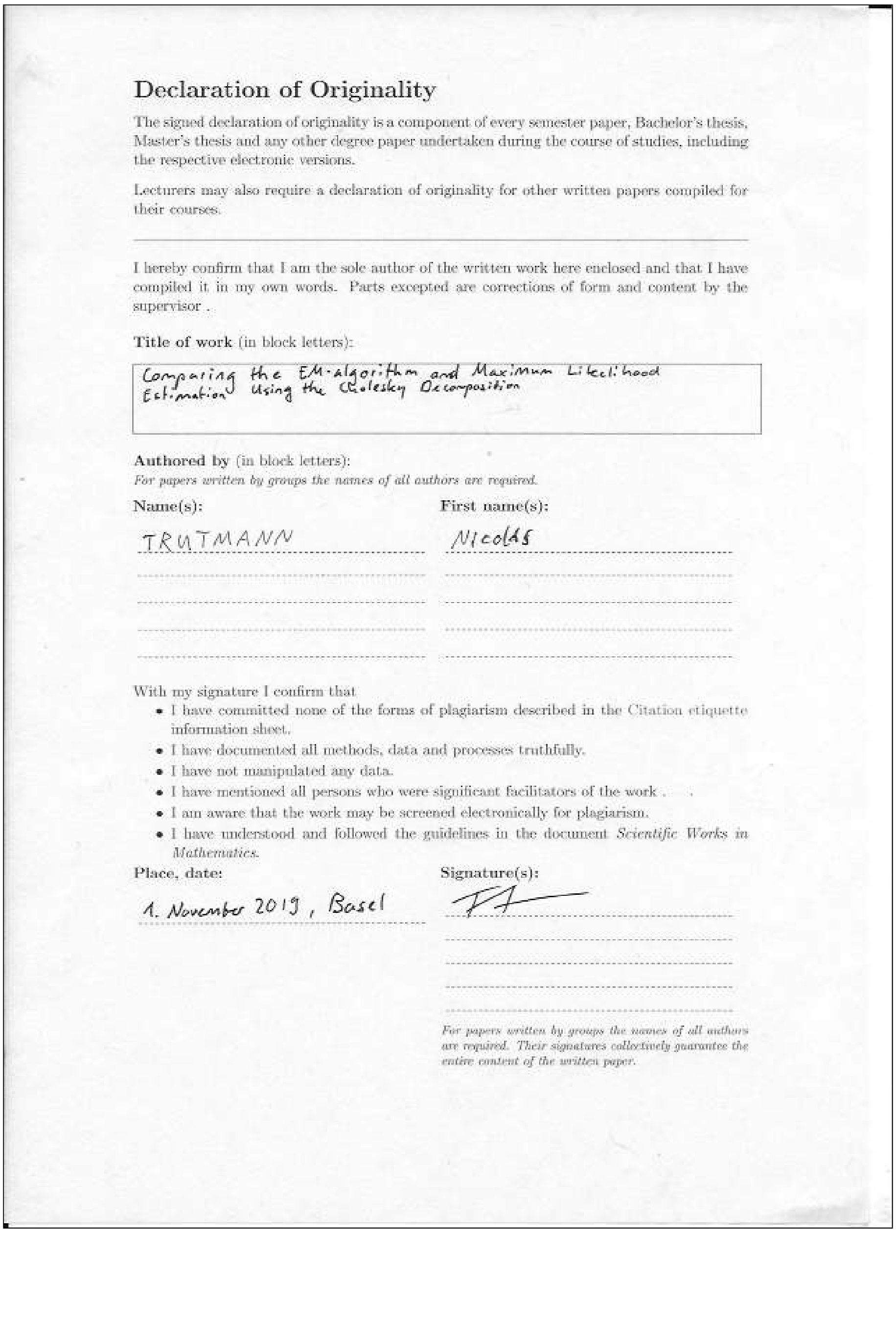

EII
3 9 15 21
VII
3 11 19 27
EEI
4 10 16 22
VEI
4 12 20 28
EVI
4 12 20 28
VVI
4 14 24 34
EEE
5 11 17 23
VEE
5 13 21 29
EVV
5 15 25 35
VVV
5 17 29 41
8000
6000
4000
1 3 5 7
clara
mclVVV
Mclust


EII
3
9
15
21
VII
3
11
19
27
EEI
4
10
16
22
VEI
4
12
20
28
EVI
4
12
20
28
VVI
4
14
24
34
EEE
5
11
17
23
VEE
5
13
21
29
EVV
5
15
25
35
VVV
5
17
29
41
1800
2000
2200
2400
2600
1
3
5
7
clara
mclVVV
Mclust


EII
3 9 15 21
VII
3 11 19 27
EEI
4 10 16 22
VEI
4 12 20 28
EVI
4 12 20 28
VVI
4 14 24 34
EEE
5 11 17 23
VEE
5 13 21 29
EVV
5 15 25 35
VVV
5 17 29 41
2300
2500
2700
1 3 5 7
■ clara
■ mclVVV
■ Mclust


EII
3 9 15 21
VII
3 11 19 27
EEI
4 10 16 22
VEI
4 12 20 28
EVI
4 12 20 28
VVI
4 14 24 34
EEE
5 11 17 23
VEE
5 13 21 29
EVV
5 15 25 35
VVV
5 17 29 41
4400 4500 4600 4700 4800
1 3 5 7
clara
mclVVV
Mclust


EII
3 9 15 21
VII
3 11 19 27
EEI
4 10 16 22
VEI
4 12 20 28
EVI
4 12 20 28
VVI
4 14 24 34
EEE
5 11 17 23
VEE
5 13 21 29
EVV
5 15 25 35
VVV
5 17 29 41
4900 5000 5100 5200 5300
1 3 5 7
clara
mclVVV
Mclust



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