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Nicolas Trutmann

Comparison of EM-algorithm and MLE using Cholesky decomposition

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Abstract

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

methods(not done)

results(not done)

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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 overlayed 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. 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.

While the theory of mixture models holds for a much broader class of distributions, we restrict ourselves here to the case of normal distributions, because this restriction fits more comfortably into the scope of this work and because normal distributions allow for a parsimonious parametrization, that is of interest to study.

This parametrization is the $\boldsymbol{LDL}^\top$ decomposition, which allows 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.

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.

$\boldsymbol{Y}_1,\ldots,\boldsymbol{Y}_n$

Definition 1.1.0.1. *Suppose we have a random sample $\boldsymbol{Y}_1,\ldots,\boldsymbol{Y}_n$ with probability density function $\boldsymbol{Y}_j \sim f(y_j)$ on $\mathbb{R}^p$ We assume that the density $f(y_j)$ of $\boldsymbol{Y}_j$ can be written in the form*

$$f(y_j) = \sum_{k=1}^{K} \pi_k \phi_k(y_k;\mu,\Sigma)$$

The π_k are called the component densities of the mixture and the ϕ_k mixture components.

For 'large' datasets there are more parsimonious parametrizations, that reduce computation time. 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 all normal mixture components.

Suppose we have a $p-$dimensional dataset of n samples $x_1, \dots, x_n$, onto which we would like to fit K normal distributions $\phi_k,\ \ k \in 1, \dots, n$. We introduce a further explaining variable $\boldsymbol{Z}$ in $\mathrm{Mat}^{n \times k}$, with entries in $[0, 1]$ which represent the expectation that observation i belongs to component k.

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.

$$\tau_i(y_j; \Psi) = \phi_i(y_j; \mu_i, \Sigma_i) / \sum_{k=1}^{K} \phi_k(y_j; \mu_k, \Sigma_k)$$

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

$$\mu_i = \sum_{j=1}^{n} \tau_{ij} y_j / \sum_{j=1}^{n} \tau_{ij}$$

$$\Sigma_i = \sum_{j=1}^{n} \tau_{ij} (y_j - \mu_i)(y_j - \mu_i)^\top / \sum_{j=1}^{n} \tau_{ij}$$

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 L, M, TB, and AE. (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 in notation between Celeux and Govaert (1995) and ours.

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 follows

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

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:

$$\begin{aligned} \boldsymbol{D} &\longmapsto \boldsymbol{Q} \\ \boldsymbol{A} &\longmapsto \boldsymbol{\Lambda} \\ \lambda &\longmapsto \alpha \\ \Sigma = \lambda\boldsymbol{D}\boldsymbol{A}\boldsymbol{D}^\top &= \alpha\boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^\top \end{aligned}$$

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 somewhat arbitrarily chosen.

1.4 Models of Covariance Matrices

As mentioned above, there are ways to constrain the covariance matrices for computational reasons. There are istances 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.

- We restrict the complexity of the decomposition components
- We restrict the variability of the mixture components

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

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

.

The second restriction simply means we hold the decomposition fixed throughout all covariance matrices. There is however an issue with the cholesky decomposition. For 10 out of 14 cases as defined by Celeux and Govaert (1995), there exists a canonical translation of decompositions. The 6 diagonal cases need no translation; the eigen and cholesky decomposition are equal to identity. For the non-diagonal cases note that for a given sym. pos. def. matrix Σ we have decompositions:

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

Since in both cases the bracketing 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 3 times 2 cases would yield the 8 out of 14 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	$\alpha\boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^\top$	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	$\alpha\boldsymbol{Q}\boldsymbol{\Lambda}_k\boldsymbol{Q}^\top$	equal	var.	equal	$\alpha, \lambda_{i,k}, q_{i,j}$	doesn't exist		$1+K(p-1)+\frac{p(p-1)}{2}$
VEE	$\alpha_k\boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^\top$	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	$\alpha_k\boldsymbol{Q}\boldsymbol{\Lambda}_k\boldsymbol{Q}^\top$	var.	var.	equal	$\alpha_k, \lambda_{i,k}, q_{i,j}$			$K+K(p-1)+\frac{p(p-1)}{2}$
EEV	$\alpha\boldsymbol{Q}_k\boldsymbol{\Lambda}\boldsymbol{Q}_k^\top$	equal	equal	var.	$\alpha, \lambda_i, q_{i,j,k}$	don't exist		$1+(p-1)+K\frac{p(p-1)}{2}$
VEV	$\alpha_k\boldsymbol{Q}_k\boldsymbol{\Lambda}\boldsymbol{Q}_k^\top$	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	reduced	$\mathcal{O}()$
EII	$K-1+pK$	1	$pK+K$	pK
VII	$K-1+pK$	K	$pK+2K-1$	pK
EEI	$K-1+pK$	$1+(p-1)$	$pK+p+K-1$	pK
VEI	$K-1+pK$	$K+(p-1)$	$pK+p+2K-2$	pK
EVI	$K-1+pK$	$1+K(p-1)$	$2pK$	pK
VVI	$K-1+pK$	$1+K(p-1)$	$2pK+1$	pK
EEE	$K-1+pK$	$1+(p-1)+\frac{p(p-1)}{2}$	$\frac{p(p-1)}{2}$	p^2
VEE	$K-1+pK$	$K+(p-1)+\frac{p(p-1)}{2}$	$K+\frac{(p+2)(p-1)}{2}$	p^2+K
EVV	$K-1+pK$	$1+K(p-1)+\frac{p(p-1)}{2}$	$\frac{(p+K)(p-1)}{2}+1$	p^2+Kp+K
VVV	$K-1+pK$	$K+K(p-1)+\frac{p(p-1)}{2}$	$Kp+\frac{p(p-1)}{2}$	p^2+Kp+K

Table 1.2: Full Table of Parameters

here explain why ldlt is so nice to parametrize; i.e. Q in QLambdaQt has as many degrees of freedom, but needs more complicated boundary conditions to work well.

1.5 Problems of the EM-algorithm

The EM-algorithm has stalling problems especially close to a local optimum. 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]. In common software implementations, 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 from CRAN.

```
>     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: Parameters of `MW.nm9`

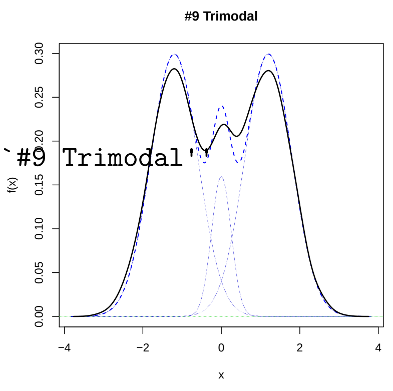


Figure 1.2: True and Estimated density

then an illustration of MW examples of pathological cases

here we see how change in loglik seems to stagnate. However, this does not stay that way, if we let EM run a bit further.

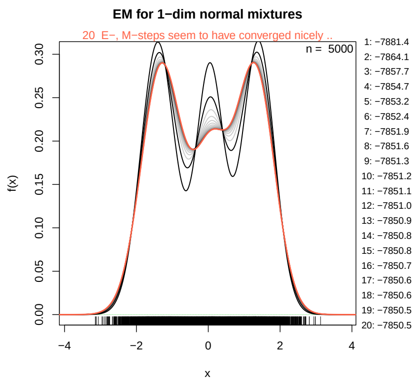


Figure 1.3: 20 EM steps

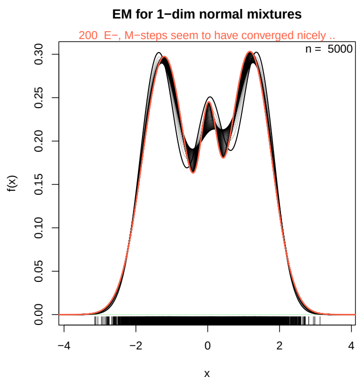


Figure 1.4: 200 EM steps

to conclude example show part of mixest that shows it takes 1200 iterations to converge

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

give 2D demonstration.

maybe show Marr Wand's examples of 'difficult' mixtures

give conclusion recapping the just demonstrated, and lead in for next chapter

Chapter 2

The `norMmix` Package

2.1 Introduction to the Package

For this thesis, an R package was developed that implements the algorithm that fits multivariate normal mixtures to given data. [1] There is a lot of unused code still in the package. These were at one point implemented used and discarded. They are still included for demonstration. 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.

The package contains the following functionality:

relies on `optim()` generic optimizer. maximizes llnormix by varying model parameters.

since mclust is one of the more popular packages implementing the EM algo, we employ a lot of functions from mclust, to keep things around EM as similar as possible.

Conceptually, at the start of a fitting algo, e.g. EM we need to initialize a mixture object. thereafter the paths diverge. at the heart of norMmix's functionality lie the functions: llnorMmix and nMm2par which are in turn employed by norMmixMLE to funnel a mixture object into optim and give optim a function to optimize.

also relies on `mixtools` package for random generating function `rnorMmix` using `rmvnorm`.

[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`

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 $\boldsymbol{LDL}^\top$ 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.

misc There are also various methods of generics, like `logLik, print, BIC, AIC` and `nobs` as well as various `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 13-th model of dimension 2.

simulations The purpose of this package is to study simulations. there are functions provided to study large collections of evaluated data. e.g `epfl`

2.2 On The Development of `norMmix`

about Cholesky decomp as ldlt. has advantages: fast, parametrically parsimonious, can easily compute loglikelihood

maybe reread section in McLachlan about accelerating EM algo

not possible to sensibly compare normal mixtures except maybe a strange sorting algorithm using Mahalanobis distance or Kullback-Leibler distance or similar (Hellinger), but not numerically sensible to integrate over potentially high-dimensional spaces.

general list of (not necessarily mathematical) dead-ends in the development life of the norMmix package. argue why this is in this section?? because, as a BScT, the learning is as much part of the research as the results.

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] -3.2617309  0.6306458  0.5682759  0.5602498  0.6616009  0.6906020  0.5707690
[8]  0.5795875
```

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`:

```
> 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.

testing of mvtnorm as proof that ldlt is in fact faster parametrization

mention, that there may be faster ways to apply backsolve. quote knuth about premature optimization?

2.3 Demonstration

Mention, that mclust doesn't depend on seed(double check) and therefore norMmix has 'advantage' of 'confidence intervals'. We can run 50 simulations and see if there might be more sensible clusters.

demonstrate things; essentially put .Rd example sections here

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, safe for restriction to 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 L 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:

$$2ln(\hat{L}) - ln(n)\theta$$

instead of the more common

$$ln(n)\theta - 2ln(\hat{L})$$

Where n is the number of observations, θ 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`.

here show bic type plots, how to read them, and what we're trying to compare i.e. clara, mclVVV, mclust.

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:

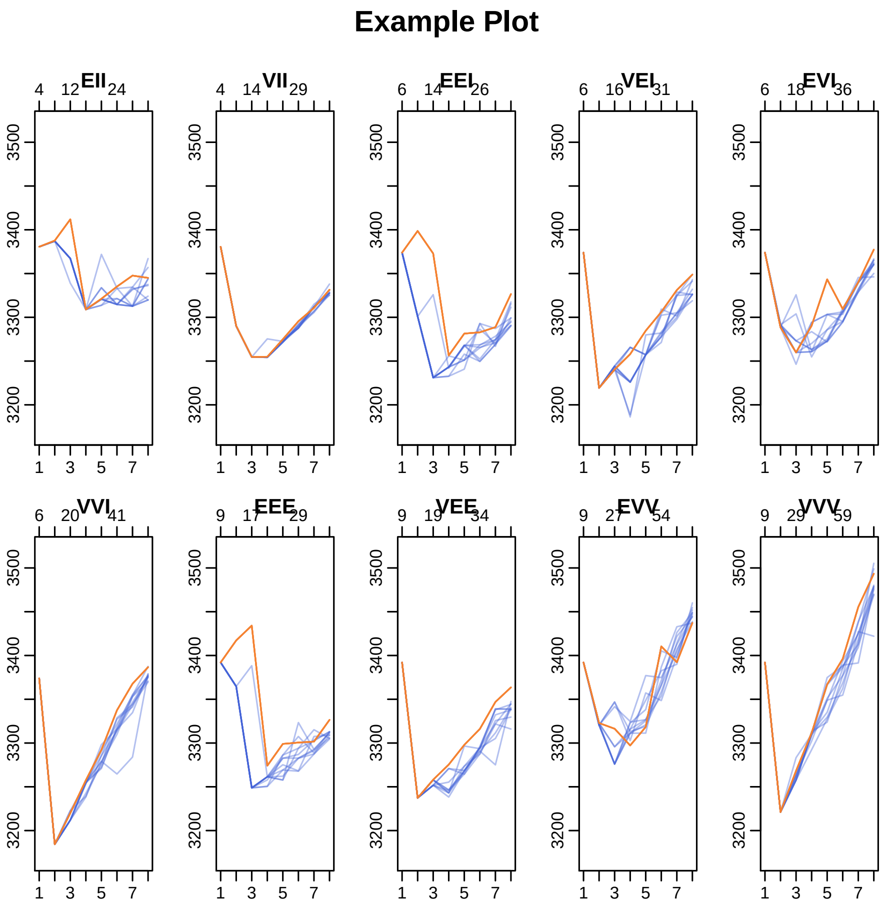


Figure 3.1: Example of Comparison Plot

As can be seen from the formula of the BIC value, 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

here explain simulations conducted, A.2 here explain the various sections: time, n, p, difficult , nonnormal

3.1 Time Analysis

here how much time they take, in p,k and n give approximate O(x) value

```
>     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)
>     ## need to split these better
>     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(log(times) ~ log(pars) + log(ddims) + log(ssize))
>     summary(r)

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

Residuals:
    Min      1Q  Median      3Q     Max
-3.4428 -0.2986  0.0671  0.4579  2.0936

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -9.74133    0.10598  -91.91   <2e-16 ***
log(pars)    2.75983    0.01181  233.75   <2e-16 ***
log(ddims)  -2.06063    0.02483  -82.99   <2e-16 ***
log(ssize)   0.61301    0.01446   42.38   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

```
Residual standard error: 0.6946 on 7196 degrees of freedom
Multiple R-squared:  0.8887,	Adjusted R-squared:  0.8887
F-statistic: 1.916e+04 on 3 and 7196 DF,  p-value: < 2.2e-16
```

```
>     plot(times~pars, log="xy", yaxt="n", xaxt="n")
>     sfsmisc::eaxis(1)
>     sfsmisc::eaxis(2)
```

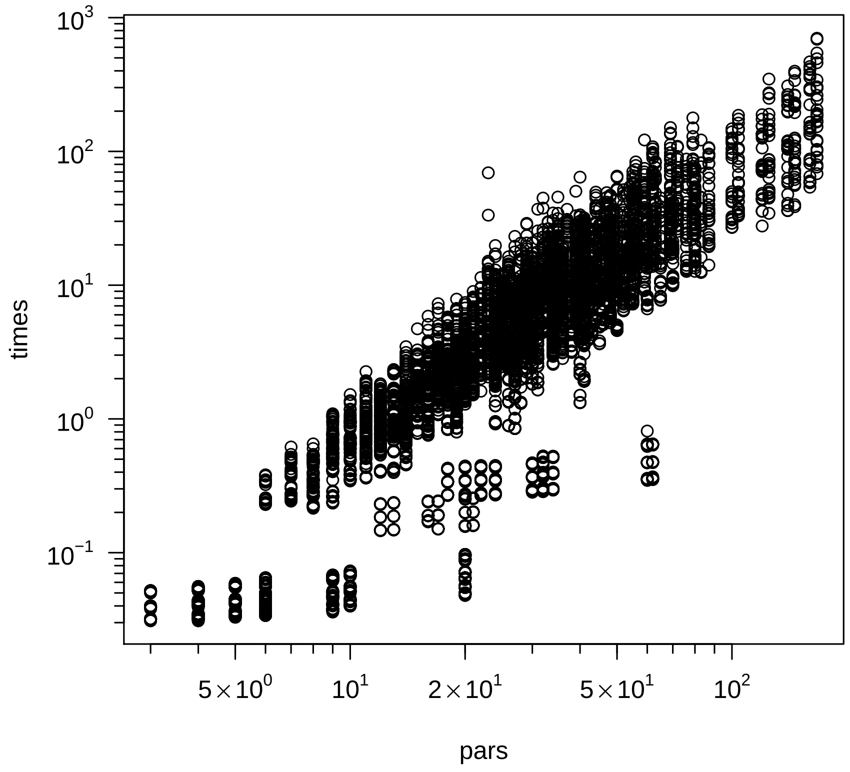


Figure 3.2: Log-log Plot of System Time against Parameter Length

can see that time is almost one to one proportional to parameter length.

3.2 Behaviour in n

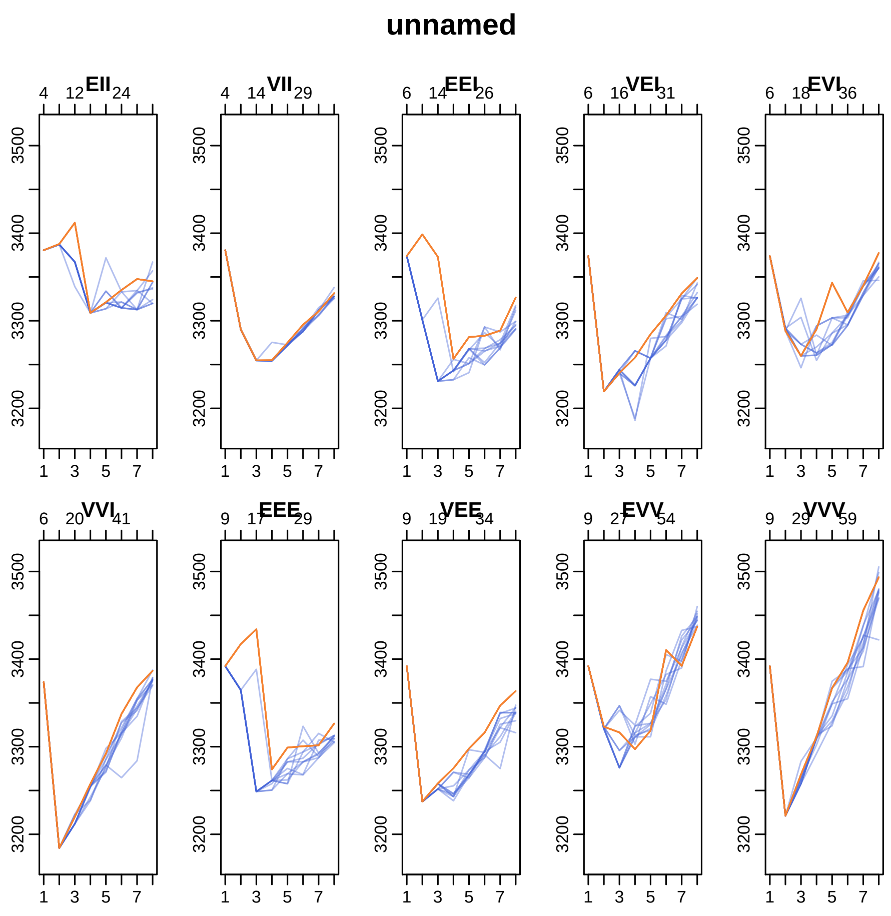
here show as expected narrower scattering as n increases

[h]

3.3 Behaviour in p

here show how norMmix is consistently competitive with mclust

```
>     compplot(s05mw34bic, m0534)
```



3.4 Diffixult Mixtures

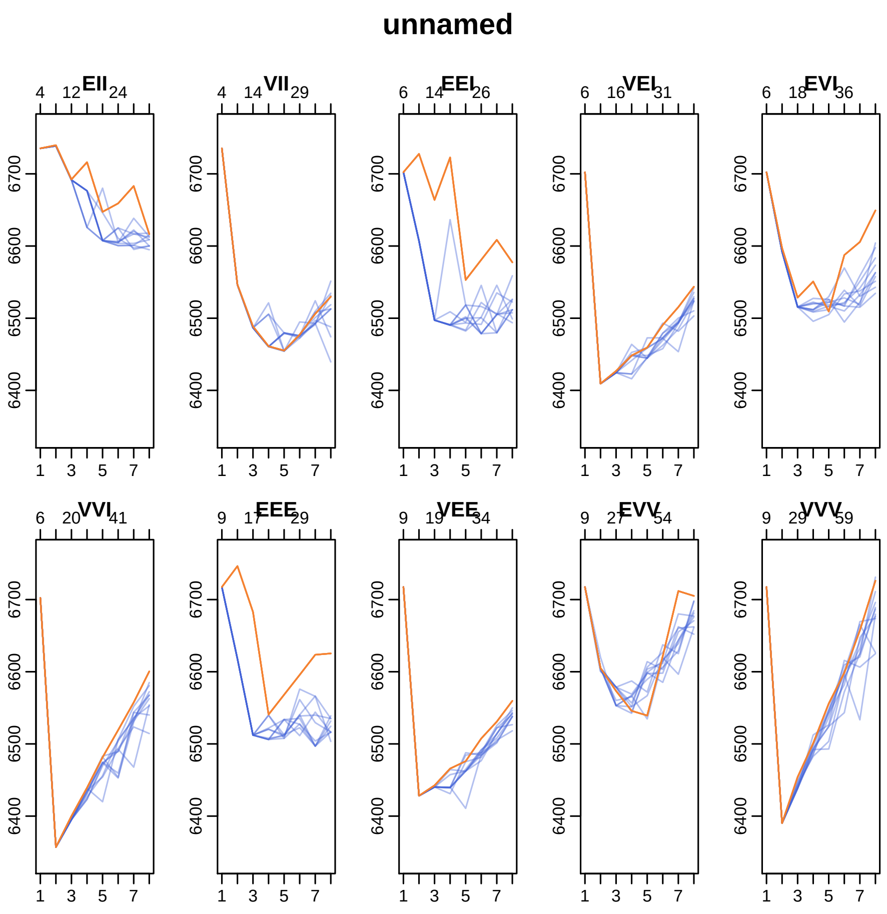
here show behaviour in difficult cases

```
>     savdir <- file.path(mainsav, "2init")
>     filenames <- list.files(savdir, pattern=".rds")
>     MW214fn <- grep("MW214", filenames, value="TRUE")
>     mclustfiles <- grep("mcl.rds", MW214fn, value=TRUE)
>     MW214fn <- grep("mcl.rds", MW214fn, value="TRUE", invert=TRUE)
>     claraMW <- grep("clara", MW214fn, value=TRUE)
>     mclMW <- grep("mclVVV", MW214fn, value=TRUE)
>     clarabic <- massbic(claraMW, savdir)
>     mclbic <- massbic(mclMW, savdir)
>     mclustbic <- readRDS(file.path(savdir,mclustfiles[1]))
```

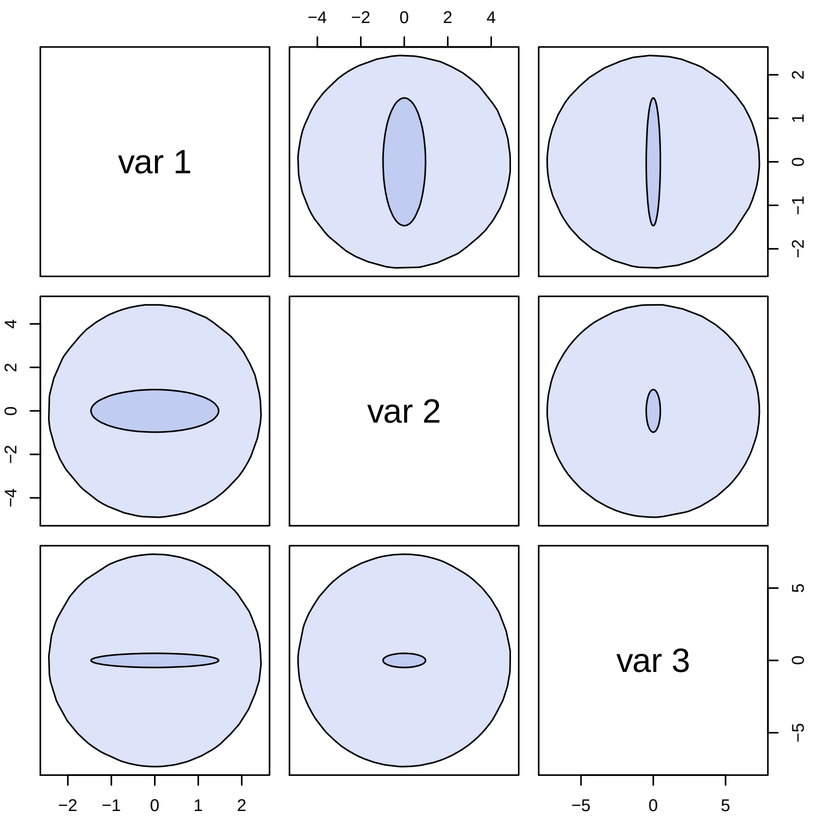
here some examples of fitted mixtures

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

```
>     compplot(s10mw34bic, m1034)
```



```
>     plot(MW34)
```



3.5 Nonnormal Mixtures

here 2smi and 2var, maybe others as well.

here 2smi:

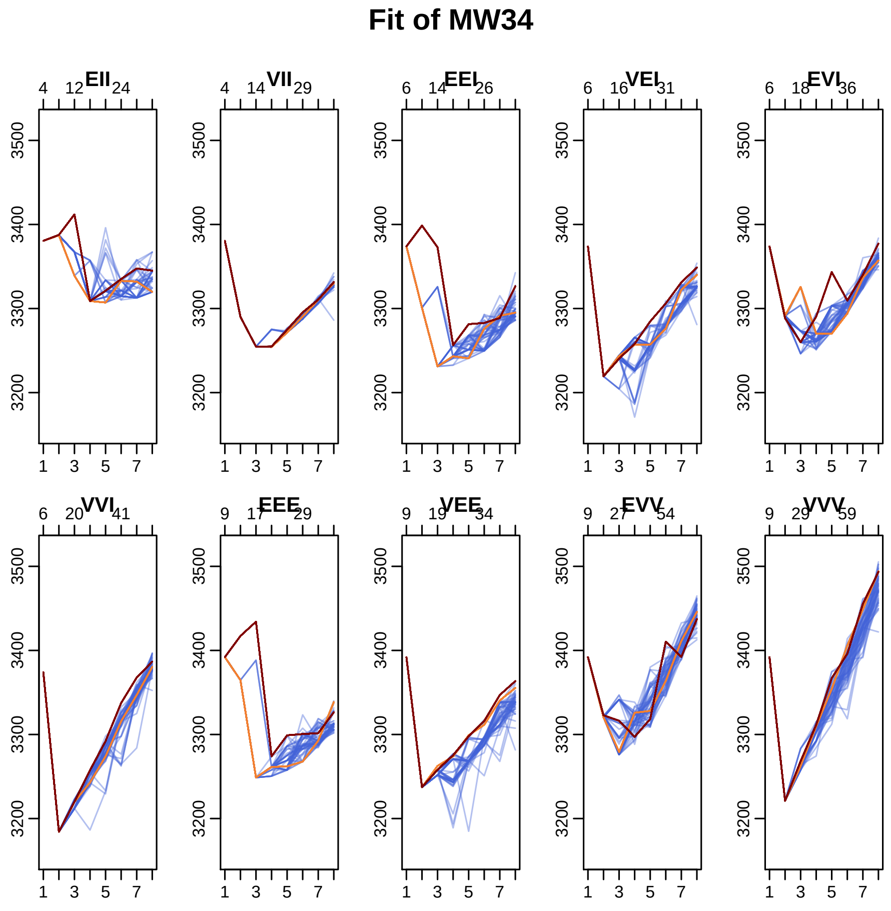
```
>     savdir <- file.path(mainsav, "2smi")
>     filenames <- list.files(savdir, pattern=".rds")
>     fnclara <- grep("clara_seed", filenames, value=TRUE)
>     fnmclVV <- grep("mclVVV_see", filenames, value=TRUE)
>     fnmclus <- grep("__mcl.rds",  filenames, value=TRUE)
```

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.

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

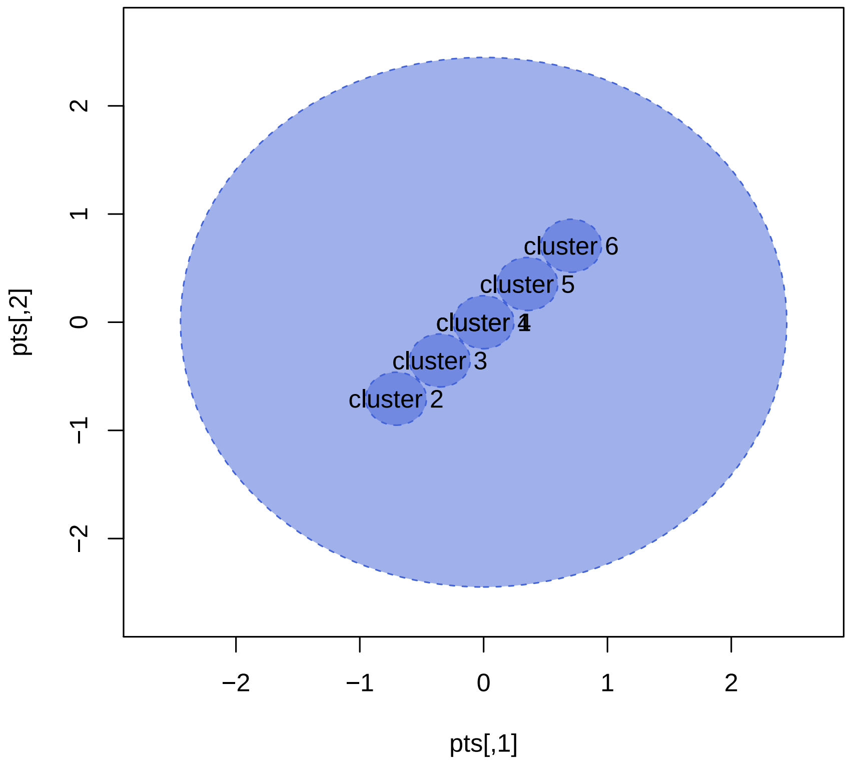
```
  EII VII EEI VEI EVI VVI EEE VEE  EVV  VVV
1  21  21  40  40  40  40 230 230  230  230
2  42  43  61  62  80  81 251 252  460  461
3  63  65  82  84 120 122 272 274  690  692
4  84  87 103 106 160 163 293 296  920  923
```

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

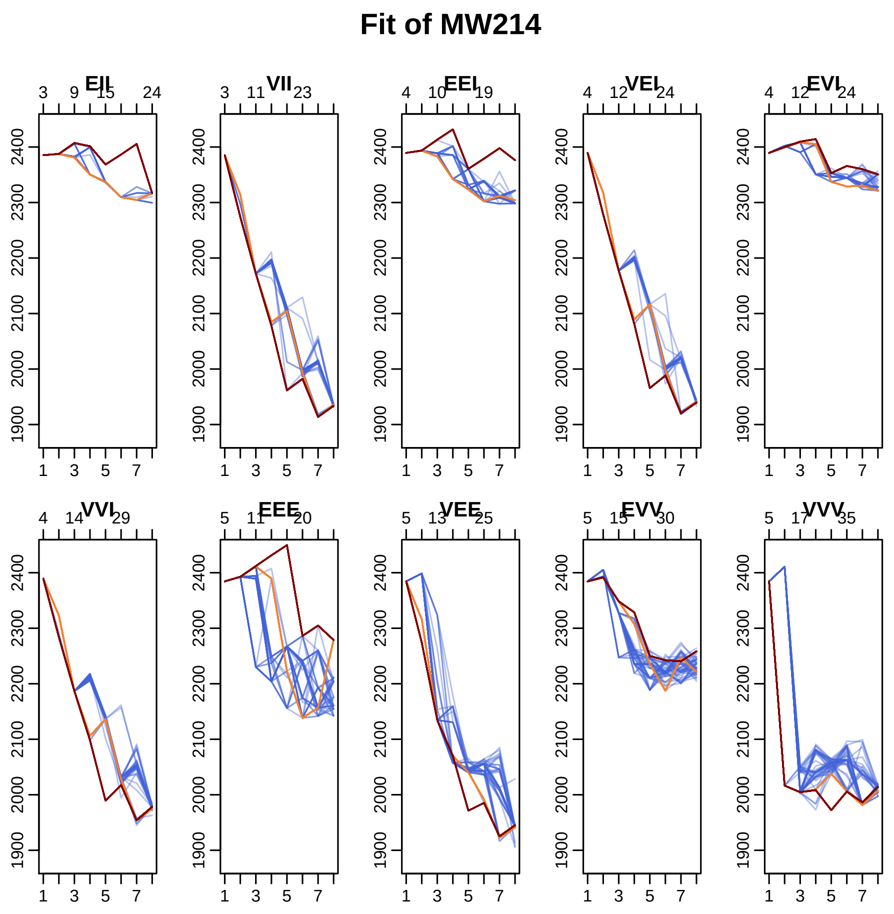


```
5 105 109 124 128 200 204 314 318 1150 1154
6 126 131 145 150 240 245 335 340 1380 1385
7 147 153 166 172 280 286 356 362 1610 1616
8 168 175 187 194 320 327 377 384 1840 1847
```

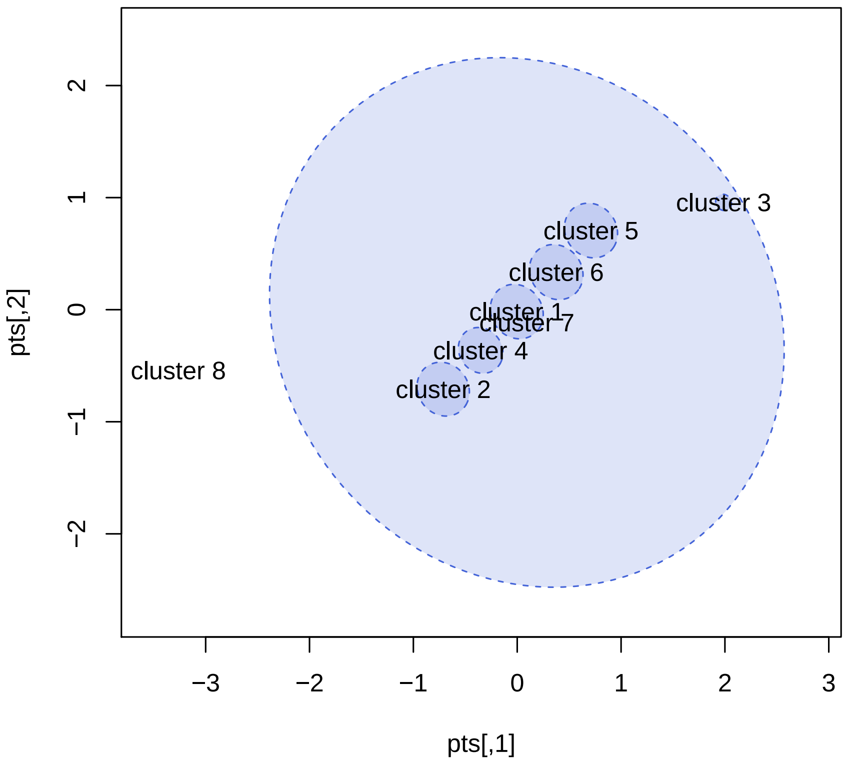
```
>     plot(MW214)
```

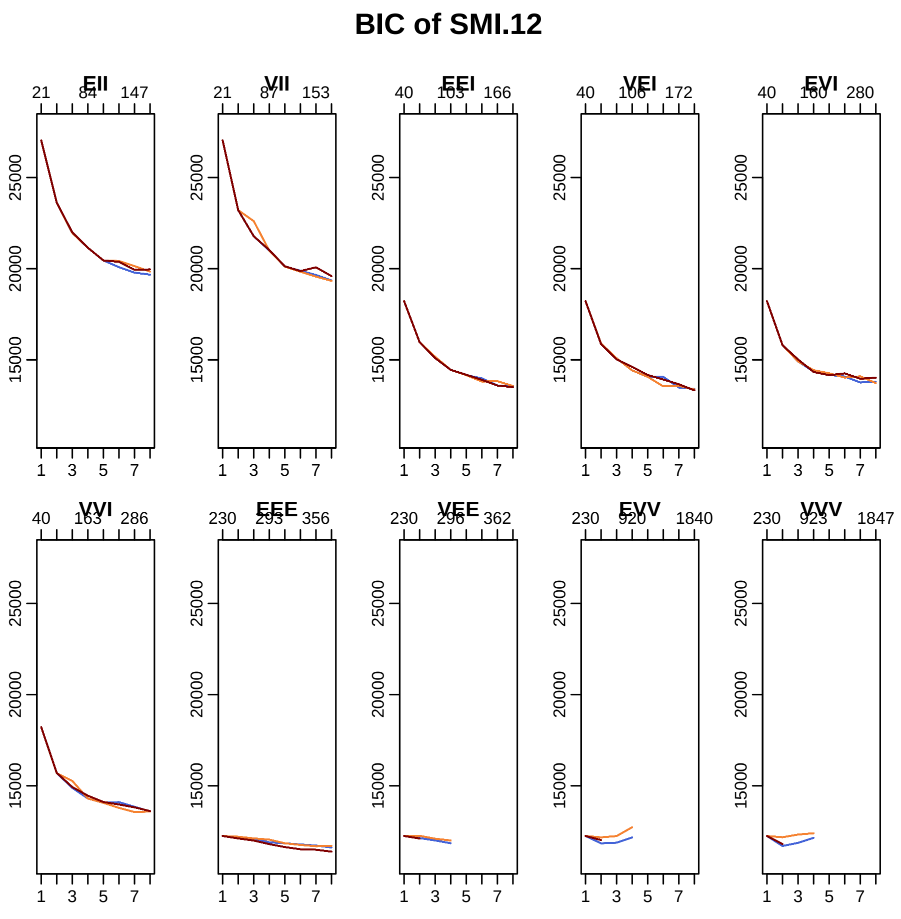

cluster 6
cluster 5
cluster 4
cluster 1
cluster 3
cluster 2
pts[,2]
pts[,1]
−2
−1
0
1
2

```
>     compplot(clarabic, mclbic, mclustbic, main="Fit of MW214")
```



```
>      f <- readRDS(file.path(savdir, claraMW[28]))
>      ff <- f$fit$nMm[8,8][[1]]
>      plot(ff$norMmix)
>      #points(ff$x)
```




BIC of SMI.12
EII
VII
EEI
VEI
EVI
VVI
EEE
VEE
EVV
VVV

Chapter 4

Discussion

one shortcoming is time inefficiency. largely due to implementation. mclust has 16'000 lines of Fortran code, impossible in the scope of this thesis.

proof of concept?? definitely possible to do model selection using a general optimizer.

strong points: 'randomness' of clara/optim allows 'confidence intervalls' for selected model flexibility of approach: given an logLik fctn can do mixture fitting w/ arbitrary models

further study might include: other presumed component distributions, 'high' dimensions

Bibliography

Celeux, G. and G. Govaert (1995). Gaussian parsimonious clustering models. *Pattern Recognition 28*(5), 781 – 793.

Dempster, A. P., N. M. Laird, and D. B. Rubin (1977). Maximum likelihood from incomplete data via the em algorithm. *Journal of the Royal Statistical Society: Series B (Methodological) 39*(1), 1–22.

L, S., F. M, M. TB, and R. AE. (2016). mclust 5: Clustering, classification and density estimation using gaussian finite mixture models. *R J.* (8(1)), 289–317.

Marron, J. S. and M. P. Wand (1992). Exact mean integrated squared error. *The Annals of Statistics 20*(2), 712–736.

McLachlan, G. and D. Peel (2000). *Finite Mixture Models* (1 ed.). Wiley Series in Probability and Statistics. Wiley-Interscience.

Pearson, K. and O. M. F. E. Henrici (1896). Vii. mathematical contributions to the theory of evolution.&#x2014;iii. regression, heredity, and panmixia. *Philosophical Transactions of the Royal Society of London. Series A, Containing Papers of a Mathematical or Physical Character 187*, 253–318.

Appendix A

R Code

A.1 llnorMmix

Here llnorMmix, since it is the central piece of the package, and 2time.R as an example of a simulation script.

```
#### 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.[,
            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))
}
sllnorMmix <- function(x, obj, trafo=c("clr1", "logit")) {
    stopifnot(is.character(model <- obj$model))
    trafo <- match.arg(trafo)
    llnorMmix(nMm2par(obj, model=model),
              tx = t(x), k = obj$k,
              model=model, trafo=trafo)
}
## log-likelihood function relying on mvtnorm function
#
# par:   parameter vector as calculated by nMm2par
# x:     matrix of samples
# k:     number of cluster
# trafo: transformation of weights
# model: assumed model of the distribution
llmvtnorm <- function(par, x, k,
                      trafo=c("clr1", "logit"),
                      model=c("EII","VII","EEI","VEI","EVI",
                              "VVI","EEE","VEE","EVV","VVV")
              ) {
    stopifnot(is.matrix(x),
              length(k <- as.integer(k)) == 1, k >= 1)
    model <- match.arg(model)
    trafo <- match.arg(trafo)
    p <- ncol(x)
    nmm <- par2nMm(par, p, k, model=model, trafo=trafo)
    ## FIXME (speed!):  dmvnorm(*, sigma= S) will do a chol(S) for each component
    ## -----  *instead* we already have LDL' and  chol(S) = sqrt(D) L' !!
    ## another par2*() function should give L and D, or from that chol(Sagma), rather than S
    w <- nmm$w
    mu <- nmm$mu
    sig <- nmm$Sigma
    y <- 0
    for (i in 1:k) {
        y <- y + w[i]*mvtnorm::dmvnorm(x,mean=mu[,i],sigma=sig[,,i])
    }
    sum(log(y))
}
```

A.2 Example Simulation Script

here e.g. 2init.R and write some remarks on it.

```
## 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)
```

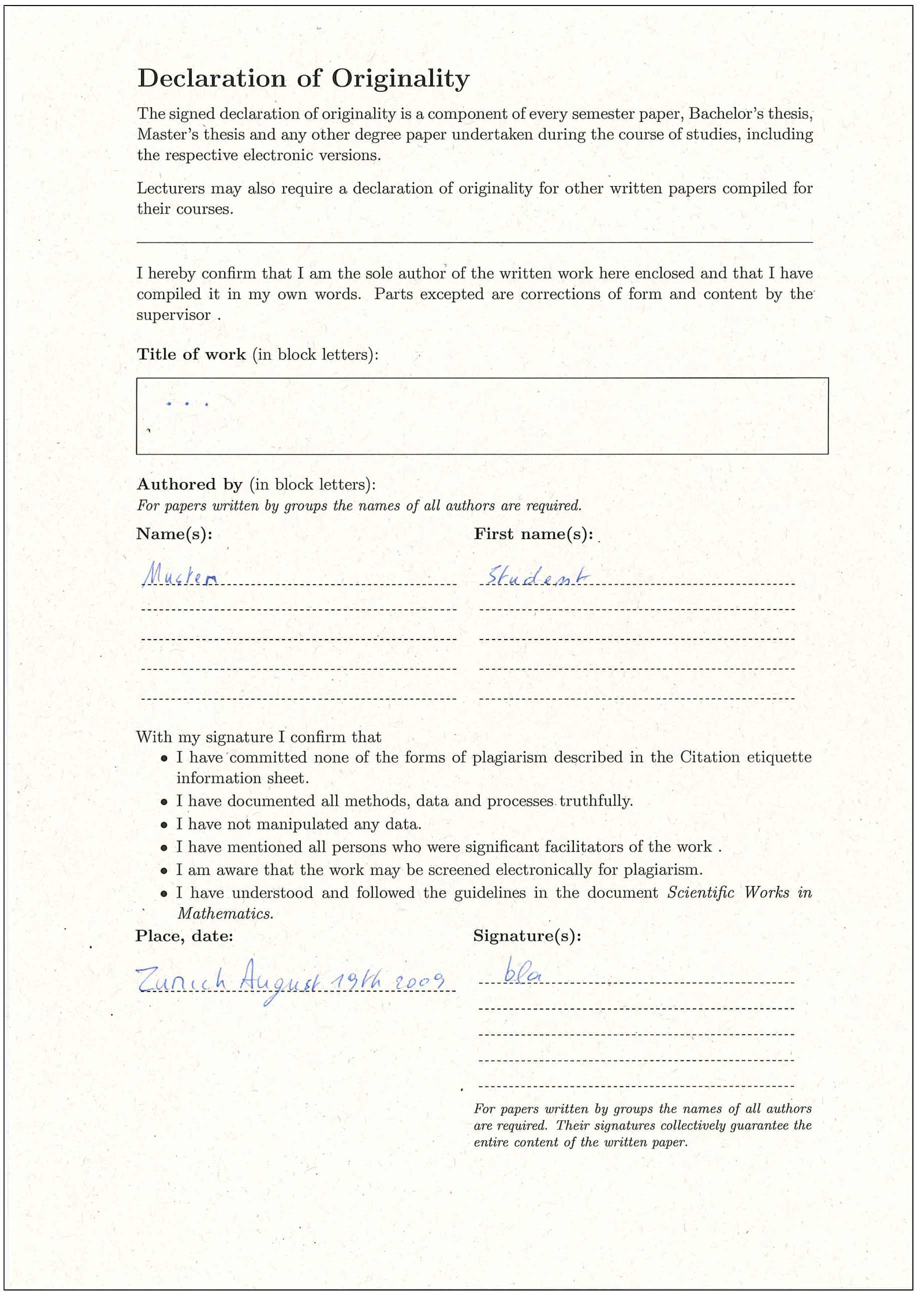
Appendix B

Further Plots

here further plots:

B.1 Ch3

dsfasdf



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