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# 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)

## Contents

<b>1</b>	<b>Introduction to normal mixture models</b>	<b>1</b>
1.1	Definitions . . . . .	1
1.2	choice of notation . . . . .	2
1.3	problems of EM . . . . .	5
<b>2</b>	<b>The <code>norMmix</code> Package</b>	<b>9</b>
2.1	concept of package . . . . .	9
2.2	finer details of <code>norMmix</code> package . . . . .	9
<b>3</b>	<b>Comparing Algorithms</b>	<b>11</b>
3.1	General Setup . . . . .	11
3.2	Findings . . . . .	11
<b>4</b>	<b>Discussion</b>	<b>13</b>
	<b>Bibliography</b>	<b>14</b>

**List of Figures**

1.1	200 EM steps . . . . .	7
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**List of Tables**

1.1 Table of Parameters . . . . .	4
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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 that to learn in depth about normal mixtures. We will here give a short overview of normal mixtures to fix notation and nomenclature.

Let  $\mu \in \mathbb{R}^p$ ,  $\Sigma \in \mathbb{R}^{p \times p}$  and  $\phi(-; \mu, \Sigma)$  be the normal distribution with mean  $\mu$  and covariance matrix  $\Sigma$ .

Normal mixture models are designed for situations where we assume that a given dataset originates from more than one population of explaining variables.

$\mathbf{Y}_1, \dots, \mathbf{Y}_n$

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

$$f(y_j) = \sum_{i=1}^K \pi_i \phi_i(y_j; \mu, \Sigma)$$

The  $\pi_i$  are called the component densities of the mixture.

explain in sketch EM algo

EM has desirable qualities like proven convergence, (give reference to Dempster 1977 paper)

explain idea to use parameter optimizer instead, EM has pathological insufficiencies, like 'getting stuck' for many iterations. We hope we need less iterations, and as consequence less time. 'special' idea: using Cholesky decomp.

## 1.2 choice of notation

describe difference in notation between celeux & govaert and our covariance matrix decomposition.

The classification of models in this paper relies heavily on the work of Celeux and Grovaert, 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 and ours.

explanation for the volume, shape and orientation descriptors

The basis of classification in Celeux & Grovaert is the decomposition of a symmetric matrix into an orthogonal and a diagonal component. A symmetric positive definite matrix  $\Sigma$  can be decomposed as follows

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

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

This decomposition has an appealing geometric interpretation, with  $\mathbf{D}$  as the *orientation* of the distribution,  $\mathbf{A}$  the *shape*, and  $\lambda$  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  $\Sigma$ , the  $\alpha \mathbf{L} \mathbf{D} \mathbf{L}^\top$  decomposition. This obviously raises some conflicts in notation.

Therefore we, from here on, when referring to the decomposition as described by cng, will use the following modification of notation:

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

These were chosen according to general conventions of linear algebra.  $\mathbf{Q}$  is usually chosen for orthonormal matrices;  $\mathbf{\Lambda}$  is often a choice for diagonal matrices eigen vectors and  $\alpha$  was somewhat arbitrarily chosen.

make clear that the models can not be translated one to one to ldlt model There is however an issue with the Cholesky decomposition. For 10 out of 14 cases as defined by Celeux & Grovaert, 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  $\Sigma$  we have decompositions:

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

Since in both cases the bracketing matrices  $\mathbf{Q}$  and  $\mathbf{L}$  have determinant 1 the determinant of  $\Sigma$  falls entirely on  $\alpha$ . Therefore  $\alpha$ , in these particular decompositions, is equal for both. Celeux & Grovaert vary  $\Sigma$  by either varying or holding fixed the volume ( $\alpha/\alpha_k$ ), shape ( $\mathbf{\Lambda}/\mathbf{\Lambda}_k$ ) and orientation ( $\mathbf{Q}/\mathbf{Q}_k$ ). 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  $\mathbf{LDL}^\top$  decomposition the lower diagonal matrix  $\mathbf{L}$  holds some of the shape of the matrix, which in the Eigen decomposition is in the  $\mathbf{\Lambda}$  matrix. In fact,  $\mathbf{L}$  is orthogonal if and only if  $\mathbf{L} = \text{Id}_{n \times n}$ . Therefore we can only decompose matrices where either both or neither shape and orientation vary. See table 1.1.

make nice table(maybe sideways to account for parameter list)

Model	$\Sigma_k$ C&G	volume	shape	orientation	parameters	count	$LDL^\top$	parameters	count
EII	$\alpha I$	equal	equal	-	$\alpha$	1	same as C&G		
VII	$\alpha_k I$	variable	equal	-	$\alpha_k$	$K$			
E EI	$\alpha \Lambda$	equal	equal	coordinate axes	$\alpha, \lambda_i$	$1 + p$			
V EI	$\alpha_k \Lambda$	variable	equal	coordinate axes	$\alpha_k, \lambda_i$	$K + p$			
E VI	$\alpha \Lambda_k$	equal	variable	coordinate axes	$\alpha, \lambda_{i,k}$	$1 + pK$			
V VI	$\alpha_k \Lambda_k$	variable	variable	coordinate axes	$\alpha_k, \lambda_{i,k}$	$K + pK$			
EEE	$\alpha Q \Lambda Q^\top$	equal	equal	equal	$\alpha, \lambda_i, q_{i,j}$	$1 + p + p^2$	$\alpha LDL^\top$		
E VE	$\alpha Q \Lambda_k Q^\top$	equal	variable	equal	$\alpha, \lambda_{i,k}, q_{i,j}$	$1 + pK + p^2$	doesn't exist		
V EE	$\alpha_k Q \Lambda Q^\top$	variable	equal	equal	$\alpha_k, \lambda_i, q_{i,j}$	$K + p + p^2$	$\alpha_k LDL^\top$		
V VE	$\alpha_k Q \Lambda_k Q^\top$	variable	variable	equal	$\alpha_k, \lambda_{i,k}, q_{i,j}$	$K + pK + p^2$			
E EV	$\alpha Q_k \Lambda Q_k^\top$	equal	equal	variable	$\alpha, \lambda_i, q_{i,j,k}$	$1 + p + Kp^2$			
V EV	$\alpha_k Q_k \Lambda Q_k^\top$	variable	equal	variable	$\alpha_k, \lambda_i, q_{i,j,k}$	$K + p + Kp^2$			
E VV	$\alpha Q_k \Lambda_k Q_k^\top$	equal	variable	variable	$\alpha, \lambda_i, q_{i,j,k}$	$1 + pK + Kp^2$	$\alpha L_k D_k L_k^\top$	$\lambda, d_{i,k}, l_{i,j,k} \quad j > i$	$1 + pK + K \frac{p(p-1)}{2}$
V VV	$\alpha_k Q_k \Lambda_k Q_k^\top$	variable	variable	variable	$\alpha_k, \lambda_i, q_{i,j,k}$	$K + pK + Kp^2$	$\alpha_k L_k D_k L_k^\top$	$\lambda_k, d_{i,k}, l_{i,j,k} \quad j > i$	$K + pK + K \frac{p(p-1)}{2}$

## 1.3 problems of EM

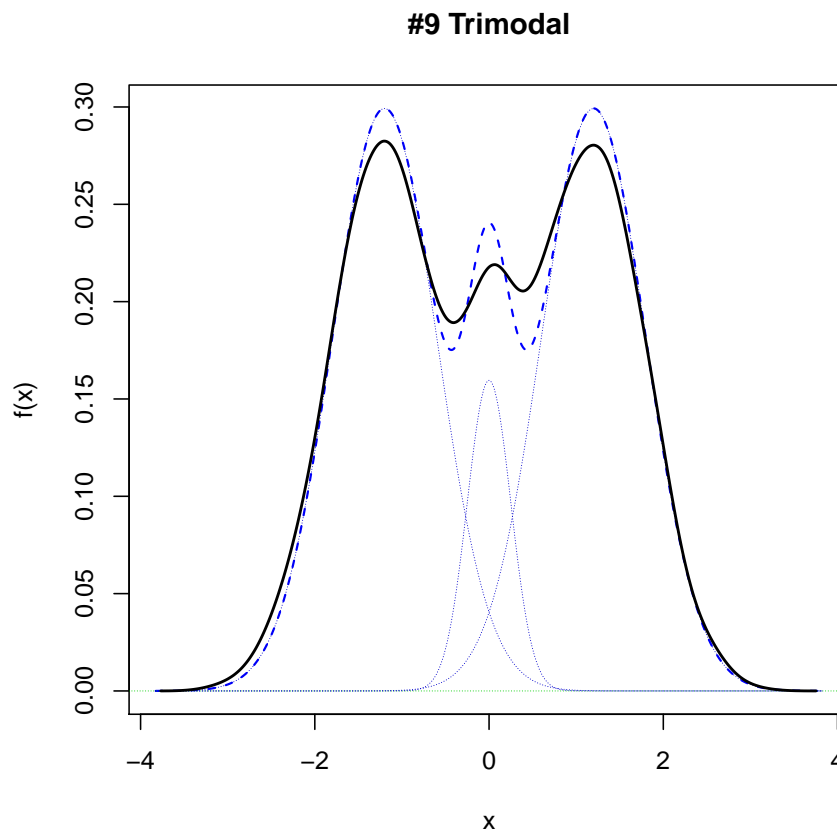
the EM-algorithm has stalling problems especially close to a local optimum. In their seminal work, [Dempster, Laird, and Rubin \(1977\)](#), have proven that the EM-algorithm converges under mild regularity conditions. However, convergence does not guarantee fast convergence. In fact, a lot of the work, 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.

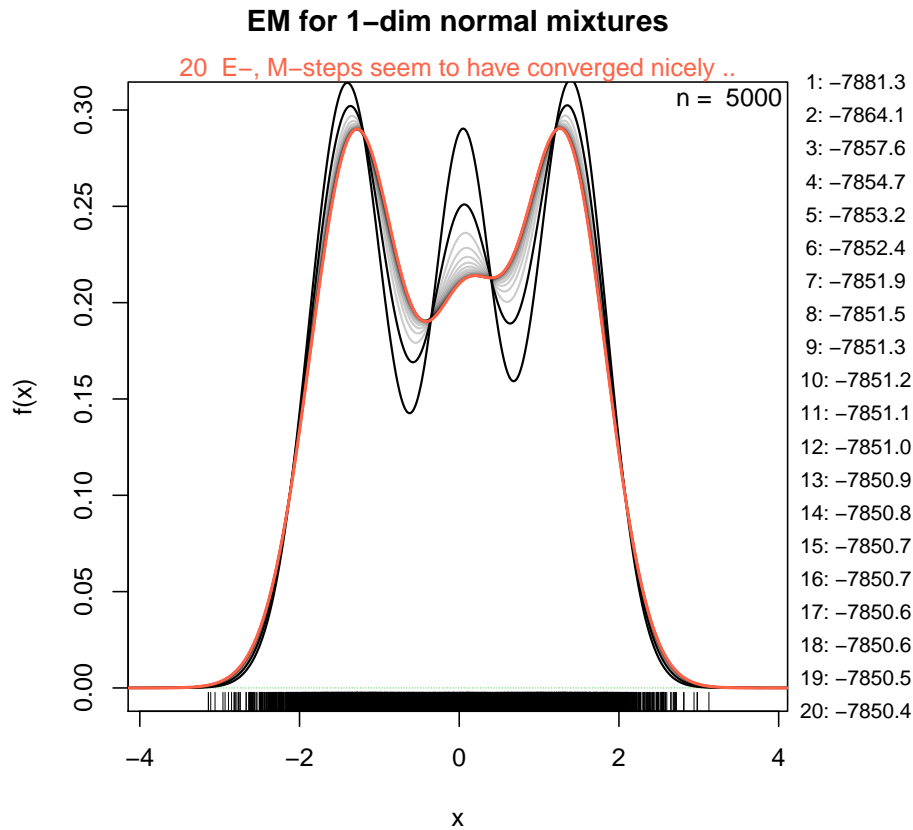
```
> library("nor1mix")
> MW.nm9 ## Trimodal mixture

'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
```

show an example using `nor1mix`



75 then an illustration of MW examples of pathological cases



76

77 yay, got figure to print. solution was use of fig=TRUE, instead of various mutations like  
78 figure=true.

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

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

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

84 should include animations?? like mix\_est\_1d.R line 249+24 lines

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

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

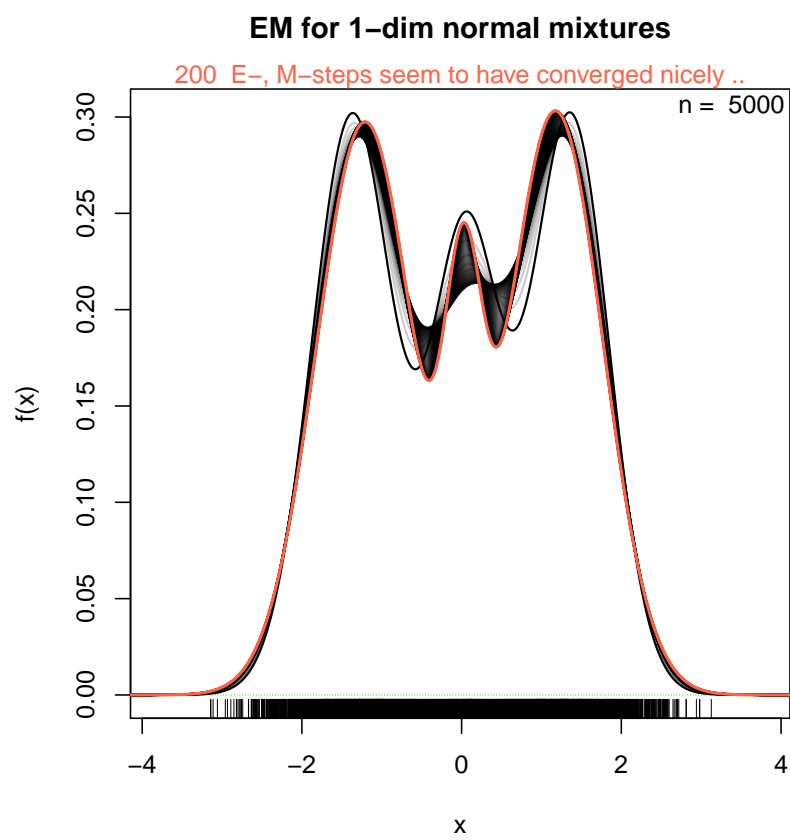


Figure 1.1: 200 EM steps



## Chapter 2

# The norMmix Package

explain, that this package was written purposefully for this paper.

The norMmix package is constructed around the `norMmix` object, that codifies a `normal` Multivariate mixture model, and the `llnorMmix()` function.

quickly list contents of `norMmix` object

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`.

## 2.1 concept of package

(this Section maybe one chapter earlier)

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.

So caomparison of algos done through throwing difficult mixtures and non-mixtures at it and hoping that `norMmix` finds better solutions than EM. So the criteria for "better fit" are 1. better log-likelihood 2. correct model, where EM fails.

## 112 2.2 finer details of norMmix package



## Chapter 3

# Comparing Algorithms

### 3.1 General Setup

display abilities of norMmix on its own. can find correct models

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.

maybe apply to MW[0-9] objects?

not sure

as in Raftery2002, Benaglia2009, Roeder 1997, maybe compare to MISE of various forms. They all did and see it as adequate method for comparing accuracy of algorithm.

also wanted is accuracy of model selection. generate from model and then compare fitted to original. either by  $\text{acc-model} = \text{fit-model}$  and  $\text{acc-k} = \text{fit-k}$  or  $\text{acc-ll} - \text{fit-ll}$ .

### 3.2 Findings



<sup>127</sup> **Chapter 4**

<sup>128</sup> **Discussion**



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