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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. MLE doesn't have this particular error, but is computationally costly. The Cholesky decomposition cuts down the necessary parameters almost in half....

methods(not done)

results(not done)

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# Chapter 1

## Introduction to normal mixture models

here intro to normal mixtures

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 model 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 1.0.0.1.** 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

$$f(y_j) = \sum_{i=1}^K \pi_i \phi_i(y_i)$$

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

explain in sketch EM algo

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.

### 1.1 choice of notation

describe difference in notation between ceuleux & 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 CnG 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  $\mathbf{LDL}^\top$  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 eigen vectors and  $\alpha$  was somewhat arbitrarily chosen.

make clear that the models can not be translated one to one to ldlt model

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



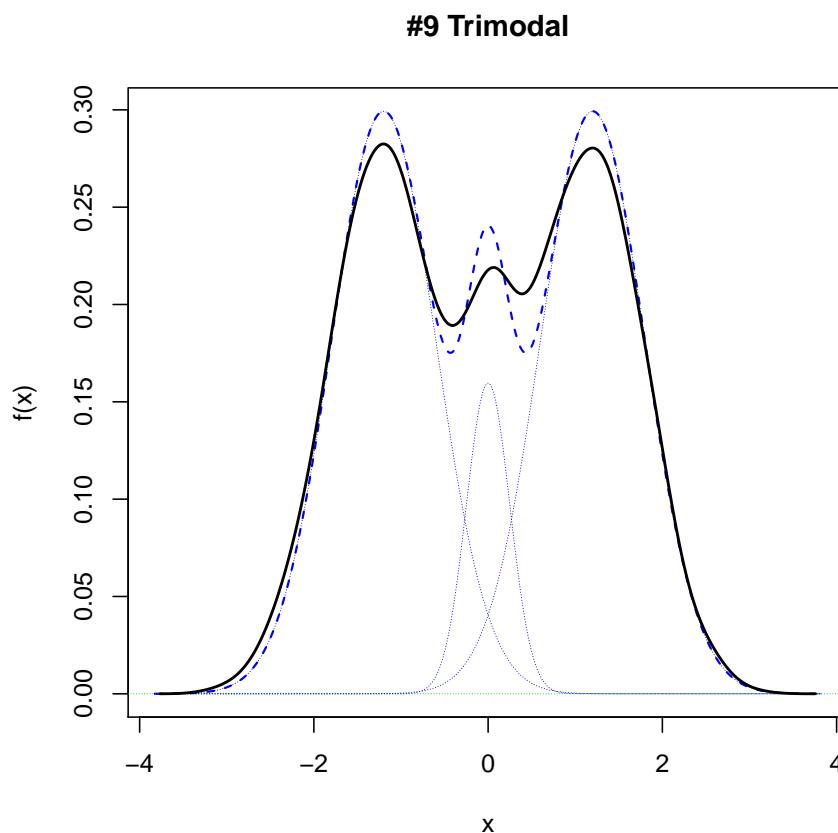
Model	$\Sigma_k$ C&G	volume	shape	orientation	parameters	count	$LDL^\top$ same as C&G	parameters	count
EII	$\alpha I$	equal	equal	-	$\alpha$	1	same as C&G		
VII	$\alpha_k I$	variable	equal	-	$\alpha_k$	$K$			
E EI	$\alpha \Lambda$	equal	equal	coordinate axes	$\alpha, \lambda_i$	$1 + p$			
VEI	$\alpha_k \Lambda$	variable	equal	coordinate axes	$\alpha_k, \lambda_i$	$K + p$			
EVI	$\alpha \Lambda_k$	equal	variable	coordinate axes	$\alpha, \lambda_{i,k}$	$1 + pK$			
VVI	$\alpha_k \Lambda_k$	variable	variable	coordinate axes	$\alpha_k, \lambda_{i,k}$	$K + pK$			
EEE	$\alpha Q \Lambda Q^\top$	equal	equal	equal	$\alpha, \lambda_i, q_{i,j}$	$1 + p + p^2$	don't exist		
EVE	$\alpha Q \Lambda_k Q^\top$	equal	variable	equal	$\alpha, \lambda_{i,k}, q_{i,j}$	$1 + pK + p^2$			
VEE	$\alpha_k Q \Lambda Q^\top$	variable	equal	equal	$\alpha_k, \lambda_i, q_{i,j}$	$K + p + p^2$			
VVE	$\alpha_k Q \Lambda_k Q^\top$	variable	variable	equal	$\alpha_k, \lambda_{i,k}, q_{i,j}$	$K + pK + p^2$			
EEV	$\alpha Q_k \Lambda Q_k^\top$	equal	equal	variable	$\alpha, \lambda_i, q_{i,j,k}$	$1 + p + Kp^2$			
VEV	$\alpha_k Q_k \Lambda Q_k^\top$	variable	equal	variable	$\alpha_k, \lambda_i, q_{i,j,k}$	$K + p + Kp^2$			
EVV	$\alpha Q_k \Lambda_k Q_k^\top$	equal	variable	variable	$\alpha, \lambda_i, q_{i,j,k}$	$1 + pK + Kp^2$	$\alpha L_k D_k L_k^\top$	$\lambda, d_{i,k}, l_{i,j,k} \quad j > i$	$1 + pK + K \frac{p(p-1)}{2}$
VVV	$\alpha_k Q_k \Lambda_k Q_k^\top$	variable	variable	variable	$\alpha_k, \lambda_i, q_{i,j,k}$	$K + pK + Kp^2$	$\alpha_k L_k D_k L_k^\top$	$\lambda_k, d_{i,k}, l_{i,j,k} \quad j > i$	$K + pK + K \frac{p(p-1)}{2}$

## 1.2 problems of EM

the EM algo has stalling problems especially close to a local optimum

show an example using `nor1mix`

```
> library("nor1mix")
> plot(MW.nm9, lty=2, col = "blue", p.norm=FALSE, p.comp=TRUE)
> set.seed(2019)
> x9 <- rnorMix(5000, MW.nm9)
> lines(density(x9), lwd=1.8) # "clearly" 3 components
```



then an illustration of MW examples of pathological cases

```
> p.EMsteps <- function(nSteps, x, nmObj,
+                         main = "EM for 1-dim normal mixtures",
+                         sleep = nSteps <= 40, sec.sleep = 0.2, col2 = "tomato",
+                         showLik = nSteps <= 80,
+                         plotIni = FALSE, # plot the initial param. ?
+                         doNote = TRUE)
+ {
+   ## Purpose: show progress of EM - steps -- only few steps
+   ## -----
+   ## Author: Martin Maechler, Date: 26 Nov 2009
+   stopifnot(is.norMix(nmObj), is.numeric(x), nSteps >= 1)
```

```

+   nm. <- nmObj
+   ll.em <- numeric(nSteps)
+   for(k in 1:nSteps) {
+       z. <- estep.nm(x9, obj = nm.)
+       nm. <- do.call(norMix, c(mstep.nm(x=x9, z=z.), name=""))
+       if(k == 1) { ## only after the first E+M - step
+           op <- par(mar = c(0,0,0, 2.) + par("mar")); on.exit(par(op))
+           plot(nm., p.norm=FALSE, main = main)
+           if(plotIni) lines(nmObj, p.norm=FALSE)
+           rug(x) ; mtext(paste("n = ", length(x)),
+                           line = -1., adj=.99)
+           nm2 <- nm. ## save the 2nd
+           if(showLik) {
+               yVal <- approxfun(x=c(nSteps,1), y=par("usr")[3:4])
+               xV <- { u <- par("usr")[1:2]; u[2] + .01*(u[2]-u[1]) }
+           }
+       } else lines(nm., p.norm=FALSE, col = rgb(0,0,0, 0.2))
+       print(ll <- llnorMix(nM2par(nm.), x=x9))
+       ll.em[k] <- ll
+       if(showLik)
+           text(xV, yVal(k), sprintf("%3d: %5.1f", k, ll),
+                cex = 0.8, adj = 0, xpd = NA)
+       if(sleep) Sys.sleep(sec.sleep)
+   }
+   ## plot the last one more visibly
+   lines(nm., p.norm=FALSE, col = col2, lwd = 2)
+   if(doNote)
+       mtext(paste(nSteps, " E-, M-steps seem to have converged nicely .."),
+             col=col2)
+   ## return final normal mixture {but invisibly}:
+   invisible(list(nm = nm., logLik = ll.em))
+ }
>

```

here figure maybe

```
> clp0 <- cluster::clara(x9, k=3, samples=1000, medoids.x = FALSE, rngR=TRUE)
> nm1 <- clus2norMix(clp0$clustering, x9) ## <-- M-step from cluster:
> p.EMsteps(20, x9, nm1, plotIni=TRUE)# 20 steps: final logLik ("ll"): -7779.5
[1] -7881.319
[1] -7864.054
[1] -7857.641
[1] -7854.718
[1] -7853.212
[1] -7852.369
[1] -7851.864
[1] -7851.543
[1] -7851.327
[1] -7851.173
[1] -7851.055
[1] -7850.961
[1] -7850.88
[1] -7850.808
[1] -7850.742
[1] -7850.679
[1] -7850.617
[1] -7850.557
[1] -7850.498
[1] -7850.439
>
```

## Chapter 2

# placeholder

placeholder



# Bibliography

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- Hampel, F. R. (1985). The breakdown points of the mean combined with some rejection rules. *Technometrics* 27(2), 95–107.
- Stahel, W. and S. Weisberg (1991). *Directions in Robust Statistics and Diagnostics*, 2 vol. N. Y.: Springer-Verlag.





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