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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. 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 overwiev of normal mixtures to fix notation and nomenclature.

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

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

$\boldsymbol{Y}_1, \ldots, \boldsymbol{Y}_n$
Definition 1.0.0.1. *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*

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

The π_i are called the component densities of the mixture.

explain in scetch 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 concequence 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 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 arbytrary and diagonal matrices respectively. Furthermore, we intend to apply a variant of the Cholesky decomposition to Σ, the $\boldsymbol{L}\boldsymbol{D}\boldsymbol{L}^\top$ decomposition. This obviously raises some conflicts in notation.

Therefore we, from here on, when reffering to the decomposition as described by cng, 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 eigen vectors and α 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)

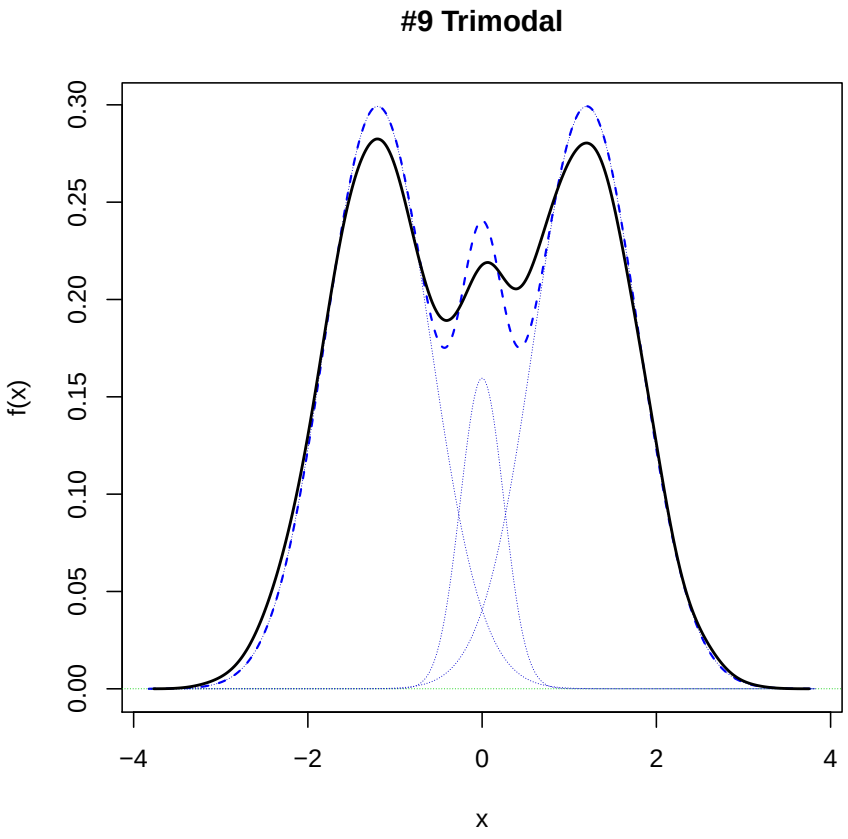
Model	$\boldsymbol{\Sigma}_k$ C&G	volume	shape	orientation	parameters	count	$\boldsymbol{LDL}^\top$	parameters	count
EII	$\alpha\boldsymbol{I}$	equal	equal	-	α	1	same as C&G		
VII	$\alpha_k\boldsymbol{I}$	variable	equal	-	α_k	K			
EEI	$\alpha\boldsymbol{\Lambda}$	equal	equal	coordinate axes	α, λ_i	$1+p$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

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

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Bibliography

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