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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)

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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 overwiev 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 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 1.1.0.1. *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*

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

The π_i are called the component densities of the mixture.

explain in scetch 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 concequence less time. 'special' idea: using cholesky decomp.

1.2 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 Celeux & Grovaert 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

$$\Sigma = \lambda \boldsymbol{DAD}^\top$$

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 $\boldsymbol{LDL}^\top$ 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:

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

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

There is howerver 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 Σ we have decompositions:

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

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.

So, for varying Σ we could vary $\alpha, \boldsymbol{Q}$ and $\boldsymbol{\Lambda}$ either holding them constant or varying them. giving 8 cases, plus 6 diagonal cases = 14. However we cannot do that in the case of a

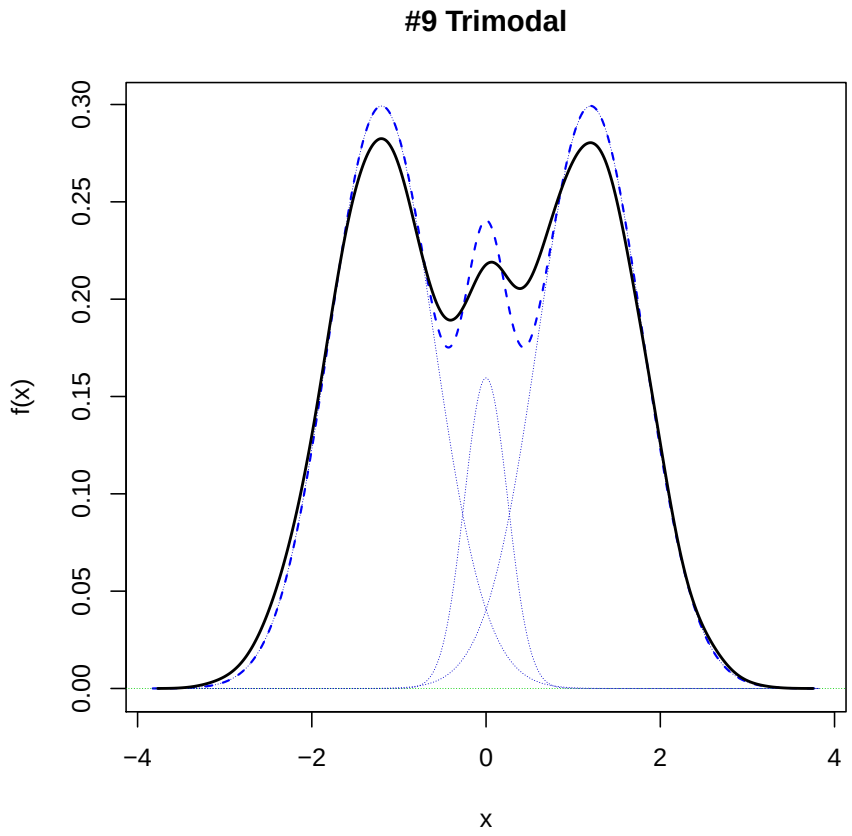
make nice table(maybe sideways to account for parameter list)

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	$\alpha, \lambda_i, q_{i,j}$	$1+p+p^2$	$\alpha\boldsymbol{LDL}^\top$		
EVE	$\alpha\boldsymbol{Q}\boldsymbol{\Lambda}_k\boldsymbol{Q}^\top$	equal	variable	equal	$\alpha, \lambda_{i,k}, q_{i,j}$	$1+pK+p^2$	doesn't exist		
VEE	$\alpha_k\boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^\top$	variable	equal	equal	$\alpha_k, \lambda_i, q_{i,j}$	$K+p+p^2$	$\alpha_k\boldsymbol{LDL}^\top$		
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	$\alpha_k, \lambda_i, q_{i,j,k}$	$K+pK+Kp^2$	$\alpha_k\boldsymbol{L}_k\boldsymbol{D}_k\boldsymbol{L}_k^\top$	$\lambda_k, d_{i,k}, l_{i,j,k}\ j>i$	$K+pK+K\frac{p(p-1)}{2}$

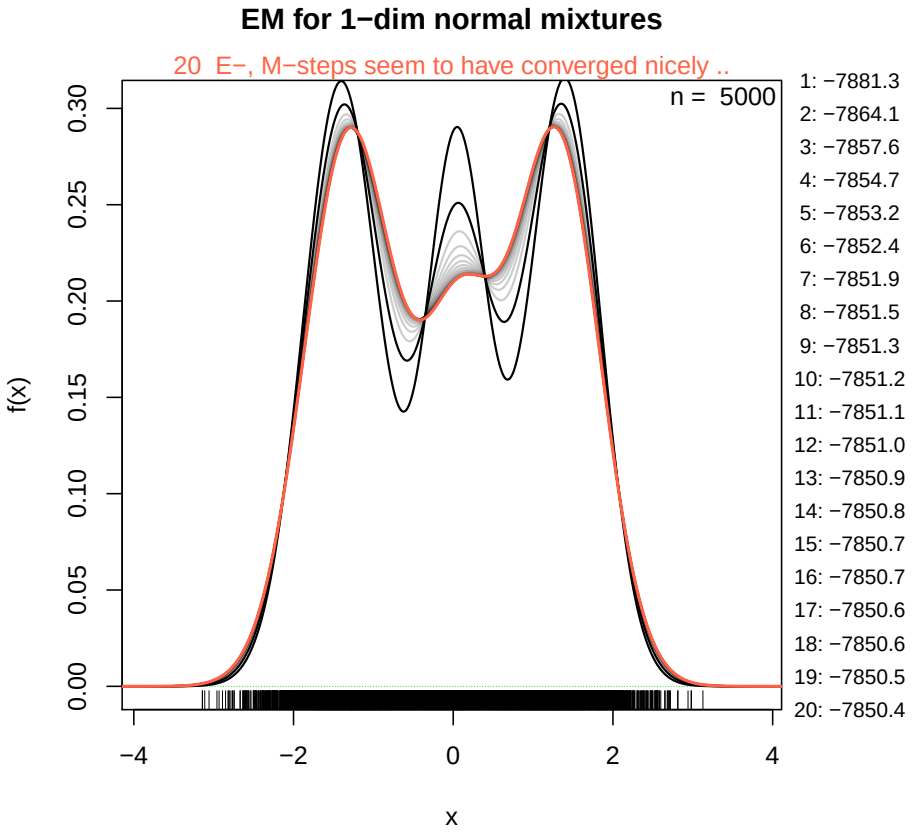
1.3 problems of EM

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

show an example using nor1mix



then an illustration of MW examples of pathological cases



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

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.

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.

should include animations?? like mix_est_1d.R line 249+24 lines

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

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

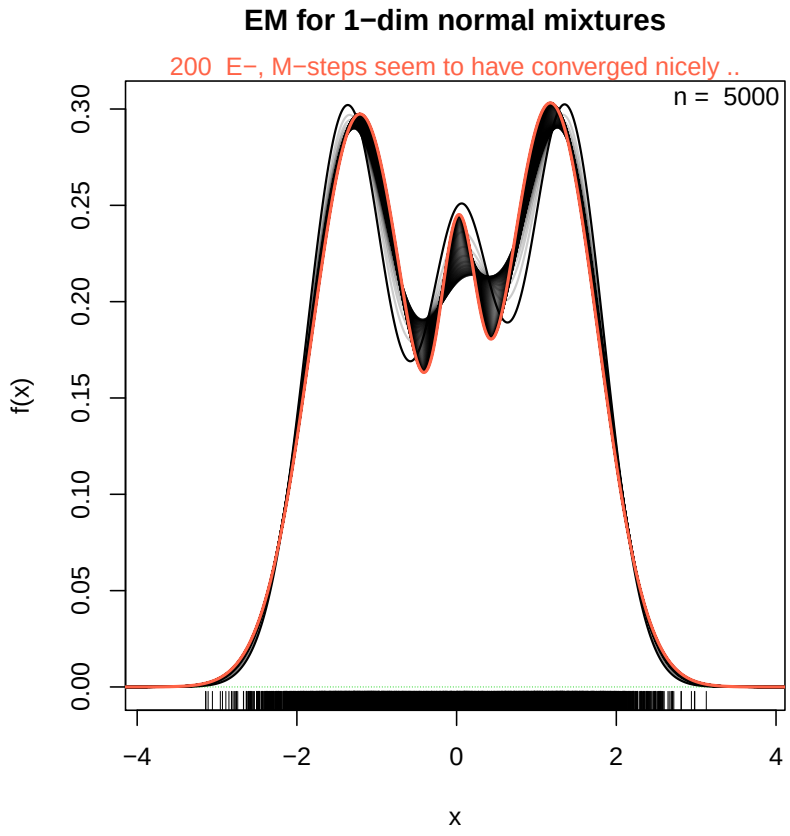


Figure 1.1: 200 EM steps

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 `nor`mal `M`ultivariate `mix`ture 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.

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.

2.2 finer details of `norMmix` package

Chapter 3

Comparing Algotithms

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

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 acc-model==fit-model and acc-k==fit-k or acc-ll - fit-ll.

Chapter 4

Conclusions

testing citations McLachlan and Peel (2000) Benaglia, Chauveau, and Hunter (2009) Roeder and Wasserman (1997)

Bibliography

Benaglia, T., D. Chauveau, and D. R. Hunter (2009). An em-like algorithm for semi- and nonparametric estimation in multivariate mixtures. *Journal of Computational and Graphical Statistics 18*(2), 505–526.

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

Roeder, K. and L. Wasserman (1997). Practical bayesian density estimation using mixtures of normals. *Journal of the American Statistical Association 92*(439), 894–902.

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