# FEMCA: A flexible clustering algorithm for noisy data

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## **Motivation**

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Group data points into clusters to understand the structure of the data.





- similar points to be in the same cluster,
- really different points to be in different clusters, and
- well separated clusters.

#### Image segmentation





#### Functions/Time-series



Bouveyron et al. (2007)

## Some challenges for clustering

#### Heterogeneous datasets

- Datasets with outliers/noise.
- Heavy tails distributions.
- Different scales/distributions.
- Continuous and discrete data.

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- Needs of parallelization / batch versions.

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#### High dimensional context $(m \gg)$

- ill-posed problems.
- Data on manifolds.
- $\Rightarrow$  Regularization/penalization, dimensionality reduction

Focus here on:

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We address "not too high dimensions" regimes (say 30-100).

**Reference paper:** [Roizman et al., 2023] Roizman, V., Jonckheere, M., & Pascal, F. (2023). A flexible EM-like clustering algorithm for noisy data. *IEEE Transactions on Pattern Analysis and Machine Intelligence*.

#### **1** SOA: Classical algorithms

**2** Robustness proposals

#### **3** A novel flexible clustering algorithm: FEMCA

- 1 Model, derivation, and properties
- 2 Experimental results

#### Applications to PolSAR images segmentation

**5** Conclusions and perspectives

## State of the art

#### **K**-means

Given  $\{\mathbf{x}_i\}_{i=1}^n$ , find  $\hat{\mathbf{C}} = \{C_1, ..., C_K\}$  with  $\boldsymbol{\mu}_k = \frac{1}{\#(C_k)} \sum_{\mathbf{x} \in C_k} \mathbf{x}$  such that

$$\hat{\mathbf{C}} = \underset{\mathbf{C} = \{C_1, \dots, C_K\}}{\operatorname{argmin}} \sum_{k=1}^K \sum_{\mathbf{x} \in C_k} \|\mathbf{x} - \boldsymbol{\mu}_k\|_2^2$$

Plain optimization problem.

Simple idea. 🗸

Very fast. 🗸

Works well only when: X

- round-shaped clusters,
- with similar variance, and
- well-separated.



#### Gaussian Mixture Model (GMM)

We model data as a mixture of Gaussian distributions  $\mathcal{N}(\mu_k, \mathbf{M}_k)$ :

$$f(\mathbf{x}) = \sum_{k=1}^{K} \pi_k f_k(\mathbf{x}),$$

with  $\pi_k$  the proportion of cluster k and  $f_k$  the normal p.d.f.



## Expectation-Maximization (EM) algorithm

Statistical algorithm to estimate parameters based on a likelihood.

In the GMM case, we would need the labels of the data points to estimate the parameters. Labels  $\rightarrow$  Latent variables

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#### E-STEP

Computation of the membership a posteriori probabilities

$$p_{ik} = P(Z_i = k | \mathbf{X}_i = \mathbf{x}_i) = \frac{\pi_k f_k(\mathbf{x}_i)}{\sum\limits_{j=1}^{K} \pi_j f_j(\mathbf{x}_i)}$$

with  $f_k$  the Gaussian p.d.f.

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#### E-STEP

Computation of the membership a posteriori probabilities

#### **M-STEP**

Estimation of the parameters

$$p_{ik} = P(Z_i = k | \mathbf{X}_i = \mathbf{x}_i) = \frac{\pi_k f_k(\mathbf{x}_i)}{\sum\limits_{j=1}^{K} \pi_j f_j(\mathbf{x}_i)}$$

with  $f_k$  the Gaussian p.d.f.

$$\widehat{\pi}_{k} = \frac{1}{n} \sum_{i=1}^{n} p_{ik}$$
$$\widehat{\mu}_{k} = \frac{1}{n\widehat{\pi}_{k}} \sum_{i=1}^{n} p_{ik} \mathbf{x}_{i}$$

$$\widehat{\mathsf{M}}_{k} = \frac{1}{n\widehat{\pi}_{k}}\sum_{i=1}^{n}p_{ik}(\mathsf{x}_{i}-\widehat{\mu}_{k})(\mathsf{x}_{i}-\widehat{\mu}_{k})^{\mathsf{T}}$$

## What happens to GMM when the data has some noise or non Gaussian data?

The GMM has problems to cluster and estimate parameters for data with noise, different distribution shapes and outliers.

Result with data contaminated:



## What happens to GMM when the data has some noise or is non Gaussian?

#### Why?

- The estimators are not robust.
- Mismatch between the model and the data.
- No outlier rejection.

There are mainly two directions to **robustify clustering methods** in the literature:

- model generalizations
  - Extra uniform cluster [Banfield and Raftery, 1993]
  - Model low density areas (RIMLE and OTRIMLE) [Coretto and Hennig, 2016]
  - Mixture of *t*-distributions (t-EM) [Peel and McLachlan, 2000]

models that introduce classical robust techniques in the estimation

- Trimming methods (TCLUST) [García-Escudero et al., 2008]
- k-tau [Gonzalez et al., 2019] and Spatial-EM [Yu et al., 2015]

Some **drawbacks** of the state of the art robust clustering methods:

- No closed equations on the M-step, reliance on non-linear optimizers (t-EM).
- Extra parameters difficult to be tuned (RIMLE, TCLUST).
   e.g., if we misspecify the proportion of noise in the TCLUST algorithm [Gonzalez et al., 2019].
- Models are too specific.

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- Models are too specific.

#### Our goal:

- flexibility to very general models
- no extra parameters

# FEMCA: Model, derivation and properties

We consider  $\mathbf{x}_1, \ldots, \mathbf{x}_n$  independent vectors.

These vectors belong to some clusters  $C_1, \ldots, C_K$ .

 $x_1, \ldots, x_n$  ARE NOT i.i.d. !

#### **Cluster characterization**

 $\mathbf{x}_i$  and  $\mathbf{x}_j$  belong to  $C_k$  if they are drawn from a distribution with the same features

 $\mu_k$  and  $\Sigma_k$ 

The **location** and the **scatter matrix** are the **features** that characterize the clusters and not a particular distribution as in GMM or t-EM.

FEMCA is based on a model where the  $\mathbf{x}_1,\ldots,\mathbf{x}_n$  independent vectors are characterized by

#### **Stochastic representation**

$$\mathbf{x}_i \in C_k \Rightarrow \mathbf{x}_i \stackrel{d}{=} \boldsymbol{\mu}_k + \sqrt{\mathcal{Q}_{ik}} \sqrt{\tau_{ik}} \mathbf{A}_k \mathbf{u}_i$$

- $\mu_k$  is the mean of the cluster k.
- $Q_{ik}$  is an independent positive random variable.
- $\tau_{ik}$  are scale (nuisance) parameters that increase the flexibility of the model.
- $\mathbf{A}_k$  is such that  $\mathbf{A}_k^T \mathbf{A}_k = \boldsymbol{\Sigma}_k$  (the scatter matrix of the cluster k).
- **u**<sub>i</sub> is a uniform vector on the unit hyper-sphere.
- $\cdot_{ik}$  represents the possible dependence on k and i.

## **Elliptical Symmetric family**

The stochastic characterization [Cambanis et al., 1981] represents vectors of the Elliptical Symmetric family [Kelker, 1970].

The density can be written as

$$f_{\mathbf{x}_i}(\mathbf{x}) = A_m |\tau_{ik} \boldsymbol{\Sigma}_k|^{-1/2} \mathbf{g}_{ik} \left( \tau_{ik}^{-1} (\mathbf{x} - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1} (\mathbf{x} - \boldsymbol{\mu}_k) \right)$$

for some function  $\mathbf{g}_{ik}$  called the **density generator**. We denote it as  $\mathbf{x} \sim \mathsf{ES}(\boldsymbol{\mu}_k, \tau_{ik} \boldsymbol{\Sigma}_k, \mathbf{g}_{ik}).$ 

#### **Distributions caracterization**

One-to-one relation between  $\mathbf{g}_{ik}$  and  $\mathcal{Q}_{ik}$ 

 $\Rightarrow$  the **shape** of the distributions

This family includes **Gaussian**, t-distribution, Generalized Gaussian distribution. Heavier and lighter (than Gaussian) tails.

We consider different scenarios based on the nature of the **density gen**erator functions:

 $g_{ik} = \begin{cases} g_i, & \text{each point might come from } \neq \text{ shaped dist.} \\ \text{BUT shapes do not depend on the cluster} \\ g_i, & \text{the density generator function is} \\ \text{always the same (e.g., Gaussian case)} \\ g_k, & \text{cluster dependent shapes} \\ \text{extra parameters have to be computed (e.g., t-EM)} \end{cases}$ 

#### Parameter space

Given  $\{\mathbf{x}_i\}_{i=1}^n \in \mathbb{R}^m$  we have to estimate the usual parameters

$$\boldsymbol{\varTheta} = \left\{ \left( \pi_k, \boldsymbol{\mu}_k, \boldsymbol{\varSigma}_k \right) \right\}_{k=1,..,K}$$

AND we now have a lot of (nuisance) parameters au

$$\widetilde{\boldsymbol{\Theta}} = \{\tau_{ik}\}_{\substack{k=1,..,K\\i=1,..,n}}$$

#### MLE

We derive the two-step (E-M) algorithm based on the likelihood of the model (using the trick of [Ollila and Tyler, 2012]).

#### Proposition

Assume  $g_{ik} = g_i$ , then the membership probabilities MLE are

$$\widehat{p}_{ik} = \frac{\widehat{\pi}_k \left( (\mathbf{x}_i - \widehat{\mu}_k)^T \widehat{\boldsymbol{\Sigma}}_k^{-1} (\mathbf{x}_i - \widehat{\mu}_k) \right)^{-m/2} |\widehat{\boldsymbol{\Sigma}}_k|^{-1/2}}{\sum_{j=1}^K \widehat{\pi}_j \left( (\mathbf{x}_i - \widehat{\mu}_j)^T \widehat{\boldsymbol{\Sigma}}_j^{-1} (\mathbf{x}_i - \widehat{\mu}_j) \right)^{-m/2} |\widehat{\boldsymbol{\Sigma}}_j|^{-1/2}}$$

**Insensitivity:** the expression of the membership **does not** depend on the particular density  $g_i$  that generates each data point, neither on the  $\tau_{ik}$ 

Proof details: see [Roizman et al., 2023]

#### Proposition (Location and scatter matrix estimators)

We almost obtain Tyler's estimators.

$$\widehat{\boldsymbol{\mu}}_{k} = \frac{\sum_{i=1}^{n} \frac{\widehat{p}_{ik} \mathbf{x}_{i}}{(\mathbf{x}_{i} - \widehat{\boldsymbol{\mu}}_{k})^{T} \widehat{\boldsymbol{\Sigma}}_{k}^{-1} (\mathbf{x}_{i} - \widehat{\boldsymbol{\mu}}_{k})}}{\sum_{i=1}^{n} \frac{\widehat{p}_{ik}}{(\mathbf{x}_{i} - \widehat{\boldsymbol{\mu}}_{k})^{T} \widehat{\boldsymbol{\Sigma}}_{k}^{-1} (\mathbf{x}_{i} - \widehat{\boldsymbol{\mu}}_{k})}}$$

$$\widehat{\boldsymbol{\Sigma}}_{k} = m \sum_{i=1}^{n} \frac{w_{ik} (\mathbf{x}_{i} - \widehat{\boldsymbol{\mu}}_{k}) (\mathbf{x}_{i} - \widehat{\boldsymbol{\mu}}_{k})^{T}}{(\mathbf{x}_{i} - \widehat{\boldsymbol{\mu}}_{k})^{T} \widehat{\boldsymbol{\Sigma}}_{k}^{-1} (\mathbf{x}_{i} - \widehat{\boldsymbol{\mu}}_{k})}, \quad \text{with} \quad w_{ik} = \hat{p}_{ik} / \sum_{i} \hat{p}_{ik}$$

#### Furthermore,

Proposition ( $\tau_{ik}$  estimator)  $\hat{\tau}_{ik} = \frac{(\mathbf{x}_i - \hat{\mu}_k)^T \hat{\boldsymbol{\Sigma}}_k^{-1} (\mathbf{x}_i - \hat{\mu}_k)}{a_{ik}},$ where  $a_{ik}$  depends only on  $g_{ik}$  $a_{ik} = \arg \sup_t \{t^{m/2} g_{i,k}(t)\}$ 

*e.g.*, for the Gaussian case  $a_{ik} = m$ .

 $\widehat{\mu}_k$  and  $\widehat{\varSigma}_k$  are like usual sample estimators with small weights for outlying points

$$\frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_{i} \Longrightarrow \frac{1}{n}\sum_{i=1}^{n}w_{i}\mathbf{x}_{i}$$

$$\frac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_{i}-\widehat{\mu})(\mathbf{x}_{i}-\widehat{\mu})^{T} \Longrightarrow \frac{1}{n}\sum_{i=1}^{n}w_{ik}(\mathbf{x}_{i}-\widehat{\mu})(\mathbf{x}_{i}-\widehat{\mu})^{T}$$

with  $w_{ik} \approx rac{\hat{
ho}_{ik}}{(\mathbf{x}_i - \widehat{oldsymbol{\mu}}_k)^{ op} \widehat{\boldsymbol{\Sigma}}_k^{-1}(\mathbf{x}_i - \widehat{oldsymbol{\mu}}_k)}$ 

**Tyler** estimators [Tyler, 1987] (classical robust estimator [Maronna, 1976]) fulfill very similar equations. **HINT** about robustness of the model.

#### Properties

- The random vectors that represent the data points are independent but not necessarily i.i.d.
- Generalizes GMM. (Gaussian ∈ ES)
- If g<sub>ik</sub> = g<sub>i</sub>, the membership probabilities do not depend on the shape of the distributions!
- If  $g_{ik} = g_k$ , we can derive extra estimators to be computed on the M-Step.
- The model leads to estimators that are similar to classical robust estimators (Tyler) [Ollila and Tyler, 2012].

When the dimension grows we can better estimate the parameters  $\tau_{ik}$ .

Convergence of  $\hat{\tau}$  when g is the Gaussian density generator Let  $\mathbf{x} \stackrel{d}{=} \mu + \sqrt{\tau} \mathbf{A} \mathbf{q}$ , with  $\mathbf{q}$  a standard Gaussian. Under some assumptions, for any  $\mathbf{a} \in \mathbb{R}$ ,  $\forall \varepsilon > 0$  and  $\mathbf{y} \sim \mathcal{N}(\tau, 2\tau^2/m)$ , then  $|\mathbb{P}(\{\hat{\tau} \leq \mathbf{a}\}) - \mathbb{P}(\mathbf{y} \leq \mathbf{a})| < \varepsilon$ , if n and m are large enough

This is in agreement with previous RMT results [Couillet et al., 2014].

We can combine this result with parsimonious restrictions on the covariance matrix to avoid issues in the case of **very large** m.

- The trace of the scatter matrix estimator is fixed.
- Four slightly different versions were propsed:
  - Version 1: the parameter μ used to compute the estimator Σ is the one obtained in the same iteration of the fixed-point loop.
  - Version 2: the μ-parameter is the one obtained in the previous iteration.
  - Version 3:  $(\mathbf{x}_i \hat{\boldsymbol{\mu}}_k)^T \widehat{\boldsymbol{\Sigma}}_k^{-1} (\mathbf{x}_i \hat{\boldsymbol{\mu}}_k)$  for  $\boldsymbol{\mu}$  are replaced by their square root (original Tyler *M*-estimators).
  - **Version 4:** Version 3 on top of the algorithm of Version 2.
- Center initialization: quick run of k-means.
- Code available: github.com/violetr/fem

#### Convergence of the fixed-point loops

Setup 1



It is possible to use some heuristic outlier rejection methods based on

$$\Delta(\mathbf{x}_i; \widehat{\boldsymbol{\mu}}_k, \widehat{\boldsymbol{\mathsf{M}}}_k) = (\mathbf{x}_i - \widehat{\boldsymbol{\mu}}_k)^T \widehat{\boldsymbol{\mathsf{M}}_k}^{-1} (\mathbf{x}_i - \widehat{\boldsymbol{\mu}}_k) \sim ?.$$

Threshold to reject =  $1 - \alpha$  quantile of the distribution.

We developed some alternatives [Roizman et al., 2020] based on a scaled Fisher distribution [Drašković and Pascal, 2018].

#### **Rejection block**

It has been implemented and plugged in at the end of the FEMCA (OPTIONAL).

## **FEMCA: Experimental results**

## Measuring the performance

#### We compare our algorithm to

- k-means
- GMM-EM
- Spectral Clustering
- Mixture of Student's t (t-EM or EMMIX)
- TClust
- RIMLE

#### Metrics

- Adjusted Mutual Information (AMI),
- Adjusted Rand Index (AR).
- Estimation error of the parameters (only for simulations).

### Some simulation results

Mixtures of t-distributions with different degrees of freedom and covariance matrix classes, mixtures of more general distributions, clusters with different  $g_i$ .



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### Some simulation results



FEMCA performs well even in the situations that do not match the model.

#### Real data clustering results



MNIST (LeCun, 1998)

NORB (LeCun, 2004)

Set	k-means	GMM	t-EM	FEMCA	spectral	TCLUST	RIMLE
MNIST38	0.2884	0.5716	0.6397	0.6887	0.6866	0.6847	0.2494
MNIST71	0.8486	0.8905	0.9432	0.9360	0.9384	0.6885	0.2493
MNIST386	0.6338	0.7332	0.8262	0.8306	0.8542	0.8366	0.4274
MNIST386+n	0.4475	0.4909	0.5296	0.5548	0.3115	0.6908	0.1498
smallNORB	0.0015	0.0468	0.4223	0.5067	$\sim 0$	0.1330	0.1472
20news	0.1883	0.2739	0.4426	0.5114	0.0987	0.2664	0.0026

Table 1: Median AMI

#### Real data clustering results - The NORB case

Dataset	kmeans	GMM-EM	t-EM	FEMCA	spectral	TCLUST	RIMLE
small NORB	0.0015	0.0468	0.4223	0.5067	$\sim$ 0	0.1330	0.1472



t-SNE embedding of the dataset colored with labels:



## **Applications to PolSAR Images**

#### Land use segmentation

Joint work with V. Roizman and G. Draskovic. [Roizman et al., 2019]



#### **Change detection**

Joint work with V. Roizman, G. Ginolhac and M. Jonckheere.

two times  $t_0 \rightarrow t_1$ 

one region, two images  $l_{t_0} 
ightarrow l_{t_1}$ CD map  $\mathsf{CD}(x_l) \in \{0,1\}$  Segment PolSAR images [Conte et al., 2002, Gini et al., 2000] with a clustering algorithm to detect land use.

Keep **flexibility** but also take advantage of **spatial structure**.

Compute by **patches**  $\rightarrow$  R-EM.



We propose a modification to include spacial information (and to deal with small dimension...). We estimate the membership probabilities  $p_{ij}$  based on  $\Delta_{ik}^{(l)}$ , computed over all the neighbors.

**For each** pixel **x**<sub>*i*</sub>:

**For each** pixel  $\mathbf{x}_t$  in the patch of  $\mathbf{x}_i$ :

$$\begin{aligned} \Delta_{tk}^{(l)} &= (\mathbf{x}_t - \boldsymbol{\mu}_k^{(l)})^T (\boldsymbol{\varSigma}_k^{(l)})^{-1} (\mathbf{x}_t - \boldsymbol{\mu}_k^{(l)}) \\ \text{Set } \Delta_{ik}^{(l)} &= h(\{\Delta_{tk}^{(l)}\}_t) \end{aligned}$$



For different patch sizes and different h(x) summary functions as mean, median and trimmed mean.

#### Simulation example - clustering results



Classes

Image example

From left to right: k-means, GMM and R-EM



## **Conclusions and Perspectives**

- We developed a very general flexible clustering algorithm based on Elliptical Symmetric distributions.
- We proved some **interesting properties**.
- We showed a good performance of FEMCA on experiments.
- We applied the flexible clustering algorithm to PolSAR image problems.

- Implementation of **regularizations** methods when m > n.
- Design a model selection method more specific than AIC/BIC.

- Study of the consistency of the estimators and the behaviour of the τ<sub>ik</sub> estimation.
- Apply the parameter τ<sub>ik</sub> addition to other similar Machine
   Learning problems that include covariance matrices.

## Thanks for your attention!

## **Questions** ?

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