A K-MEANS CLUSTERING ALGORITHM FOR MULTIVARIATE BIG DATA WITH CORRELATED COMPONENTS

GIACOMO ALETTI AND ALESSANDRA MICHELETTI

Abstract. Common clustering algorithms require multiple scans of all the data to achieve convergence, and this is prohibitive when large databases, with millions of data, must be processed. Some algorithms to extend the popular K-means method to the analysis of big data are present in literature since 1998 ([1]), but they assume that the random vectors which are processed and grouped have uncorrelated components. Unfortunately this is not the case in many practical situations. We here propose an extension of the algorithm of Bradley, Fayyad and Reina to the processing of massive multivariate data, having correlated components.

Keywords: *Big data; Clustering; K-means; Mahalanobis distance.*

1. Introduction

Clustering is the (unsupervised) division of a collection of data into groups, or *clusters*, such that points in the same cluster have a small distance from one another, while points in different clusters are at a large distance from one another. When the data are not very high dimensional, but are too many to fit in memory, because they are part of a huge dataset, or because they arrive in streams and must be processed immediately or they are lost, specific algorithms are needed to analyze progressively the data, store in memory only a small number of summary statistics, and then discard the already processed data and free the memory. Situations like this, in which clustering plays a fundamental role, recur in many applications, like customer segmentation in big e-commerce web sites, image analysis of video frames for objects recognition, recognition of human movements from data provided by sensors placed on the body or on a smartphone, etc. In all such cases, popular clustering algorithms for complex data like PAM, CLARA, CLARANS ([6, 9]) can not be efficiently applied, since they either require multiple scans of the sample, or the extraction of a subsample to identify the centroids or medoids, and then all data are scanned according to such identification and the medoids are not any more updated with the information coming from the whole dataset. Actually such popular methods are suited for data which are very high dimensional (e.g. functions) or for geometrical or spatial random objects, but not for datasets with an high number of data.

The key element in smart algorithms to treat the type of big data on which we focus our attention is to find methods by which the summary statistics that are retained in memory can be updated when each new observation, or group of observations, is processed. A first and widely recognized method to cluster big data of this type is the Bradley-Fayyad-Reina (BFR) algorithm ([1, 8]), which is an extension of the classical K-means algorithm. The BFR algorithm responds to the following *data mining desiderata*:

(1) Require one scan of the database and thus ability to operate on forward-only cursor.
(2) On-line anytime behavior: a "best" answer is always available, with status information on progress, expected remaining time, etc. provided.

(3) Suspendable, stoppable, resumable; incremental progress can be saved in memory to resume a stopped job.
(4) Ability to incrementally incorporate additional data with existing models efficiently.
(5) Work within confines of a limited RAM buffer.
(6) Utilize a variety of possible scan modes: sequential, index, and sampling scan, if available.

The BRF Algorithm for clustering is based on the definition of three different sets of data:

a) the *retained set* (RS): the set of data points which are not recognized to belong to any cluster, and need to be retained in the buffer;
b) the *discard set* (DS): the set of data points which can be discarded after updating the sufficient statistics;
c) the *compression set* (CS): the set of data points which form smaller clusters among themselves, far from the principal ones and can be represented with other sufficient statistics.

Each data point is assigned to one of these sets on the basis of its distance from the center of each cluster.

The main weakness of the BFR Algorithm resides in the assumption that the covariance matrix of each cluster is diagonal, which means that the components of the analyzed multivariate data should be uncorrelated. In this way at each step of the algorithm only the means and variances of each component of the cluster centers must be retained.

Actually the data points could be transformed into vectors with uncorrelated components by performing a principal component analysis (PCA). But in order to accomplish this task in our situation, where the different clusters have different covariance matrices, we would need to know a priori the cluster to which each new observation belongs, in order to use the correct covariance matrix to perform the PC transformation. We would thus need an algorithm of supervised learning, which is not our case.

In the following we will describe an extension of the BFR algorithm to the case of clusters having "full" covariance matrix. Since with our method also the covariance terms of the clusters centers must be retained, there is an increase in the computational costs, but such increase can be easily controlled and is affordable if the processed data are not extremely high dimensional. Thus our algorithm is targeted to problems with many data points of "medium" dimension, i.e. not so small to apply visualization techniques to identify the clusters (2D or 3D problems), which usually work better, but much smaller than the number of available data.

We will use the same three sets of data a)-c) introduced in the BFR algorithm, but using different summary statistics to define the discard set and the compression set.

2. Data Compression

Like in the BFR algorithm, primary data compression determines items to be discarded (discard set DS), and updates the compression set CS with the sufficient summary statistics of the identified clusters. Secondary data-compression takes place over data points not compressed in primary phase. Data compression refers to representing groups of points by their sufficient statistics and purging these points from RAM.

In the following we will always represent vectors as column vectors.

Assume that data points $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^p$ must be compressed in the same cluster. We will retain only the sample mean $\bar{\mathbf{x}}_n = \sum_{i=1}^n \mathbf{x}_i$, and the unbiased sample covariance matrix $S_n = \frac{1}{n-1}\sum_{i=1}^n (\mathbf{x} - \bar{\mathbf{x}})(\mathbf{x} - \bar{\mathbf{x}})^\top$. These two sufficient statistics can be easily computed by keeping in memory the following quantities:

$$n, \quad sumprod_{kl}(n) = \sum_{i=1}^{n} x_{ik}x_{il}, \quad sumprodcross_{kl}(n) = \sum_{i=1}^{n}\sum_{j=1}^{n} x_{ik}x_{jl},$$

$$sumsq_k(n) = \sum_{j=1}^{n} x_{jk}^2, \quad sum_k(n) = \sum_{j=1}^{n} x_{jk}, \quad k,l = 1,\dots,p,\ k<l. \tag{1}$$

In fact note that the element s_{kl} of S_n, when $k \neq l$, is given by

$$\begin{aligned}
s_{kl} &= \frac{1}{n-1}\sum_{i=1}^{n}(x_{ik}-\bar{x}_k)(x_{il}-\bar{x}_l) \\
&= \frac{1}{n-1}\sum_{i=1}^{n}(x_{ik}x_{il}-\bar{x}_k x_{il}-x_{ik}\bar{x}_l+\bar{x}_k\bar{x}_l) \\
&= \frac{1}{n-1}\sum_{i=1}^{n}x_{ik}x_{il}-\frac{1}{(n-1)^2}\sum_{i=1}^{n}\sum_{j=1}^{n}x_{ik}x_{jl}-\frac{1}{(n-1)^2}\sum_{i=1}^{n}\sum_{j=1}^{n}x_{jk}x_{il}+\frac{1}{(n-1)^2}(\sum_{i=1}^{n}x_{ik})(\sum_{j=1}^{n}x_{jl}) \\
&= \frac{1}{n-1}sumprod_{kl}(n)-\frac{2}{(n-1)^2}sumprodcross_{kl}(n)+\frac{1}{(n-1)^2}sum_k(n)sum_l(n),
\end{aligned}$$

while when $k = l$ we have

$$\begin{aligned}
s_{kk} &= \frac{1}{n-1}[\sum_{i=1}^{n}x_{ik}^2-(\frac{1}{n}\sum_{i=1}^{n}x_{ik})^2] \\
&= \frac{1}{n-1}[sumsq_k(n)-(\frac{1}{n}sum_k(n))^2]
\end{aligned}$$

The sufficient statistics listed in (1) can be easily updated when a new data point $\mathbf{x}_{n+1}$ must be added to the cluster, without processing again the already compressed points. In fact, for $k,l = 1,\dots,n,\ k<l$, we have

$$\begin{aligned}
sumprod_{kl}(n+1) &= \sum_{i=1}^{n+1}x_{ik}x_{il} = sumprod_{kl}(n)+x_{(n+1)k}x_{(n+1)l} \\
sumprodcross_{kl}(n+1) &= \sum_{i=1}^{n+1}\sum_{j=1}^{n+1}x_{ik}x_{jl} = sumprodcross_{kl}(n)+x_{(n+1)k}sum_l(n) \\
&\quad +x_{(n+1)l}sum_k(n)+x_{(n+1)k}x_{(n+1)l} \\
sumsq_k(n+1) &= \sum_{j=1}^{n+1}x_{jk}^2 = sumsq_k(n)+x_{(n+1)k}^2 \\
sum_k(n+1) &= \sum_{j=1}^{n+1}x_{jk} = sum_k(n)+x_{(n+1)k}
\end{aligned}$$

Thus at each step of the algorithm we have to retain in memory only p^2+p+1 sufficient statistics for each cluster, where p is the dimension of the data points. In addition, note that we should simply sum the corresponding statistics if we want to merge two clusters.

2.1. **The covariance matrices of the clusters.** Note that when a new cluster is formed, it contains too few data points to obtain a positive definite estimate of the covariance matrix, using the sample covariance matrix, at least until $n \leq p$. This is a problem since we need to invert or calculate the determinant of this matrix, in order to compute the Mahalanobis distance, that we will use to assign the observations to the clusters. Recent research methods in estimating covariance matrices include banding, tapering, penalization and shrinkage. We have focused on the Steinian shrinkage method since, as underlined in [11], it leads to covariance matrix estimators that are non-singular, well-conditioned, expressed in closed form and computationally cheap regardless of p. We use the diagonal matrix D_S of the sample covariance matrix S as "target matrix" of the shrinkage method, noting that D_S was the BRF estimate of the covariance of each cluster used in [1]. In other words, in presence of few data, our method coincides with that of [1], and we allow a progressive influence of correlation as the number of data increases. Summing up, we use a linear shrinkage estimator for the covariance matrix, like that proposed in [2, 4, 5, 11] of the form

$$\hat{S} = (1-\lambda)S + \lambda D_S,$$

where S is the sample covariance matrix, D_S is its diagonal matrix, and λ is a parameter in $[0,1]$, whose optimal value depends on the number n of data in the cluster. The parameter λ is initially settled to 1, and then its value is decreasing to 0 when $n \to \infty$.

In the following we will describe the details of our method and the assumptions that must be satisfied to apply it.

2.2. **A model for the estimate of the covariance matrices.** Our dataset is given by a sequence of p-dimensional vectors $\mathbf{x}_1, \mathbf{x}_2, \ldots$. Each observation $\mathbf{x}_n$ is independent on the others and, if belonging to the cluster $\underline{k}$, it is generated as

$$\mathbf{x}_n = \boldsymbol{\mu}_{\underline{k}} + \Sigma_{\underline{k}}^{\frac{1}{2}} \mathbf{z}_n$$

where $\boldsymbol{\mu}_{\underline{k}}$ is the mean vector and $\Sigma_{\underline{k}}^{\frac{1}{2}}$ is a matrix such that $\Sigma_{\underline{k}} = \Sigma_{\underline{k}}^{\frac{1}{2}} (\Sigma_{\underline{k}}^{\frac{1}{2}})^\top$ is strictly positive definite. The following hypothesis of uncorrelation is assumed on the first four moments:

$$E[\mathbf{z}_n] = \mathbf{0}, \qquad \mathrm{Cov}(\mathbf{z}_n) = E[\mathbf{z}_n \mathbf{z}_n^\top] = \mathbf{I}, \qquad E[\prod_{i=1}^{q} z_{n,i}^{\gamma_i}] = \prod_{i=1}^{q} E[z_{n,i}^{\gamma_i}], \tag{2}$$

for any integers $\gamma_1, \ldots, \gamma_q$ satisfying $0 \leq \sum_1^q \gamma_i \leq 4$, and where $z_{n,i}$ is the i-th component of the vector $\mathbf{z}_n = (z_{n,1}, \ldots, z_{n,q})^\top$.

Assume that the sequence $\mathbf{x}_1, \mathbf{x}_2, \ldots$ belongs to the same cluster with $\Sigma_{\underline{k}}^{\frac{1}{2}} = \Sigma^{\frac{1}{2}}$. Then the sequence $\mathbf{y}_1, \mathbf{y}_2, \ldots$ defined as $\mathbf{y}_n = \mathbf{x}_n - \boldsymbol{\mu}_{\underline{k}} = \Sigma^{\frac{1}{2}} \mathbf{z}_n$, is formed by independent vectors with null expectation. Then, as a consequence of (2), we have that

$$E[\mathbf{y}_i^\top \mathbf{y}_j] = \begin{cases} E[\mathbf{z}_i^\top (\Sigma^{\frac{1}{2}})^\top \Sigma^{\frac{1}{2}} \mathbf{z}_i] = \mathrm{tr}((\Sigma^{\frac{1}{2}})^\top \Sigma^{\frac{1}{2}}) = \mathrm{tr}(\Sigma^{\frac{1}{2}} (\Sigma^{\frac{1}{2}})^\top) = \mathrm{tr}(\Sigma) & \text{if } i = j; \\ 0 & \text{otherwise.} \end{cases}$$

Moreover, $E[\mathbf{y}_i^\top \mathbf{y}_j \mathbf{y}_k^\top \mathbf{y}_l] \neq 0$ only in the following situation:

when $i = j = k = l$**:** then

$$E[\mathbf{y}_i^\top \mathbf{y}_j \mathbf{y}_k^\top \mathbf{y}_l] = E[(\mathbf{y}_i^\top \mathbf{y}_i)^2] = \kappa_{11} + 2\mathrm{tr}(\Sigma^2) + (\mathrm{tr}\Sigma)^2, \tag{3a}$$

where κ_{11} is defined in [4];

when $(i=j)\neq(k=l)$**:** then

$$E[\mathbf{y}_i^\top\mathbf{y}_j\mathbf{y}_k^\top\mathbf{y}_l]=E[(\mathbf{y}_i^\top\mathbf{y}_i)(\mathbf{y}_k^\top\mathbf{y}_k)]=E[(\mathbf{y}_i^\top\mathbf{y}_i)]E[(\mathbf{y}_k^\top\mathbf{y}_k)]=(\mathrm{tr}\Sigma)^2; \tag{3b}$$

when $(i=l)\neq(j=k)$**:** then

$$\begin{aligned}E[\mathbf{y}_i^\top\mathbf{y}_j\mathbf{y}_k^\top\mathbf{y}_l]&=E[\mathbf{z}_i^\top(\Sigma^{\frac12})^\top\Sigma^{\frac12}(\mathbf{z}_j\mathbf{z}_j^\top)(\Sigma^{\frac12})^\top\Sigma^{\frac12}\mathbf{z}_i]\\&=E[\mathbf{z}_i^\top(\Sigma^{\frac12})^\top\Sigma^{\frac12}E[\mathbf{z}_j\mathbf{z}_j^\top](\Sigma^{\frac12})^\top\Sigma^{\frac12}\mathbf{z}_i]\\&=E[\mathbf{z}_i^\top(\Sigma^{\frac12})^\top\Sigma^{\frac12}(\Sigma^{\frac12})^\top\Sigma^{\frac12}\mathbf{z}_i]\\&=\mathrm{tr}((\Sigma^{\frac12})^\top\Sigma^{\frac12}(\Sigma^{\frac12})^\top\Sigma^{\frac12})=\mathrm{tr}(\Sigma^{\frac12}(\Sigma^{\frac12})^\top\Sigma^{\frac12}(\Sigma^{\frac12})^\top)=\mathrm{tr}(\Sigma^2);\end{aligned} \tag{3c}$$

when $(i=k)\neq(j=l)$**:** the same as above, since $\mathbf{y}_k^\top\mathbf{y}_l=\mathbf{y}_l^\top\mathbf{y}_k$, hence

$$E[\mathbf{y}_i^\top\mathbf{y}_j\mathbf{y}_k^\top\mathbf{y}_l]=\mathrm{tr}(\Sigma^2). \tag{3d}$$

Lemma 2.1. *As a consequence of* (3d)*,*

$$E\Big[\Big(\mathbf{y}_N^\top\sum_{i=1}^{N-1}\mathbf{y}_i\Big)^2\Big]=(N-1)\mathrm{tr}(\Sigma^2).$$

Lemma 2.2. *As a consequence of all the relations* (3)*,*

$$E\Big[\sum_{i,j,k,l=1}^{N-1}\mathbf{y}_i^\top\mathbf{y}_j\mathbf{y}_k^\top\mathbf{y}_l\Big]=(N-1)\kappa_{11}+2(N-1)^2\mathrm{tr}(\Sigma^2)+(N-1)^2(\mathrm{tr}\Sigma)^2.$$

Lemma 2.3. *As a consequence of* (3b)*,*

$$E\Big[\sum_{i,j=1}^{N-1}\mathbf{y}_N^\top\mathbf{y}_N\mathbf{y}_i^\top\mathbf{y}_j\Big]=(N-1)(\mathrm{tr}\Sigma)^2.$$

2.3. **Optimal shrinkage estimation.** The optimal weight for the nonparametric linear shrinkage estimation, in terms of minimizing the risk function relative to the quadratic loss, is computed as follows (see, e.g., [2, 4, 11, 5])

$$\frac{E[\mathrm{tr}(S(S-D_S))]-E[\mathrm{tr}(\Sigma(S-D_S))]}{E[\mathrm{tr}((S-D_S)^2)]}$$

It is obvious that $E[\mathrm{tr}(S(S-D_S))]$ and $E[\mathrm{tr}((S-D_S)^2)]$ may be directly unbiasedly estimated.

The problem here is the unbiased estimation of the term

$$E[\mathrm{tr}(\Sigma(S-D_S))]=\mathrm{tr}(\Sigma E[S-D_S])=\mathrm{tr}(\Sigma(\Sigma-D_\Sigma))=\mathrm{tr}(\Sigma^2)-\mathrm{tr}(D_\Sigma^2).$$

In [11, 5], the estimation is based on the statistic Q given for the first time in [4] as

$$Q=\frac{\sum_{n=1}^N\big((\mathbf{x}_n-\overline{\mathbf{x}})^\top(\mathbf{x}_n-\overline{\mathbf{x}})\big)^2}{N-1}$$

to obtain, e.g. in [5, Eq. (2.17)]

$$\hat\lambda=0\vee\frac{\mathrm{tr}(S^2)/p-\mathrm{tr}(SD_S)/p-\big(\widehat{\mathrm{tr}(\Sigma^2)-\mathrm{tr}}(D_\Sigma^2)\big)/p}{\mathrm{tr}(S^2)/p-(\mathrm{tr}S/p)^2}\wedge1.$$

The statistics Q was added to correct a bias due to non-gaussian models. In fact (see, e.g., [4, 5]), we may make use of the following additional relations to estimate $\mathrm{tr}(\Sigma^2) - \mathrm{tr}(D_\Sigma^2)$,

$$E[\mathrm{tr}(S^2)] = \frac{1}{N}\kappa_{11} + \frac{N}{N-1}\mathrm{tr}(\Sigma^2) + \frac{1}{N-1}(\mathrm{tr}\Sigma)^2 \tag{4a}$$

$$E[(\mathrm{tr}S)^2] = \frac{1}{N}\kappa_{11} + \frac{2}{N-1}\mathrm{tr}(\Sigma^2) + (\mathrm{tr}\Sigma)^2 \tag{4b}$$

$$E[\mathrm{tr}(D_S^2)] = \frac{1}{N-1}\kappa_{11} + \frac{N+1}{N-1}\mathrm{tr}(D_\Sigma^2) + \frac{R_N}{N-1}, \tag{4c}$$

once we have recalled that the quantity R_N is neglegible (see, again, [11, 5]). When the model is gaussian, a direct computation without Q may be done (see [2]), since $\kappa_{11} = 0$. Unfortunately, the statistic Q cannot be updated by keeping in memory only simple sufficient statistics when two clusters are merged together or when a single point is added to a cluster. With this problem in mind, we define a modification of Q, that can be simply updated, while, on the other hand, we loose the exchangeability property of Q. More precisely, we define the statistics Q_N inductively as

$$Q_N = \begin{cases} \big((\mathbf{x}_2 - \mathbf{x}_1)^\top(\mathbf{x}_2 - \mathbf{x}_1)\big)^2 & \text{if } N = 2; \\ Q_{N-1} + \big((\mathbf{x}_N - \overline{\mathbf{x}}^{(N)})^\top(\mathbf{x}_N - \overline{\mathbf{x}}^{(N)})\big)^2 & \text{if a new point } \mathbf{x}_N \text{ is added} \\ & \quad \text{to a cluster of } N-1 \text{ points}; \\ Q_{N_1} + Q_{N_2} & \text{if a cluster is made by merging} \\ & \quad \text{two clusters of } N_1 \text{ and } N_2 \text{ points}; \end{cases} \tag{5}$$

where

$$\overline{\mathbf{x}}^{(N)} = \frac{1}{N-1}\sum_{n=1}^{N-1}\mathbf{x}_n, \tag{6}$$

is the centroid of the cluster at the time of the update. Accordingly, we define two quantities $\mathbb{S}_N$ and $\mathbb{T}_N$ and we will prove in Lemma 2.4 that

$$E[Q_N] = \mathbb{S}_N\kappa_{11} + \mathbb{T}_N(2\mathrm{tr}(\Sigma^2) + (\mathrm{tr}\Sigma)^2), \tag{7}$$

where $\mathbb{S}_N$ and $\mathbb{T}_N$ may be simply updated:

$$\mathbb{S}_N = \begin{cases} 2 & \text{if } N = 2; \\ \mathbb{S}_{N-1} + \left(1 + \frac{1}{(N-1)^3}\right) & \text{if a new point is added} \\ & \quad \text{to a cluster of } N-1 \text{ points}; \\ \mathbb{S}_{N_1} + \mathbb{S}_{N_2} & \text{if a cluster is made by merging} \\ & \quad \text{two clusters of } N_1 \text{ and } N_2 \text{ points}; \end{cases} \tag{8}$$

$$\mathbb{T}_N = \begin{cases} 4 & \text{if } N = 2; \\ \mathbb{T}_{N-1} + \left(1 + \frac{1}{(N-1)}\right)^2 & \text{if a new point is added} \\ & \quad \text{to a cluster of } N-1 \text{ points}; \\ \mathbb{T}_{N_1} + \mathbb{T}_{N_2} & \text{if a cluster is made by merging} \\ & \quad \text{two clusters of } N_1 \text{ and } N_2 \text{ points}; \end{cases} \tag{9}$$

Now, given the system (4) and (7), it is sufficient to solve the following linear system to get an unbiased estimator of $\mathrm{tr}(\Sigma^2) - \mathrm{tr}(D_\Sigma^2)$

$$\begin{pmatrix} a_N & b_N & c_N & d_N \end{pmatrix} \begin{pmatrix} \frac{1}{N} & \frac{N}{N-1} & \frac{1}{N-1} & 0 \\ \frac{1}{N} & \frac{2}{N-1} & 1 & 0 \\ \frac{1}{N-1} & 0 & 0 & \frac{N+1}{N-1} \\ \mathbb{S}_N & 2\mathbb{T}_N & \mathbb{T}_N & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & -1 \end{pmatrix} \tag{10}$$

The previous linear system has the following solution:

$$\begin{aligned} a_N &= \Big(\frac{(N+1+\frac{2}{N-2})\mathbb{S}_N - (3+\frac{1}{N-2}-\frac{2}{N+1})\mathbb{T}_N}{(N+2+\frac{2}{N-1})\mathbb{S}_N - 3\mathbb{T}_N} \Big); \\ b_N &= \Big(\frac{-(1+\frac{2}{N-2})\mathbb{S}_N + (\frac{1}{N-2}+\frac{1}{N+1})\mathbb{T}_N}{(N+2+\frac{2}{N-1})\mathbb{S}_N - 3\mathbb{T}_N} \Big); \\ c_N &= -1 + \frac{2}{N+1}; \\ d_N &= \Big(\frac{\frac{1}{N-1}}{(N+2+\frac{2}{N-1})\mathbb{S}_N - 3\mathbb{T}_N} \Big). \end{aligned}$$

Then an almost unbiased estimator of $\mathrm{tr}(\Sigma^2) - \mathrm{tr}(D_\Sigma^2)$ is

$$\widehat{\mathrm{tr}(\Sigma^2) - \mathrm{tr}}(D_\Sigma^2) = a_N \mathrm{tr}(S^2) + b_N (\mathrm{tr}S)^2 + c_N \mathrm{tr}(D_S^2) + d_N Q_N$$

since

$$E[a_N \mathrm{tr}(S^2) + b_N (\mathrm{tr}S)^2 + c_N \mathrm{tr}(D_S^2) + d_N Q_N] = \mathrm{tr}(\Sigma^2) - \mathrm{tr}(D_\Sigma^2) + \Big(1 + \frac{2}{N+1}\Big)\frac{R_N}{N-1}.$$

Lemma 2.4. *With the notation of* (5), (6), (8) *and* (9) *we have*

$$E[Q_N] = \begin{cases} 2\kappa_{11} + 4(2\mathrm{tr}(\Sigma^2) + (\mathrm{tr}\Sigma)^2) & \text{if } N = 2; \\ E[Q_{N-1}] + \big(1 + \frac{1}{(N-1)^3}\big)\kappa_{11} & \text{if a new point is added} \\ \quad +(1+\frac{1}{N-1})^2(2\mathrm{tr}(\Sigma^2) + (\mathrm{tr}\Sigma)^2) & \quad \text{to a cluster of } N-1 \text{ points}; \\ E[Q_{N_1}] + E[Q_{N_2}] & \text{if a cluster is made by merging} \\ & \quad \text{two clusters of } N_1 \text{ and } N_2 \text{ points}; \end{cases}$$

and hence

$$E[Q_N] = \mathbb{S}_N \kappa_{11} + \mathbb{T}_N (2\mathrm{tr}(\Sigma^2) + (\mathrm{tr}\Sigma)^2).$$

See the Appendix for the proof.

2.4. **Model update.** Like in the BFR algorithm, the second step of our algorithm consists of performing K-means iterations over sufficient statistics of compressed, discarded and retained points. In order to assign a point to a cluster we use the squared Mahalanobis distance from its center (sample mean), i.e. we assign a new data point $\mathbf{x}$ to cluster h with center $\bar{\mathbf{x}}_h$ and estimated covariance matrix $\hat{S}_h$, if h is the index which minimizes

$$\Delta^2_{\hat{S}_h}(\mathbf{x}, \bar{\mathbf{x}}_h) = (\mathbf{x} - \bar{\mathbf{x}}_h)^T (\hat{S}_h)^{-1} (\mathbf{x} - \bar{\mathbf{x}}_h),$$

and if $\Delta^2_{\hat{S}_h}(\mathbf{x}, \bar{\mathbf{x}}_h)$ is smaller than a fixed threshold δ. In order to avoid the inversion of a matrix and thus to reduce the computational costs, we observe that the Mahalanobis distance between

two points $\mathbf{x}, \mathbf{y}$, computed with respect to a covariance matrix S, can be rewritten as follows (see e.g. [10, Expression A.7.10]):

$$\Delta^2_S(\mathbf{x},\mathbf{y}) = (\mathbf{x}-\mathbf{y})^T S^{-1}(\mathbf{x}-\mathbf{y}) = \frac{\det[S+(\mathbf{x}-\mathbf{y})(\mathbf{x}-\mathbf{y})^T]}{\det(S)} - 1 \tag{11}$$

In our algorithm we will actually use expression (11) for the computation of all the Mahalanobis distances.

We also compare $\mathbf{x}$ with each point $\mathbf{x}_o$ in the retained set (RS), by computing

$$\Delta^2_{\hat{S}_P}(\mathbf{x},\mathbf{x}_o) = (\mathbf{x}-\mathbf{x}_o)^T(\hat{S}_P)^{-1}(\mathbf{x}-\mathbf{x}_o),$$

where $\hat{S}_P$ matrix is the pooled covariance matrix based on all $\hat{S}_h$:

$$\hat{S}_P = \frac{(n_{h_1}-1)\hat{S}_{h_1} + (n_{h_2}-1)\hat{S}_{h_2} + \cdots (n_{h_M}-1)\hat{S}_{h_M}}{n_{h_1}+n_{h_2}+\cdots+n_{h_M}-M}, \tag{12}$$

and where n_h is the number of points in cluster h. With $\hat{S}_P$, we emphasize the weighted importance of directions that are more significant for the clusters when we compute the distance between two "isolated" points.

We then approximate locally the distribution of the clusters with a $p-$variate Gaussian and we build confidence regions around the centers of the clusters (see [**?**]). Following the approach stated in [1], which is motivated by the assumption that the mean is unlikely to move outside of the computed confidence interval, we perturb $\bar{\mathbf{x}}_h$ by moving it in the farthest position from $\mathbf{x}$ in its confidence region, while we perturb the centers of the other clusters by moving them in the closest positions with respect to $\mathbf{x}$ and we check if the cluster center closer to $\mathbf{x}$ is still $\bar{\mathbf{x}}_h$. If yes, we assign $\mathbf{x}$ to cluster h, we update the corresponding sufficient statistics and we put $\mathbf{x}$ in the discard set; if the point is closer to a point $\mathbf{x}_o$ of the retained set than to any cluster, we form a new secondary cluster (CS) with the two points and we put $\mathbf{x}$ and $\mathbf{x}_o$ in the discard set; otherwise, we put $\mathbf{x}$ in the retained set (RS).

Let us see this procedure in deeper detail.

2.4.1. *Confidence regions.* It is well-known ([**?**]) that a confidence interval for the mean $\boldsymbol{\mu}$ based on $\overline{\mathbf{x}}$ and S may be based on the Hotelling's T-squared distribution

$$t^2 = n(\overline{\mathbf{x}}-\boldsymbol{\mu})^\top S^{-1}(\overline{\mathbf{x}}-\boldsymbol{\mu}) \sim T^2_{p,n-1} = \frac{p(n-1)}{n-p}F_{p,n-p},$$

where $F_{p,n-p}$ is the F-distribution with parameters p and $n-p$.

Then, if we denote by $CI_{\underline{k}}$ the confidence interval of the mean of cluster $\underline{k}$, i.e.

$$CI_{\underline{k}} = \{\boldsymbol{\mu}\colon n(\overline{\mathbf{x}}_{\underline{k}}-\boldsymbol{\mu})^\top {S_{\underline{k}}}^{-1}(\overline{\mathbf{x}}_{\underline{k}}-\boldsymbol{\mu}) \le T^2_{p,n-1}(1-\alpha)\}$$

then the perturbation $p_{\underline{k}}(\mathbf{x})$ for the data point $\mathbf{x}$ is

$$p_{\underline{k}}(\mathbf{x}) = \begin{cases} \sup_{\boldsymbol{\mu}\in CI_{\underline{k}}}(\mathbf{x}-\boldsymbol{\mu})^\top {S_{\underline{k}}}^{-1}(\mathbf{x}-\boldsymbol{\mu}) & \text{if } \underline{k}=j; \\ \inf_{\boldsymbol{\mu}\in CI_{\underline{k}}}(\mathbf{x}-\boldsymbol{\mu})^\top {S_{\underline{k}}}^{-1}(\mathbf{x}-\boldsymbol{\mu}) & \text{if } \underline{k}\neq j; \end{cases}$$

Denoting by $t_\alpha = T^2_{p,n-1}(1-\alpha)$, if we introduce a Lagrange multiplier λ^*, the problems of minimization or maximization stated in the definition of $p_{\underline{k}}(\mathbf{x})$ can be solved by differentiating the following lagrangian form $\mathcal{L}$:

$$\mathcal{L}(\boldsymbol{\mu},\lambda) = (\mathbf{x}-\boldsymbol{\mu})^\top {S_{\underline{k}}}^{-1}(\mathbf{x}-\boldsymbol{\mu}) - n\lambda^*\big((\overline{\mathbf{x}}_{\underline{k}}-\boldsymbol{\mu})^\top {S_{\underline{k}}}^{-1}(\overline{\mathbf{x}}_{\underline{k}}-\boldsymbol{\mu}) - \tfrac{t_\alpha}{n}\big).$$

The resolution $\nabla_{\boldsymbol{\mu}}\mathcal{L} = \mathbf{0}$ gives $\boldsymbol{\mu} = \frac{\mathbf{x}-\lambda\overline{\mathbf{x}}_{\underline{k}}}{1-\lambda}$, where $\lambda = n\lambda^*$. In particular, the optimal $\boldsymbol{\mu}$ is the linear combination of $\mathbf{x}$ and $\overline{\mathbf{x}}_{\underline{k}}$ in $CI_{\underline{k}}$ which is farther from $\mathbf{x}$ or closer to $\mathbf{x}$, when $\underline{k} = j$ or $\underline{k} \neq j$, respectively. The constrain reads

$$(\overline{\mathbf{x}}_{\underline{k}} - \frac{\mathbf{x}-\lambda\overline{\mathbf{x}}_{\underline{k}}}{1-\lambda})^\top {S_{\underline{k}}}^{-1}(\overline{\mathbf{x}}_{\underline{k}} - \frac{\mathbf{x}-\lambda\overline{\mathbf{x}}_{\underline{k}}}{1-\lambda}) = \frac{t_\alpha}{n} \quad \Longrightarrow \quad \frac{t_\alpha}{n} = \frac{(\overline{\mathbf{x}}_{\underline{k}} - \mathbf{x})^\top {S_{\underline{k}}}^{-1}(\overline{\mathbf{x}}_{\underline{k}} - \mathbf{x})}{(1-\lambda)^2}.$$

Denoting by $\Delta^2_{\underline{k},\mathbf{x}} = (\overline{\mathbf{x}}_{\underline{k}} - \mathbf{x})^\top {S_{\underline{k}}}^{-1}(\overline{\mathbf{x}}_{\underline{k}} - \mathbf{x})$, we have $\lambda = 1 \pm \sqrt{n\Delta^2_{\underline{k},\mathbf{x}}/t_\alpha}$ and

$$p_{\underline{k}}(\mathbf{x}) = (\mathbf{x} - \frac{\mathbf{x}-\lambda\overline{\mathbf{x}}_{\underline{k}}}{1-\lambda})^\top {S_{\underline{k}}}^{-1}(\mathbf{x} - \frac{\mathbf{x}-\lambda\overline{\mathbf{x}}_{\underline{k}}}{1-\lambda}) = \frac{\lambda^2}{(1-\lambda)^2}\Delta^2_{\underline{k},\mathbf{x}}.$$

Summarizing we obtain the following perturbations of the cluster centers, referred to the data point $\mathbf{x}$,

$$p_{\underline{k}}(\mathbf{x}) = \begin{cases} (\sqrt{\Delta^2_{\underline{k},\mathbf{x}}} + \sqrt{t_\alpha/n})^2 & \text{if } \underline{k} = j; \\ (\sqrt{\Delta^2_{\underline{k},\mathbf{x}}} - \sqrt{t_\alpha/n})^2 & \text{if } \underline{k} \neq j \text{ and } \Delta^2_{\underline{k},\mathbf{x}} \geq t_\alpha. \\ 0 & \text{if } \underline{k} \neq j \text{ and } \Delta^2_{\underline{k},\mathbf{x}} < t_\alpha. \end{cases}$$

3. Secondary data compression

The purpose of secondary data compression is to identify "tight" sub-clusters of points among the data that we can not discard in the primary phase. In [1] this is made in two phases. In the first one, a K-means algorithm tries to locate subclusters that could be merged if they meet a "density" condition. The candidate merging clusters are chosen sequentially based on a hierarchical agglomerative clustering built on the subclusters. In all this procedure, the euclidean metric is adopted. Finally, the number of clusters is initialized to K, and it can increase or decrease during the procedure.

We adopt the same general idea, but we modify the procedure. First, we change the metric, by taking the Mahalanobis distance based on the pooled covariance matrix $\hat{S}_P$. We think that this metric is more precise than the euclidean one for this stage, since it takes into account the specific variability of each cluster. Then, a hierarchical clustering is performed using the Ward's method [3, 7]: the distance between two clusters h_1 and h_2 with $n_{h_1} > 1, n_{h_2} > 1$ points and centroids $\bar{\mathbf{x}}_{h_1}$ and $\bar{\mathbf{x}}_{h_2}$, is given by

$$\Delta^2(h_1, h_2) = \frac{n_{h_1} n_{h_2}}{n_{h_1} + n_{h_2}} (\bar{\mathbf{x}}_{h_1} - \bar{\mathbf{x}}_{h_2})^\top \hat{S}_P (\bar{\mathbf{x}}_{h_1} - \bar{\mathbf{x}}_{h_2}).$$

where $\hat{S}_P = \frac{n_{h_1} S_{h_1} + n_{h_2} S_{h_2}}{n_{h_1} + n_{h_2} - 2}$ is the pooled sample covariance matrix of the two clusters.

The distance between a single retained point and a cluster is computed by the squared Mahalanobis distance between the point and the cluster centroid, based on the sample covariance matrix of the cluster, while the distance between two retained points is computed by their squared Mahalanobis distance based on the pooled covariance matrix (12) of all the clusters.

We sequentially merge two clusters only if a suitable density condition is fulfilled. This condition is different for the different types of merging that we can perform:

- we merge two clusters h_1 and h_2 if $\Delta^2(h_1, h_2) < \theta(tr(S_{h_1}) + tr(S_{h_2}))$;
- we merge a retained point $\mathbf{x}$ and a cluster h if $\Delta^2(\mathbf{x}, h) < \theta(tr(S_h))$;
- we merge two retained points $\mathbf{x}_1$ and $\mathbf{x}_2$ if $\Delta^2(\mathbf{x}_1, \mathbf{x}_2) < \theta_0$.

Here θ is a threshold, chosen by the user, corresponding to a proportion of the total variances of the groups and θ_0 a fixed value. We suggest a significant quantile of the χ-square distribution that arises under the null hypothesis
H_0: the retained points comes from a gaussian distribution with covariance matrix given by the pooled covariance matrix (12) of all the clusters.

4. Results on simulated data

Synthetic data were created for the cases of 5 and 20 clusters. Data were sampled from 5 or 20 independent p-variate Gaussians, with elements of their mean vectors (the true means) uniformly distributed on $[-5, 5]$. The covariance matrices were generated by computing products of the type $\Sigma = UHU^T$, where H is a diagonal matrix with elements on the diagonal distributed as a $Beta(0.5, 0.5)$ rescaled to the interval on $[0.5, 2.5]$, and U is the orthonormal matrix obtained by the singular value decomposition of a symmetric matrix MM^T, where the elements of the $p \times p$ matrix M are uniformly distributed on $[-2, 2]$. In either cases of 5 or 20 clusters, we generated 10.000 vectors for each cluster, having dimensions $p = 5, 10, 20$.

This procedure guarantees that these clusters are rather well-separated Gaussians, in particular for higher vector dimensions, an ideal situation for K-Means.

We applied both our procedure and the BFR algorithm to these synthetic data, to compare the performance of the two methods. In both cases, we computed the secondary data compression once out of 25, or out of 50 data points. We choose a fixed threshold $\theta = 2.5$ for all our test cases, and in the tests on data from 20 clusters we started from a lower number of initial clusters (equal to 10), in order to check the ability of our algorithm to detect the correct number of clusters. The results are reported in Table 1.

We note that the number of clusters is sometimes overestimated, in particular when the dimension p of the data points is small, which corresponds to the case where the clusters are less separated. In such cases, if the point clouds in different clusters are gathered in particularly "elongated" and rather close ellipsoids, then the correct detection of the clusters may be more difficult. Anyway in such cases the results of our algorithm are better than those obtained with the BFR algorithms. We also note that in the case of 20 clusters with $p = 10$ the overestimation of the number of clusters is compensated by the presence of one small cluster, composed by 2 data points, which can then be revisited as a small group of outliers.

The method seems to be sensitive to the frequency of the secondary compression only for data dimension smaller than the number of clusters.

Finally both algorithms underestimate the true number of clusters in the case of 20 clusters with data dimension $p = 20$, but our proposed algorithm gives slightly better results. Anyway if we initialize both algorithms with 20 clusters, both of them detect the correct number of clusters with no retained points.

We tested also cases with bigger values of p, but in such cases both algorithms are able to detect the correct number of clusters, in an equivalent way.

5. Conclusion

We have introduced an extension of the BFR algorithm to cluster data with correlated components. The algorithm uses a k-means approach, based on the computation of the Mahalanobis distance. In order to compute such distance, positive definite estimators of the covariance matrices of the clusters are needed, also when the clusters contain just a few data points. We obtained such

n. of true clusters	algorithm	dimension p of data points	n. of data in each chunk	n. of estimated clusters	n. of small clusters	n. of retained points (outliers)
5	PA	5	25	10	0	0
5	BFR	5	25	14	0	1
5	PA	5	50	10	0	0
5	BFR	5	50	35	2	3
5	PA	10	25	5	0	1
5	BFR	10	25	5	0	1
5	PA	10	50	5	0	1
5	BFR	10	50	5	0	1
5	PA	20	25	5	0	0
5	BFR	20	25	5	0	0
5	PA	20	50	5	0	0
5	BFR	20	50	5	0	0
20	PA	10	25	18	0	0
20	BFR	10	25	12	0	0
20	PA	10	50	21	1	2
20	BFR	10	50	11	0	0
20	PA	20	25	14	0	0
20	BFR	20	25	13	0	0
20	PA	20	50	14	0	0
20	BFR	20	50	13	0	0

TABLE 1. Results of the application of our proposed algorithm (PA) and of the BFR algorithm to synthetic data. We call chunk the number of processed data out of which we apply secondary compression. By small clusters we mean clusters containing less than 10 data points

estimators by considering a Steinian shrinkage method, which leads to covariance matrix estimators that are non-singular, well-conditioned, expressed in a recursive way and thus computationally cheap.

We applied both our proposed method and the BFR algorithm to synthetic gaussian data, and we compared their performance. From the numerical results we conclude that our method provides rather good clustering on synthetic data, and performs better than the BFR algorithm in particular in presence of many clusters in spaces of rather low dimension. This is reasonable since the BFR algorithm approximates the "clouds" of data with ellipsoids having axes parallel to the reference system, and this leads to a wrong classification when the clusters are elongated, not much separated, and with axes rotated with respect to the reference system. In such situations our algorithm is able to capture in a more proper way the geometry of the clusters, and thus improves the classification.

APPENDIX A. PROOFS

Proof of Lemma 2.4

For $N=2$, as a consequence of the model:

$$\begin{aligned}E[\big((\mathbf{x}_2-\mathbf{x}_1)^\top(\mathbf{x}_2-\mathbf{x}_1)\big)^2] &= E[\big((\mathbf{y}_2-\mathbf{y}_1)^\top(\mathbf{y}_2-\mathbf{y}_1)\big)^2]\\ &= E[(\mathbf{y}_2^\top\mathbf{y}_2)^2]+4E[(\mathbf{y}_2^\top\mathbf{y}_1)^2]+E[(\mathbf{y}_1^\top\mathbf{y}_1)^2]+2E[(\mathbf{y}_2^\top\mathbf{y}_2)(\mathbf{y}_1^\top\mathbf{y}_1)]\\ &\quad -2E[(\mathbf{y}_2^\top\mathbf{y}_2)(\mathbf{y}_2^\top\mathbf{y}_1)]-2E[(\mathbf{y}_2^\top\mathbf{y}_1)(\mathbf{y}_1^\top\mathbf{y}_1)^2]\\ &= 2E[(\mathbf{y}_1^\top\mathbf{y}_1)^2]+4E[(\mathbf{y}_2^\top\mathbf{y}_1)^2]+2E[(\mathbf{y}_1^\top\mathbf{y}_1)]^2\\ &\quad -2E[(\mathbf{y}_2^\top\mathbf{y}_2)\mathbf{y}_2^\top]E[\mathbf{y}_1]-2E[\mathbf{y}_2^\top]E[\mathbf{y}_1(\mathbf{y}_1^\top\mathbf{y}_1)^2]\\ &= 2E[(\mathbf{y}_1^\top\mathbf{y}_1)^2]+4E[(\mathbf{y}_2^\top\mathbf{y}_1)^2]+2E[(\mathbf{y}_1^\top\mathbf{y}_1)]^2.\end{aligned}$$

Since $E[(\mathbf{y}_1^\top\mathbf{y}_1)]=\mathrm{tr}\Sigma$, by (3a) and (3d), we obtain the first part of the thesis.

Let us add a point to a cluster of $N-1$ points. We obtain

$$\begin{aligned}E[Q_N]-E[Q_{N-1}] &= E[Q_N-Q_{N-1}]\\ &= E\big[\big((\mathbf{x}_N-\overline{\mathbf{x}}^{(N)})^\top(\mathbf{x}_N-\overline{\mathbf{x}}^{(N)})\big)^2\big]=E\big[\big((\mathbf{y}_N-\overline{\mathbf{y}}^{(N)})^\top(\mathbf{y}_N-\overline{\mathbf{y}}^{(N)})\big)^2\big]\\ &= E[(\mathbf{y}_N^\top\mathbf{y}_N-2\mathbf{y}_N^\top\overline{\mathbf{y}}^{(N)}+\overline{\mathbf{y}}^{(N)\top}\overline{\mathbf{y}}^{(N)})^2]\\ &= \underbrace{E[(\mathbf{y}_N^\top\mathbf{y}_N)^2]}_{A}+\underbrace{E[4(\mathbf{y}_N^\top\overline{\mathbf{y}}^{(N)})^2]}_{B}+\underbrace{E[(\overline{\mathbf{y}}^{(N)\top}\overline{\mathbf{y}}^{(N)})^2]}_{C}+\underbrace{E[2\mathbf{y}_N^\top\mathbf{y}_N\overline{\mathbf{y}}^{(N)\top}\overline{\mathbf{y}}^{(N)}]}_{D}\\ &\quad -\underbrace{E[4\mathbf{y}_N^\top\mathbf{y}_N\mathbf{y}_N^\top\overline{\mathbf{y}}^{(N)}]}_{E}-\underbrace{E[4\overline{\mathbf{y}}^{(N)\top}\overline{\mathbf{y}}^{(N)}\mathbf{y}_N^\top\overline{\mathbf{y}}^{(N)}]}_{F}.\end{aligned}$$

As above, the fact that $\mathbf{y}_n$ is independend from $\overline{\mathbf{y}}^{(n)}$, and both have expectation null, imply

$$\begin{aligned}E &= 4E[\mathbf{y}_n^\top\mathbf{y}_n\mathbf{y}_n^\top\overline{\mathbf{y}}^{(n)}]=4E[\mathbf{y}_n^\top\mathbf{y}_n\mathbf{y}_n^\top]E[\overline{\mathbf{y}}^{(n)}]=0\\ F &= E[4\overline{\mathbf{y}}^{(n)\top}\overline{\mathbf{y}}^{(n)}\mathbf{y}_n^\top\overline{\mathbf{y}}^{(n)}]=4E[\overline{\mathbf{y}}^{(n)\top}\overline{\mathbf{y}}^{(n)}\overline{\mathbf{y}}^{(n)\top}\mathbf{y}_n]=4E[\overline{\mathbf{y}}^{(n)\top}\overline{\mathbf{y}}^{(n)}\overline{\mathbf{y}}^{(n)\top}]E[\mathbf{y}_n]=0\end{aligned}$$

By (3a), $A=\kappa_{11}+2\mathrm{tr}(\Sigma^2)+(\mathrm{tr}\Sigma)^2$. By Lemma 2.1, $B=\frac{4}{N-1}\mathrm{tr}(\Sigma^2)$. By Lemma 2.2, $C=\frac{1}{(N-1)^3}\kappa_{11}+\frac{2}{(N-1)^2}\mathrm{tr}(\Sigma^2)+\frac{1}{(N-1)^2}(\mathrm{tr}\Sigma)^2$. By Lemma 2.3, $D=\frac{2}{N-1}(\mathrm{tr}\Sigma)^2$. Then

$$\begin{aligned}E[Q_N]-E[Q_{N-1}] &= \Big(1+\frac{1}{(N-1)^3}\Big)\kappa_{11}+\Big(1+\frac{2}{N-1}+\frac{1}{(N-1)^2}\Big)(2\mathrm{tr}(\Sigma^2)+(\mathrm{tr}\Sigma)^2)\\ &= \Big(1+\frac{1}{(N-1)^3}\Big)\kappa_{11}+\Big(1+\frac{1}{N-1}\Big)^2(2\mathrm{tr}(\Sigma^2)+(\mathrm{tr}\Sigma)^2).\end{aligned}$$

The case of merging two clusters is a simple consequence of (5), (8) and (9).

□

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Department of Environmental Science and Policy & ADAMSS Center, Università degli Studi di Milano, Milan, Italy
E-mail address: giacomo.aletti@unimi.it

Department of Environmental Science and Policy & ADAMSS Center, Università degli Studi di Milano, Milan, Italy
E-mail address: alessandra.micheletti@unimi.it