K-bMOM: a robust Lloyd-type clustering algorithm based on bootstrap Median-of-Means

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Abstract
We propose a new clustering algorithm that is robust to the presence of outliers in the dataset. We perform Lloyd-type iterations with robust estimates of the centroids. More precisely, we build on the idea of median-of-means statistics to estimate the centroids, but allow for replacement while constructing the blocks. We call this methodology the bootstrap median-of-means (bMOM) and prove that if enough blocks are generated through the bootstrap sampling, then it has a better breakdown point for mean estimation than the classical median-of-means (MOM), where the blocks form a partition of the dataset. From a clustering perspective, bMOM enables to take many blocks of a desired size, thus avoiding possible disappearance of clusters in some blocks, a pitfall that can occur for the partition-based generation of blocks of the classical median-of-means. Experiments on simulated datasets show that the proposed approach, called K-bMOM, performs better than existing robust K-means based methods. It is also recommended to the practitioner to use such a robust approach to initialize their clustering algorithm.

1 Introduction
Data scientists have nowadays to deal with massive and complex datasets, that are often corrupted by outliers. Classical data mining procedures such as K-means or more general EM algorithms for instance are however sensitive to the presence of outliers, which can induce a time consuming pre-processing of the data.

In this context, robust versions of data mining procedures are particularly relevant and we investigate a way to produce a Lloyd-type algorithm for hard clustering that is robust to the presence of outliers. To do this, we propose to use a variant of median-of-means (MOM) statistics, that we call bootstrap median-of-means (bMOM). MOM principle has been the object of recent active research in mean estimation, regression, high-dimensional framework and also supervised classification and machine learning ([17, 9, 15, 18, 20, 22]). Note that other approaches to robustness for K-means exist in the literature, such as for instance K-median or trimmed K-means (see for instance the survey [10] and references therein ; see also [5]).

Given a dataset, the boostrap median-of-means consists in first generating a (large) bootstrap sample and then perform a classical median-of-means on this bootstrap sample. We prove in Section 2 that if enough blocks are generated from the bootstrap sampling, then for a fixed block size, bMOM has a higher breakdown point than MOM.

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We propose a robust-to-outliers version of K-means, that we call K-bMOM, and that performs Lloyd-type iterations through the use of bMOM estimates of the K-means distortion, as further explained in Section 3.

In Section 4 a bMOM based procedure is considered to initialize clustering algorithms and is compared to existing initialization on simulated datasets. Practical considerations to choose the number and size of blocks are discussed and a heuristic is proposed. Finally, the K-bMOM algorithm is compared to existing robust k-means based clustering approach on simulated datasets with the presence of outliers.

While completing the editing of this work, we became aware of the recent preprint [14] that investigates the use of median-of-means statistics to produce a robust K-means clustering. However, the latter work is theoretical and the authors study probabilistic performance bounds for the minimizer of the median-of-means of the K-means distortion loss. In particular the authors do not discuss the use of median-of-means through Lloyd-type iterations nor a practical way to compute the estimator. Neither do they discuss the possibility of generating blocks with replacement in the dataset.

2 Robust mean estimation by the bootstrap median-of-means

2.1 Median-of-Means and bootstrap Median-of-Means

The median-of-means (MOM) estimator of the mean in dimension one consists in taking a median of some arithmetic means computed on a collection - say of size $B$ - of disjoint blocks $(x_i)_{i \in b_k}$, where $\{b_k : k \in \{1, ..., B\}\}$ form a partition of the set of indices $\{1, ..., n\}$ of a real valued sample $x^n_1 = (x_1, ..., x_n)$. The length of the blocks are generally taken to be equal, eventually up to one data. We thus have, by denoting $b^n_B$ the collection of blocks,

$$\text{MOM}(x^n_1, b^n_B) = \text{med} \left\{ \sum_{j \in b_k} x_j : k \in \{1, ..., B\} \right\}.$$  

where med is a median, that is $\# \{k \in \{1, ..., B\} : a_k \leq \text{med} \{a_i\} \} \geq B/2$ and $\# \{k \in \{1, ..., B\} : a_k \geq \text{med} \{a_i\} \} \geq B/2$.

We can consider that the blocks are generated according to a random drawing process, that proceeds without replacements (disjoint blocks) and according to the uniform distribution at each step on the remaining data. This formulation naturally leads to consider more general random block generating processes.

For any positive integers $n_B$ and $B$, denote $m = Bn_B$ and generate a bootstrap sample $y^n_1 = (y_1, ..., y_m)$ from the dataset $x^n_1$. More precisely, each $y_i$ is taken uniformly at random from the values $(x_1, ..., x_n)$ and independently from the $(y_j)_{j \neq i}$. Then the bootstrap median-of-means (bMOM) of the dataset $x^n_1$ with parameters $n_B$ and $B$ is the (classical) MOM estimator on the bootstrap sample $y^n_1$ with blocks $b_j = (n_B(j - 1) + 1, ..., n_Bj)$ for $j \in \{1, ..., B\}$,

$$\text{bMOM}(x^n_1, n_B, B) = \text{MOM}(y^n_1, b^n_B).$$

We can notice that bMOM is a randomized estimator. Also, for any fixed sample size $n$, we can choose any block size $n_B$ and number of blocks $B$ to define a bMOM estimator, on contrary to the classical MOM, where the product of the block size with the number of blocks should be equal to the sample size. This will turn out to be precious in the clustering context, where we do not want too small sample block sizes in order to avoid disappearance of some clusters in the blocks.
We prove below that taking enough blocks in the definition of bMOM enables to perform a more robust estimation than with MOM and same block size, in the sense that the breakdown point of the bMOM is higher. This also provides an interest to bMOM compared to MOM for mean estimation in general. We leave as an interesting problem the question of sub-gaussian deviation bounds for mean estimation using bMOM.

2.2 Breakdown points

The breakdown point is a classical concept in the robust statistics literature ([11, 21]), that gives the maximal proportion of outliers that is allowed so that the deviations of the estimator stay bounded compared to the no-corruption setting. 

Assume that we are given a sample \( x_n = (x_1, \ldots, x_n) \) of real valued random variables.

**Definition 1** (Deterministic Breakdown point). The (deterministic) breakdown point \( \delta_n( T_n, x_1^n ) \) of an estimator \( T_n \) given the sample \( x_1^n \) is the maximal proportion of outliers that leave the value of the estimator bounded.

\[
\delta_n( T_n, x_1^n ) = \frac{1}{n} \max \left\{ m; \max_{i_1, \ldots, i_m} \sup_{y_1, \ldots, y_m} | T_n(z_{i_1}, \ldots, z_n)| < +\infty \right\},
\]

where the sample \((z_1, \ldots, z_n)\) is obtained by replacing the \( m \) data points \( x_{i_1}, \ldots, x_{i_m} \) of the sample \( x_1^n \) by arbitrary values \( y_1, \ldots, y_m \).

One can notice that Definition 1 corresponds to a worst case analysis, the outliers potentially appearing at the worst places for the estimator \( T_n \). If the estimator \( T_n \) is randomized - we rather denote it \( T_n^\omega \) in this case -, then its breakdown point is a random variable.

For a median \( \text{med} \), it holds \( \delta_n( T_n, x_1^n ) = \lfloor n/2 \rfloor / n \) and for the empirical mean \( \bar{x}_n = 1/n \sum_{i=1}^n x_i \), \( \delta_n( T_n, x_1^n ) = 1/n \). For the median-of-means estimator,

\[
\delta_n( \text{MOM}(x_1^n, b_B^n), x_1^n ) = \lfloor B/2 \rfloor / n \ a.s.,
\]

since it suffices to have one outlier in a majority of blocks to make MOM diverge. Note that [9, Section 4.2] proposes to automatically select the number of blocks of the MOM estimator by a Lepskii-type procedure that consists in choosing the smallest number of blocks such that the intersection of some confidence intervals constructed for MOM with greater number of blocks is empty. Then, it is easily seen that the resulting estimator will inherit from the value of the breakdown point corresponding to the highest number of blocks in the considered collection. If the highest number of blocks is \( n \), the sample size, thus corresponding to a median, then the method of intersection of confidence intervals gives an optimal value of breakdown point, corresponding \( \lfloor n/2 \rfloor / n \). However, computing such selection procedure is time consuming and as we want to make an iterative use of (bootstrap) MOM estimates, this method seems out of the scope for us. Instead, we show below that the use of replacements while constructing the blocks already gives an improvement of the breakdown point if enough blocks are considered, compared to the use of disjoint blocks when applied to median-of-means statistics.

**Proposition 2.** We have

\[
\delta_n( \text{bMOM}(x_1^n, n_B, B), x_1^n ) \leq \delta_n( \text{MOM}(x_1^n, b_B^n), x_1^n ) \ a.s.
\]

and

\[
\lim_{B \to +\infty} \delta_n( \text{bMOM}(x_1^n, n_B, B), x_1^n ) = 1 - \frac{1}{2^{1/n_B}} > \frac{1}{2n_B} \ a.s.
\]
Note that $1 - \frac{1}{2^{1/n_B}} \sim n_B \to +\infty \frac{\log 2}{n_B} \sim \frac{0.69}{n_B}$.

On the one hand, the first display in Proposition 2 states that when the number of blocks in bMOM is equal to the number of blocks in MOM, bMOM has a breakdown point that is smaller than or equal to the breakdown point of MOM (this is due to the possible repetitions of outliers along the blocks for bMOM). On the other hand, the second display in Proposition 2 states that for a fixed block size, when the number of blocks in bMOM tends to infinity, its breakdown point tends to a value that is strictly greater than the breakdown point of MOM with the same block size.

**Proof.** For the second display. Assume that the sample is corrupted by $m$ outliers. Denote $S_i$ the indicator that the block $B_i$ is not corrupted. Then $S_i$ is a Bernoulli random variable of mean $(1 - m/n)^{n_B}$. Then $\sup_{y_1, \ldots, y_m} |bMOM(x_1^n, n_B, B)|$ is finite if the proportion of corrupted blocks smaller than 1/2. This corresponds to the condition $\sum_{i=1}^B S_i/B > 1/2$. By the strong law of large numbers, the latter is almost surely realized asymptotically if $(1 - m/n)^{n_B} > 1/2$, hence the result.

Considering that the contaminated sample is fixed, it is interesting to evaluate the probability that a randomized estimator does not diverge under divergence of the outliers. It can indeed happen that the indices of the outliers are not the worst with respect to the block drawing process. This leads to the following definition.

**Definition 3** (Probabilistic Breakdown point). The probabilistic breakdown point of a randomized estimator $T_n^\omega$ given the sample $x_1^n$ is

$$p_n(T_n^\omega, x_1^n, (i_1, \ldots, i_m)) = P \left( \left\{ \omega : \sup_{y_1, \ldots, y_m} |T_n^\omega(z_1, \ldots, z_n)| < +\infty \right\} \right)$$

where the sample $(z_1, \ldots, z_n)$ is obtained by replacing the $m$ data points $x_1, \ldots, x_{i_m}$, for some fixed indices $(i_1, \ldots, i_m)$, by the arbitrary values $y_1, \ldots, y_m$.

As $p_n(bMOM(x_1^n, n_B, B), x_1^n, (i_1, \ldots, i_m))$ only depends on $n$ and $m$, but not on the values of $(i_1, \ldots, i_m)$ or $x_1^n$, we will rather denote it $p_n(bMOM(x_1^n, n_B, B), m)$. We have the following bound.

**Proposition 4.** It holds

$$p_n(bMOM(x_1^n, n_B, B), m) \geq 1 - \exp \left( -2B ((1 - m/n)^{n_B} - 1/2)^2 \right).$$

If $m$ and $n$ are fixed then the block length $n_B$ should be such that $(1 - m/n)^{n_B} > 1/2$, that is $n_B < \log(2)/\log((1 - m/n)^{-1})$. In this case, by denoting $D = (1 - m/n)^{n_B} - 1/2$, we have that $p_n(bMOM(x_1^n, n_B, B), m) \geq 1 - R$ is equivalent to $B > \log(1/R) / (2D^2)$.

**Proof.** As in the proof of Proposition 2 denote $S_i$ the indicator that the block $B_i$ is not corrupted. We have, by Hoeffding’s inequality ([4, Theorem 2.27]),

$$P \left( \left\{ \omega : \sup_{y_1, \ldots, y_m} |bMOM(x_1^n, n_B, B)| = +\infty \right\} \right) = P \left( \sum_{i=1}^B (1 - S_i) > B/2 \right) \leq \exp \left( -2B ((1 - m/n)^{n_B} - 1/2)^2 \right).$$

\[ \square \]
3 K-bMOM algorithm

This Section proposes an estimation procedure based on the MOM principle for clustering unlabeled data. Moreover, since the resulting partition of most of clustering approaches depends on the starting centers, we propose also a MOM-based initialization procedure.

Let us introduce the following notations. Let \( x_1, \ldots, x_n \in \mathbb{R}^p \) denote a dataset of \( n \) observations that we want to cluster into \( K \) homogenous groups. \( b \in \{1, \ldots, B\} \) stands for the index of a block \( b \) and \( B \in \mathbb{N}^* \) the number of blocks containing at least \( n_B > K \) datapoints. We define the empirical risk of the block \( b \) as:

\[
R_b(c) = \sum_{k=1}^{K} \sum_{i \in C_k(b)} \| x_i^{(b)} - c_k^{(b)} \|^2
\]

where \( x_i^{(b)} \) stands for the \( i \)th datapoint contained in the block \( b \), \( C_k^{(b)} \) stands for the set of datapoints belonging to cluster \( k \) in the block \( b \) and \( \| . \|^2 \) is the Euclidean norm. \( c_k^{(b)} \) stands for the mean vector of the cluster \( k \) in the block \( b \) and we denote by \( v_k^{(b)} \) its within variance. Finally, we denote by \( P(c) \) the partition obtained from the matrix of centroids \( c \).

A robust initialisation

It is well-known that since the clustering problem is non convex, then the initialisation step is a key step for the resulting partition. We propose therefore a robust variant of traditional initialisation strategies by applying the MOM principle. To do so, the idea is to build uniformly and with replacement \( B \) blocks of \( n_B \) datapoints where the number of points is strictly superior to the number of groups. In each block a traditional k-means++ initialisation \([2]\) is operated. Such an approach proceeds iteratively : it starts with a centroid picked at random among the datapoints. Then, iteratively and until the number of groups \( K \) is reached, a new centroid is chosen from the datapoints with a probability which increases exponentially with the distance \( D^2(x, c) \) to the closest centers already chosen. In each block, the empirical risk is therefore computed and the centers linked to the median empirical risk, called the median block, is selected as the initial centers.

We define the following algorithm :

**Algorithm 1 Initialisation strategy**

**Input:** the dataset \( \{x_1, \ldots, x_n\} \), \( B \) the number of blocks and \( n_B > K \) size of blocks

1. Iterate from 1 until \( B \) blocks:
   (a) Select at random, uniformly and with replacement \( n_B \) datapoints
   (b) Proceed a kmeans++ initialisation
   (c) Compute the empirical risk \( \hat{R}_b(c) \) of the block \( b \)

2. Select the centers from the block having the median empirical risk and get: \( \left( \hat{c}_{bmed}^{(1)}, \ldots, \hat{c}_{bmed}^{(K)} \right) \), \( \left( \hat{v}_{bmed}^{(1)}, \ldots, \hat{v}_{bmed}^{(K)} \right) \).

**Output:** \( \left( \hat{c}_{bmed}^{(1)}, \ldots, \hat{c}_{bmed}^{(K)} \right) \), \( \left( \hat{v}_{bmed}^{(1)}, \ldots, \hat{v}_{bmed}^{(K)} \right) \).
The $K$-bMOM algorithm

Due to the nature of the MOM principle and the clustering goal, the algorithm we propose alternates 3 main steps. At iteration $t$, and given the centers fitted in the median block of the previous iteration, $B$ blocks of $n_B$ data are built by uniform sampling with replacement. Then, a partition per block is computed by assigning each data point to its closest centroids fitted on the median block at $(t-1)$. The centroids of each block are updated according to their block partition and the empirical risk $\hat{R}_b(c)$ is returned. The block with the median empirical risk is selected and the fitted centers of this median block become the current ones. This is done until the empirical risk of the median block $\hat{R}_{b_{med}}(c)$ remains stable. The final partition on all the dataset is obtained by assigning each data point to its nearest closest centroid $(\hat{c}_1^{(med)}, \ldots, \hat{c}_K^{(med)})$ of the current median block.

A pseudo algorithm of this procedure is detailed in Algorithm 2.

Algorithm 2 Iteration phase structure
Input: $\{x_1, \ldots, x_n\}$, $B$ the number of blocks and $n_B$ size of blocks ($n_B > K$)
Initialisation step: Algorithm 1.
Set: $q = 0$ and $crit >> \varepsilon$.
Main Loop: while $crit > \varepsilon$ or $q < q_{\text{max}}$:
1. Create $B$ blocks of the data of size $n_B$ randomly and uniformly with replacement
2. In each block $b$:
   - Assign each datapoint to its closest centroid.
   - If $n_k^{(b)} \geq 1$, $\forall k \in \{1, \ldots, K\}$:
     - for $k \in \{1, \ldots, K\}$: $\hat{c}_k^{(b)} \leftarrow 1/n_k^{(b)} \sum_{i \in C_k^{(b)}} x_i^{(b)}$
     - $\hat{R}_b(c) \leftarrow \sum_{k=1}^{K} \sum_{i \in C_k^{(b)}} \|x_i^{(b)} - \hat{c}_k^{(b)}\|^2$
3. Get the median empirical risk $\hat{R}_{b_{med}}(c)$ and the associated quantities of the median block: $b_{med}$, $(\hat{c}_1^{(med)}, \ldots, \hat{c}_K^{(med)})$.
4. if $q > 2$:
   (a) $A^{(q)} \leftarrow (\hat{R}_{b_{med}}^{(q+1)} - \hat{R}_{b_{med}}^{(q)})/\hat{R}_{b_{med}}^{(q)} - \hat{R}_{b_{med}}^{(q-1)}$
   (b) $\text{crit} \leftarrow 1/(1 - A^{(q)})(\hat{R}_{b_{med}}^{(q+1)} - \hat{R}_{b_{med}}^{(q)})$
5. $q \leftarrow q + 1$
Output: $(\hat{c}_1^{(med)}, \ldots, \hat{c}_K^{(med)})$ and $P(\hat{c}_{med})$

Stopping criterion and convergence monitoring

In order to decide whether the algorithm has converged or not, we propose to use a criterion based on the Aitken’s criterion defined by $A^{(q)} = (\hat{R}_{b_{med}}^{(q+1)} - \hat{R}_{b_{med}}^{(q)})/(\hat{R}_{b_{med}}^{(q)} - \hat{R}_{b_{med}}^{(q-1)})$ where $\hat{R}_b^{(q)}$ is the empirical distortion computed on the median bloc at iteration $q$. Then asymptotic estimate of the empirical distortion maximum
is given by:

\[ R^{(q+1)} = R^{(q)} + \frac{1}{1 - A^{(q)}} \left( R^{(q+1)} - R^{(q)} \right) \]

and the algorithm can be considered to have converged if \( |R^{(q+1)} - R^{(q)}| < \varepsilon \) where \( \varepsilon \) is a small positive number (set to \( \varepsilon = 0.001 \)). In practice, if the criterion is not satisfied after a given number of maximum iterations, the algorithm is stopped.

Model selection

In model-based clustering, it is frequent to consider several models in order to find the most appropriate one for the considered data. In particular, for most of clustering algorithms, the model is specified by its number of clusters \( K \). There are lots of ad-hoc approaches in the literature to select the number of components \( K \) and we can therefore think of the Gap statistics from [24], the Silhouette criterion and so one. However, since the k-means algorithm can be seen as a hard version of an EM-like algorithm which tries to estimate a mixture of \( K \) Gaussians with isotropic covariance matrices, we can therefore apply classical tools for model selection including BIC, ICL criteria and the heuristic slope [3] for example. We can therefore use such criteria on the proposed robust version of the kmeans by processing the K-b-MOM on several values of \( K \), computing the chosen criterion for each model and select the model defined by its number of components which either maximizes the BIC or ICL criteria or follow the principle of the heuristic slope.

4 Simulations and practical considerations

4.1 Comparing initialisation strategies for the clustering task

It is well-known that the resulting partition of most clustering approaches such as for example the k-means or the Gaussian Mixture models, heavily depends on the starting centers. Therefore, a bad initialisation leads to a poor partitioning of the data. This is particularly true in the context of data with outliers where most of traditional and state-of-the-art initialisation techniques behave poorly in such a context. We propose in this section to apply the MOM principle to the most widely used initialisation methods among which kmeans++ and kmedians++. We evaluate and compare them to their traditional use.

These different strategies will be compared on simulated data in two different contexts of outliers: punctual, spread out outliers and a cluster of outliers.

Simulation contexts: The data are generated from \( K = 3 \) multivariate Gaussian distributions of dimension \( p = 2 \) and length \( n_1 = n_2 = n_3 = 300 \) with variance \( \sigma^2 = 0.6 \) and average vectors \( \mu_1 = [1, 4], \mu_2 = [2, 1] \) and \( \mu_3 = [-2, 3] \). Figure 1.a illustrates one realisation of the simulated context.

- **simulation 1:** punctual outliers. From these \( n = 600 \) datapoints, we randomly select \( n_{\text{outlier}} \) as potential outliers and their coordinates are multiplied by a constant term \( \beta \) which quantifies how far these outliers are from their own distribution. We consider different level of pollution of data \( n_{\text{outlier}} \in \{9, 27\} \) and different degrees of outliers \( \beta \in \{5, 20\} \). Figure 1.b illustrates the data polluted by \( n_{\text{outlier}} = 9 \) with degree \( \beta = 20 \).

- **simulation 2:** cluster of outliers. A cluster of outliers of size \( n_{\text{outlier}} \) is generated according to a 2-dimensional Gaussian distribution with average \( \mu_{\text{outlier}} = \beta[1, 1] \) and variance fixed to \( \sigma^2 = 1 \). Note
that, the size of the cluster of outliers varies among \( n_{\text{outlier}} \in \{9, 27\} \) and the level distance varies such that \( \beta \in \{5, 20\} \). Figure 1c illustrates the cluster of outliers with \( n_{\text{outlier}} = 9 \) and degree \( \beta = 5 \).

For all the methods, the number of clusters is supposed to be known and fixed to \( K = 3 \).

![Figure 1: Illustrations of simulated data generated according to a Gaussian Mixture Model in order to compare initialisation methods if the context of outliers](image)

**Initialisation strategies:** We consider the following 3 traditional initialisation strategies:

- **Random initialisation:** we select \( K \) datapoints randomly and without replacement as initial centers.

- **kmeans++** proposed by [2] which is maybe the most widely used technique to initialise clustering algorithm. The first center is taken from the data uniformly at random. Then iteratively and until the number \( K \) of chosen clusters is reached, a new center is chosen from the datapoints with a probability which increases exponentially with the distance \( D^2(x, c) \) to the closest centers already chosen.

- **kmedians++** is a variant of kmeans++. The same process is iterated but the probability is computed with respect to \( D(x, c) \) instead of \( D^2(x, c) \).

and a robust initialisation strategy developed by Hasan et al. in 2009 named ROBIN [3] which is a density-based approach:

- **ROBIN** (ROBust INitialisation) uses the Local Outlier Factor approach (LOF) [7] to select, as initial centroids, data points far away from each other and representative of dense regions in the dataset. This approach requires to know the number of clusters \( K \) and the number of neighboring data points in order to compute the LOF of each data point. In the experiment, the number of neighboring datapoints has been fixed to 10. According to the chosen method, selected datapoints changes drastically and it has to be noted that the best approach is obtained for the approximation method where the algorithm looks for the first LOF value that falls in \( [1 - \varepsilon, 1 + \varepsilon] \). We chose this method and set \( \varepsilon = 0.2 \).

We propose a robust variant of kmeans++ and kmedians++ by applying the MOM principle as described in Section 3. In particular, let \( B \) be the number of blocks of data, \( n_B \) the size of each block and \( \mathcal{R}_b(c) \) the empirical risk of the \( b \)th block. Then, we define the following algorithm:
1. Iterate from 1 until $B$ blocks:
   (a) Select at random, uniformly and with replacement $n_B$ datapoints
   (b) Proceed a $k$means++ (or $k$medians++) initialisation
   (c) Compute the empirical risk of the block $b$

2. Select the centers from the block having the median empirical risk

3. Affect the datapoints to their nearest centroid of the selected (median) block.

Note that the size of each block is chosen equal to 18 and the number of blocks is fixed to 250. These parameters follow the breakdown point bounds presented in Section 2.2.

For the rest of the paper, we will call K-bMOM-km++ (respectively K-bMOM-kmed++) the robust strategy based on k-means++ (respectively $k$medians++).

**Performance criteria:** In order to compare the different starting strategies in terms of performance, we compute 4 criteria:

- the Root Mean Square Error (RMSE) in order to evaluate the robustness of fitted centers once the initialisation step is performed. This criterion is calculated between the centers proposed by the initialisation process and the ones used to simulate the data, given by:
  \[
  \text{RMSE} = \sqrt{\frac{\sum_{k=1}^{K} \|\hat{c}_k - \mu_k\|^2}{K}}
  \]
  where $\hat{c}_k$ stands for the started center the most probable for the class $k$ and $\mu_k$ the average parameter of the $k$th mixture.

- the accuracy (acc) of the initial partition obtained by the nearest initial centers and computed on the non-polluted data. This is equivalent to a classification rate.

- the Adjusted Rand Index (ARI) computed between the partition obtained by the nearest initial centers and computed on the non-polluted data.

- the empirical distortion obtained at the end of the initialisation step and computed on the non polluted data:
  \[
  \hat{R} (\hat{c}) = \sum_{k=1}^{K} \sum_{x_i \in C_k} \|x_i - \hat{c}_k\|^2
  \]
  - the number of clusters obtained on the non polluted data named $nb$.

The experience has been repeated 300 times and for all these criteria, average and standard deviations have been computed for each initialisation method.

**Empirical Results for simulation 1:** The results of simulation 1 are summarized in Table 1.

As we can observe, except for the random approach which behaves roughly the same manner according to the different contexts, all the starting approaches behave quite well when the number of outliers is small ($n_{\text{outlier}} \leq 9$) and their distance level is low (cases $\beta = 5$): accuracies vary between 0.92 to 0.98. However, ROBIN and the K-bMOM based initialisation are the more stable approaches with a standard deviation
around 2 to 5% whereas the 3 other methods remains up to 8.4%. Besides, as soon as the context becomes harder (more outliers and further), only the K-bMOM approaches have their accuracies and ARI\'s unchanged whereas the performances of the 4 other methods decrease drastically.

The level of the RMSE computed on the initial centers depends on the strategy used: in particular, it remains under 1 in average for the kmedians++, ROBIN, K-bMOM-km++ and K-bMOM-kmed++ strategies when the simulated context is simple ($n_{\text{outlier}} = 9$, $\beta = 5$). As the distance level of outliers and the number of outliers increase, the kmeans++ strategy propose poor centers since at least one of them is stuck on an outlier. Indeed, its RMSE is up to 50 and the number of clusters fitted on the non polluted data is below the true number of components. The kmedians++ is more robust to outliers, by construction, but its performances decrease drastically when both the number of outliers and the distance level become higher ($n_{\text{outlier}} = 27$, $\beta = 20$). The RMSE becomes up to 30 and the accuracy is about 0.77. At the opposite, K-bMOM-km++ and K-bMOM-kmed++, well-perform in every contexts of simulations even when the number of outliers reaches 27 and the distance level 20. In average, the initialisation by K-bMOM-km++ is 95 % accurate at the end of the initialisation step and the proposed centers remain really close to theoretical ones (RMSE < 1 in average).

Finally, Figures 2 and 3 stand for violinplots of accuracies and distortions respectively for each initialisation method from the less noisy simulation context to the noisiest one. Several information are displayed in these violinplots: the interquartile range (black bold vertical line), the median (orange point), the percentile 95 (navy blue horizontal line) and the probability density of accuracies (resp. distortions) for each method. In the context ($n_{\text{outlier}}, \beta = (20, 27)$, one can observe the erratic behavior of ROBIN represented by the bimodal distribution of its accuracy: it is true that in median this approach reaches 95% of accuracy but 10% of the time, the initialisation present poor results (under 60% of accuracy) compared to K-bMOM which does not decrease below 65%. The same kind of observations can be done on the distortions (see Figure 3).

Finally, by combining the results in distortions and accuracies K-bMOM-km++ and K-bMOM-kmed++ are the initialisation procedures which performs the best in terms of stability and the accuracy of initial centers. They are totally insensitive to the distance of outliers with the rest of data and remain quite effective even when the number of outliers increases (around 3% of data in our context).

**Empirical Results for simulation 2:** The results of simulation 2 are summarized in Table 2.

Again, in this situation the random initialization is not as bad as we could expect in average, however such a starting approach is very instable as we can observe via its standard deviations. On the other hand, the standard initialization methods based on kmeans++ and kmedians++ (at least in accuracy) present comparable performances to their robust version for a low number of outliers (see case $n_{\text{outlier}} = 9$ for $\beta = 5$). This can be explained simply by the fact that the outliers are grouped together in the same area of the space and therefore kmeans++ and kmedians++ are going to chose started centers well-spread among the datasets by construction. However, when the number of outliers increases and so does their distance to the grouped data, then they are outperformed by their robust versions. Finally, Figure 4 stands for boxplots of all accuracies (left) and all RMSE (right) over the noisiest versions of the simulation context of a cluster of outliers which groups together $n_{\text{outlier}} = 27$ and $\beta = \{5, 20\}$. Again, the K-bMOM-km++ initialisation presents better and stable results in both accuracy and RMSE compared to the rest of methods.
| $n_{\text{outlier}}$ | $\beta$ | Initialisation | RMSE | accuracy | ari | distortion | nb |
|-----------------|--------|----------------|------|----------|-----|------------|----|
| 9               | 5      | random         | 1.738 (1.697) | 0.763 (0.133) | 0.564 (0.212) | 3399.1 (1785.4) | 3.0 (0.2) |
| 9               | 5      | kmeans++       | 2.538 (3.598) | 0.91 (0.13) | 0.84 (0.187) | 1559.1 (897.9) | 2.8 (0.4) |
| 9               | 5      | kmedians++     | 1.009 (1.365) | 0.95 (0.084) | 0.891 (0.141) | 1306.6 (619.8) | 3.0 (0.2) |
| 9               | 5      | ROBIN          | 0.951 (0.45)  | 0.973 (0.028) | 0.925 (0.063) | 1385.0 (326.3) | 3.0 (0.1) |
| 9               | 5      | K-bMOM-km++    | **0.457 (0.947)** | **0.988 (0.029)** | **0.968 (0.044)** | **790.0 (234.5)** | **3.0 (0.1)** |
| 9               | 5      | K-bMOM-kmed++  | **0.488 (0.815)** | **0.981 (0.053)** | **0.956 (0.088)** | **832.3 (342.3)** | **3.0 (0.1)** |
| 9               | 20     | random         | 2.432 (5.659) | 0.771 (0.143) | 0.58 (0.238) | 3421.4 (2079.7) | 3.0 (0.2) |
| 9               | 20     | kmeans++       | 54.734 (10.795) | 0.427 (0.147) | 0.141 (0.226) | 6807.2 (2869.2) | 1.3 (0.5) |
| 9               | 20     | kmedians++     | 7.884 (15.954) | 0.907 (0.13) | 0.835 (0.192) | 1593.5 (952.0) | 2.8 (0.4) |
| 9               | 20     | ROBIN          | 1.317 (3.876)  | 0.972 (0.037) | 0.924 (0.073) | 1412.3 (376.2) | 3.0 (0.1) |
| 9               | 20     | K-bMOM-km++    | **0.402 (0.162)** | **0.989 (0.009)** | **0.969 (0.026)** | **789.2 (150.7)** | **3.0 (0.0)** |
| 9               | 20     | K-bMOM-kmed++  | **0.393 (0.171)** | **0.987 (0.031)** | **0.966 (0.052)** | **801.5 (287.5)** | **3.0 (0.0)** |
| 27              | 20     | random         | 4.175 (9.975) | 0.752 (0.143) | 0.549 (0.229) | 3506.7 (1891.5) | 2.9 (0.3) |
| 27              | 20     | kmeans++       | 57.84 (7.832)  | 0.343 (0.05) | 0.012 (0.077) | 8810.5 (2902.3) | 1.0 (0.2) |
| 27              | 20     | kmedians++     | 31.532 (19.748) | 0.734 (0.156) | 0.604 (0.222) | 2782.4 (1378.7) | 2.2 (0.5) |
| 27              | 20     | ROBIN          | 25.71 (29.783) | 0.738 (0.289) | 0.585 (0.42) | 4199.2 (3936.4) | 2.3 (0.9) |
| 27              | 20     | K-bMOM-km++    | **3.361 (10.576)** | **0.951 (0.094)** | **0.903 (0.143)** | **1005.0 (507.3)** | **2.9 (0.3)** |
| 27              | 20     | K-bMOM-kmed++  | **4.786 (12.513)** | **0.934 (0.115)** | **0.882 (0.172)** | **1117.7 (677.9)** | **2.9 (0.3)** |

Table 1: Average (and standard deviation in parentheses) of accuracies and RMSE computed on 300 repetitions of the simulation 1 for the 6 proposed initialisation methods for different number of outliers and distance levels.

Figure 2: Violinplots of accuracies of 6 initialisation approaches according to the level of pollution of data in the context of punctual outliers. From the less noisy context (left) to the noisiest one (right).

Figure 3: Violinplots of distortions of 6 initialisation approaches according to the level of pollution of data in the context of punctual outliers. From the less noisy context (left) to the noisiest one (right).
| $n_{\text{outlier}}$ | $\beta$ | Initialisation | RMSE | accuracy | ari | distortion | nb |
|----------------|--------|----------------|------|----------|-----|------------|----|
| 9             | 5      | random         | 1.429 (0.663) | 0.791 (0.138) | 0.609 (0.226) | 3239.7 (1795.4) | 3.0 (0.1) |
| 9             | 5      | kmeans++       | 0.743 (0.307) | 0.962 (0.077) | 0.912 (0.122) | 1193.9 (464.1) | 3.0 (0.1) |
| 9             | 5      | kmedians++     | 0.777 (0.347) | 0.955 (0.077) | 0.896 (0.137) | 1239.6 (517.0) | 3.0 (0.1) |
| 9             | 5      | ROBIN          | 0.948 (0.161) | 0.97 (0.079) | 0.916 (0.074) | 1437.3 (369.1) | 3.0 (0.1) |
| 9             | 5      | K-bMOM-km++    | 0.368 (0.141) | 0.99 (0.008) | 0.971 (0.023) | 772.6 (125.5) | 3.0 (0.0) |
| 9             | 5      | K-bMOM-kmed++  | 0.376 (0.197) | 0.987 (0.034) | 0.965 (0.06)  | 790.8 (244.6) | 3.0 (0.0) |
| 9             | 20     | random         | 1.4 (0.608)   | 0.771 (0.131) | 0.582 (0.211) | 3220.1 (1577.0) | 3.0 (0.2) |
| 9             | 20     | kmeans++       | 1.058 (0.608) | 0.666 (0.039) | 0.513 (0.074) | 3280.9 (779.8) | 2.0 (0.1) |
| 9             | 20     | kmedians++     | 0.795 (0.32)  | 0.94 (0.098) | 0.877 (0.152) | 1359.4 (648.8) | 2.9 (0.3) |
| 9             | 20     | ROBIN          | 0.921 (0.132) | 0.974 (0.032) | 0.928 (0.066) | 1401.6 (348.9) | 3.0 (0.1) |
| 9             | 20     | K-bMOM-km++    | 0.37 (0.147)  | 0.989 (0.011) | 0.969 (0.029) | 772.3 (141.8) | 3.0 (0.0) |
| 9             | 20     | K-bMOM-kmed++  | 0.359 (0.132) | 0.99 (0.007) | 0.971 (0.02)  | 763.5 (106.7) | 3.0 (0.0) |
| 27            | 20     | random         | 1.455 (0.705) | 0.755 (0.137) | 0.552 (0.22)  | 3656.2 (2096.8) | 2.9 (0.3) |
| 27            | 20     | kmeans++       | 0.962 (0.552) | 0.661 (0.019) | 0.506 (0.059) | 3264.6 (756.5) | 2.0 (0.0) |
| 27            | 20     | kmedians++     | 0.925 (0.494) | 0.807 (0.156) | 0.707 (0.214) | 2179.2 (1084.5) | 2.5 (0.5) |
| 27            | 20     | ROBIN          | 2.036 (1.295) | 0.38 (0.115)  | 0.068 (0.17)  | 8219.6 (2931.6) | 1.1 (0.3) |
| 27            | 20     | K-bMOM-km++    | 0.548 (0.354) | 0.94 (0.108)  | 0.89 (0.161)  | 1106.5 (652.8) | 2.9 (0.3) |
| 27            | 20     | K-bMOM-kmed++  | 0.658 (0.429) | 0.893 (0.141) | 0.821 (0.207) | 1329.6 (762.6) | 2.8 (0.4) |

Table 2: Average (and standard deviation in parentheses) of RMSE, accuracies, distortions and number of clusters computed on 300 repetitions of the simulation 2 for the 6 proposed initialisation methods for different number of outliers in the cluster of outliers and different distance levels.

Figure 4: Violinplots of accuracies of 6 initialisation approaches according to the level of pollution of data in the context of cluster of outliers. From the less noisy context (left) to the noisiest one (right).

Figure 5: Violinplots of distortions of 6 initialisation approaches according to the level of pollution of data in the context of cluster of outliers. From the less noisy context (left) to the noisiest one (right).
**Conclusion:** We showed in this Section that it seems therefore preferable to use the robust version of popular initialization methods whatever is the context (with or without outlier).
4.2 Discussion about the selection of hyperparameters linked to blocks

The good behavior of our algorithm with respect to outliers is linked to an appropriate choice of the size of blocks \( n_B \) and the number of blocks \( B \). For a known level of noise, we are able to compute lower and upper bounds respectively for the within-block size and the number of blocks as presented in Section 2.2 enabling therefore to guide the practitioner. However, when the number of outlier is unknown, it is important to propose a heuristic which selects automatically the size of the blocks \( n_B \).

The proposed strategy is the following: the within block size varies a priori from \( K \) to \( n/K \) at its maximum and for each level of within block size, the empirical risk of each block is computed and the median one is kept and plotted. We choose \( n_B^* \) the level of the size block linked to a cutting-point of the curve. Indeed, as the within block size increases the likelihood of picking an outlier in the block and among all \( B \) blocks increases and this should drastically impact the empirical risk of the median block, hence the search of breakpoints in this empirical risk.

In order to illustrate such a strategy, we consider a 2-dimensional Gaussian mixture models of \( K = 3 \) components with equal size \( n_1 = n_2 = n_3 = 300 \). The mean vectors are set to \( \mu_1 = [3, 12] \), \( \mu_2 = [6, 3] \) and \( \mu_3 = [-6, 9] \) and the variance parameter is set to \( \sigma^2 = 0.6 \). Twenty outliers are selected randomly from the data and their coordinates are multiplied by 50. We look for 2 situations where we fix the number of blocks to \( B = 50 \) and \( B = 100 \).

Figure 6, Figure 7, and Figure 8 depict respectively the evolution of the median empirical risk, the number of outliers present in the median block and the Adjusted Rand Index (ARI) computed on the partitionning of data obtained by the nearest centroid selected in the median block, according to the number of data in the blocks.

We get \( n_B^* \leq 25 \) for both cases as we can observe the evolution of the empirical risk of the median block in Figure 6a. for the case with a number of blocks \( B = 50 \) and in Figure 6b. for the case \( B = 100 \).

Note that the selection of \( n_B^* \) works well in both examples and the associated clustering seems also good. Indeed, under the selected \( n_{B=50}^* = 20 \) and \( n_{B=100}^* = 25 \), there is no outlier present in the median block and the resulting partitionning of data is perfect on the non polluted data (ARI = 1). Above this cutting-point, the number of outliers in the median block increases with the within block size whereas the ARI index decreases.

These results show that, in practice, if one chooses a small size of blocks and a high number of blocks, then the initialisation step is likely to be robust.
Figure 6: Evolution of the empirical risk of the median block for $B = 50$ blocks (left) and $B = 100$ blocks (right).

Figure 7: Evolution of the number of outliers selected in the median block for $B = 50$ blocks (left) and $B = 100$ blocks (right).

Figure 8: Evolution of the ARI obtained by the partitioning associated the median block for $B = 50$ blocks (left) and $B = 100$ blocks (right).
4.3 Benchmark among the robust kmeans-based algorithms

The objective of that section is to compare the performance of the K-bMOM strategy with the robust clustering algorithms based on k-means approaches on a framework with outliers. To do so, we dispose of \(N = 1500\) points of dimension \(p = 3\) which are generated according to a mixture of \(K = 5\) multivariate Gaussian density functions with isotropic covariance matrix. The average vectors for the 5 components are respectively \(\mu_1 = [0, 1, 4], \mu_2 = [2, 1, 0], \mu_3 = [0, -2, 3], \mu_4 = [0, 5, -5]\) and \(\mu_5 = [-1, -2, 0]\). An example of data generated according to this framework is displayed in Figure 9a. Outliers have been generated by randomly taken 30 datapoints from which their coordinates have been multiplied by a factor of +/-10, An example of the final polluted data are illustrated in Figure 9b.

Given this context, three variations from this framework have been considered in this Section:

Variation 1 The clusters have equal size and dispose of the same spherical covariance matrix. These assumptions are well-suited for the k-means procedure.

Variation 2 The clusters have unequal size but dispose of the same spherical covariance matrix.

Variation 3 The clusters have unequal size and dispose of different scaling parameters.

Simulation parameters for each of these variations are detailed below:

| variation | size | scaling parameter : \(\sigma_k^2\) |
|-----------|------|----------------------------------|
| 1         | \(\forall k \in \{1, \ldots, 5\} : n_k = n = 300\) | \(\forall k \in \{1, \ldots, 5\} : \sigma_k^2 = \sigma^2 = 0.6\) |
| 2         | \(n_1 = 300, n_2 = n_5 = 100, n_3 = 400, n_4 = 600\) | \(\forall k \in \{1, \ldots, 5\} : \sigma_k^2 = \sigma^2 = 0.6\) |
| 3         | \(n_1 = 300, n_2 = n_5 = 100, n_3 = 400, n_4 = 600\) | \(\sigma_1^2 = \sigma_4^2 = 1, \sigma_2^2 = 0.4, \sigma_3^2 = 0.6, \sigma_5^2 = 0.5\) |

These variations have been repeated 50 times and each time, the kmeans-based algorithms have been initialized in the same manner with a kmeans++ procedure iterated 10 times.
We consider 6 different algorithms: our proposed robust clustering algorithm based on MOM principle, a variant and also, 4 well-known robust versions of the k-means. These methods are described below:

**K-bmom** k-mom algorithm introduced in Section 3.

**Block-k-mom** $B$ blocks of $n_B$ data are randomly selected with replacement. In each block, a k-means is processed initialized with a kmeans++ strategy and the block with the median empirical distortion is selected to define the centroids and therefore the final partition of data.

These $k$-MOM type approaches are compared to the traditional k-means algorithm and 4 other robust kmeans approaches well-known in the literature such as:

**k-medoids** aims at finding $k$ data points as centers such as the within inertia is minimized. The partition around medoids algorithm named PAM [13] aims to achieve this in two steps: an assignment step where each datapoint is assigned to its closest medoid; a refinement step which looks for better medoids than the current ones. The search is each time exhaustive in the data PAM has a complexity dominated by $O\left(n^2kp\right)$. Faster versions have been proposed in [23]. The number of clusters $K$ needs to be set in the procedure.

**k-medians** is a robust variant of the $k$-means algorithm [12]: in the aggregation step, instead of computing the barycenter of each group ad in the $k$-means procedure, the $k$-medians compute in each single dimension the median in the Manhattan-distance formulation. This makes the algorithm more reliable for outlier for extreme values. The number of clusters $K$ needs to be specified by the practitioner.

**trimmed-kmeans** (Trim-km) implementation is an EM-like algorithm introduced by [8] in the late 90s. It is derived from the $k$-means and benefits robustness properties from the trimming action during the maximisation step where only a proportion $1 - \alpha$ of the closest data point from their assigned centroid is taken into account. Since the trimming needs to sort the data points according to their distance to centroid, it leads therefore to an overall complexity of $O\left(nkp + n \log n\right)$ at each iteration. Besides, note that in practice, the user needs to choose a value for the number of datapoints to be discarded and no practical information is given to calibrate such an hyperparameter. In the simulations, $\alpha$ is set to the true value of the number of outliers ie $n_{\text{outlier}}$. A more general framework has been proposed by [Brecheteau, Fisher and Levrard]. They extend the previous trimming approaches to the general framework of clustering with Bregman divergences. They propose a Lloyd-type algorithm with a trimming parameter $\alpha$ which is automatically selected from sample by a heuristic using the notion of breakdown point.

**k-PDTM** is a robust quantization algorithm introduced by [5, 6] that aims to infer the manifold from which the data points are drawn. This inference is done by means of $K$ centroids that should be on the manifold if the algorithm runs well. It is based also on a Lloyd-type algorithm where in the updating step, the centroid is computed as the barycenter of the $q$ nearest neighbours of the barycenter of the cluster. In the assignement step, the data point is assigned according to a Bregman divergence. This algorithm has two hyperparameters: $q$, the number of neighbors used to compute the centroid and the number of clusters $K$.

Finally, by default, for all the proposed methods having the number of clusters as hyperparameter, we set it to its true value ie $K = 5$. 
In order to compare the performances of these algorithms, the distortion and the Adjusted Rand Index (ARI) have been computed based on the true parameters of data distribution and their label membership. Moreover, the average number of clusters found among the non polluted data have also been displayed.

Results and Analysis

The results of 3 simulated contexts presented above are summarized in Tables 3a, 3b and 3c where averages and standard deviations of distortion, ARI and number of clusters describing the non polluted data are displayed. Besides, the whole distribution of 50 repetitions for each metric and tested algorithm are illustrated according to violinplots in Figures 10a, 10b and 10c where the median of each distribution is depicted by an orange dot and the interquartile range by a thick black vertical line.

First of all, one can observe that the k-means, k-median and k-medoids methods fail to discover the right number of clusters among the non polluted data. Indeed, in average the outliers are grouped in 2 clusters and the rest of the data in 3 instead of 5 groups in the first case as it is illustrated in Table 3a. On the violinplot in left side Figure 10c we can observe that none of these 3 procedures is able to find the real structure of data: the maximum number of clusters found on the non polluted data is about 4. This is mainly due to the initialisation process via the kmeans++ procedure which instantiates the algorithm on one or two outliers. Thus, the Lloyd type algorithm whatever is the aggregation method used, is stucked in a local minima. This situation gets worse in cases 2 and 3 since all 3 centers among 5 are located towards outliers as one can see in Table 3b and Table 3c but also on the middle and right side of Figure 10c where the associated violinplots can be summarized by a point. The cluster assignment in the last context for the kmedians procedure is depicted in Figure 11a.

By looking at the number of clusters found among the non polluted data, trimmed k-means and k-pdtm algorithms seem to have a better behavior. They tend to find the intrinsic structure all the times (5 clusters) whatever is the situation considered since the average number of clusters found among the non polluted data is around 4.9 in average with a very low standard deviation. However, the relevance of the data grouping decreases with the complexity of the simulated situation and is really dependant of the algorithm. Indeed, for the 3 simulated contexts, trimmed-k-means dispose of an average ARI about 0.60 and an average distortion which is quite huge and reaches approximately 12000 ie 6 times more than k-pdtm distortion and twice more than kmeans distortion as we can observe in Tables 3a, 3b and 3c. The cluster assignment in Figure 11b illustrates the failure of the algorithm to discover the true partition of data.

On the other side, the ARI for k-pdtm reaches in average 0.88 in Table 3a. Moreover, on the associated violinplot in the left side of Figure 10a we can see that this method is really performant since 50% of the time (the median is represented by an orange dot), the ARI on the non polluted data is perfect and equals to 1 and the empirical distortion is low. However, the performance of this method decreases and becomes more erratic as the complexity of the situation increases. As we can observe in the middle and left side in Figure 10a the median ARI is as the same level as the average one which is about 0.71 and the distribution of ARI are spread almost uniformly between 0.2 and 1. An example of cluster assignment resulting from the k-pdtm procedure after 300 iterations is depicted in Figure 11c.

Finally, even if the average performance tends to slowly decrease according to the different situations, both robust versions based on the MOM principle perform well in the presence of outliers. Indeed, the intrinsic structure is almost all the time found in the easiest context (Case 1) as the ARI, the distortions and the number of clusters show it. The average ARI is up to 0.98 for the K-bmom algorithm with a standard deviation around 0.03 whereas the ARI of the Block-k-mom version reaches almost 0.97. For both algorithms
the ARI median reaches 1 as it is illustrated in the left hand side of Figure 10a. In the same manner, the
distortion is slightly better and more stable for the K-bmom algorithm than the Block-k-mom version as it
can be observed in Table 3a and Figure 10b. This remark remains true for the more complex contexts where
the distortion is more favorable for the K-bmom algorithm both in average, in medians and in variation.
In the less constraint context (case 3), the K-bmom algorithm outperforms the rest of approaches even if it
remains less stable than in the easiest simulated context as it can be seen in the right-hand side and left hand
side of Figure 10a.

To conclude, this work provides a benchmark of robust k-means-based clustering algorithms. Although it
is still necessary to test their performances on other different settings, our simulations give a preliminary
overview of performances of using MOM principle in clustering context.

Though the algorithmic principle of K-bMOM is the simplest one one can think of when merging the
Lloyd’s algorithm and the Median-Of-Means design, it has good performances compared to already known
robust k-means based algorithm in the presence of outliers.

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| methods       | ari (std)       | distortion (std) | nb groups (std) |
|---------------|-----------------|------------------|-----------------|
| k-means       | 0.427 (0.185)   | 7236.4 (1677.8)  | 2.56 (0.49)     |
| k-pdtm        | 0.879 (0.176)   | 2168.5 (1263.9)  | 4.90 (0.36)     |
| trim-km       | 0.598 (0.110)   | 14456.5 (8554.6) | 4.84 (0.36)     |
| k-median      | 0.351 (0.151)   | 12066.5 (3859.1) | 2.52 (0.50)     |
| k-medoids     | 0.418 (0.178)   | 7688.4 (1889.1)  | 2.56 (0.49)     |
| K-bmom        | 0.982 (0.034)   | 1990.9 (164.2)   | 4.98 (0.14)     |
| block-k-mom   | 0.967 (0.076)   | 2189.2 (828.6)   | 4.96 (0.19)     |

(a) Case 1: equal cluster size and same covariance matrix ($\forall k, n_k = n$ and $\sigma_k = \sigma$)

| methods       | ari (std)       | distortion (std) | nb groups (std) |
|---------------|-----------------|------------------|-----------------|
| k-means       | 0.529 (6.6e-16) | 5879.8 (13.1)    | 2.00 (0.0)      |
| k-pdtm        | 0.704 (0.246)   | 2734.4 (1265.4)  | 4.88 (0.32)     |
| trim-km       | 0.626 (0.184)   | 12352.3 (12304.9)| 4.94 (0.24)     |
| k-median      | 0.530 (0.002)   | 8309.3 (971.0)   | 2.00 (0.0)      |
| k-medoids     | 0.529 (6.6e-16) | 5980.7 (24.9)    | 2.00 (0.0)      |
| K-bmom        | 0.863 (0.131)   | 2263.7 (419.6)   | 4.94 (0.27)     |
| block-k-mom   | **0.914 (0.102)** | 2544.0 (789.3)   | 4.78 (0.41)     |

(b) Case 2: unequal cluster size but same covariance matrix ($\forall k, \sigma_k = \sigma$)

| methods       | ari (std)       | distortion (std) | nb groups (std) |
|---------------|-----------------|------------------|-----------------|
| k-means       | 0.529 (6.6e-16) | 5881.7 (15.1)    | 2.0 (0.0)       |
| k-pdtm        | 0.655 (0.257)   | 2948.5 (1369.4)  | 4.92 (0.27)     |
| trim-km       | 0.570 (0.197)   | 12336.3 (11705.1)| 4.94 (0.23)     |
| k-median      | 0.530 (0.001)   | 8561.9 (1986.6)  | 2.0 (0.0)       |
| k-medoids     | 0.529 (6.6e-16) | 5981.9 (33.4)    | 2.0 (0.0)       |
| K-bmom        | **0.922 (0.122)** | **2114.2 (454.4)** | **5.0 (0.0)**  |
| block-k-mom   | 0.879 (0.111)   | 2776.6 (841.4)   | 4.8 (0.44)      |

(c) Case 3: unequal cluster size and different spherical covariance matrix among clusters.

Table 3: Distortions, ARI and number of clusters represented in the dataset without outliers averaged among 50 repetitions of the k-means-based approaches and their standard deviation according to 3 frameworks.
Figure 10: Violinplots of different metrics computed on 50 repetitions of 6 kmeans-based algorithms according to 3 frameworks. The median of each distribution is depicted by an orange dot and the interquartile range by a thick black vertical line.
Figure 11: Examples of cluster assignment according to several procedures in the more complex simulation case (unequal cluster size and unequal scaling parameter in the covariance matrix). Note: Outliers have been removed from the pictures to ease the interpretation.
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