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B3: An efficient approximation to the K-means clustering for massive data

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Contents

Chapter 1

Introduction

This project consists on the implementation of the paper [1], which was developed by Marco Capó and Aritz Pérez and Jose A. Lozano in the Knowledge-Based Systems journal. The paper aims to approximate the performance of KMeans, one of the most widely used clustering methods for massive datasets, while reducing the number of distance computations required to achieve a good clustering solution. The solution proposed by the authors is based on the recursive partition of the dataset following an heuristic that they call Recursive Partition based K-Means.

1.1 Definitions

In their paper, the authors start by defining mathematically a partition, subset and the cardinality of the subset and the center of mass. They define a partition P as a collection of disjoint subsets S which the union of them results in the whole dataset D. They define the weight of the subset as the cardinality of it $|S|$ and the center of mass as the mean of all the points in the subset $\bar{S} = \frac{\sum_{x \in S} x}{|S|}$.

1.2 Proposed solution

The solution proposed by the authors uses partitions as the units for fitting weighted Lloyd algorithms instead of using the data points from the dataset. The dataset is split into subsets each of them is represented by a representative sample and the cardinality of the subset.

The authors propose to divide the space where the dataset lies and partition it recursively using a quadtree, where the entire space of the subset is divided into 2^d subspaces. In a $2D$ space, the plane would be divided into quadrants, then each of the quadrants would be divided into 4 "subquadrants" and so on. Thanks to kthis heuristic, the number of elements is controlled, always satisfying $|P| < n$ or in other words, that the length of the partition ant every given moment is smaller than the number of instances in the dataset.

In 1.1 we show a $2D$ gaussian mixture with 3 gaussian and an overlap of 5%. Each partition has the subsets in different colors to be able to discriminate them easily. Each partition contains subsets thinner than the previous one, and the subsets of the partition P_{i+1} are generated by spliiting subsets from the partition P_i. The authors define that a partition P_i is thinner than P_j if every subset of P_i can be written as the union of subsets of P_j which applies in the case of the RPKM algorithm.

The authors propose an approach where for each one of the partitions mentioned above, a weighted Lloyd (WL) algorithm is trained and the centers extracted in each of the iterations is used

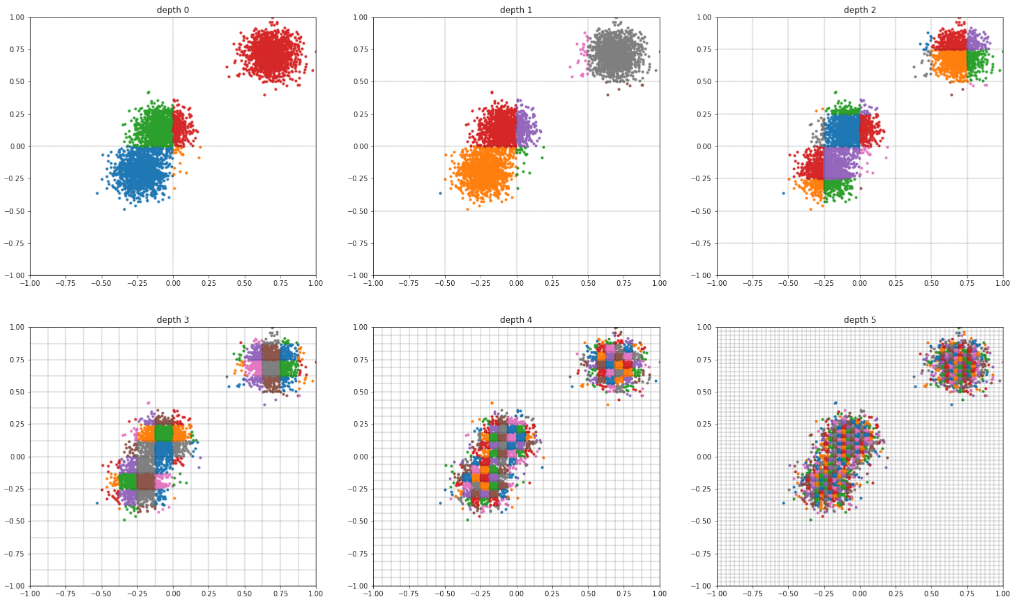


Figure 1.1: Partition example for a 2d gaussian mixture

as initialization for the next partition. This drastically reduces the number of distance computations that the algorithm realizes as the number of representative samples that will be used to fit the WL algorithm is always smaller than n.

```
**Algorithm 1:** WL algorithm
  **Input:** Set of representatives $\{\bar{S}\}_{S \in P}$ and weights $\{|S|\}_{S \in P}$, for the partition $P$. Number
         of clusters K and initial set of centroids $C_0$.
  **Output:** Set of centroids $C_r$ and the Corresponding clustering pattern $G_r$
  $G_0 \leftarrow C_0; r = 0;$
  **while** *not Stopping Condition* **do**
      $r = r + 1;$
      $C_r \leftarrow G_{r-1};$
      $G_r \leftarrow C_r;$
  **end**
  **return** $C_r$ *and* $G_r$
```

The weighted Lloyd algorithm is shown in 1 and it shows that given a set of representatives, a set of weights, a number of clusters and an initial set of centroids C_0, it iteratively improves the centers by assigining the weighted mean of all the instances in a group or cluster as their centroid and then computing the group of each instance as the center index that is closer to each instance.

```
Algorithm 2: RPKM algorithm
Input: Dataset D, number of clusters K, maximum number of iterations m
Output: Set of centroids approximation $C_i$
Compute the set of weights and representatives of the sequence of thinner partitions,
  $P_1, \dots, P_m$, backwards. ;
i := 1;
while not Stopping Criterion do
    Update the centroid's set approximation, $C_i = \{c^i_j\}_{j=1}^K$:
      $C_i = WL(\{\bar{S}\}_{S \in P_i}, \{|S|\}_{S \in P_i}, K, C_{i-1})$;
    $i = i + 1$
end
return $C_i$
```

The RPKM algorithm is exposed in 2. In the algorithm we can appreciate that the autors compute all the weights and representatives for the given dataset D and then iteratively update the centers for each iteration by performing a WL computation on the representative samples and cardinality of the subsets. Additionally, they use the cluster centers from the previous RPKM iteration as initialization.

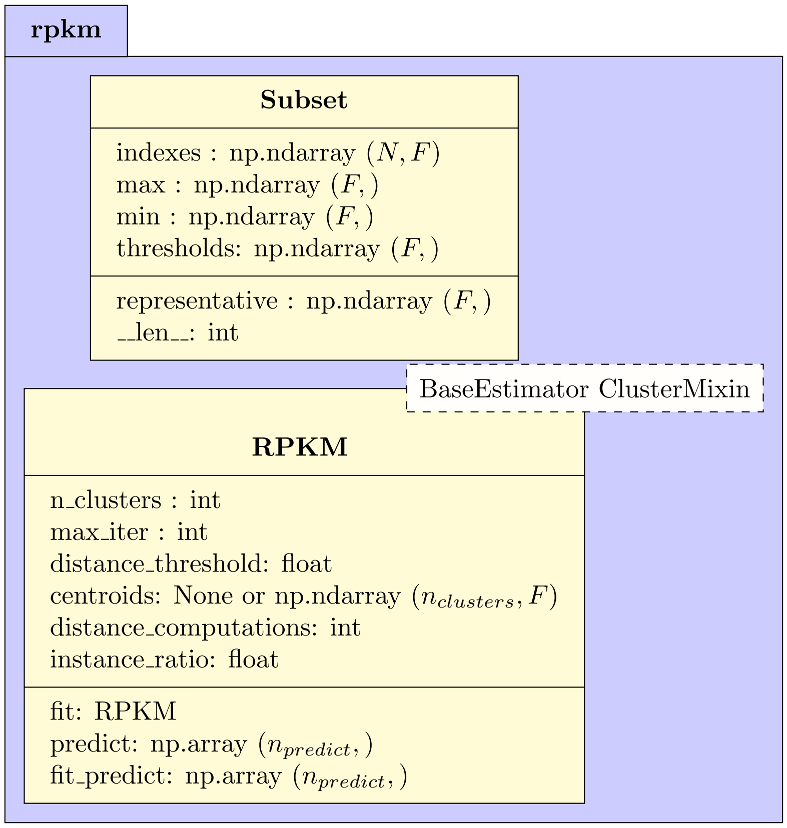
Both algorithms hav similar stop criteria, a threshold on the distance between the centers of the previous and new iteration and a maximum number of iterations. However, the authours have removed the distance limitation in their implementation in order to see the effects of the algorithm fully.

Chapter 2

Implementation

2.1 Implementation

The algorithm was created in python 3 using scikit-learn coding guidelines and API conventions. The Classes will be defined as shown in 2.1 UML diagram.


rpkm
Subset
indexes : np.ndarray (N, F)
max : np.ndarray $(F,)$
min : np.ndarray $(F,)$
thresholds: np.ndarray $(F,)$
representative : np.ndarray $(F,)$
__len__: int
BaseEstimator ClusterMixin
RPKM
n_clusters : int
max_iter : int
distance_threshold: float
centroids: None or np.ndarray $(n_{clusters}, F)$
distance_computations: int
instance_ratio: float
fit: RPKM
predict: np.array $(n_{predict},)$
fit_predict: np.array $(n_{predict},)$

Only the public methods are specified in the diagram. N in the diagram represents the number of instances in a subset. The F value indicates the number of features in the dataset. $n_{predict}$ represents the number of instances to be predicted in the inference dataset.

2.2 Subset

Subset would be a struct in other programming languages but in python it is defined as a class. The class contains:

1. **The indexes of the original data in this subset.** This is done in order to store pointers to a data structure instead of cloning the memory on the numpy arrays, as for massive datasets this can lead to memory issues.
2. **The minimum and maximum range** per each of the dimensions on the dataset and the thresholds used to build the next partition from this subset.
3. The threshold t is defined as the value that divides the range in to equal size subspaces for each dimension $\overrightarrow{t} = \frac{\overrightarrow{max}+\overrightarrow{min}}{2}$.
4. A method to compute the **cardinality**. In this case python's __len__ method is used to return the length of the index array.
5. A method to compute the **representative** for the cluster. As mentioned before, this is computed as the mean of the instances in the subset. The *np.mean* function was used to perform the operation effectively.

The Subset class has been created to follow an obejct oriented approach to the data structures.

2.3 RPKM

The RPKM algorithm was implemented in another class which inherits from *sklearn's BaseEstimator , ClassifierMixin and ClusterMixin* classes. The *BaseEstimator* is the main base class that all sklearn estimators inherit from. it provides parameter setters and getters for the class as well as a string representation of the class as well as some utility methods.

1. **set_params(**params)**: Set the parameters of this estimator.
2. **get_params()**: Get parameters for this estimator.
3. **__repr__()**: String representation of the estimator
4. **_validate_data(X)**: Validate input data and set or check the *n_features_in_* attribute, also of BaseEstimator.

The ClassifierMixin provides methods for all classifiers in the scikit-learn package. It implements the **score(X, y)** method to predict the labels for the data X and then compute the accuracy wrt y.

The ClusterMixin provides methods for all clustering methods in the scikit-learn package. It implements the **fit_predict(X, y=None)** method to fit the estimator and return the labels for the training data.

In the following subsections we will explain parts of RPKM's fit method that implements the method described by the authors to recursively partition the feature space into hypercubes.

2.3.1 fit

The fit method is the responsible of computing the partition and it's subsets for each RPKM iteration and apply a WL algorithm in every step. The algorithm in pseudocode is presented in 3.

Algorithm 3: RPKM Fit

```
Input: Dataset D, number of clusters K, maximum number of iterations m
Output: Self
reset centers;
Initialize $P_0 = \{D\}$;
i := 0;
while $i < m$ do
    create next partition (_create_partition);
    compute $R$ and cardinality of the subsets (_compute_partition_meta);
    if $|P_i| < K$ then
        there are not enough partitions to initialize clusters.;
        continue;
    else if centroids not initialized then
        choose K random representatives as cluster centers;
    else if $|P_i| >= K$ then
        there are as many subsets as samples, no point in continuing.;
        break;
    update clusters with WL (_cluster);
    i += 1;
end
return Self
```

The fit algorithm contains the main loop for the RPKM algorithm. One notable difference between the proposal of the authors and the implementation presented in this work is the change in the partition creation. The authors propose the creation of the partitions outside of the loop, creating always m partitions of the dataset. The method proposed here is to generate only the partitions that we require by integrating the creation of the partitions in the while loop. By doing this we are only computing the partitions that are required for the run (in case we reach the number of instances earlier than the iteration m).

The fit method calls internally to 3 methods: **_create_partition(X, partition)**, **_compute_partition_meta(X, partition)**, and **_cluster(R, cardinality)**. Each of the methods will be now explained.

2.3.2 _create_partition

The create partition method is the one reponsible of, given a list of sets that constitute a partition, perform a binary partition on each subset and create a list containing the new subsets. For the sake of brevity, the binary partition methodology will be explained in this section.

The binary partition method segments the data given as an input that constutes a subset S of the previous iteration's partition P_{i-1}. The subsets are created by taking the input data and a set of thresholds defined as the values that partition a dimension in two equally sized hypercubes. This operation is done for each of the dimensions in the dataset. The operation is performed by the following numpy operation:

```
comps = X > subset.thresholds[None, :]
```

This operation will generate a numpy matrix with boolean values with shape (n_{subset}, n_{dim}) where each row will contain the binary representation of a numerical index assigned to each hypercube. This matrix will be converted to an array of integer indexes containing the assignation of each of the elements to a subset. The conversion from binary to int is performed by the *np.packbits* method.

After the indexes are computed, the subsets initialized using the Subset struct described above, where the min, max and threshold arrays are modified to suit the new subset's instances. The range is modified in the following way:

If the binary representation for the cluster integer value has the value 1 in a dimension position, it means that the comparison performed before was true, so all instances are in the positive half of the spatial partitions. Because of that, the minimum for that dimension is updated to be the threshold value for that dimension. On the other hand, if the value is 0 for that dimension, the max for that dimension is set to be the threshold value for that dimension. Then the threshold values are updated to be the mean between the min and the max arrays. The subsets are then returned for the create partition function to concatenate them all and build the new partition.

2.3.3 _compute_partition_meta

The compute partition meta method is responsible for the generation of the representatives for each subset in the partition as well as the cardinality values for each subset. This method initializes the R vector to be of shape $(n_{subsets}, n_{features})$ and the cardinality array to be of shape $(n_{subsets},)$. Once the arrays are initialized it procedes to populate the arrays with the result of the **representative** function of the Subset class and the length of the Subset class respectively.

2.3.4 _cluster

The cluster method is in charge of updating the centroids of the RPKM algorithm by fitting a WL algorithm with the representatives as data points and the cardinality of the subsets as the weights. In the implementation, *scikit-learn's KMeans* object was used with the *n_iter* parameter set to 1 and giving as argument the weights into the fit method. It's also important to note that KMeans supports Lloyd's algorithm as well as Elkan optimization. In order to ensure the usage of Lloyd's algorithm, the *algorithm* parameter must be set to *full*. As initialization for the KMeans algorithm, the centroids of the previous RPKM iteration are passed. After the algorithm is fitted, the cluster centers are extracted by accessing the *cluster_centers_* attribute of KMeans.

2.4 fit results

Once the implementation was done, we demonstrate the operation of the algorithm. We will use a 2 dimensional gaussian mixture with 3 gaussian distributions. The RPKM algorithm was performed with the max iterations of $m = 6$. On the first figure 2.1 we represent the creation of the partitions. where the dataset comprised in the range -1, 1 for both dimensions. In the first iteration, the subsets are the 4 quadrants of the subspace, on the next iteration, each quadrant is divided in 4, and so on. We represent each subset with different colors for better interpretability.

In the next figure 2.2 we represent the data in light gray, the representative sampels for each of the subsets in black and the centers with more vivid colors.

Finally, the last figure 2.3 represent the evolution of the centers from iteration of iteration. And how the centers approximate more and more the centers of the gaussian distributions.

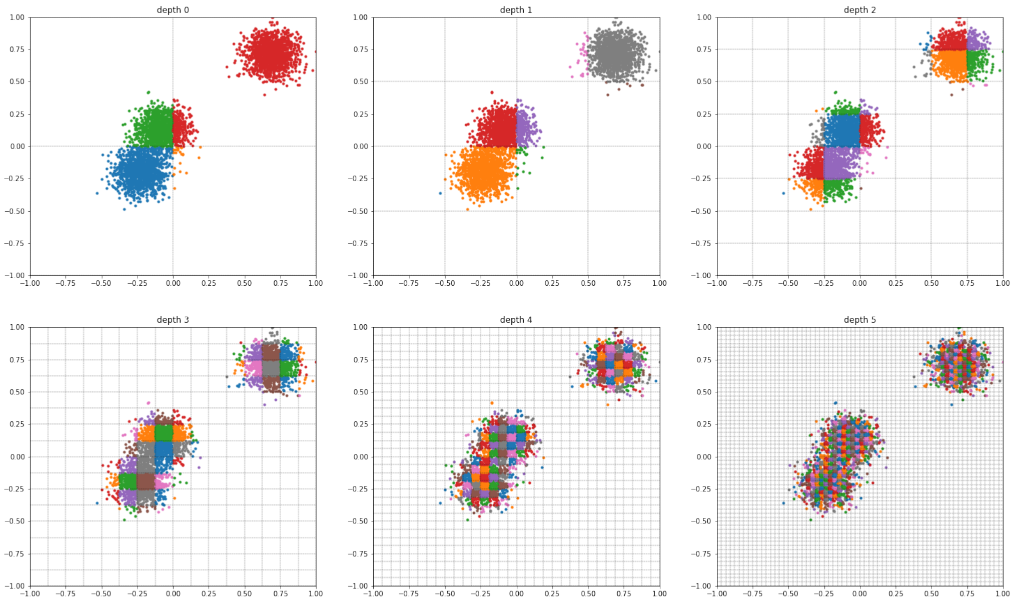


Figure 2.1: Partition example for a 2d gaussian mixture

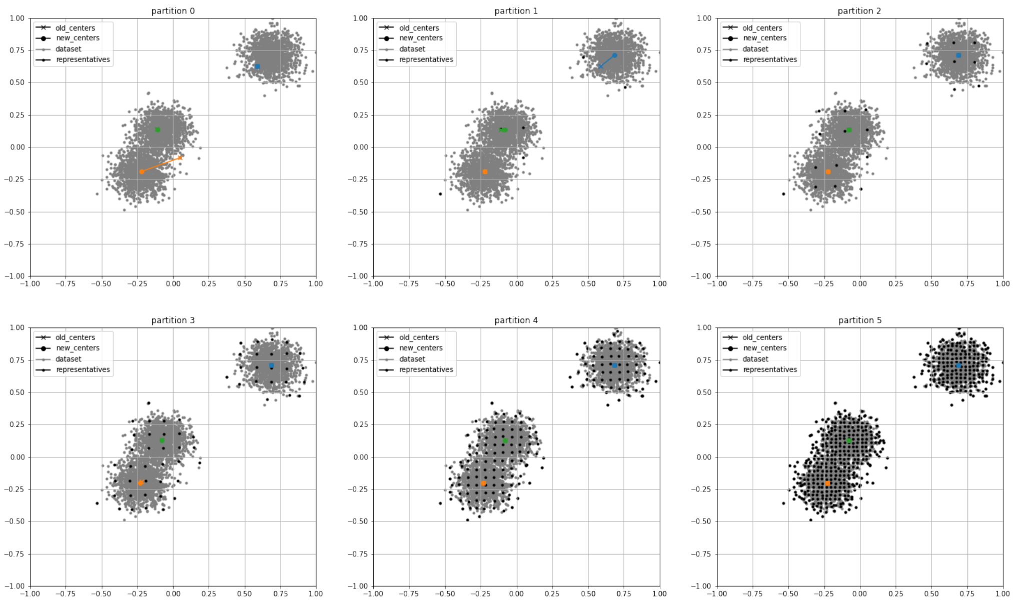


Figure 2.2: Centers and representatives in each iteration

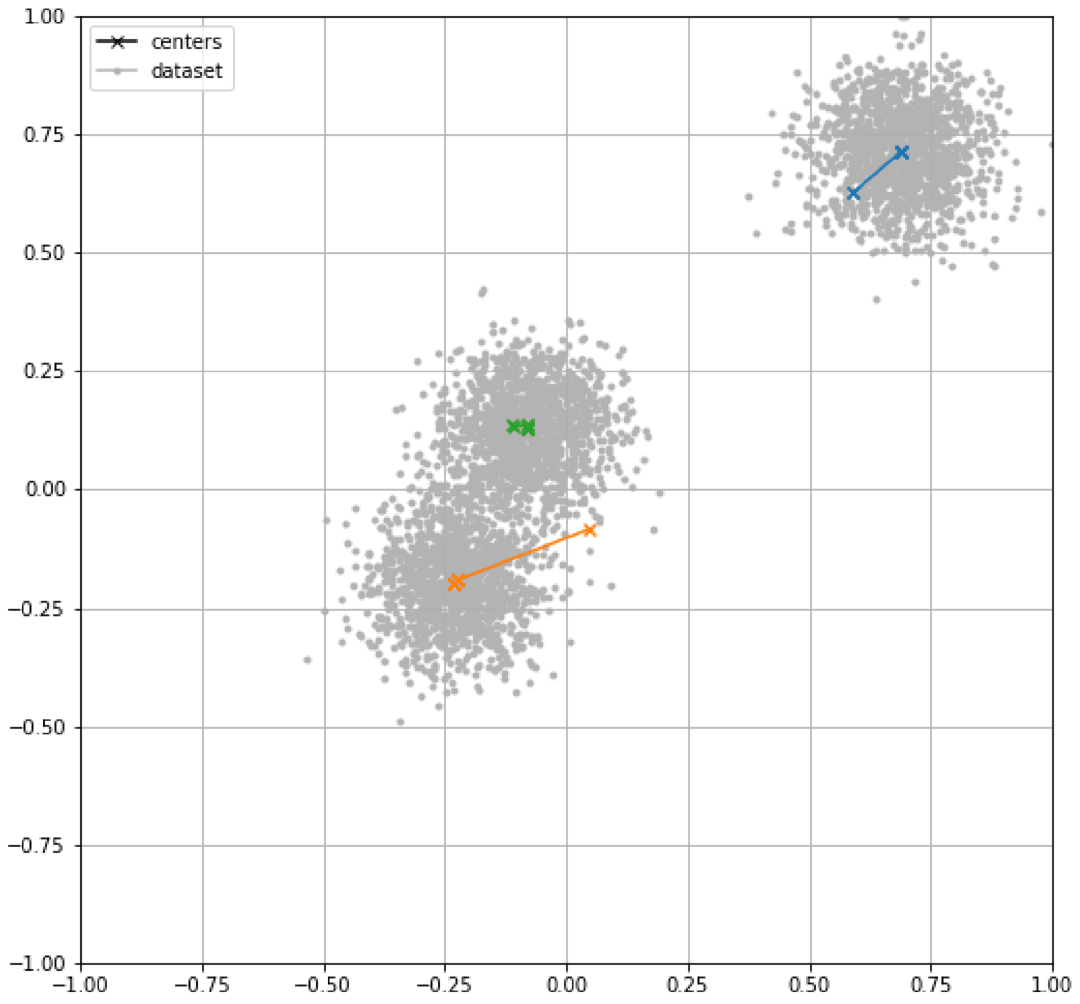


Figure 2.3: Center evolution

Chapter 3

Experiments

3.1 Experiments

Experiments

Chapter 4

Conclusions

4.1 Conclusions

Conclusions

Chapter 5

Annex

5.1 Annex

Tables and figures not in the document

Bibliography

[1] Marco Capó, Aritz Pérez, and Jose A. Lozano. "An efficient approximation to the K-means clustering for massive data". In: *Knowledge-Based Systems* 117 (2017). Volume, Variety and Velocity in Data Science, pp. 56–69. ISSN: 0950-7051. DOI: `https://doi.org/10.1016/j.knosys.2016.06.031`. URL: `https://www.sciencedirect.com/science/article/pii/S0950705116302027`.