

- 2. Initialize centroids by first shuffling the dataset and then randomly selecting *K* data points for the centroids without replacement.
- 3. Keep iterating until there is no change to the centroids. i.e assignment of data points to clusters isn't changing.
- Compute the sum of the squared distance between data points and all centroids.
- Assign each data point to the closest cluster (centroid).
- Compute the centroids for the clusters by taking the average of the all data points that belong to each cluster.

The approach kmeans follows to solve the problem is called **Expectation-Maximization**. The E-step is assigning the data points to the closest cluster. The Mstep is computing the centroid of each cluster. Below is a break down of how we can solve it mathematically (feel free to skip it).

The objective function is:

$$
J = \sum_{i=1}^{m} \sum_{k=1}^{K} w_{ik} ||x^{i} - \mu_{k}||^{2}
$$
 (1)

where wik=1 for data point xi if it belongs to cluster *k*; otherwise, wik=0. Also, μk is the centroid of xi's cluster.

It's a minimization problem of two parts. We first minimize J w.r.t. wik and treat μk fixed. Then we minimize J w.r.t. μk and treat wik fixed. Technically speaking, we differentiate J w.r.t. wik first and update cluster assignments (*E-step*). Then we

differentiate J w.r.t. μk and recompute the centroids after the cluster assignments from previous step (*M-step*). Therefore, E-step is:

$$
\frac{\partial J}{\partial w_{ik}} = \sum_{i=1}^{m} \sum_{k=1}^{K} ||x^{i} - \mu_{k}||^{2}
$$
  
\n
$$
\Rightarrow w_{ik} = \begin{cases} 1 & \text{if } k = argmin_{j} ||x^{i} - \mu_{j}||^{2} \\ 0 & \text{otherwise.} \end{cases}
$$
 (2)

In other words, assign the data point xi to the closest cluster judged by its sum of squared distance from cluster's centroid.

And M-step is:

$$
\frac{\partial J}{\partial \mu_k} = 2 \sum_{i=1}^m w_{ik} (x^i - \mu_k) = 0
$$
  

$$
\Rightarrow \mu_k = \frac{\sum_{i=1}^m w_{ik} x^i}{\sum_{i=1}^m w_{ik}}
$$
 (3)

Which translates to recomputing the centroid of each cluster to reflect the new assignments.

Few things to note here:

- Since clustering algorithms including kmeans use distance-based measurements to determine the similarity between data points, it's recommended to standardize the data to have a mean of zero and a standard deviation of one since almost always the features in any dataset would have different units of measurements such as age vs income.
- Given kmeans iterative nature and the random initialization of centroids at the start of the algorithm, different initializations may lead to different clusters since kmeans algorithm may *stuck in a local optimum and may not converge to global optimum*. Therefore, it's recommended to run the



Bayes theorem came into existence after Thomas Bayes, who first utilized conditional probability to provide an algorithm that uses evidence to calculate limits on an unknown parameter.

Bayes's theorem is expressed mathematically by the following equation that is given below.

$$
P\big(X/Y\big)~=~\frac{P(Y/X)P(X)}{P(Y)}
$$

Where X and Y are the events and P (Y)  $\neq$  0

P(X/Y) is a **conditional probability** that describes the occurrence of event **X** is given that **Y** is true.

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P(X) and P(Y) are the probabilities of observing X and Y independently of each other. This is known as the **marginal probability**.

## **Bayesian interpretation:**

In the Bayesian interpretation, probability determines a "**degree of belief**." Bayes theorem connects the degree of belief in a hypothesis before and after accounting for evidence. For example, Lets us consider an example of the coin. If we toss a coin, then we get either heads or tails, and the percent of occurrence of either heads and tails is 50%. If the coin is flipped numbers of times, and the outcomes are observed, the degree of belief may rise, fall, or remain the same depending on the outcomes.

For proposition X and evidence Y,

- $\circ$  P(X), the prior, is the primary degree of belief in X
- $\circ$  P(X/Y), the posterior is the degree of belief having accounted for Y.  $P(Y/X)$
- The quotient  $\overline{P(Y)}$  represents the supports Y provides for X.

Bayes theorem can be derived from the conditional probability:

$$
P(X/Y) = \frac{P(X \cap Y)}{P(Y)}, \text{ if } P(Y) \neq 0
$$
  

$$
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$$





In this diagram,  $minPts = 4$ . Point A and the other red points are core points, because the area surrounding these points in an *ε* radius contain at least 4 points (including the point itself). Because they are all reachable from one another, they form a single cluster. Points B and C are not core points, but are reachable from A (via other core points) and thus belong to the cluster as well. Point N is a noise point that is neither a core point nor directly-reachable.

Reachability is not a symmetric relation: by definition, only core points can reach non-core points. The opposite is not true, so a non-core point may be reachable, but nothing can be reached from it. Therefore, a further notion of *connectedness* is needed to formally define the extent of the clusters found by DBSCAN. Two points *p* and *q* are density-connected if there is a point *o* such that both *p* and *q* are reachable from *o*. Density-connectedness *is* symmetric.

A cluster then satisfies two properties:

- 1. All points within the cluster are mutually density-connected.
- 2. If a point is density-reachable from some point of the cluster, it is part of the cluster as well.

## Algorithm<sub>[\[edit\]](https://en.wikipedia.org/w/index.php?title=DBSCAN&action=edit§ion=3)</sub>

## **Original query-based algorithm**[\[edit\]](https://en.wikipedia.org/w/index.php?title=DBSCAN&action=edit§ion=4)

DBSCAN requires two parameters: ε (eps) and the minimum number of points required to form a dense region<sup>[\[a\]](https://en.wikipedia.org/wiki/DBSCAN#cite_note-minpts-7)</sup> (minPts). It starts with an arbitrary starting point that has not been visited. This point's ε-neighborhood is retrieved, and if it contains sufficiently many points, a cluster is started. Otherwise, the point is labeled as noise. Note that this point might later be found in a sufficiently sized ε-environment of a different point and hence be made part of a cluster.

If a point is found to be a dense part of a cluster, its  $\varepsilon$ -neighborhood is also part of that cluster. Hence, all points that are found within the ε-neighborhood are added, as is their own εneighborhood when they are also dense. This process continues until the density-connected cluster is completely found. Then, a new unvisited point is retrieved and processed, leading to the discovery of a further cluster or noise.

DBSCAN will also require a distance function $114$  (as well as similarity functions or other predicates).<sup>[\[7\]](https://en.wikipedia.org/wiki/DBSCAN#cite_note-:0-8)</sup> The distance function (dist) can therefore be seen as an additional parameter.

The algorithm can be expressed in [pseudocode](https://en.wikipedia.org/wiki/Pseudocode) as follows:<sup>[\[4\]](https://en.wikipedia.org/wiki/DBSCAN#cite_note-tods-4)</sup>

DBSCAN(DB, distFunc, eps, minPts) {

 C := 0 */\* Cluster counter \*/* **for each** point P **in** database DB { **if** label(P) ≠ undefined **then [continue](https://en.wikipedia.org/wiki/Continue_(keyword))** */\* Previously processed in inner loop \*/* Neighbors N := RangeQuery(DB, distFunc, P, eps) */\* Find neighbors \*/* **if** |N| < minPts **then** { */\* Density check \*/* label(P) := Noise */\* Label as Noise \*/* **continue** } C := C + 1 */\* next cluster label \*/* label(P) := C */\* Label initial point \*/* SeedSet S := N \ {P} */\* Neighbors to expand \*/* **for each** point Q **in** S { */\* Process every seed point Q \*/* **if** label( $Q$ ) = Noise **then** label( $Q$ ) := C /\* Change *Noise to border point \*/* **if** label(Q) ≠ undefined **then continue** */\* Previously processed (e.g., border point) \*/* label(Q) := C */\* Label neighbor \*/* Neighbors N := RangeQuery(DB, distFunc, Q, eps) */\* Find neighbors \*/* **if** |N| ≥ minPts **then** { */\* Density check (if Q is a core point) \*/* S := S ∪ N */\* Add new neighbors to seed set \*/* } } } } where RangeQuery can be implemented using a database index for better performance, or using a slow linear scan: RangeQuery(DB, distFunc, Q, eps) { Neighbors N := empty list **for each** point P **in** database DB { */\* Scan all points in the database \*/* **if** distFunc( $Q$ ,  $P$ )  $\leq$  eps **then** {  $\frac{1}{2}$  /\* Compute *distance and check epsilon \*/* N := N ∪ {P} */\* Add to result \*/* } } **return** N } 6 Explain the following: Agglomerative Hierarchical Clustering and Divisive hierarchical method  $[1|CO3| L3]$ 0]

Agglomerative Hierarchical Clustering (AHC) is a **clustering (or classification) method** which has the following advantages: It works from the dissimilarities between the objects to be grouped together. A type of dissimilarity can be suited to the subject studied and the nature of the data.



The agglomerative clustering is **the most common type of hierarchical clustering used to group objects in clusters based on their similarity**. It's also known as AGNES (Agglomerative Nesting). ... Next, pairs of clusters are successively merged until all clusters have been merged into one big cluster containing all objects. Divisive Clustering:

The divisive clustering algorithm is a **top-down clustering approach**, initially, all the points in the dataset belong to one cluster and split is performed recursively as one moves down the hierarchy.

## **Divisive clustering**

So far we have only looked at agglomerative clustering, but a cluster hierarchy can also be generated top-down. This variant of hierarchical clustering is called *top-down clustering* or *divisive clustering* . We start at the top with all documents in one cluster. The cluster is split using a flat clustering algorithm. This procedure is applied recursively until each document is in its own singleton cluster.

Top-down clustering is conceptually more complex than bottom-up clustering since we need a second, flat clustering algorithm as a ``subroutine''. It has the advantage of being more efficient if we do not generate a complete hierarchy all the way down to individual document leaves. For a fixed number of top levels, using an efficient flat

algorithm like  $\equiv$ -means, top-down algorithms are linear in the number of documents and clusters. So they run much faster than HAC algorithms, which are at least quadratic.

There is evidence that divisive algorithms produce more accurate hierarchies than

bottom-up algorithms in some circumstances. See the references on bisecting  $\equiv$ means in Section [17.9](https://nlp.stanford.edu/IR-book/html/htmledition/references-and-further-reading-17.html#sec:hclstfurther) . Bottom-up methods make clustering decisions based on local patterns without initially taking into account the global distribution. These early decisions cannot be undone. Top-down clustering benefits from complete information about the global distribution when making top-level partitioning decisions.





