Breathing KMeans vs KMeans

Robustify KMeans with centroid addition and removal.

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KMeans is widely used for its simplicity and effectiveness as a clustering algorithm.

Yet, we all know that its performance is entirely dependent on the centroid initialization step.

Thus, it is likely that we may obtain inaccurate clusters, as depicted below:

KMeans produces inaccurate clustering results

Of course, rerunning with different initialization does help at times.

But I have never liked the unnecessary run-time overhead it introduces.

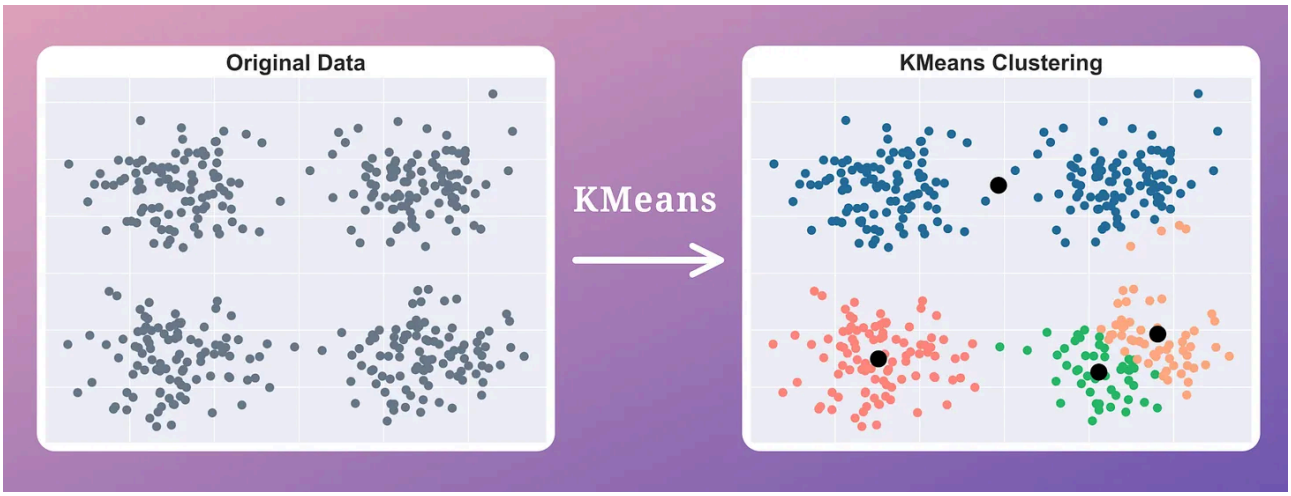
So today, let me share a neat and supercharged upgrade to KMeans, which addresses this issue while also producing better clustering results.

It's called the **Breathing KMeans** algorithm.

Let's understand how it works.

Step 1: Run Kmeans

First, we run the usual KMeans clustering only once, i.e., **without rerunning the algorithm with a different initialization.**



Clustering results of KMeans after running the algorithm without repetition and until convergence

This gives us the location of "k" centroids, which may or may not be accurate.

Step 2: Breathe in step

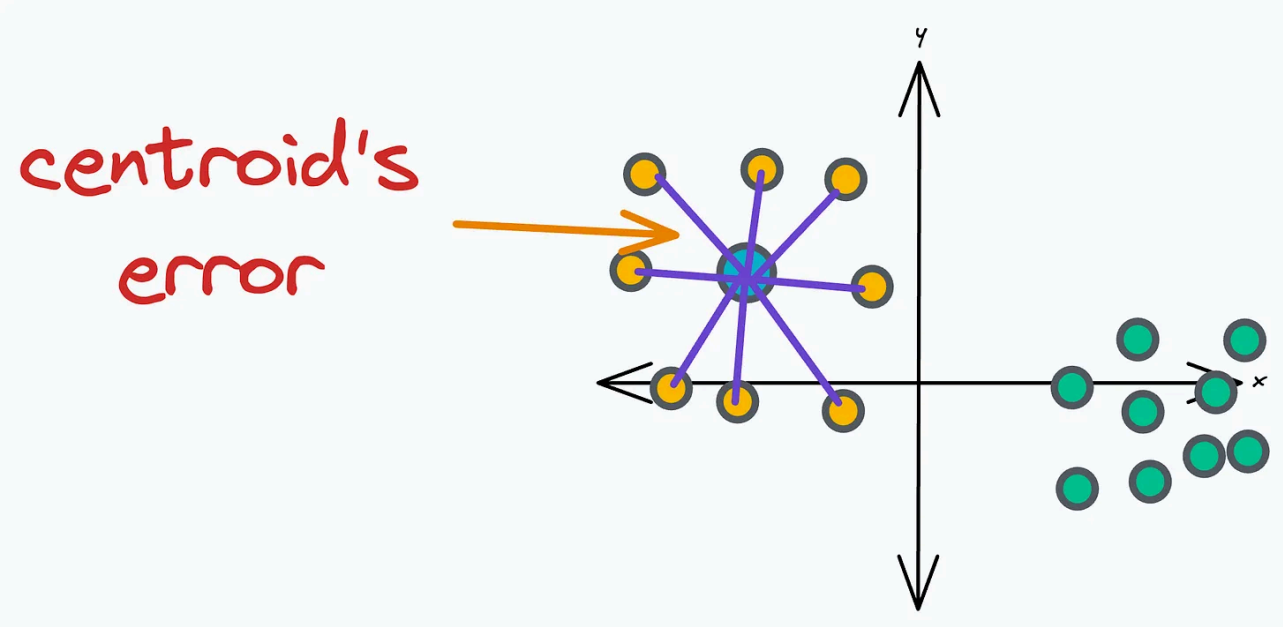
To the "k" centroids obtained from Step 1, we add "m" new centroids.

> As per the research paper of Breathing Kmeans, `m=5` was found to be good value.

Now, you might be thinking, **where do we add these "m" centroids?**

The addition of new centroids is decided based on the error associated with a centroid.

Simply put, a centroid's error is the sum of the squared distance to the points associated with that centroid.



The error of a centroid

Thus, we add “m” centroids in the vicinity of centroids with high error.

Let’s understand more intuitively why this makes sense.

Centroids with high and low error

In the above KMeans clustering results:

- The centroid at the top has a high error.
- All other centroids have relatively low error.

Intuitively speaking, if a centroid has a very high error, it is possible that multiple clusters are associated with it.

Thus, we would want to split this cluster.

Adding new centroids near clusters with high error will precisely fulfill this objective.

After adding "m" new centroids, we get a total of "k+m" centroids.

Finally, we run KMeans again with "k+m" centroids **only once**.

This gives us the location of "k+m" centroids.

Step 3: Breathe out step

Next, we want to remove "m" centroids from the "k+m" centroids obtained above.

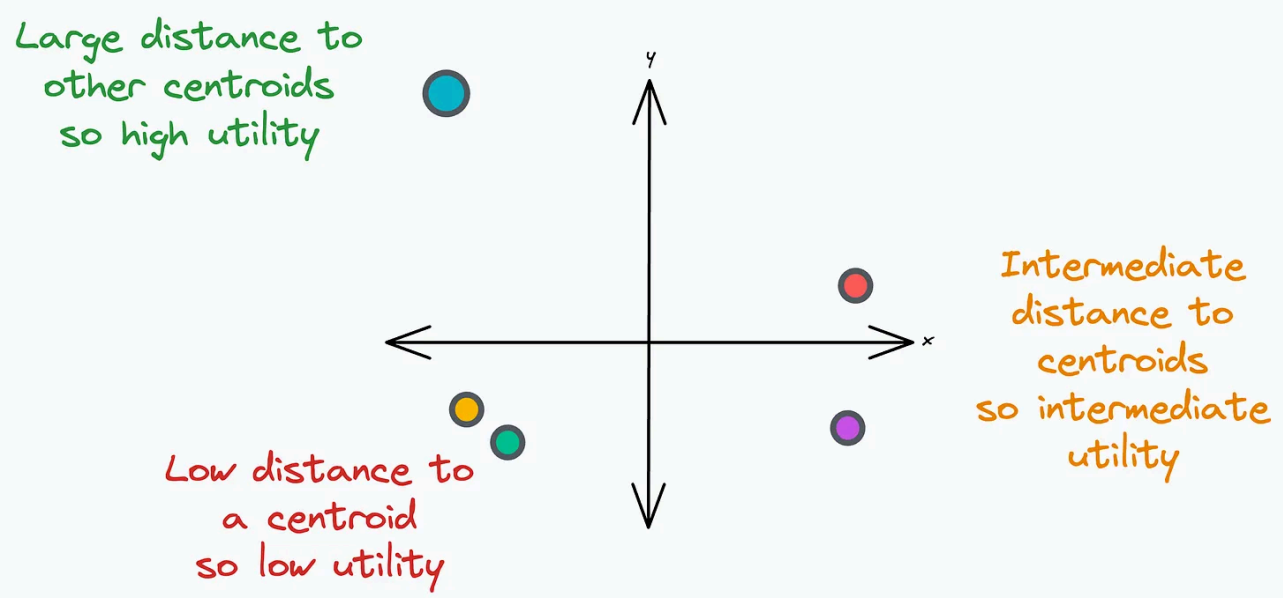
Here, you might be thinking, **which "m" centroids should we remove?**

The removal of centroids is decided based on the "utility" of a centroid.

Simply put, a centroid's utility is proportional to its distance from all other centroids.

The greater the distance, the more isolated it will be.

Hence, the more the utility.



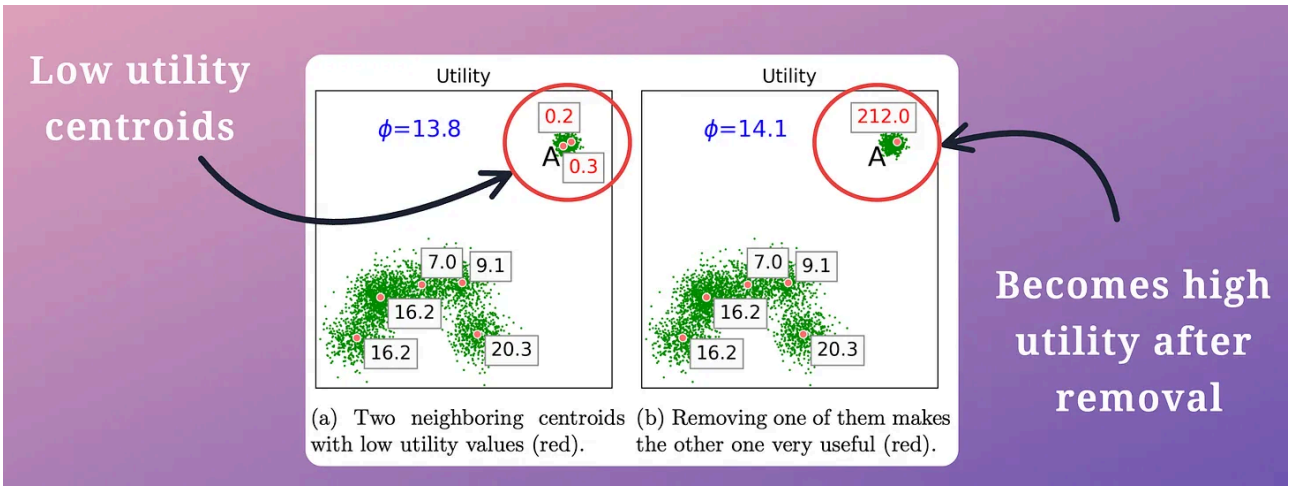
Utility of centroids

This makes intuitive sense as well.

If two centroids are pretty close, they will have low utility.

Thus, they are likely in the same cluster, and we must remove one of them.

This is demonstrated below:



Remove low utility centroid

After removing one of the low-utility centroids, the other centroid becomes very useful.

So, in practice, after removing one centroid, we update the utility values of all other centroids.

We repeat the process until all “m” low-utility centroids have been removed.

This gives back “k” centroids.

Finally, we run KMeans with these “k” centroids **only once**.

Step 4: Decrease `m` by 1.

Step 5: Repeat Steps 2 to 4 until `m=0`.

Done!

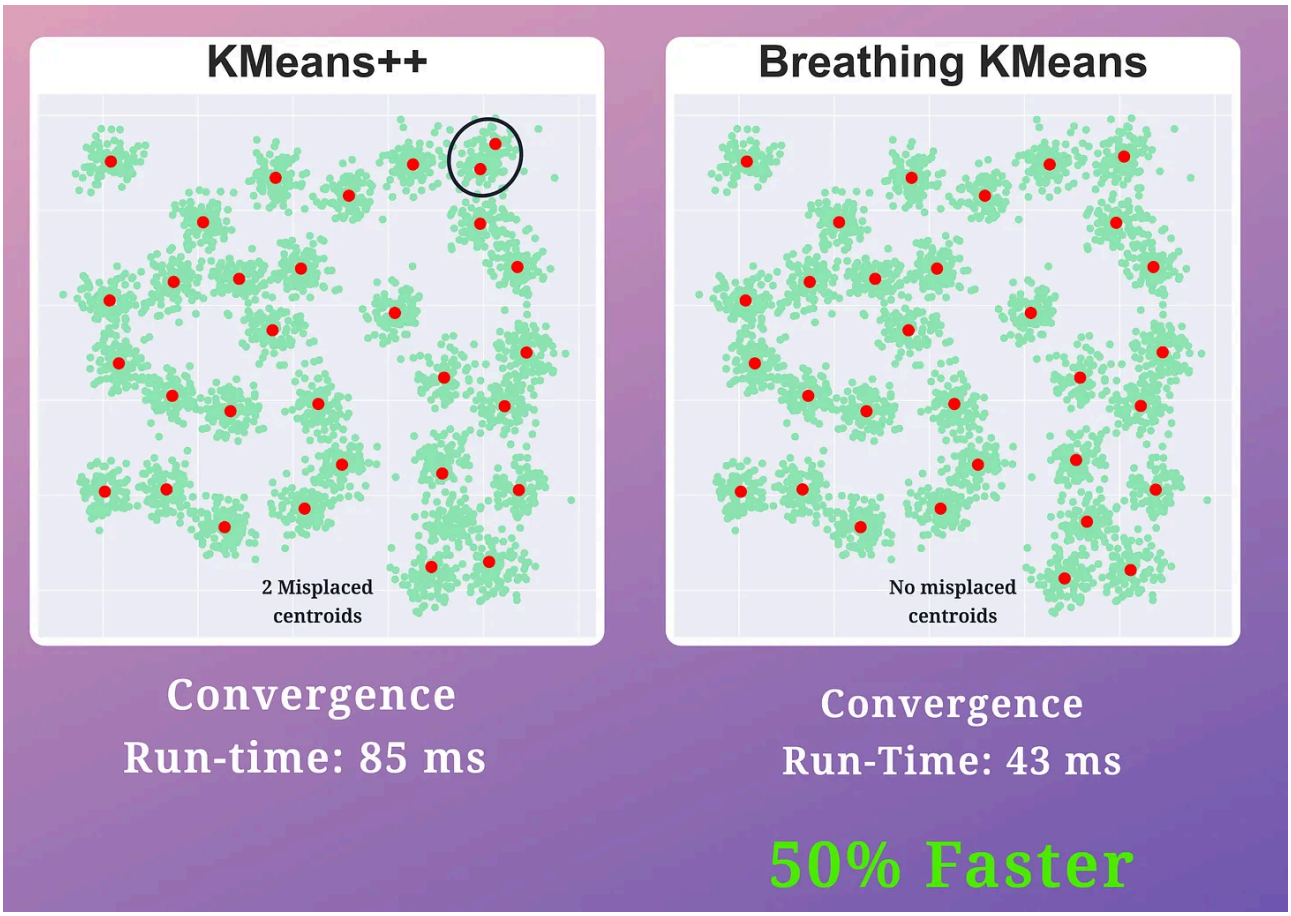
These repeated breathing cycles (breathe-in and breathe-out steps) **almost always** provide a faster and better solution than standard KMeans with repetitions.

In each cycle:

- New centroids are added at "good" locations. This helps in splitting clusters occupied by a single centroid.
- Low-utility centroids are removed. This helps in eliminating centroids that are likely in the same cluster.

As a result, it is expected to converge to the optimal solution faster.

The effectiveness of Breathing KMeans over KMeans is evident from the image below:



KMeans vs. Breathing KMeans results

- KMeans produced two misplaced centroids

- Breathing KMeans accurately clustered the data with a 50% run-time improvement.

There is also an open-source implementation of Breathing KMeans, with a sklearn-like API.

To get started, install the **bkmeans** library:

```
pip install bkmeans
```

Next, run the algorithm as follows:

```
from bkmeans import BKMeans

bkm = BKMeans(n_clusters = 100)

bkm.fit(X)
```

Isn't that a cool upgrade to KMeans?

That said, data conformity is another big issue with KMeans, which makes it highly inapplicable in many data situations.

These two guides cover distribution-based and density-based clustering, which address KMeans' limitations in specific data situations:

- Gaussian Mixture Models (GMMs)
- DBSCAN++: The Faster and Scalable Alternative to DBSCAN Clustering

👉 Over to you: What are some other ways to improve KMeans' clustering and its run-time?

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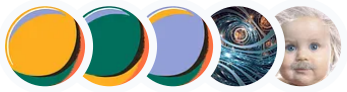

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