K-Density-Based-Means (KDB-Means)

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Algorithm

A deep dive into KDB-Means

The problem…

K-Means

An unsupervised machine learning algorithm that partitions data into k number of distinct clusters by assigning points to the nearest centroid and updating centroids periodically based on distances between data points in their respective cluster.

Its Benefits:

- Scalable and Easy to implement
- Guaranteed convergence
- Interpretable clustering results

Its Drawbacks:

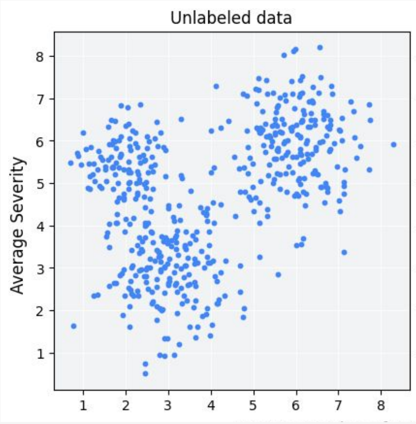
- Highly sensitive to centroid initialization
- Random initialization → unstable clustering results
- Poor initialization increases iterations and runtime

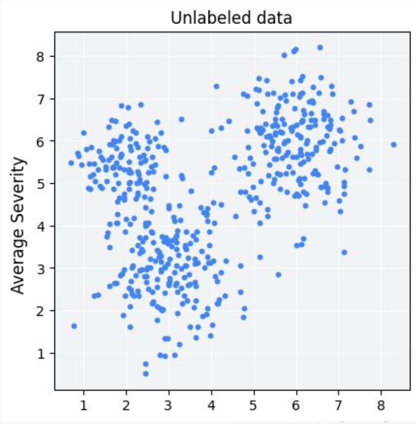
The Solution

KDB-Means

Aiming to solve the inherent issues of the normal K-Means algorithm, we present KDB-Means, a deterministic extension of K-Means that initializes centroids in high-density regions while enforcing separation. Combining local density estimates with distance-based selection to calculate centroids allows for faster convergence and improved clustering on unevenly distributed data.

Here is a quick example:





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Algorithm and Pseudocode

Pseudocode:

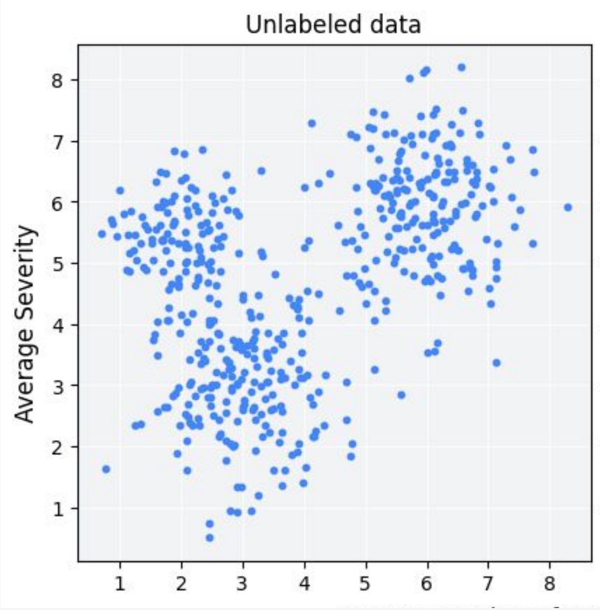
1. Normalize features of the dataset
2. Computer measure of spread of the entire dataset with the average distance
3. Define density radius r_o based on the spread of the dataset; average distance * an alpha value (0.2 through trial-and-error)
4. For each instance x_i in dataset X:

    Look in neighborhood around data point in the radius r_o: count how many points fall inside that neighborhood, record as density value

5. Select the point with highest density as first centroid
6. Until k centroids are picked:

    Choose next centroid by calculating the distance of every node to its closest centroid, select the node with the highest density * distance^2 value

7. Record centroids and use in SciKit's K-Means algorithm



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Related Work

K-Means++ and DBSCAN

K-Means++

A modification of the K-means algorithm that improves standard K-Means by carefully initializing centroids so they are well separated, reducing poor initializations and speeding up convergence.

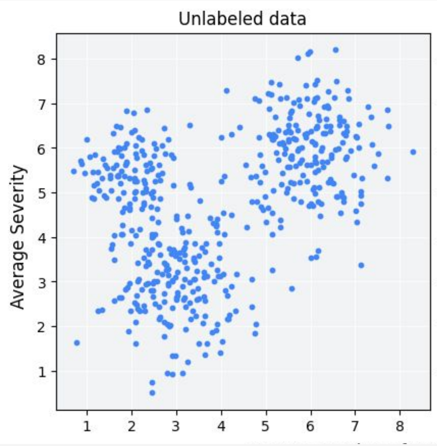
Its Benefits:

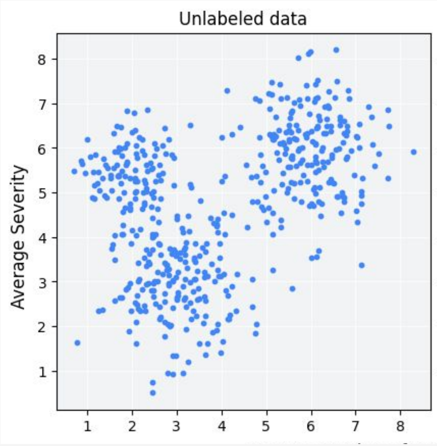
- Faster than regular K-Means
- Guaranteed convergence
- Interpretable clustering results

Its Drawbacks:

- Does not take valuable info such as local data density into account

Example:





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DBSCAN

DBSCAN is clustering algorithm that clusters data by grouping dense regions of points and identifying sparse points as noise, without requiring the number of clusters in advance.

Benefits:

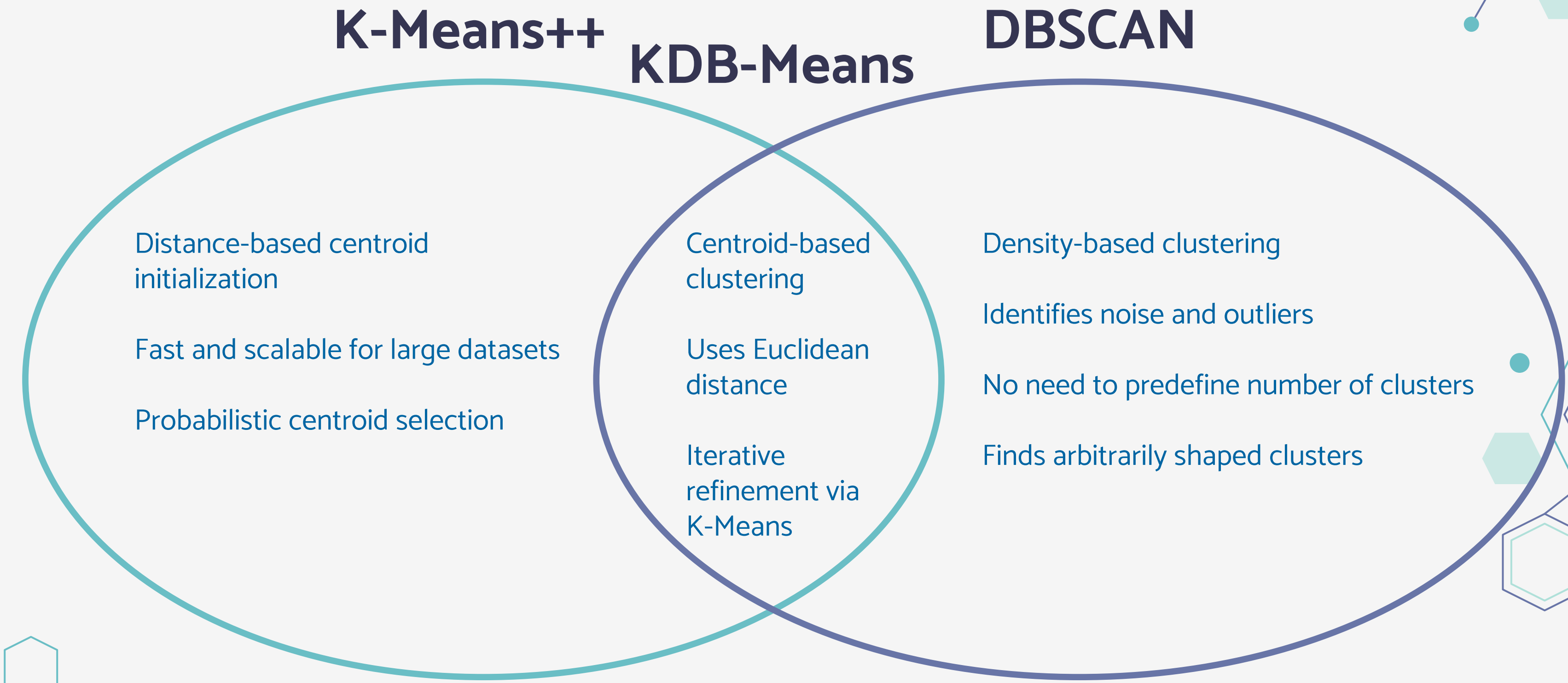
- No need to predefined number of clusters
- Can identify arbitrarily shaped clusters

Drawbacks:

- Sensitive to parameter selection
- Doesn’t create centroid-based clusters
- Less suitable for applications needing centroid refinement

KDB-Means vs. DBSCAN and K-Means++

“KDB-Means can be viewed as a hybrid that combines key ideas from K-Means++ and DBSCAN.”



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Our Dataset

Dataset

Source: UCI Machine Learning Repository

Name: User Knowledge Modeling (UNS) [8]

Domain: Student knowledge assessment in *Electrical DC Machines*

Instances: 403 students

Features: 5 continuous attributes (values in [0,1][0,1][0,1])

Features

STG: Study time for target subject

SCG: Frequency of repetition of target material

STR: Study time for related subjects

LPR: Performance in related subject exams

PEG: Performance in elective exams

Class Label (UNS)

Ordinal categories: *Very Low, Low, Middle, High*

Used only for evaluation, not for clustering

Preprocessing

- **Combined training and testing sets**
  - Dataset is used in an **unsupervised** setting
  - All instances treated as unlabeled during clustering
- **Standardized class labels (UNS)**
  - Resolved capitalization inconsistency:
    - "very_low" and "Very Low"
  - Encoded labels as ordinal values *(0–3)*
  - **Labels were used only for evaluation**, not clustering
- **Feature normalization**
  - All continuous features normalized prior to clustering
  - Prevents features with larger variances from dominating:
    - Distance calculations
    - Density estimation
  - Essential for fair centroid initialization

Toy Datasets

What are they? Why did we use them?

In addition to our User Knowledge Modeling dataset, we created a number of toy (example) datasets for visualization purposes. Due to the higher-dimensional nature of the User Knowledge dataset, no visualizations were created.

The toy dataset visualizations provide much more understandable and communicable results.

Description of our Toy Datasets:

- Created with Scikit-Learn's make_blobs [11] function
- Each toy dataset has a random number of instances between 100 - 500 (inclusive)
- Each dataset has a random number of clusters between 3 and 10 (inclusive)

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Results & Analysis

Results & Analysis

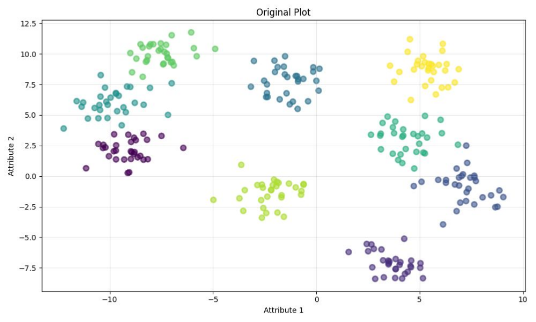

Fig. 1: Initial cluster formation in a 2D toy dataset with # nodes=271, k=9.

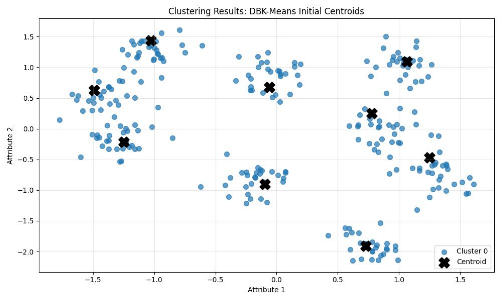

Fig. 2: DBK-Means initial centroid positions.

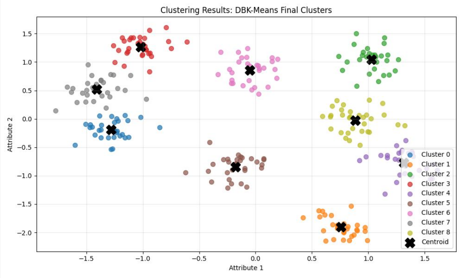

Fig. 3: DBK-Means final centroid positions with final clusters.

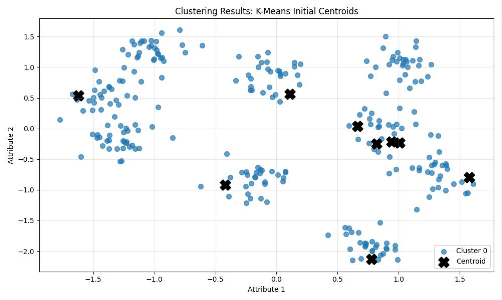

Fig. 4: K-Means initial centroid positions.

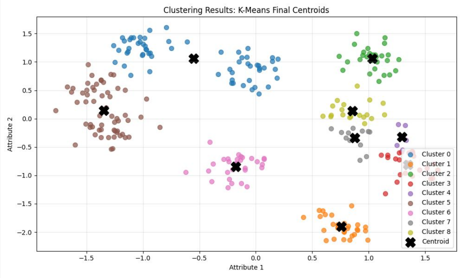

Fig. 5: K-Means final centroid positions with clusters.

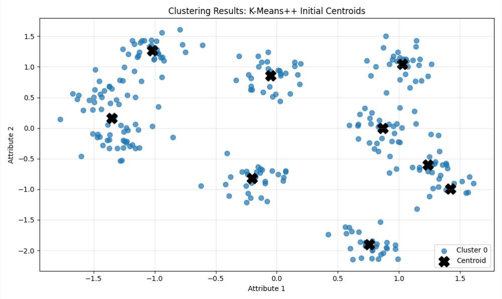

Fig. 6: K-Means++ initial centroid positions.

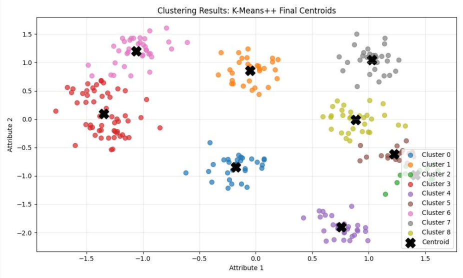

Fig. 7: K-Means++ final centroid positions with final clusters.

Results & Analysis

	KDB-Means	K-Means	K-Means++
AMI	0.2930	0.2225	0.2217
ARI	0.2108	0.1579	0.1556
Silhouette	0.1755	0.1703	0.1697
Iterations	12.0000	18.8400	16.2000

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Conclusion + Future Work

Key Findings

- Integrating density weighting improves clustering quality
- KDB-Means produces better formed clusters
- Achieves faster convergence

Strengths & Limitations

Strengths:

- Performs well on datasets with uneven cluster density
- Outperforms K-Means and K-Means++ in density-imbalanced data

Limitations:

- Performance degrades in very high dimensions due to density estimation within an n-dimensional radius r_o

Future Work

- Explore applications with Variants of K-Means and DBSCAN-inspired hybrids
- Tune density radius parameter α for higher-dimensional datasets
- Investigate better scalable density estimation methods for large feature spaces

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Thank you for listening!

Questions?