K-MEANS++ OPTIMAL INITIALIZATION ALGORITHM

An Improved K-means Clustering Method

OVERVIEW

- K-means Clustering Algorithm
- K-means++ Initialization Algorithm
- Experiment
- Datasets
- Conclusion

K-MEANS CLUSTERING ALGORITHM

- A well-known naïve clustering method.
- Designed to find natural clusters in unclassified datasets.
- Only requires a single input parameter K
- Uses random initialization technique for centroids.
- Uses Euclidean distance to determine instances' cluster assignments.
- Calculates means of finished clusters then starts over.

CLUSTERING EXAMPLE



MEAN CALCULATION AND RE-CLUSTERING



K-MEANS++ INITIALIZATION ALGORITHM

- Arbitrarily selects the first centroid.
- Every other centroids selected based on distance from other centroids.



EXPERIMENT

- Compared standard K-means and K-means++ methods.
- Goal: to discover if either one of them produces better results than the other.
- Setup:
 - Both methods run against 3 datasets with classes Cluster, Iris, and Wine.
 - Each set has 3 classes which are used to verify the quality of the resulting clusters.
 - Quality in clusters is also determined by majority class
 - Fixed "arbitrary" setup to create a optimal and worst random centroid selection.
 - Both methods run against both centroid setups 3 times with a different K value.
 - Total of 36 trials.

MULTIDIMENSIONAL DATA - CLUSTER



MULTIDIMENSIONAL DATA - IRIS



MULTIDIMENSIONAL DATA - WINE

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RESULTS

- K-means++ proven to be better.
- No reason to use standard K-means.
- Still not perfect.

	K-means				K-means++			
	Cluster Dataset	t		Cluster Dataset				
	Optimal	Worst			Optimal	Worst		
3 Clusters	1	1		3 Clusters	1	1		
5 Clusters	0	1		5 Clusters	1	1		
7 Clusters	1	1		7 Clusters	1	1		
	Iris Dataset				Iris Dataset			
	Optimal	Worst			Optimal	Worst		
3 Clusters	17	18		3 Clusters	17	17		
5 Clusters	23	24		5 Clusters	19	19		
7 Clusters	10	17		7 Clusters	3	4		
	Wine Dataset			Wine Dataset				
	Optimal	Worst			Optimal	Worst		
3 Clusters	46	53		3 Clusters	45	45		
5 Clusters	39	44		5 Clusters	25	26		
7 Clusters	42	43		7 Clusters	42	42		

IMPORTANT NOTES

- Imperfect simulation of K-means++
- Results could be better.
- Results should give clearer favor to K-means++

REVIEW

- K-means Clustering Algorithm
- K-means++ Initialization Algorithm
- Comparison Experiment
- Multidimensional Datasets
- Results

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