K-Nearest Neighbors based on the Nk Interaction Graph

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Abstract. The K-Nearest Neighbors (KNN) is a simple and intuitive non-parametric classification algorithm. In KNN, the K nearest neighbors are determined according to the distance to the example to be classified. Generally, the Euclidean distance is used, which facilitates the formation of hyper-ellipsoid clusters. In this work, we propose using the Nk interaction graph to return the K-nearest neighbors in KNN. The Nk interaction graph, originally used in clustering, is built based on the distance between examples and spatial density in small groups formed by k examples of the training dataset. By using the distance combined with the spatial density, it is possible to form clusters with arbitrary shapes. We propose two variations of the KNN based on the Nk interaction graph. They differ in the way in which the vertices associated with the N examples of the training dataset are visited. The two proposed algorithms are compared to the original KNN in experiments with datasets with different properties.

1. Introduction

Machine learning is often successfully applied in problems where discovering relationships between multiple examples in a dataset is important. If those examples carry a label, predetermining the groups they are in, the learning is called supervised [KOTSIANTIS et al., 2007]. One of the most important supervised learning problems is classification, which is a pre-requisite for different technologies that are present on our daily lives, such as speech recognition, biometrical identification, computational vision, recommendation systems and more.

Many classification algorithms are implemented using a distance metric for comparing examples, especially the Euclidean distance. This metric induces the formation of hyper ellipsoidal decision boundaries. Therefore, examples that belong to arbitrary clusters, defined by both distance and spatial density [RODRIGUEZ & LAIO, 2014], [ESTER et al., 1996] are often incorrectly classified by those algorithms.

The Euclidean distance is used the *K-Nearest Neighbors algorithm* (KNN). The KNN classifies a new example according to the majority class of the *K* nearest neighbors. The *K* nearest neighbors are determined by the Euclidean distance of the new example to the examples of the training dataset. KNN still is one of the simplest and most efficient algorithms for supervised learning, being one of the first efficient non-parametrical classification methods [FIX, 1985]. The KNN strategy is used in many other supervised and unsupervised learning algorithms.

In this work, we propose using the Nk interaction graph to find the K-nearest neighbors in KNN. We also propose two variations of the KNN based on the Nk

interaction graph that differ in the way in which the vertices associated with the N examples of the training dataset are visited. The Nk interaction graph is built based on the distance and spatial density in small groups formed by k examples of the training dataset. By using the distance combined with the spatial density, it is possible to form clusters with arbitrary shapes. The Nk interaction graph was initially proposed in the NK Hybrid Genetic Algorithm (NKGA) for clustering [TINÓS et al., 2018]. In [MORAES & TINÓS, 2020], the Nk interaction graph was used for the similarity search problem. Basically, the method proposed in [MORAES & TINÓS, 2020] returns K examples of a dataset similar to the queried example by visiting K vertices of the interaction graph. The proposed similarity search method showed to be interesting for querying examples in datasets with clusters with arbitrary shapes.

In the methods previously proposed for clustering [TINÓS et al., 2018] and similarity search [MORAES & TINÓS, 2020], for $k \ge 1$, only one edge of each vertex of the Nk interaction graph depends on the spatial density of the respective example of the training dataset. All the other edges depend only on the distance between examples. Here, for the modified KNN, we propose changing the ratio between the number of edges depending on spatial density and distance for creating the Nk interaction graph.

2. Methodology

Both variations of the proposed KNN utilize the Nk interaction graph to build a KNN algorithm that can classify examples based on both Euclidian distance and spatial density. The original KNN and the Nk interaction graph, with modifications, are explained in sections 2.1 and 2.2. The proposed KNN based on the Nk interaction graph is presented in Section 2.3.

2.1. K-Nearest Neighbors

The KNN is a supervised learning algorithm that classifies a new example x based on the majority class (label) of the K dataset examples that are closest to x [AHA et al., 1991]. The K nearest examples are those with minimum Euclidean distance to x. The KNN can be modified for regression, be weighted [ALTMAN, 1992], and be modified to follow another approach of neighbor selection, where K is the radius of a hyper sphere that selects the examples that will be analyzed. For any version or modification, the parameter K has an important impact on the performance, efficiency, and definition of the decision boundaries produced by the classifier in the decision space.

2.2. Nk Interaction Graph

Most machine learning algorithms use one single metric to define the groups for clustering or decision boundaries in classification. On clustering, the Euclidean distance is often used, as in the *k-means* algorithm [MACQUEEN, 1967]. But other metrics can be employed, such as the spatial density, used in the *density-based spatial clustering of applications with noise* (DBSCAN) [ESTER et al., 1996]. The NKGA [TINÓS et al., 2018] uses both metrics, computed on examples in *N* small groups, each one with *k* examples, given a dataset with *N* examples. The groups are defined by using the Nk interaction graph.

The Nk interaction graph is a directed graph with N vertices with outdegree k. Each vertex is associated to an example of the training set. Originally, each vertex of the graph has an auto-loop, an output edge defined by spatial density and k-2 output edges defined by the Euclidean distance between examples of the training dataset. In this work, we propose to use a parameter α , which specifies the ratio of edges defined by density. Let $A = \lceil \alpha k \rceil$, where A is an integer number that represents the quantity of output edges defined by spatial density for each edge. As said before, in the original Nk graph, α always leads to A=1 and, therefore, there was one auto-loop, one density defined edge and k-2 edges defined by distance, for $k \ge 2$. For k=1, there will be only the auto-loop edge and, therefore, A=0. Here we propose using α that can result in $A\ne 1$, changing the number of edges defined by both spatial density and Euclidean distance. Each edge (v_j, v_i) of the graph indicates that the j-th example is related to the i-th example. The spatial density ρ_i for the i-th example (v_i) of the dataset with N examples is given by:

$$\rho_i = \sum_{j=i}^{N} \mathbf{K}(y_i - y_j) \tag{1}$$

where \mathbf{K} is the kernel function, here defined by:

$$\mathbf{K}(y_i - y_j) = e^{\frac{-\left|\left|y_i - y_j\right|\right|^2}{2\epsilon^2}} \tag{2}$$

where ϵ is the parameter that defines the cutting distance. Here, this parameter is equal to 2%, as suggested in [RODRIGUEZ & LAIO, 2014].

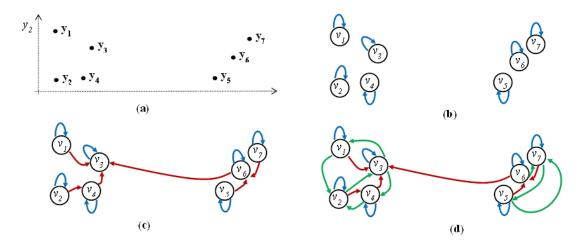


Figure 1. Building the Nk interaction graph for k=3, $\alpha=1/3$, and N=7 two-dimensional examples. Each example of the dataset (a) is associated with a vertex with auto-loop (b). The density of the examples is calculated and each vertex is connected to the $A= \lceil \alpha k \rceil$ nearest examples with higher density then itself (c). Then, the remaining edges are connected to the closest vertices, resulting in the interaction graph (d) with N=7 vertices and Nk edges.

For the construction of the Nk interaction graph, given a dataset with N examples, first a vertex v_i with an auto-loop is added for each example y_i of the dataset. Second, the remainder k-l edges are defined by both spatial density and Euclidean

distance, whereas its ratio is defined by an α parameter. This parameter sets the percentage of edges defined by spatial density, connecting them to the closest examples with a density greater than y_i . The number of edges connected this way is equal to A, let $A = \lceil \alpha k \rceil$, and $A \le k$ (one of the edges must be the auto-loop). Then, remaining k - A - I edges are connected by distance, to the vertex of the closest examples to y_i . Figure 1 shows an example for building the Nk interaction graph with k = 2, $\alpha = 1/3$, and N = 7.

2.3. KNN based on the Nk Interaction Graph

The proposed KNN uses the Nk interaction graph to return the K nearest neighbors of a new example (to be classified) x. Two variations are proposed: they differ in the way the vertices associated to the N examples of the training dataset are visited. In both variations: given N examples of a training dataset and the parameters k and α , the Nk interaction graph is built (see Section 2.2); parameter k is equal to k, i.e., the outdegree for each vertex (k) is equal to the number of nearest neighbors (k) of KNN; for each new example (to be classified) k, the spatial density of k (considering all examples of the training dataset) and distances of k to all examples of the training dataset are computed; given an example k, the k visited vertices (see next paragraph) define the k nearest neighbors of k; given the k nearest neighbors of k (defined by using the Nk interaction graph), the classification is performed as in the original KNN, i.e., the KNN based on the Nk interaction graph differs from the original KNN only in the way the k nearest neighbors are defined.

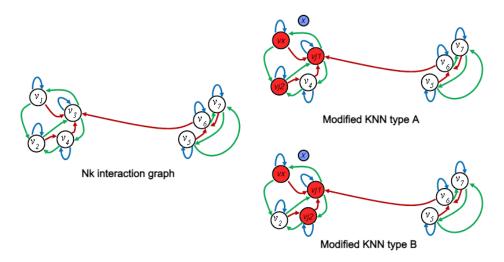


Figure 2. Examples of finding the K-nearest neighbors for modified KNN types A and B, when classifying an example x. On modified KNN type A, the neighbors are defined by the adjacency list of v_x On modified KNN type B, the neighbors are defined by the vertex adjacent to v_x related to the example that is the closest to x, followed by $v_i = v_x$ and iteratively repeating the process.

When classifying a new example x, the vertex v_x related to the example (according to the Euclidean Distance) of the training dataset that is closest to x is chosen from the training dataset to represent x on the Nk interaction graph. In the first variation of the algorithm, named *modified KNN type A*, the adjacency list of v_x is obtained by using the spatial density and distances of x to the examples of the dataset. The k=K

examples associated to vertices in the adjacency list of v_x are then taken as the nearest neighbors of x and, therefore, used to classify it.

The second variation, named *modified KNN type B*, consists in finding and saving the vertex v_j , from the adjacency list of v_x , whose example y_j is the closest (according to the Euclidean distance) to x, ignoring the auto-loop. Then the operation $v_x=v_j$ is performed, and the same step is repeated, totalizing k times. The list of vertices v_j generated through this process is taken as the nearest neighbors of x and, therefore, used to classify it. Figure 2 exemplifies the difference of modified KNN types A and B.

3. Experimental Results

The proposed algorithms¹ are compared to the original KNN in two experiments. The experiments were designed to test the effects of changing parameters K and α . Datasets from the UCI Machine Learning Repository [DUA & GRAFF, 2019], and S-sets and Shape Datasets [FRÄNTI & SIERANOJA, 2018] are used to test the original and modified KNNs (types A and B). The 2-dimensional S-sets and Shape datasets contain clusters with different properties, e.g., clusters with non hyper-ellipsoid shapes and with different overlapping degree.

In the first experiment, the performance of the algorithms is tested for changing parameter K in the range [1, 10]. In the proposed KNN variations, we set α to a value that leads to A=I, i.e., only one output edge for each vertex is defined by spatial density. In the second experiment, we test the impact of changing parameter α . In this case, results were generated for two values of parameter K (5 and 10). When K=5, parameter α changes resulting in A in the range [0, 4]; when K=I0, parameter α changes resulting in A in the range [0, 9]. In the second experiment, the original KNN is tested only one time for each dataset and respective K value because it does not have α as a parameter.

The results presented in the tables are for 10-fold cross-validation. Each table shows the number of test examples that are corrected classified (n) and the respective accuracy (ACC). The algorithms (modified KNN type A, modified KNN type A, and original KNN) are tested for datasets: Aggregation, Compound, D31, ecoli, flame, ionosphere, iris, jain, pathbased, R15 and spiral; for K = 10 in the second experiment, we also tested the algorithms for S-sets datasets s1, s2, s3 and s4.

In the tables, the results highlighted by dark gray background are the overall best results for the respective dataset, while the results highlighted in light gray background represent the best results for the respective row (for a given value of K or α , depending on the experiment).

3.1. Experiment 1: Impact of changing K

Table 1 shows the results for the experiment designed for testing the impact of changing parameter *K*. The results indicate that, in general, better performance is obtained by modified KNN type B in the UCI Machine Learning Repository datasets (*iris*, *ecoli* and

¹ The codes and results of this work can be found at https://github.com/gusfcc/ScientificResearch KNN NkGraph .

ionosphere). These are the only datasets with dimension higher than 2. It is also possible to observe that the modified KNN type A and the original KNN presents similar results for higher values of K. This is explained by the small number of neighbors defined by density (A=1). We also observe that, in most of the datasets with hyper-ellipsoidal clusters, modified KNN type A and original KNN algorithms generally present better accuracy; the exception is for datasets with many clusters with overlap (D31), where better results were obtained by modified KNN type B.

3.2. Experiment 2: Impact of changing α

Tables 2 and 3 show the results for the experiment designed for testing the impact of changing α . Table 2 shows the results for K=5, while Table 3 shows the results for K=10. It is possible to observe that the modified KNN type B obtained the overall best results for datasets D31, ionosphere, and flame in Table 2, and in datasets D31, s3 and s4 in Table 3. The experimental results indicate that worse performance was obtained in most of the datasets for higher values of α , i.e., when all or most of the K neighbors are defined by spatial density. It is also possible to observe that better results were generally obtained for higher values of α on datasets with overlapping clusters (D31, s3 and s4). The overlapping degree increases from s1 to s4 in the S-set datasets; one can observe that better results are obtained in s3 and s4 for higher values of α , i.e., choosing more neighbors by spatial density in the modified KNN impacts positively the performance when cluster overlapping degree increases. Finally, one can observe that modified KNN type A behaves like the original KNN when A=0.

4. Conclusions

In this work, we propose using the Nk interaction graph to find the K-nearest neighbors in KNN. We also propose changing the ratio between the number of edges depending on the spatial density and those depending only on distance in the Nk Interaction Graph. A parameter α controls the ratio between the number of edges depending on the spatial density and edges depending only on distance between examples.

The experimental results indicate that the best performance is generally obtained by the original KNN or the proposed KNN with a small value for α in datasets with 2 dimensions and non-overlapping clusters. In these cases, choosing nearest neighbors by using spatial density neutrally or negatively affects the performance of the proposed KNN. However, better results are obtained in datasets with more dimensions and/or with overlapping clusters. The results for experiments investigating the impact of α indicate that better results are generally obtained for small values of α . The exception is for datasets with overlapping clusters. Selecting more neighbors based on spatial density generally results in better performance for datasets with overlapping clusters.

The automatic selection of α in the proposed KNN is a possible future work. Another future work is to investigate the performance of the proposed KNN in high-dimensional datasets in Medicine. Finally, an important topic of research is to reduce the time and memory complexity of KNN. The use of the Nk interaction graph can be investigated in the future to reduce the number of examples of the training dataset analyzed by the algorithm when finding the K-nearest neighbors.

Table 1. Results for Experiment 1.

							Compound								
<u> </u>	T	A		gation B		NN			T	A	Comp			NN	
К	n	A ACC	n	ACC	n	ACC	Total	К	n	ACC	n	ACC	n	ACC	Total
1	787	0.999	787	0.999	787	0.999		1	389	0.975	389	0.975	389	0.975	
2	783	0.994	783	0.994	786	0.997		2	384	0.962	384	0.962	389	0.975	
3	786	0.997	785	0.996	786	0.997	1	3	382	0.957	381	0.955	382	0.957	i i
4	784	0.995	784	0.995	784	0.995		4	387	0.970	381	0.955	387	0.970	
5	786	0.997	783	0.994	786	0.997	788	5	381	0.955	373	0.935	381	0.955	399
6	786	0.997	784	0.995	786	0.997	, , , ,	6	383	0.960	372	0.932	383	0.960	333
7	786	0.997	784	0.995	786	0.997		7	379	0.950	372	0.932	379	0.950	
8	787	0.999	784	0.995	787	0.999		8	379	0.950	372	0.932	379	0.950	
9 10	786 786	0.997	786 784	0.997 0.995	786 786	0.997		9 10	377 377	0.945	369 369	0.925	377 377	0.945 0.945	
10	700	0.997		31	780	0.997		10	3//	0.945		oli	3//	0.945	
К		Α		В	KI	NN	Total	К		Α		В	KI	NN	Total
	n	ACC	n	ACC	n	ACC			n	ACC	n	ACC	n	ACC	
1	2981	0.962	2981	0.962	2981	0.962		1	274	0.815	274	0.815	274	0.815	
2	2965	0.956	2965	0.956	2991	0.965		2	265	0.789	265	0.789	274	0.815	
3	2992	0.965	2997	0.967	2989	0.964		3	285	0.848	288	0.857	285	0.848	
4	2991	0.965	2998	0.967	2989	0.964		4	285	0.848	287	0.854	286	0.851	
5	3001	0.968	3006	0.970	3000	0.968	3100	5	285	0.848	283	0.842	286	0.851	336
6 7	3004	0.969	3001 2997	0.968	3004	0.969		6 7	286	0.851	282	0.839	286	0.851	
8	3000 3000	0.968	2997 2997	0.967 0.967	3000	0.968		8	287 291	0.854	286 285	0.851	287 290	0.854 0.863	
9	2997	0.967	3003	0.969	2997	0.967	1	9	287	0.854	287	0.854	288	0.857	1
10	2999	0.967	3007	0.970	2999	0.967	1	10	288	0.857	278	0.827	289	0.860	l i
			fla	me							ionos	phere			
К		A		В	KI	NN	Total	К		A		В	KI	NN	Total
	n	ACC	n	ACC	n	ACC			n	ACC	n	ACC	n	ACC	
1	240	1	240	1	240	1		1	306	0.872	306	0.872	306	0.872	
2	237	0.988	237	0.988	238	0.992		2	310	0.883	310	0.883	307	0.875	
3	239	0.996	238	0.992	239	0.996		3	291	0.829	295	0.840	291	0.829	
5	238	0.992	240	1.000	238	0.992		4 5	298	0.849	300	0.855	298 293	0.849	
6	239 239	0.996	240 237	1.000 0.988	239 239	0.996	240	6	293 297	0.835 0.846	296 296	0.843 0.843	293 297	0.835 0.846	351
7	238	0.992	236	0.983	238	0.992		7	293	0.835	298	0.849	293	0.835	1
8	238	0.992	236	0.983	238	0.992	1	8	295	0.840	292	0.832	295	0.840	
9	238	0.992	237	0.988	238	0.992	1	9	293	0.835	290	0.826	293	0.835	1
10	238	0.992	236	0.983	238	0.992		10	293	0.835	291	0.829	293	0.835	
				ris							ja	in			
К		A		В		NN	Total	К		A	-			NN	Total
_	n	ACC	n	ACC	n	ACC			n	ACC	n	ACC	n	ACC	
2	144 139	0.960 0.927	144 139	0.960 0.927	144	0.960		2	373 370	0.992	373 370	0.992	373 373	1.000	1
3	143	0.953	144	0.960	144	0.960		3	373	1.000	373	1.000	373	1.000	1
4	142	0.947	142	0.947	142	0.947	1	4	373	1.000	373	1.000	373	1.000	1
5	143	0.953	143	0.953	143	0.953		5	373	1.000	373	1.000	373	1.000	
6	142	0.947	142	0.947	143	0.953	150	6	373	1.000	373	1.000	373	1.000	373
7	143	0.953	144	0.960	143	0.953		7	373	1.000	373	1.000	373	1.000	
8	140	0.933	145	0.967	141	0.940		8	373	1.000	373	1.000	373	1.000	
9	141	0.940	146	0.973	141	0.940		9	373	1.000	373	1.000	373	1.000	
10	142	0.947	143	0.953	143	0.953		10	373	1.000	373 R:	1.000	373	1.000	
к		A		based B	KI	NN	Total	К		Α.	R		KI	NN	Total
	n	ACC	n	ACC	n	ACC	iotai	^	n	ACC	n	ACC	n	ACC	iotai
1	300	1.000	300	1.000	300	1.000		1	597	0.995	597	0.995	597	0.995	
2	299	0.997	299	0.997	300	1.000		2	589	0.982	589	0.982	597	0.995	
3	298	0.993	298	0.993	298	0.993		3	598	0.997	598	0.997	598	0.997	
4	297	0.990	296	0.987	297	0.990		4	597	0.995	596	0.993	597	0.995	
5	298	0.993	297	0.990	298	0.993	300	5	598	0.997	597	0.995	598	0.997	600
6	297	0.990	297	0.990	297	0.990		6	598	0.997	596	0.993	598	0.997	
7 8	297	0.990	295	0.983	297	0.990 0.987		7 8	598 598	0.997 0.997	596	0.993	598 598	0.997	
9	296 297	0.987 0.990	297 296	0.990 0.987	296 297	0.987		9	598	0.997	596 596	0.993	598	0.997 0.997	
10	296	0.990	295	0.987	296	0.990		10	598	0.997	596	0.993	598	0.997	
							sn	iral							
				К		A		В	KI	NN	Total	Ì			
					n	ACC	n	ACC	n	ACC		1			

	spiral														
K	-	4		В	KI	NN	Total								
	n	n ACC		ACC n ACC		ACC	n	ACC							
1	312	1.000	312	1.000	312	1.000									
2	312	1.000	312	1.000	312	1.000									
3	312	1.000	312	1.000	312	1.000									
4	312	312 1.000		1.000	312	1.000									
5	312	1.000	312	1.000	312	1.000	312								
6	312	1.000	311	0.997	312	1.000	312								
7	312	1.000	311	0.997	312	1.000									
8	311	0.997	307	0.984	311	0.997									
9	311 0.997		304	304 0.974		0.997									
10	308	0.987	302	0.968	308	0.987									

Table 2. Results for Experiment 2 with K=5.

		Aggregation -> K = 5								Compound -> K = 5							
α α*Κ		4		В	KI	NN	Total	α α*Κ		A		В	KI	NN	Total		
	n	ACC	n	ACC	n	ACC			n	ACC	n	ACC	n	ACC			
0.0 0	786	0.997	783	0.994				0.0 0	381	0.955	372	0.932					
0.2 1	786	0.997	783	0.994				0.2 1	381	0.955	372	0.932					
0.4 2	786	0.997	783	0.994	786	0.997	788	0.4 2	381	0.955	372	0.932	381	0.955	399		
0.6 3	778	0.987	781	0.991				0.6 3	372	0.932	368	0.922					
0.8 4	773	0.981	763	0.968				0.8 4	366	0.917	344	0.862					
			D31 -	> K = 5							ecoli -	> K = 5					
α α*K	Α		В		KNN		Total	α α*Κ	Α		В		KNN		Total		
	n	ACC	n	ACC	n	ACC			n	ACC	n	ACC	n	ACC			
0.0 0	3000	0.968	3006	0.970				0.0 0	286	0.851	284	0.845					
0.2 1	3000	0.968	3006	0.970				0.2 1	286	0.851	284	0.845					
0.4 2	3002	0.968	3007	0.970	3000	0.968	3100	0.4 2	285	0.848	285	0.848	286	0.851	336		
0.6 3	2960	0.955	2987	0.964				0.6 3	284	0.845	281	0.836					
0.8 4	2932	0.946	2863	0.924				0.8 4	279	0.830	254	0.756					
			flame	-> K = 5							ionosphe	re -> K = 5					
α α*Κ		Α		В	KI	NN	Total	α α*Κ		A		В	KI	NN	Total		
	n	ACC	n	ACC	n	ACC			n	ACC	n	ACC	n	ACC			
0.0 0	239	0.996	240	1.000				0.0 0	293	0.835	296	0.843					
0.2 1	239	0.996	240	1.000				0.2 1	293	0.835	296	0.843					
0.4 2	239	0.996	240	1.000	239	0.996	240	0.4 2	293	0.835	297	0.846	293	0.835	351		
0.6 3	239	0.996	240	1.000				0.6 3	290	0.826	289	0.823					
0.8 4	238	0.992	238	0.000				0014			077	0.700					
	20	0.552	238	0.992				0.8 4	281	0.801	277	0.789					
	250	0.992		0.992 • K = 5				0.8 4	281	0.801		0.789 > K = 5					
α α*K		0.552	iris ->		KI	NN	Total	α α*Κ		0.801 A	jain -:		KI	NN	Total		
α α*Κ	n		iris ->	K = 5 B ACC	KI n	NN ACC	Total		n		jain -: n	> K = 5	KI n	NN ACC	Total		
	n 143	A ACC 0.953	iris -> n 143	K=5			Total		n 373	A	jain -	> K = 5		_	Total		
α α*Κ	n	A ACC	iris ->	K = 5 B ACC			Total	α α*Κ	n	A ACC	jain -: n	> K = 5 B ACC		_	Total		
α α*K	n 143	A ACC 0.953	iris -> n 143	K = 5 B ACC 0.953			Total	α α*K	n 373	A ACC 1.000	jain -: n 373	> K = 5 B ACC 1.000		_	Total		
α α*K 0.0 0 0.2 1	n 143 143	ACC 0.953 0.953	iris -> n 143	ACC 0.953 0.953	n	ACC		α α*K 0.0 0 0.2 1	n 373 373	A ACC 1.000 1.000	jain -: n 373 373	ACC 1.000	n	ACC			
α α*K 0.0 0 0.2 1 0.4 2	n 143 143	ACC 0.953 0.953 0.953	iris -> n 143 143 143	ACC 0.953 0.953 0.953	n	ACC		α α*K 0.0 0 0.2 1 0.4 2	n 373 373 373	A ACC 1.000 1.000	jain -: n 373 373 373	ACC 1.000 1.000	n	ACC			
α α*K 0.0 0 0.2 1 0.4 2 0.6 3	n 143 143 143 141	ACC 0.953 0.953 0.953 0.940	iris -> n 143 143 143 143 143	ACC 0.953 0.953 0.953 0.953	n	ACC		α α*K 0.0 0 0.2 1 0.4 2 0.6 3	n 373 373 373 372	A ACC 1.000 1.000 1.000 0.997	n 373 373 373 371 365	ACC 1.000 1.000 1.000 0.995	n	ACC			
α α*K 0.0 0 0.2 1 0.4 2 0.6 3	n 143 143 143 141 139	ACC 0.953 0.953 0.953 0.940	iris -> n 143 143 143 143 143 146 pathbase	ACC 0.953 0.953 0.953 0.953 0.953	n 143	ACC		α α*K 0.0 0 0.2 1 0.4 2 0.6 3	n 373 373 373 373 372 371	A ACC 1.000 1.000 1.000 0.997 0.995	jain -: n 373 373 373 371 365 R15 -:	ACC 1.000 1.000 1.000 0.995 0.979	n 373	ACC			
α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 α α*K	n 143 143 143 141 139	ACC 0.953 0.953 0.953 0.940 0.927	143 143 143 143 143 136 pathbase	ACC 0.953 0.953 0.953 0.953 0.953 0.907 d -> K = 5 B ACC	n 143	0.953	150	0.0 0 0.2 1 0.4 2 0.6 3 0.8 4	n 373 373 373 372 371	A ACC 1.000 1.000 0.997 0.995	jain -: n 373 373 373 371 365 R15 -:	ACC 1.000 1.000 1.000 0.995 0.979 K = 5	n 373	1.000	373		
α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4	n 143 143 143 141 139	A ACC 0.953 0.953 0.953 0.940 0.927 A ACC 0.993	n 143 143 143 136 pathbase n 297	ACC 0.953 0.953 0.953 0.953 0.907 d -> K = 5	n 143	0.953	150	α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 α α*K	n 373 373 373 372 371	A ACC 1.000 1.000 0.997 0.995 A ACC 0.997	jain -: n 373 373 373 371 365 R15 -: n 597	ACC 1.000 1.000 1.000 0.995 0.979 K = 5	n 373 KI	1.000	373		
α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 α α*K	n 143 143 143 141 139	ACC 0.953 0.953 0.953 0.940 0.927	143 143 143 143 143 136 pathbase	ACC 0.953 0.953 0.953 0.953 0.953 0.907 d -> K = 5 B ACC	n 143	0.953	150	0.0 0 0.2 1 0.4 2 0.6 3 0.8 4	n 373 373 373 372 371	A ACC 1.000 1.000 0.997 0.995	jain -: n 373 373 373 371 365 R15 -:	> K = 5 B	n 373 KI	1.000	373		
α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 α α*K	n 143 143 143 141 139	A ACC 0.953 0.953 0.953 0.940 0.927 A ACC 0.993	n 143 143 143 136 pathbase n 297	ACC 0.953 0.953 0.953 0.953 0.907 d -> K = 5 B ACC 0.990	n 143	0.953	150	α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 α α*K	n 373 373 373 372 371	A ACC 1.000 1.000 0.997 0.995 A ACC 0.997	jain -: n 373 373 373 371 365 R15 -: n 597	ACC 1.000 1.000 1.000 0.995 0.979 >K=5 B ACC 0.995	n 373 KI	1.000	373		
α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 α α*K 0.0 0 0.2 1 0.4 2 0.6 3	n 143 143 143 141 139 n 298 298 298 298	A ACC 0.953 0.953 0.953 0.940 0.927 A ACC 0.993 0.993 0.993 0.993	n 143 143 143 143 143 126 pathbase n 297 296 295	ACC 0.953 0.953 0.953 0.953 0.953 0.953 0.953 0.904 0.907 0.990 0.990	143 KI	0.953	150	α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 α α*K 0.0 0 0.2 1 0.4 2 0.6 3	n 373 373 373 372 371 n 598 598 598 598	A ACC 1.000 1.000 0.997 0.995 A ACC 0.997 0.997 0.997 0.997	jain -: n 373 373 373 371 365 R15 -: n 597	ACC 1.000 1.000 0.995 0.979 B ACC 0.995 0.995 0.995 0.995 0.980	n 373 KI	1.000	373 Total		
α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 α α*K 0.0 0 0.2 1 0.4 2	n 143 143 143 141 139 n 298 298 298	A ACC 0.953 0.953 0.953 0.940 0.927 A ACC 0.993 0.993 0.993	n 143 143 143 143 136 pathbase n 297 297 296	ACC 0.953 0.953 0.953 0.953 0.953 0.953 0.953 0.953 0.953 0.96d -> K = 5 B ACC 0.990 0.990 0.987	143 KI	0.953	150 Total	α α*K 0.0 0 0.2 1 0.6 3 0.8 4 0.0 0 0 0 0 0 0 0 0	n 373 373 373 372 371 n 598 598	A ACC 1.000 1.000 0.997 0.995 A ACC 0.997 0.997 0.997	jain -: n 373 373 373 371 365 R15 -: n 597 597	ACC 1.000 1.000 1.000 0.995 0.979	n 373 KI	1.000	373 Total		
α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 α α*K 0.0 0 0.2 1 0.4 2 0.6 3	n 143 143 143 141 139 n 298 298 298 298	A ACC 0.953 0.953 0.953 0.940 0.927 A ACC 0.993 0.993 0.993 0.993	n 143 143 143 143 143 126 pathbase n 297 296 295	ACC 0.953 0.953 0.953 0.953 0.953 0.953 0.953 0.904 0.907 0.990 0.990	n 143 Kn n 298	0.953 NN ACC 0.993	Total 300 spiral	0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4	n 373 373 373 372 371 n 598 598 598 598 586	A ACC 1.000 1.000 0.997 0.995 A ACC 0.997 0.997 0.997 0.995	jain -: n 373 373 373 371 365 R15 -: n 597 597 588 532	ACC 1.000 1.000 0.995 0.979 B ACC 0.995 0.995 0.995 0.995 0.980	n 373 KI	1.000	373 Total		
α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 α α*K 0.0 0 0.2 1 0.4 2 0.6 3	n 143 143 143 141 139 n 298 298 298 298	A ACC 0.953 0.953 0.953 0.940 0.927 A ACC 0.993 0.993 0.993 0.993	n 143 143 143 143 143 126 pathbase n 297 296 295	ACC 0.953 0.953 0.953 0.953 0.953 0.953 0.953 0.904 0.907 0.990 0.990	n 143 Kn n 298	0.953 NN ACC 0.993	Total 300 spiral	0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4	n 373 373 373 372 371 n 598 598 598 598 586 567	A ACC 1.000 1.000 0.997 0.995 A ACC 0.997 0.997 0.997 0.997 0.997 0.945	jain -: n 373 373 373 371 365 R15 -: n 597 597 597 588	ACC 1.000 1.000 0.995 0.979 B ACC 0.995 0.995 0.995 0.995 0.980	n 373 KI	1.000	373 Total		
α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 α α*K 0.0 0 0.2 1 0.4 2 0.6 3	n 143 143 143 141 139 n 298 298 298 298	A ACC 0.953 0.953 0.953 0.940 0.927 A ACC 0.993 0.993 0.993 0.993	n 143 143 143 143 143 126 pathbase n 297 296 295	K = 5 B ACC 0.953 0.953 0.953 0.953 0.907 d -> K = 5 B ACC 0.990 0.987 0.983 0.957 α α*K	143 Kf	0.953 NN ACC 0.993	Total 300 spiral	α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4	n 373 373 373 372 371 n 598 598 598 598 586	A ACC 1.000 1.000 0.997 0.995 A ACC 0.997 0.997 0.997 0.995	jain -: n 373 373 373 371 365 R15 -: n 597 597 588 532	ACC 1.000 1.000 0.995 0.979 B ACC 0.995 0.995 0.995 0.995 0.980	n 373 KI	1.000	373 Total		
α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 α α*K 0.0 0 0.2 1 0.4 2 0.6 3	n 143 143 143 141 139 n 298 298 298 298	A ACC 0.953 0.953 0.953 0.940 0.927 A ACC 0.993 0.993 0.993 0.993	n 143 143 143 143 143 126 pathbase n 297 296 295	K = 5 B ACC 0.953 0.953 0.953 0.907 d > K = 5 B ACC 0.990 0.987 0.983 0.957 α α*K α*K 0.0 0 0	n 143 Kf	0.953 NN ACC 0.993 A ACC 1.000	150 Total 300 spiral	α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 ACC 1.000	n 373 373 373 372 371 n 598 598 598 598 586 567	A ACC 1.000 1.000 0.997 0.995 A ACC 0.997 0.997 0.997 0.997 0.997 0.945	jain -: n 373 373 373 371 365 R15 -: n 597 597 588 532	ACC 1.000 1.000 0.995 0.979 B ACC 0.995 0.995 0.995 0.995 0.980	n 373 KI	1.000	373 Total		
α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 α α*K 0.0 0 0.2 1 0.4 2 0.6 3	n 143 143 143 141 139 n 298 298 298 298	A ACC 0.953 0.953 0.953 0.940 0.927 A ACC 0.993 0.993 0.993 0.993	n 143 143 143 143 143 126 pathbase n 297 296 295	ACC 0.953 0.953 0.953 0.953 0.953 0.953 0.953 0.953 0.957 dd -> K = 5 B ACC 0.990 0.990 0.9957 0.983 0.957 0.983 0.957	n 143 KH n 298 N 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	0.953 NN ACC 0.993 A ACC 1.000 1.000	150 Total 300 spiral n 312 312	\(\alpha \) \(n 373 373 373 372 371 n 598 598 598 598 567	A ACC 1.000 1.000 0.997 0.995 A ACC 0.997 0.995 0.997 0.995 NNN ACC	jain n 373 373 371 365 R15 n 597 597 597 588 532	ACC 1.000 1.000 0.995 0.979 B ACC 0.995 0.995 0.995 0.995 0.980	n 373 KI	1.000	373 Total		
α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 α α*K 0.0 0 0.2 1 0.4 2 0.6 3	n 143 143 143 141 139 n 298 298 298 298	A ACC 0.953 0.953 0.953 0.940 0.927 A ACC 0.993 0.993 0.993 0.993	n 143 143 143 143 143 126 pathbase n 297 296 295	K = 5 B ACC 0.953 0.953 0.953 0.953 0.953 0.957 d -> K = 5 B ACC 0.990 0.987 0.983 0.957	n 143 Kr n 298 312 312 312 312	0.953 NN ACC 0.993 A ACC 1.000 1.000	150 Total 300 spiral n 312 312 312 312	α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 Δ α*K Α α α*K Α α α α α α α α α α	n 373 373 373 372 371 n 598 598 598 598 586 567	A ACC 1.000 1.000 0.997 0.995 A ACC 0.997 0.997 0.997 0.997 0.997 0.945	jain -: n 373 373 373 371 365 R15 -: n 597 597 588 532	ACC 1.000 1.000 0.995 0.979 B ACC 0.995 0.995 0.995 0.995 0.980	n 373 KI	1.000	373 Total		
α α*K 0.0 0 0.2 1 0.4 2 0.6 3 0.8 4 α α*K 0.0 0 0.2 1 0.4 2 0.6 3	n 143 143 143 141 139 n 298 298 298 298	A ACC 0.953 0.953 0.953 0.940 0.927 A ACC 0.993 0.993 0.993 0.993	n 143 143 143 143 143 126 pathbase n 297 296 295	ACC 0.953 0.953 0.953 0.953 0.953 0.953 0.953 0.953 0.957 dd -> K = 5 B ACC 0.990 0.990 0.9957 0.983 0.957 0.983 0.957	n 143 KH n 298 N 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	0.953 NN ACC 0.993 A ACC 1.000 1.000	150 Total 300 spiral n 312 312	\(\alpha \) \(n 373 373 373 372 371 n 598 598 598 598 567	A ACC 1.000 1.000 0.997 0.995 A ACC 0.997 0.995 0.997 0.995 NNN ACC	jain n 373 373 371 365 R15 n 597 597 597 588 532	ACC 1.000 1.000 0.995 0.979 B ACC 0.995 0.995 0.995 0.995 0.980	n 373 KI	1.000	373 Total		

Table 3. Results for Experiment 2 with K=10.

			Aggregation	on -> K = 10)			Compound -> K = 10								
α α*Κ	A B		В	KNN		Total	α α*K		A	В		KNN		Total		
	n	ACC	n	ACC	n	ACC			n	ACC	n	ACC	n	ACC		
0.0 0	786	0.997	784	0.995				0.0 0	377	0.945	369	0.925				
0.1 1	786	0.997	784	0.995				0.1 1	377	0.945	369	0.925				
0.2 2	786	0.997	784	0.995				0.2 2	377	0.945	369	0.925				
0.3 3	786	0.997	784	0.995				0.3 3	377	0.945	369	0.925				
0.4 4	786	0.997	784	0.995	700	0.007	700	0.4 4 377 0.945 369 0.925	277	0.045	200					
0.5 5	781	0.991	784	0.995	786	0.997	/88	0.5 5	374	0.937	369	0.925	377 -	0.945	399	
0.6 6	775	0.984	785	0.996				0.6 6	369	0.925	367	0.920				
0.7 7	775	0.984	785	0.996				0.7 7	369	0.925	367	0.920				
0.8 8	767	0.973	774	0.982				0.8 8	350	0.877	341	0.855				
0.9 9	760	0.964	698	0.886				0.9 9	342	0.857	277	0.694	1			

			D31 ->	K = 10				ecoli -> K = 10								
α α*K		4		В		KNN		α α*K	Α		В		KNN		Total	
	n	ACC	n	ACC	n	ACC			n	ACC	n	ACC	n	ACC		
0.0 0	2999	0.967	3007	0.970				0.0 0	289	0.860	278	0.827				
0.1 1	2999	0.967	3007	0.970				0.1 1	289	0.860	278	278 0.827				
0.2 2	2999	0.967	3007	0.970				0.2 2	289	0.860	278	0.827				
0.3 3	2999	0.967	3007	0.970				0.3 3	286	0.851	278	0.827	l i			
0.4 4	2999	0.967	3009	0.971	2999	0.967	3100	0.4 4	0.4 4 285 0.848 278 0.827	289	0.860	225				
0.5 5	2982	0.962	3012	0.972	2999	0.967	3100	0.5 5	281	0.836	279	0.830	269	0.860	336	
0.6 6	2952	0.952	3014	0.972				0.6 6	282	0.839	275	0.818				
0.7 7	2952	0.952	3014	0.972				0.7 7	282	0.839	275	0.818				
0.8 8	2876	0.928	2923	0.943				0.8 8	270	0.804	264	0.786				
0.9 9	2842	0.917	2492	0.804				0.9 9	265	0.789	174	0.518				

Table 3. (continuation)

			flame -	> K = 10							ionosphe	re -> K = 10			
α α*K	-	4		3	KI	IN	Total	α α*K		Α		В	KI	NN	Total
	n	ACC	n	ACC	n	ACC			n	ACC	n	ACC	n	ACC	
0.0 0	238	0.992	236	0.983				0.0 0	293	0.835	291	0.829			
0.1 1	238	0.992	236	0.983				0.1 1	293	0.835	291	0.829			
0.2 2	238	0.992	236	0.983				0.2 2	293	0.835	291	0.829			
0.3 3	238	0.992	236	0.983				0.3 3	293	0.835	291	0.829			
0.4 4	238	0.992	236	0.983	238	0.992	240	0.4 4	293	0.835	291	0.829	293	0.835	351
0.5 5	238	0.992	236	0.983	230	0.552	240	0.5 5	290	0.826	291	0.829	255	0.055	331
0.6 6	238	0.992	236	0.983				0.6 6	288	0.821	290	0.826			
0.7 7	238	0.992	236	0.983				0.7 7	288	0.821	290	0.826			
0.8 8	234	0.975	233	0.971				0.8 8	281	0.801	272	0.775			
0.9 9	234	0.975	217	0.904				0.9 9	279	0.795	242	0.689			
			iris ->	K = 10							jain ->	> K = 10			
α α*K		4	ı	3	KI	IN	Total	α α*K		A		В	KI	NN	Total
	n	ACC	n	ACC	n	ACC			n	ACC	n	ACC	n	ACC	
0.0 0	143	0.953	143	0.953				0.0 0	373	1.000	373	1.000			
0.1 1	143	0.953	143	0.953				0.1 1	373	1.000	373	1.000			
0.2 2	142	0.947	142	0.947				0.2 2	373	1.000	373	1.000	1		
0.3 3	142	0.947	142	0.947			0.3 3	373	1.000	373	1.000	4			
0.4 4	141	0.940	142	0.947	143	0.953	150	0.4 4	373	1.000	373	1.000	373	1.000	373
0.5 5	140	0.933	143	0.953	2.0		250	0.5 5	372	0.997	373	1.000	3,3		3,3
0.6 6	141	0.940	142	0.947				0.6 6	371	0.995	372	0.997			
0.7 7	141	0.940	142	0.947				0.7 7	371	0.995	372	0.997			
0.8 8	136	0.907	132	0.880				0.8 8	365	0.979	364	0.976			
0.9 9	134	0.893	90	0.600				0.9 9	361	0.968	336	0.901			
				d -> K = 10								K = 10			
α α*K		4		3	KI		Total	α α*K		A		В		NN	Total
	n	ACC	n	ACC	n	ACC			n	ACC	n	ACC	n	ACC	
0.0 0	296	0.987	295	0.983				0.0 0	598	0.997	596	0.993			
0.1 1	296	0.987	295	0.983				0.1 1	598	0.997	596	0.993			
0.2 2	296	0.987	295	0.983				0.2 2	598	0.997	596	0.993			
0.3 3	296	0.987	295	0.983				0.3 3	598	0.997	596	0.993			
0.4 4	296	0.987	295	0.983	296	296 0.987 3	300	0.4 4	598	0.997	596	0.993	598	0.997	600
0.5 5	296	0.987	295	0.983				0.5 5	593	0.988	596	0.993			
0.6 6	295	0.983	294	0.980				0.6 6	576	0.960	596	0.993			
0.7 7	295	0.983	294	0.980				0.7 7	576	0.960	596	0.993			
0.8 8	290	0.967	280	0.933				0.8 8	548	0.913	544	0.907			
0.9 9	285	0.950	222	0.740				0.9 9	531	0.885	383	0.638			

	•••				0.0							
				spiral -	piral -> K = 10							
α	α*K	-	A		В	KI	NN	Total				
		n	ACC	n	ACC	n	ACC					
0.0	0 0	308	0.987	302	0.968							
0.3	1 1	308	0.987	302	0.968							
0.2	2 2	308	0.987	302	0.968							
0.3	3 3	308	0.987	301	0.965							
0.4	1 4	308	0.987	301	0.965	308	0.987	312				
0.	5 5	308	0.987	299	0.958	308	0.987	312				
0.0	5 6	305	0.978	297	0.952							
0.7	7 7	305	0.978	297	0.952							
0.8	8 8	296	0.949	271	0.869							
0.9	9 9	286	0.917	233	0.747							

				\$2 -> K = 10											
L			_	K = 10											
α α*K		Α		В	KI	NN	Total	α α*K		4		3	KN	IN	Total
	n	ACC	n	ACC	n	ACC			n	ACC	n	ACC	n	ACC	
0.0 0	2986	0.597	2973	0.595				0.0 0	2843	0.569	2819	0.564			
0.1 1	2986	0.597	2973	0.595				0.1 1	2843	0.569	2819	0.564			
0.2 2	2986	0.597	2973	0.595				0.2 2	2843	0.569	2819	0.564			
0.3 3	2986	0.597	2973	0.595				0.3 3	2843	0.569	2819	0.564			
0.4 4	2986	0.597	2973	0.595	2986	0.597	5000	0.4 4	2843	0.569	2815	0.563	2843	0.569	5000
0.5 5	2946	0.589	2973	0.595	2986	0.597	5000	0.5 5	2816	0.563	2808	0.562	2843	0.569	5000
0.6 6	2881	0.576	2976	0.595				0.6 6	2787	0.557	2808	0.562			
0.7 7	2881	0.576	2976	0.595				0.7 7	2787	0.557	2808	0.562			
0.8 8	2823	0.565	2865	0.573				0.8 8	2719	0.544	2677	0.535			
0.9 9	2786	0.557	2440	0.488				0.9 9	2694	0.539	2263	0.453			
			S3 ->	K = 10					S4 -> K = 10						
α α*K		4		В	KI	NN	Total	α α*K		4	В		KN	IN	Total
	n	ACC	n	ACC	n	ACC			n	ACC	n	ACC	n	ACC	
0.0 0	2320	0.464	2329	0.466				0.0 0	2010	0.402	2007	0.401			
0.1 1	2320	0.464	2329	0.466				0.1 1	2010	0.402	2007	0.401			
0.2 2	2318	0.464	2327	0.465				0.2 2	2009	0.402	1999	0.400			
0.3 3	2320	0.464	2329	0.466				0.3 3	2017	0.403	1991	0.398			
0.4 4	2323	0.465	2321	0.464	2222			0.4 4	2015	0.403	1985	0.397	2040	0.400	
0.5 5	2314	0.463	2318	0.464	2320	0.464	5000	0.5 5	2015	0.403	1992	0.398	2010	0.402	5000
0.6 6	2302	0.460	2328	0.466				0.6 6	2019	0.404	1992	0.398			
0.7 7	2302	0.460	2328	0.466				0.7 7	2019	0.404	1992	0.398			
0.8 8	2264	0.453	2306	0.461				0.8 8	1949	0.390	1954	0.391			
	2252	0.450	1968	0.394				0.9 9	1939	0.388	1615	0.323		l	

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