

Dataset	Objects	Features	Clusters	0% CS					
				PCCC-N2-S	COPKM	LCC	CSC	DILS	KMEANS
Banana	5,300	2	2	0.019	0.018	–	<b>0.030</b>	0.008	0.017
Letter	20,000	16	26	0.149	<b>0.156</b>	–	–	0.000	0.149
Shuttle	57,999	9	7	0.193	<b>0.429</b>	–	–	–	0.411
CIFAR 10	60,000	3,072	10	<b>0.039</b>	–	–	–	–	0.040
CIFAR 100	60,000	3,072	100	<b>0.021</b>	–	–	–	–	0.021
MNIST	70,000	784	10	<b>0.304</b>	0.193	–	–	–	0.312
Mean				0.121	<b>0.133*</b>	0.000*	0.005*	0.001*	0.159

\*Nan values (–) are replaced with 0 before computing the mean.

Table W31: Average Adjusted Rand Index (ARI) values of the PCCC-N2-S algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 0% CS. Higher values indicate more overlap with the ground truth assignment. The highest values are stated in bold. The column KMEANS reports the average ARI values that were obtained with the unconstrained k-means algorithm. The hyphen indicates that the respective algorithm returned no solution within the time limit of 3,600 seconds. We noticed that the LCC algorithm stops with a runtime error when the constraint set is empty. This is why the LCC algorithm did not return any solutions for the constraint sets of size 0% CS. The differences between the results of the PCCC version and the results of the COPKM and the KMEANS algorithms can be explained as follows. The COPKM algorithm uses a different implementation of the kmeans++ algorithm, and the PCCC version uses the Euclidean distance for parameter  $d_{il}$  and not the squared Euclidean distance which can lead to different assignments for some instances.

Dataset	Objects	Features	Clusters	0.5% CS					
				PCCC-N2-S	COPKM	LCC	CSC	DILS	KMEANS
Banana	5,300	2	2	<b>0.018</b>	–	0.006	0.000	0.003	0.017
Letter	20,000	16	26	0.154	<b>0.156</b>	0.148	–	0.000	0.149
Shuttle	57,999	9	7	<b>0.503</b>	–	0.312	–	–	0.411
CIFAR 10	60,000	3,072	10	<b>0.044</b>	–	–	–	–	0.040
CIFAR 100	60,000	3,072	100	<b>0.022</b>	–	–	–	–	0.021
MNIST	70,000	784	10	<b>0.387</b>	0.217	–	–	–	0.312
Mean				<b>0.188</b>	0.062*	0.078*	0.000*	0.000*	0.159

\*Nan values (–) are replaced with 0 before computing the mean.

Table W32: Average Adjusted Rand Index (ARI) values of the PCCC-N2-S algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 0.5% CS. Higher values indicate more overlap with the ground truth assignment. The highest values are stated in bold. The column KMEANS reports the average ARI values that were obtained with the unconstrained k-means algorithm. The hyphen indicates that the respective algorithm returned no solution within the time limit of 3,600 seconds.

Dataset	Objects	Features	Clusters	1% CS					
				PCCC-N2-S	COPKM	LCC	CSC	DILS	KMEANS
Banana	5,300	2	2	<b>0.013</b>	–	0.011	-0.000	0.004	0.017
Letter	20,000	16	26	0.150	0.154	<b>0.162</b>	–	0.000	0.149
Shuttle	57,999	9	7	<b>0.974</b>	–	–	–	–	0.411
CIFAR 10	60,000	3,072	10	<b>0.060</b>	–	–	–	–	0.040
CIFAR 100	60,000	3,072	100	<b>0.021</b>	–	–	–	–	0.021
MNIST	70,000	784	10	<b>0.594</b>	–	–	–	–	0.312
Mean				<b>0.302</b>	0.026*	0.029*	-0.000*	0.001*	0.159

\*Nan values (–) are replaced with 0 before computing the mean.

Table W33: Average Adjusted Rand Index (ARI) values of the PCCC-N2-S algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets 1%. Higher values indicate more overlap with the ground truth assignment. The highest values are stated in bold. The column KMEANS reports the average ARI values that were obtained with the unconstrained k-means algorithm. The hyphen indicates that the respective algorithm returned no solution within the time limit of 3,600 seconds.

Dataset	Objects	Features	Clusters	5% CS					
				PCCC-N2-S	COPKM	LCC	CSC	DILS	KMEANS
Banana	5,300	2	2	<b>1.000</b>	–	–	0.996	0.100	0.017
Letter	20,000	16	26	<b>0.588</b>	–	–	–	0.000	0.149
Shuttle	57,999	9	7	<b>0.985</b>	–	–	–	–	0.411
CIFAR 10	60,000	3,072	10	<b>0.570</b>	–	–	–	–	0.040
CIFAR 100	60,000	3,072	100	<b>0.303</b>	–	–	–	–	0.021
MNIST	70,000	784	10	<b>0.745</b>	–	–	–	–	0.312
Mean				<b>0.699</b>	0.000*	0.000*	0.166*	0.017*	0.159

\*Nan values (–) are replaced with 0 before computing the mean.

Table W34: Average Adjusted Rand Index (ARI) values of the PCCC-N2-S algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 5% CS. Higher values indicate more overlap with the ground truth assignment. The highest values are stated in bold. The column KMEANS reports the average ARI values that were obtained with the unconstrained k-means algorithm. The hyphen indicates that the respective algorithm returned no solution within the time limit of 3,600 seconds.

Dataset	Objects	Features	Clusters	0% CS					KMEANS	GT
				PCCC-N2-S	COPKM	LCC	CSC	DILS		
Banana	5,300	2	2	<b>0.389</b>	<b>0.389</b>	–	0.388	0.185	0.389	0.032
Letter	20,000	16	26	<b>0.145</b>	0.141	–	–	-0.020	0.145	0.010
Shuttle	57,999	9	7	0.356	<b>0.459</b>	–	–	–	0.463	0.300
CIFAR 10	60,000	3,072	10	<b>0.048</b>	–	–	–	–	0.051	-0.053
CIFAR 100	60,000	3,072	100	<b>0.015</b>	–	–	–	–	0.015	-0.114
MNIST	70,000	784	10	0.003	<b>0.012</b>	–	–	–	0.007	-0.043
Mean				<b>0.159</b>	-0.167*	-1.000*	-0.769*	-0.639*	0.178	0.022

\*Nan values (–) are replaced with -1 before computing the mean.

Table W35: Average Silhouette coefficients of the PCCC-N2-S algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 0% CS. Higher values indicate better separated clusters. The highest values are stated in bold. The column KMEANS reports the average Silhouette coefficients that were obtained with the unconstrained k-means algorithm. The column GT reports the Silhouette coefficients of the ground truth assignment. The hyphen indicates that the respective algorithm returned no solution within the time limit of 3,600 seconds. We noticed that the LCC algorithm stops with a runtime error when the constraint set is empty. This is why the LCC algorithm did not return any solutions for the constraint sets of size 0% CS. The differences between the results of the PCCC version and the results of the COPKM and the KMEANS algorithms can be explained as follows. The COPKM algorithm uses a different implementation of the kmeans++ algorithm, and the PCCC version uses the Euclidean distance for parameter  $d_{il}$  and not the squared Euclidean distance which can lead to different assignments for some instances.

Dataset	Objects	Features	Clusters	0.5% CS					KMEANS	GT
				PCCC-N2-S	COPKM	LCC	CSC	DILS		
Banana	5,300	2	2	<b>0.358</b>	–	0.347	0.284	0.143	0.389	0.032
Letter	20,000	16	26	<b>0.135</b>	0.134	0.117	–	-0.020	0.145	0.010
Shuttle	57,999	9	7	<b>0.145</b>	–	0.005	–	–	0.463	0.300
CIFAR 10	60,000	3,072	10	<b>0.030</b>	–	–	–	–	0.051	-0.053
CIFAR 100	60,000	3,072	100	<b>0.014</b>	–	–	–	–	0.015	-0.114
MNIST	70,000	784	10	<b>-0.015</b>	-0.018	–	–	–	0.007	-0.043
Mean				<b>0.111</b>	-0.647*	-0.422*	-0.786*	-0.646*	0.178	0.022

\*Nan values (–) are replaced with -1 before computing the mean.

Table W36: Average Silhouette coefficients of the PCCC-N2-S algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 0.5% CS. Higher values indicate better separated clusters. The highest values are stated in bold. The column KMEANS reports the average Silhouette coefficients that were obtained with the unconstrained k-means algorithm. The column GT reports the Silhouette coefficients of the ground truth assignment. The hyphen indicates that the respective algorithm returned no solution within the time limit of 3,600 seconds.

Dataset	Objects	Features	Clusters	1% CS					KMEANS	GT
				PCCC-N2-S	COPKM	LCC	CSC	DILS		
Banana	5,300	2	2	<b>0.280</b>	–	0.261	-0.118	0.103	0.389	0.032
Letter	20,000	16	26	<b>0.113</b>	0.111	0.110	–	-0.020	0.145	0.010
Shuttle	57,999	9	7	<b>0.320</b>	–	–	–	–	0.463	0.300
CIFAR 10	60,000	3,072	10	<b>-0.010</b>	–	–	–	–	0.051	-0.053
CIFAR 100	60,000	3,072	100	<b>0.008</b>	–	–	–	–	0.015	-0.114
MNIST	70,000	784	10	<b>-0.039</b>	–	–	–	–	0.007	-0.043
Mean				<b>0.112</b>	-0.815*	-0.605*	-0.853*	-0.653*	0.178	0.022

\*Nan values (–) are replaced with -1 before computing the mean.

Table W37: Average Silhouette coefficients of the PCCC-N2-S algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 1% CS. Higher values indicate better separated clusters. The highest values are stated in bold. The column KMEANS reports the average Silhouette coefficients that were obtained with the unconstrained k-means algorithm. The column GT reports the Silhouette coefficients of the ground truth assignment. The hyphen indicates that the respective algorithm returned no solution within the time limit of 3,600 seconds.

Dataset	Objects	Features	Clusters	5% CS						GT
				PCCC-N2-S	COPKM	LCC	CSC	DILS	KMEANS	
Banana	5,300	2	2	0.032	–	–	<b>0.033</b>	0.004	0.389	0.032
Letter	20,000	16	26	-0.049	–	–	–	<b>-0.017</b>	0.145	0.010
Shuttle	57,999	9	7	<b>0.350</b>	–	–	–	–	0.463	0.300
CIFAR 10	60,000	3,072	10	<b>-0.203</b>	–	–	–	–	0.051	-0.053
CIFAR 100	60,000	3,072	100	<b>-0.127</b>	–	–	–	–	0.015	-0.114
MNIST	70,000	784	10	<b>-0.116</b>	–	–	–	–	0.007	-0.043
Mean				<b>-0.019</b>	-1.000*	-1.000*	-0.828*	-0.669*	0.178	0.022

\*Nan values (–) are replaced with -1 before computing the mean.

Table W38: Average Silhouette coefficients of the PCCC-N2-S algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 5% CS. Higher values indicate better separated clusters. The highest values are stated in bold. The column KMEANS reports the average Silhouette coefficients that were obtained with the unconstrained k-means algorithm. The column GT reports the Silhouette coefficients of the ground truth assignment. The hyphen indicates that the respective algorithm returned no solution within the time limit of 3,600 seconds.

Dataset	Objects	Features	Clusters	0% CS					
				PCCC-N2-S	COPKM	LCC	CSC	DILS	KMEANS
Banana	5,300	2	2	6.7	<b>1.0</b>	–	5,208.4	3,849.2	0.1
Letter	20,000	16	26	<b>74.1</b>	1,007.8	–	–	4,450.1	0.5
Shuttle	57,999	9	7	<b>18.3</b>	227.7	–	–	–	0.3
CIFAR 10	60,000	3,072	10	<b>375.6</b>	–	–	–	–	18.0
CIFAR 100	60,000	3,072	100	<b>3,546.9</b>	–	–	–	–	84.5
MNIST	70,000	784	10	<b>199.1</b>	3,655.5	–	–	–	4.2
Sum				<b>4,220.9</b>	12,092.0*	21,600.0*	23,208.4*	22,699.4*	107.6

\*Nan values (–) are replaced with 3,600 before computing the sum.

Table W39: Average running times (in seconds) of the PCCC-N2-S algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) for the constraint sets of size 0% CS. The lowest values are stated in bold. The column KMEANS reports the average running time of the unconstrained k-means algorithm. The hyphen indicates that the respective algorithm returned no solution within the time limit of 3,600 seconds. We noticed that the LCC algorithm stops with a runtime error when the constraint set is empty. This is why the LCC algorithm did not return any solutions for the constraint sets of size 0% CS.

Dataset	Objects	Features	Clusters	0.5% CS					
				PCCC-N2-S	COPKM	LCC	CSC	DILS	KMEANS
Banana	5,300	2	2	<b>4.1</b>	–	94.1	4,415.0	3,622.2	0.1
Letter	20,000	16	26	<b>70.9</b>	846.9	3,642.4	–	4,459.9	0.5
Shuttle	57,999	9	7	<b>25.8</b>	–	4,926.2	–	–	0.3
CIFAR 10	60,000	3,072	10	<b>382.5</b>	–	–	–	–	18.5
CIFAR 100	60,000	3,072	100	<b>3,576.8</b>	–	–	–	–	82.3
MNIST	70,000	784	10	<b>241.9</b>	3,884.6	–	–	–	4.3
Sum				<b>4,302.1</b>	19,131.5*	19,462.7*	22,415.0*	22,482.1*	106.1

\*Nan values (–) are replaced with 3,600 before computing the sum.

Table W40: Average running times (in seconds) of the PCCC-N2-S algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) for the constraint sets of size 0.5% CS. The lowest values are stated in bold. The column KMEANS reports the average running time of the unconstrained k-means algorithm. The hyphen indicates that the respective algorithm returned no solution within the time limit of 3,600 seconds.

Dataset	Objects	Features	Clusters	1% CS					
				PCCC-N2-S	COPKM	LCC	CSC	DILS	KMEANS
Banana	5,300	2	2	<b>7.6</b>	–	114.5	3,774.8	3,629.6	0.1
Letter	20,000	16	26	<b>115.6</b>	841.7	3,785.3	–	4,568.9	0.5
Shuttle	57,999	9	7	<b>10.0</b>	–	–	–	–	0.4
CIFAR 10	60,000	3,072	10	<b>3,085.1</b>	–	–	–	–	16.7
CIFAR 100	60,000	3,072	100	<b>3,575.2</b>	–	–	–	–	87.1
MNIST	70,000	784	10	<b>3,342.5</b>	–	–	–	–	4.3
Sum				<b>10,136.0</b>	18,841.7*	18,299.8*	21,774.8*	22,598.5*	109.0

\*Nan values (–) are replaced with 3,600 before computing the sum.

Table W41: Average running times (in seconds) of the PCCC-N2-S algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) for the constraint sets of size 1% CS. The lowest values are stated in bold. The column KMEANS reports the average running time of the unconstrained k-means algorithm. The hyphen indicates that the respective algorithm returned no solution within the time limit of 3,600 seconds.

Dataset	Objects	Features	Clusters	5% CS					KMEANS
				PCCC-N2-S	COPKM	LCC	CSC	DILS	
Banana	5,300	2	2	<b>0.4</b>	–	–	4,386.9	4,283.3	0.1
Letter	20,000	16	26	<b>229.5</b>	–	–	–	4,109.1	0.5
Shuttle	57,999	9	7	<b>21.0</b>	–	–	–	–	0.3
CIFAR 10	60,000	3,072	10	<b>21.8</b>	–	–	–	–	17.5
CIFAR 100	60,000	3,072	100	<b>3,759.6</b>	–	–	–	–	85.2
MNIST	70,000	784	10	<b>20.7</b>	–	–	–	–	4.3
Sum				<b>4,053.1</b>	21,600.0*	21,600.0*	22,386.9*	22,792.4*	108.0

\*Nan values (–) are replaced with 3,600 before computing the sum.

Table W42: Average running times (in seconds) of the PCCC-N2-S algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) for the constraint sets of size 5% CS. The lowest values are stated in bold. The column KMEANS reports the average running time of the unconstrained k-means algorithm. The hyphen indicates that the respective algorithm returned no solution within the time limit of 3,600 seconds.