	5% CS		10% CS		15% CS		20% CS	
	ML	CL	ML	CL	ML	CL	ML	CL
Appendicitis	13	2	39	16	71	49	164	67
Breast Cancer	216	190	876	720	1,965	1,690	3,487	2,954
Bupa	79	74	323	272	699	627	1,201	1,145
Circles	50	55	208	227	502	488	853	917
Ecoli	30	106	163	398	357	918	609	1,669
Glass	11	44	52	179	139	389	259	644
Haberman	76	44	304	161	634	401	1,135	756
Hayesroth	12	16	39	81	102	174	177	319
Heart	41	50	178	173	396	424	744	687
Ionosphere	92	61	330	300	732	646	1,299	1,186
Iris	6	22	25	80	57	196	94	341
Led7Digit	25	275	126	1,099	267	2,508	460	4,490
Monk2	101	130	473	473	979	1,101	1,917	1,824
Moons	55	50	200	235	494	496	900	870
Movement Libras	6	147	27	603	112	1,319	158	2,398
Newthyroid	25	30	108	123	270	258	449	454
Saheart	152	124	595	486	1,292	1,123	2,330	1,948
Sonar	29	26	100	110	245	251	436	425
Spectfheart	56	35	233	118	543	277	965	466
Spiral	52	53	224	211	487	503	918	852
Soybean	0	3	4	6	6	22	12	33
Tae	8	20	40	80	82	171	151	314
Vehicle	221	682	874	2,696	1,955	6,046	3,589	10,776
Wine	8	28	31	122	70	281	143	487
Zoo	7	8	21	34	29	91	41	169

Table W1: Number of must-link (ML) and cannot-link (CL) constraints in the different constraint sets of collection COL1.

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	5% CS		10% CS		15% CS		20% CS	
	ML	CL	ML	CL	ML	CL	ML	CL
n500-k2	147	153	607	618	1,380	1,395	2,465	2,485
n500-k5	56	244	233	992	594	2,181	999	3,951
n500–k10	26	274	134	1,091	280	2,495	482	4,468
n500-k20	16	284	58	1,167	129	2,646	270	4,680
n500-k50	6	294	28	1,197	45	2,730	105	4,845
n500-k100	4	296	7	1,218	23	2,752	46	4,904
n1000-k2	607	618	2,494	2,456	5,559	5,616	10,007	9,893
n1000-k5	245	980	989	3,961	2,249	8,926	3,966	15,934
n1000-k10	127	1,098	449	4,501	1,119	10,056	1,996	17,904
n1000-k20	50	1,175	229	4,721	522	10,653	929	18,971
n1000-k50	26	1,199	91	4,859	203	10,972	404	19,496
n1000-k100	1	1,224	55	4,895	104	11,071	189	19,711
n2000-k2	2,472	2,478	9,984	9,916	22,405	22,445	39,612	40,188
n2000-k5	972	3,978	3,860	16,040	8,943	35,907	15,928	63,872
n2000-k10	472	4,478	1,978	17,922	4,405	40,445	7,950	71,850
n2000-k20	229	4,721	950	18,950	2,175	42,675	4,009	75,791
n2000-k50	90	4,860	363	19,537	860	43,990	1,594	78,206
n2000-k100	58	4,892	201	19,699	411	44,439	807	78,993
n5000-k2	15,632	15,493	62,161	62,589	140,016	140,859	249,040	250,460
n5000-k5	6,252	24,873	24,892	99,858	56,001	224,874	99,497	400,003
n5000-k10	3,106	28,019	12,458	112,292	27,954	252,921	49,307	450,193
n5000-k20	1,546	29,579	6,075	118,675	14,097	266,778	25,003	474,497
n5000-k50	607	30,518	2,440	122,310	5,536	275,339	9,762	489,738
n5000-k100	292	30,833	1,229	123,521	2,694	278,181	4,854	494,646

Table W2: Number of must-link (ML) and cannot-link (CL) constraints in the different constraint sets of collection COL2.

	0.5% CS		1% CS		5% CS	
	ML	CL	ML	CL	ML	CL
Banana	160	191	707	671	17,797	17,183
Letter	190	4,760	743	19,157	19,165	480,335
Shuttle	27,099	14,806	108,254	59,656	2,707,873	1,495,677
Cifar 10	4,511	40,339	17,840	161,860	450,153	4,048,347
Cifar 100	467	44,383	1,760	177,940	44,792	4,453,708
Mnist	6,074	55,001	24,592	220,058	612,630	5,510,620

Table W3: Number of must-link (ML) and cannot-link (CL) constraints in the different constraint sets of collection COL3.

	5% CS					
	PCCC	COPKM	CSC	DILS	LCC	KMEANS
Dataset						
Appendicitis	**0.467**	0.182	-0.074	0.031	0.459	0.330
Breast Cancer	**0.931**	–	-0.001	0.568	0.655	0.675
Bupa	-0.000	–	-0.009	0.021	**0.040**	-0.005
Circles	0.001	–	0.001	**0.163**	0.015	-0.003
Ecoli	**0.425**	0.277	0.006	0.022	0.322	0.387
Glass	0.233	**0.237**	0.012	-0.025	0.226	0.239
Haberman	**0.029**	–	-0.037	0.006	0.004	0.094
Hayesroth	0.068	0.025	0.003	-0.015	**0.122**	0.062
Heart	0.600	–	0.002	0.227	**0.617**	0.407
Ionosphere	**0.359**	–	0.004	0.030	0.194	0.170
Iris	0.698	0.660	0.002	0.623	**0.702**	0.626
Led7Digit	**0.456**	0.407	-0.000	0.129	–	0.429
Monk2	**0.715**	–	-0.002	0.202	0.176	0.051
Moons	**0.675**	0.536	0.001	0.417	0.622	0.470
Movement Libras	0.296	**0.307**	-0.000	0.087	0.297	0.307
Newthyroid	**0.790**	0.779	-0.017	-0.071	0.789	0.593
Saheart	**0.431**	–	0.005	0.068	0.238	0.072
Sonar	0.012	–	0.001	0.040	**0.088**	0.005
Soybean	**0.896**	0.854	-0.000	0.183	0.723	0.896
Spectfheart	0.066	–	-0.043	**0.236**	0.023	-0.103
Spiral	0.074	–	0.002	**0.107**	0.079	0.027
Tae	0.055	0.024	-0.000	0.009	**0.068**	0.035
Vehicle	**0.122**	–	0.000	0.040	0.062	0.084
Wine	**0.927**	**0.927**	0.004	0.352	0.921	0.852
Zoo	**0.826**	0.804	0.052	0.117	0.783	0.794
Mean	**0.406**	0.241*	-0.003	0.143	0.329*	0.300

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

Table W4: Average Adjusted Rand Index (ARI) values of the PCCC 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 1,800 seconds.

	10% CS					
	PCCC	COPKM	CSC	DILS	LCC	KMEANS
Dataset						
Appendicitis	**0.60**	–	-0.11	0.52	0.01	0.33
Breast Cancer	0.99	–	-0.00	**1.00**	0.79	0.67
Bupa	0.91	–	-0.01	**0.95**	0.68	-0.00
Circles	0.87	–	**0.89**	0.84	0.50	-0.00
Ecoli	**0.69**	0.50	0.10	0.13	0.61	0.39
Glass	0.21	0.19	0.03	0.02	**0.26**	0.24
Haberman	**0.97**	0.92	0.01	0.85	0.62	0.09
Hayesroth	**0.15**	–	0.04	0.04	0.10	0.06
Heart	**0.89**	–	0.02	0.88	0.09	0.41
Ionosphere	**0.95**	–	0.08	0.92	0.45	0.17
Iris	**0.68**	0.54	0.12	0.61	0.67	0.63
Led7Digit	**0.68**	0.52	0.01	0.11	0.56	0.43
Monk2	**0.97**	**0.97**	0.96	**0.97**	0.56	0.05
Moons	0.99	–	**1.00**	0.99	0.86	0.47
Movement Libras	**0.32**	0.30	0.01	0.08	**0.32**	0.31
Newthyroid	**0.92**	**0.92**	0.19	0.03	0.41	0.59
Saheart	**0.98**	0.97	0.73	0.97	0.64	0.07
Sonar	**0.74**	–	-0.00	0.63	0.09	0.00
Soybean	**0.86**	0.85	-0.03	0.21	0.61	0.90
Spectfheart	0.81	–	-0.02	**0.97**	0.59	-0.10
Spiral	**0.87**	–	0.21	0.84	0.44	0.03
Tae	**0.15**	–	0.01	0.02	0.05	0.03
Vehicle	**0.96**	–	0.49	0.30	–	0.08
Wine	**0.93**	**0.93**	0.22	0.58	0.85	0.85
Zoo	**0.93**	0.82	0.14	0.17	0.88	0.79
Mean	**0.76**	0.34*	0.20	0.55	0.47*	0.30

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

Table W5: Average Adjusted Rand Index (ARI) values of the PCCC algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 10% 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 1,800 seconds.

	15% CS					
	PCCC	COPKM	CSC	DILS	LCC	KMEANS
Dataset						
Appendicitis	**1.00**	–	0.97	0.73	0.05	0.33
Breast Cancer	**1.00**	**1.00**	0.00	**1.00**	**1.00**	0.67
Bupa	**1.00**	**1.00**	-0.01	**1.00**	0.99	-0.00
Circles	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	-0.00
Ecoli	**0.93**	–	0.24	0.62	0.80	0.39
Glass	**0.79**	–	0.01	0.38	0.45	0.24
Haberman	**1.00**	**1.00**	0.01	**1.00**	0.96	0.09
Hayesroth	**0.98**	–	0.11	0.51	0.44	0.06
Heart	**1.00**	**1.00**	0.65	**1.00**	0.83	0.41
Ionosphere	**1.00**	**1.00**	0.08	**1.00**	**1.00**	0.17
Iris	**0.62**	0.59	0.56	0.57	**0.62**	0.63
Led7Digit	**0.88**	–	0.01	0.11	–	0.43
Monk2	**1.00**	**1.00**	0.97	**1.00**	**1.00**	0.05
Moons	**1.00**	**1.00**	**1.00**	**1.00**	0.84	0.47
Movement Libras	**0.33**	0.30	0.02	0.07	0.32	0.31
Newthyroid	**1.00**	**1.00**	0.56	0.82	0.68	0.59
Saheart	**1.00**	**1.00**	0.78	**1.00**	–	0.07
Sonar	**1.00**	–	-0.00	**1.00**	0.78	0.00
Soybean	**1.00**	0.82	0.03	0.55	0.77	0.90
Spectfheart	**1.00**	0.98	-0.04	**1.00**	**1.00**	-0.10
Spiral	**1.00**	–	0.97	**1.00**	0.93	0.03
Tae	**0.70**	–	0.20	0.59	0.16	0.03
Vehicle	**1.00**	**1.00**	0.63	0.81	–	0.08
Wine	**0.93**	**0.93**	0.54	0.58	0.78	0.85
Zoo	0.89	0.75	0.33	0.71	**0.92**	0.79
Mean	**0.92**	0.61*	0.39	0.76	0.65*	0.30

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

Table W6: Average Adjusted Rand Index (ARI) values of the PCCC algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 15% 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 1,800 seconds.

	20% CS					
	PCCC	COPKM	CSC	DILS	LCC	KMEANS
Dataset						
Appendicitis	**1.00**	–	**1.00**	**1.00**	0.57	0.33
Breast Cancer	**1.00**	**1.00**	0.00	**1.00**	–	0.67
Bupa	**1.00**	**1.00**	-0.01	**1.00**	**1.00**	-0.00
Circles	**1.00**	**1.00**	**1.00**	**1.00**	–	-0.00
Ecoli	**0.98**	–	0.32	0.81	0.80	0.39
Glass	**0.94**	–	0.12	0.79	0.74	0.24
Haberman	**1.00**	**1.00**	0.01	**1.00**	**1.00**	0.09
Hayesroth	**0.93**	–	0.23	0.92	0.78	0.06
Heart	**1.00**	**1.00**	0.93	**1.00**	**1.00**	0.41
Ionosphere	**1.00**	**1.00**	0.05	**1.00**	–	0.17
Iris	**0.65**	0.60	0.56	0.57	0.63	0.63
Led7Digit	**1.00**	–	0.05	0.13	0.50	0.43
Monk2	**1.00**	**1.00**	0.89	**1.00**	–	0.05
Moons	**1.00**	**1.00**	0.96	**1.00**	**1.00**	0.47
Movement Libras	**0.48**	–	0.03	0.10	0.31	0.31
Newthyroid	**1.00**	0.98	0.86	**1.00**	0.85	0.59
Saheart	**1.00**	**1.00**	0.01	**1.00**	–	0.07
Sonar	**1.00**	**1.00**	-0.00	**1.00**	**1.00**	0.00
Soybean	**1.00**	**1.00**	0.13	0.70	0.79	0.90
Spectfheart	**1.00**	**1.00**	-0.01	**1.00**	**1.00**	-0.10
Spiral	**1.00**	–	**1.00**	**1.00**	**1.00**	0.03
Tae	**0.96**	–	0.36	0.94	0.54	0.03
Vehicle	**1.00**	**1.00**	0.30	0.82	–	0.08
Wine	**0.96**	0.95	0.73	0.61	0.90	0.85
Zoo	**0.93**	0.73	0.35	0.63	0.84	0.79
Mean	**0.95**	0.65*	0.39	0.84	0.61*	0.30

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

Table W7: Average Adjusted Rand Index (ARI) values of the PCCC algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 20% 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 1,800 seconds.

	5% CS						
	PCCC	COPKM	CSC	DILS	LCC	KMEANS	GT
Dataset							
Appendicitis	**0.35**	0.26	-0.05	-0.25	0.34	0.40	0.25
Breast Cancer	0.30	–	**0.38**	0.19	0.24	0.34	0.29
Bupa	**0.15**	–	-0.09	-0.02	0.14	0.45	0.00
Circles	0.17	–	**0.20**	-0.02	0.17	0.29	0.21
Ecoli	**0.22**	0.17	-0.27	-0.18	0.15	0.28	0.09
Glass	**0.29**	0.26	-0.35	-0.35	0.23	0.34	-0.03
Haberman	**0.13**	–	0.04	0.05	0.12	0.34	0.07
Hayesroth	0.16	0.14	-0.10	-0.15	**0.17**	0.21	0.01
Heart	0.13	–	**0.34**	0.07	0.13	0.16	0.11
Ionosphere	0.18	–	**0.41**	0.03	0.16	0.27	0.16
Iris	**0.44**	0.43	-0.25	0.35	**0.44**	0.46	0.38
Led7Digit	**0.35**	0.31	-0.11	-0.02	–	0.40	0.21
Monk2	**0.09**	–	-0.02	0.04	0.05	0.11	0.08
Moons	**0.44**	0.40	-0.09	0.32	0.38	0.50	0.38
Movement Libras	**0.22**	0.20	-0.30	-0.11	0.19	0.24	0.02
Newthyroid	0.51	**0.52**	-0.33	-0.36	0.51	0.60	0.46
Saheart	0.09	–	**0.30**	0.05	0.06	0.20	0.07
Sonar	0.13	–	**0.32**	-0.01	0.10	0.16	0.04
Soybean	**0.34**	0.32	-0.26	-0.07	0.23	0.34	0.36
Spectfheart	0.12	–	-0.05	-0.05	**0.13**	0.46	-0.08
Spiral	**0.21**	–	0.02	0.17	0.19	0.34	0.05
Tae	**0.20**	0.19	-0.16	-0.13	**0.20**	0.23	-0.02
Vehicle	**0.04**	–	**0.04**	-0.00	0.03	0.29	-0.01
Wine	**0.28**	**0.28**	-0.17	-0.02	**0.28**	0.28	0.28
Zoo	**0.34**	0.32	-0.20	-0.30	**0.34**	0.35	0.37
Mean	**0.24**	-0.33*	-0.03	-0.03	0.16*	0.32	0.15

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

Table W8: Average Silhouette coefficients of the PCCC 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 1,800 seconds.

	10% CS						
	PCCC	COPKM	CSC	DILS	LCC	KMEANS	GT
Dataset							
Appendicitis	**0.33**	–	0.05	0.22	0.09	0.40	0.25
Breast Cancer	0.30	–	**0.65**	0.29	0.24	0.34	0.29
Bupa	0.01	–	**0.61**	0.00	0.01	0.45	0.00
Circles	0.18	–	**0.21**	0.15	0.14	0.29	0.21
Ecoli	**0.15**	0.10	-0.11	-0.14	0.12	0.28	0.09
Glass	0.08	0.03	**0.17**	-0.24	0.05	0.34	-0.03
Haberman	0.07	0.07	**0.68**	0.06	0.02	0.34	0.07
Hayesroth	**0.07**	–	-0.06	0.01	**0.07**	0.21	0.01
Heart	0.12	–	**0.20**	0.12	0.00	0.16	0.11
Ionosphere	0.17	–	**0.36**	0.15	0.12	0.27	0.16
Iris	**0.45**	0.40	0.22	0.25	**0.45**	0.46	0.38
Led7Digit	**0.26**	0.19	-0.06	-0.08	0.24	0.40	0.21
Monk2	**0.08**	**0.08**	**0.08**	**0.08**	0.04	0.11	0.08
Moons	0.38	–	0.38	0.38	**0.39**	0.50	0.38
Movement Libras	**0.19**	0.15	-0.13	-0.10	0.17	0.24	0.02
Newthyroid	**0.48**	**0.48**	0.06	-0.09	0.19	0.60	0.46
Saheart	0.07	0.07	**0.10**	0.07	0.04	0.20	0.07
Sonar	0.04	–	**0.39**	0.03	0.02	0.16	0.04
Soybean	**0.34**	0.32	-0.21	-0.01	0.20	0.34	0.36
Spectfheart	-0.05	–	**0.55**	-0.08	-0.06	0.46	-0.08
Spiral	**0.06**	–	0.03	**0.06**	0.03	0.34	0.05
Tae	**0.10**	–	-0.01	0.03	0.05	0.23	-0.02
Vehicle	**-0.01**	–	**-0.01**	-0.03	–	0.29	-0.01
Wine	**0.29**	**0.29**	0.08	0.07	0.28	0.28	0.28
Zoo	**0.35**	0.31	-0.06	-0.27	**0.35**	0.35	0.37
Mean	**0.18**	-0.42*	0.17	0.04	0.09*	0.32	0.15

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

Table W9: Average Silhouette coefficients of the PCCC algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 10% 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 1,800 seconds.

	15% CS						
Dataset	PCCC	COPKM	CSC	DILS	LCC	KMEANS	GT
Appendicitis	**0.25**	–	0.24	0.19	0.04	0.40	0.25
Breast Cancer	0.29	0.29	**0.66**	0.29	0.29	0.34	0.29
Bupa	0.00	0.00	**0.62**	0.00	0.00	0.45	0.00
Circles	**0.21**	**0.21**	**0.21**	**0.21**	**0.21**	0.29	0.21
Ecoli	**0.16**	–	-0.10	-0.04	0.13	0.28	0.09
Glass	0.02	–	**0.24**	-0.23	-0.03	0.34	-0.03
Haberman	0.07	0.07	**0.68**	0.07	0.07	0.34	0.07
Hayesroth	**0.01**	–	**0.01**	-0.05	-0.00	0.21	0.01
Heart	0.11	0.11	**0.19**	0.11	0.09	0.16	0.11
Ionosphere	0.16	0.16	**0.36**	0.16	0.16	0.27	0.16
Iris	0.46	0.43	**0.49**	0.24	0.46	0.46	0.38
Led7Digit	**0.24**	–	-0.03	-0.09	–	0.40	0.21
Monk2	0.08	0.08	**0.09**	0.08	0.08	0.11	0.08
Moons	**0.38**	**0.38**	**0.38**	**0.38**	0.31	0.50	0.38
Movement Libras	**0.06**	0.03	-0.11	-0.12	**0.06**	0.24	0.02
Newthyroid	0.46	0.46	**0.49**	0.36	0.35	0.60	0.46
Saheart	0.07	0.07	**0.11**	0.07	–	0.20	0.07
Sonar	0.04	–	**0.39**	0.04	0.02	0.16	0.04
Soybean	**0.36**	0.31	-0.04	0.15	0.23	0.34	0.36
Spectfheart	-0.08	-0.08	**0.54**	-0.08	-0.08	0.46	-0.08
Spiral	**0.05**	–	**0.05**	**0.05**	0.04	0.34	0.05
Tae	-0.00	–	**0.08**	-0.02	-0.02	0.23	-0.02
Vehicle	**-0.01**	**-0.01**	**-0.01**	-0.02	–	0.29	-0.01
Wine	**0.29**	**0.29**	0.24	0.09	0.27	0.28	0.28
Zoo	0.33	0.23	-0.02	-0.12	**0.35**	0.35	0.37
Mean	0.16	-0.20*	**0.23**	0.07	0.00*	0.32	0.15

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

Table W10: Average Silhouette coefficients of the PCCC algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 15% 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 1,800 seconds.

	20% CS						
	PCCC	COPKM	CSC	DILS	LCC	KMEANS	GT
Dataset							
Appendicitis	**0.25**	–	**0.25**	**0.25**	0.14	0.40	0.25
Breast Cancer	0.29	0.29	**0.66**	0.29	–	0.34	0.29
Bupa	0.00	0.00	**0.63**	0.00	0.00	0.45	0.00
Circles	**0.21**	**0.21**	**0.21**	**0.21**	–	0.29	0.21
Ecoli	**0.16**	–	-0.07	0.04	0.08	0.28	0.09
Glass	0.01	–	**0.04**	-0.09	0.03	0.34	-0.03
Haberman	0.07	0.07	**0.68**	0.07	0.07	0.34	0.07
Hayesroth	0.01	–	**0.11**	0.01	0.01	0.21	0.01
Heart	0.11	0.11	**0.12**	0.11	0.11	0.16	0.11
Ionosphere	0.16	0.16	**0.38**	0.16	–	0.27	0.16
Iris	0.45	0.43	**0.50**	0.24	0.45	0.46	0.38
Led7Digit	**0.21**	–	-0.04	-0.08	0.00	0.40	0.21
Monk2	0.08	0.08	**0.09**	0.08	–	0.11	0.08
Moons	0.38	0.38	**0.40**	0.38	0.38	0.50	0.38
Movement Libras	**0.01**	–	-0.11	-0.11	-0.02	0.24	0.02
Newthyroid	0.46	**0.47**	0.38	0.46	0.43	0.60	0.46
Saheart	0.07	0.07	**0.44**	0.07	–	0.20	0.07
Sonar	0.04	0.04	**0.39**	0.04	0.04	0.16	0.04
Soybean	**0.36**	**0.36**	-0.01	0.13	0.24	0.34	0.36
Spectfheart	-0.08	-0.08	**0.58**	-0.08	-0.08	0.46	-0.08
Spiral	**0.05**	–	**0.05**	**0.05**	**0.05**	0.34	0.05
Tae	-0.02	–	**0.09**	-0.02	-0.03	0.23	-0.02
Vehicle	-0.01	-0.01	**0.05**	-0.02	–	0.29	-0.01
Wine	**0.28**	**0.28**	0.24	0.11	**0.28**	0.28	0.28
Zoo	**0.34**	0.22	0.06	0.01	0.29	0.35	0.37
Mean	0.16	-0.20*	**0.25**	0.09	-0.14*	0.32	0.15

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

Table W11: Average Silhouette coefficients of the PCCC algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 20% 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 1,800 seconds.

	5% CS					
Dataset	PCCC	COPKM	CSC	DILS	LCC	KMEANS
Appendicitis	0.1	**0.0**	5.1	501.4	6.4	0.2
Breast Cancer	**0.3**	–	5.3	1,818.9	104.4	0.2
Bupa	**0.4**	–	2.6	1,658.8	18.9	0.2
Circles	**0.1**	–	1.8	1,346.8	8.6	0.1
Ecoli	1.4	**0.4**	2.0	1,447.1	41.9	0.1
Glass	0.4	**0.2**	1.7	969.1	28.9	0.2
Haberman	**0.4**	–	4.4	1,331.1	9.2	0.2
Hayesroth	0.3	**0.0**	1.7	716.5	7.3	0.2
Heart	**0.6**	–	4.1	1,391.3	22.4	0.2
Ionosphere	**0.4**	–	5.8	1,810.6	71.3	0.2
Iris	0.6	**0.0**	6.4	615.5	6.2	0.3
Led7Digit	1.4	**0.4**	6.1	1,810.3	–	0.2
Monk2	**0.7**	–	4.9	1,801.8	23.6	0.1
Moons	0.3	**0.0**	9.0	1,259.3	6.3	0.2
Movement Libras	**2.1**	5.9	7.5	1,809.3	853.1	0.3
Newthyroid	0.5	**0.0**	4.0	980.6	11.0	0.2
Saheart	**0.6**	–	8.1	1,811.1	39.0	0.2
Sonar	**0.5**	–	5.8	1,480.5	73.0	0.2
Soybean	0.3	**0.0**	1.6	229.7	17.2	0.2
Spectfheart	**0.4**	–	6.8	1,809.9	64.6	0.2
Spiral	**0.4**	–	4.2	1,280.8	7.7	0.3
Tae	0.4	**0.0**	2.8	670.0	8.7	0.2
Vehicle	**2.2**	–	15.3	1,826.6	274.1	0.1
Wine	0.2	**0.1**	5.3	906.4	17.7	0.2
Zoo	0.5	**0.1**	1.4	456.4	23.4	0.3
Sum	**15.8**	21,607.3*	123.5	31,739.7	3,545.2*	5.0

*Nan values (–) are replaced with 1,800 before computing the sum.

Table W12: Average running times (in seconds) of the PCCC 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 1,800 seconds.

	10% CS					
Dataset	PCCC	COPKM	CSC	DILS	LCC	KMEANS
Appendicitis	**0.2**	–	1.5	488.8	7.4	0.2
Breast Cancer	**0.2**	–	6.9	1,808.1	445.1	0.2
Bupa	**0.3**	–	4.4	1,795.4	224.0	0.1
Circles	**0.2**	–	2.9	1,397.8	246.7	0.2
Ecoli	1.5	**0.4**	5.1	1,525.9	34.6	0.2
Glass	**0.8**	1.9	5.3	972.2	42.8	0.2
Haberman	0.2	**0.1**	2.7	1,456.0	176.9	0.2
Hayesroth	**0.4**	–	2.7	734.2	11.7	0.2
Heart	**0.1**	–	7.4	1,464.7	117.9	0.3
Ionosphere	**0.3**	–	4.4	1,809.2	1,815.1	0.2
Iris	0.5	**0.0**	3.8	647.8	6.8	0.2
Led7Digit	3.4	**0.5**	4.9	1,808.5	107.0	0.2
Monk2	**0.2**	3.3	3.3	1,809.3	631.6	0.2
Moons	**0.3**	–	4.6	1,396.1	46.1	0.2
Movement Libras	5.3	6.3	**4.9**	1,806.2	1,007.9	0.3
Newthyroid	0.4	**0.1**	2.2	977.6	21.6	0.2
Saheart	**0.2**	2.7	7.0	1,812.8	852.4	0.2
Sonar	**0.3**	–	3.6	1,516.7	269.5	0.2
Soybean	0.2	**0.0**	1.0	246.6	16.4	0.2
Spectfheart	**0.3**	–	5.1	1,809.2	267.0	0.2
Spiral	**0.2**	–	4.7	1,396.3	188.0	0.2
Tae	**0.5**	–	3.7	696.7	11.5	0.3
Vehicle	**0.7**	–	14.3	1,811.9	–	0.2
Wine	0.3	**0.1**	3.5	912.2	19.5	0.2
Zoo	0.4	**0.1**	1.4	481.9	19.1	0.3
Sum	**17.4**	23,415.6*	111.5	32,581.7	8,386.6*	5.3

*Nan values (–) are replaced with 1,800 before computing the sum.

Table W13: Average running times (in seconds) of the PCCC algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) for the constraint sets of size 10% 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 1,800 seconds.

	15% CS					
Dataset	PCCC	COPKM	CSC	DILS	LCC	KMEANS
Appendicitis	**0.2**	–	5.3	567.2	16.7	0.2
Breast Cancer	**0.1**	36.1	5.5	1,815.7	27.6	0.2
Bupa	**0.1**	6.4	2.2	1,805.8	1,953.1	0.2
Circles	**0.1**	2.8	5.2	1,552.0	1,850.0	0.3
Ecoli	**1.2**	–	8.0	1,787.9	238.9	0.2
Glass	**0.7**	–	1.9	1,090.4	537.3	0.2
Haberman	**0.1**	1.7	10.7	1,705.6	167.4	0.2
Hayesroth	**0.3**	–	3.4	782.7	59.2	0.2
Heart	**0.3**	1.9	5.1	1,625.7	501.0	0.2
Ionosphere	**0.2**	5.0	2.0	1,807.2	809.4	0.2
Iris	0.6	**0.0**	7.6	759.5	9.5	0.3
Led7Digit	**5.4**	–	12.2	1,817.7	–	0.2
Monk2	**0.3**	15.2	8.3	1,811.8	6.6	0.2
Moons	**0.1**	2.8	5.4	1,568.5	46.7	0.2
Movement Libras	**7.7**	8.8	7.9	1,815.2	1,513.9	0.2
Newthyroid	**0.1**	**0.1**	6.1	1,114.6	192.6	0.2
Saheart	**0.3**	15.5	5.9	1,816.4	–	0.2
Sonar	**0.4**	–	7.3	1,605.9	1,433.7	0.2
Soybean	0.1	**0.0**	0.9	236.1	19.4	0.2
Spectfheart	**0.4**	6.5	6.8	1,812.0	531.7	0.2
Spiral	**0.1**	–	5.5	1,626.3	91.5	0.2
Tae	**0.5**	–	1.9	797.8	83.3	0.2
Vehicle	**0.4**	92.7	16.9	1,847.4	–	0.2
Wine	0.4	**0.1**	3.7	1,027.0	63.1	0.2
Zoo	0.6	**0.1**	6.0	508.5	20.4	0.2
Sum	**20.6**	14,595.9*	151.4	34,704.9	15,573.0*	5.2

*Nan values (–) are replaced with 1,800 before computing the sum.

Table W14: Average running times (in seconds) of the PCCC algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) for the constraint sets of size 15% 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 1,800 seconds.

	20% CS					
Dataset	PCCC	COPKM	CSC	DILS	LCC	KMEANS
Appendicitis	**0.2**	–	4.4	606.1	42.8	0.3
Breast Cancer	**0.4**	65.7	5.4	1,847.9	–	0.2
Bupa	**0.2**	11.4	3.5	1,811.6	5.5	0.2
Circles	**0.3**	6.3	4.9	1,807.2	–	0.3
Ecoli	**0.7**	–	7.3	1,806.4	1,360.9	0.2
Glass	**0.4**	–	1.7	1,239.5	1,018.3	0.2
Haberman	**0.3**	4.3	8.7	1,803.4	7.4	0.2
Hayesroth	**0.1**	–	6.4	865.3	68.4	0.2
Heart	**0.2**	4.3	7.2	1,810.7	6.2	0.3
Ionosphere	**0.3**	10.3	2.6	1,815.9	–	0.2
Iris	0.4	**0.0**	5.4	814.4	16.7	0.3
Led7Digit	**2.3**	–	5.0	1,826.6	1,843.0	0.3
Monk2	**0.5**	24.5	5.9	1,818.8	–	0.3
Moons	**0.1**	6.3	4.0	1,804.3	2.9	0.2
Movement Libras	10.0	–	**6.1**	1,815.9	1,850.7	0.3
Newthyroid	0.3	**0.2**	2.8	1,357.8	546.0	0.2
Saheart	**0.4**	28.1	6.2	1,817.4	–	0.2
Sonar	**0.4**	1.5	6.6	1,777.1	19.5	0.4
Soybean	0.4	**0.0**	2.2	243.8	29.0	0.3
Spectfheart	**0.3**	7.9	5.7	1,815.4	760.2	0.2
Spiral	**0.5**	–	4.8	1,811.0	7.5	0.2
Tae	**0.3**	–	5.9	835.5	693.2	0.2
Vehicle	**0.4**	157.0	14.0	1,840.1	–	0.4
Wine	0.4	**0.1**	6.5	1,115.9	658.8	0.2
Zoo	0.5	**0.1**	3.9	539.5	28.5	0.2
Sum	**20.1**	14,728.0*	137.2	36,647.4	19,765.6*	6.3

*Nan values (–) are replaced with 1,800 before computing the sum.

Table W15: Average running times (in seconds) of the PCCC algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) for the constraint sets of size 20% 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 1,800 seconds.

	0% CS									
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	CSC	DILS	LCC	KMEANS
n500-k2	0.960	0.960	0.960	0.960	0.960	0.968	**1.000**	0.992	–	0.968
n500-k5	0.774	0.774	0.774	0.774	0.774	0.766	**0.866**	0.782	–	0.773
n500–k10	0.874	0.874	0.874	0.874	0.874	0.775	**0.897**	0.458	–	0.874
n500-k20	**0.562**	**0.562**	**0.562**	**0.562**	**0.562**	0.529	0.500	0.155	–	0.563
n500-k50	0.376	0.376	0.376	0.376	0.376	**0.394**	0.355	0.037	–	0.376
n500-k100	**0.221**	**0.221**	**0.221**	**0.221**	**0.221**	0.209	0.205	0.009	–	0.221
n1000-k2	0.984	0.984	0.984	0.984	0.984	0.984	**1.000**	**1.000**	–	0.984
n1000-k5	**0.857**	**0.857**	**0.857**	**0.857**	**0.857**	0.764	0.855	0.623	–	0.860
n1000-k10	0.801	0.801	0.801	0.801	0.801	0.772	**0.896**	0.294	–	0.801
n1000-k20	**0.574**	**0.574**	**0.574**	**0.574**	**0.574**	0.573	0.519	0.097	–	0.574
n1000-k50	0.398	0.398	0.398	0.398	0.398	**0.399**	0.391	0.022	–	0.398
n1000-k100	**0.238**	**0.238**	**0.238**	**0.238**	**0.238**	0.237	0.235	0.007	–	0.238
n2000-k2	0.966	0.966	0.966	0.966	0.966	0.965	**0.994**	0.990	–	0.963
n2000-k5	0.771	0.771	0.771	0.771	0.771	**0.867**	0.865	0.330	–	0.770
n2000-k10	0.835	0.835	0.835	0.835	0.835	0.751	**0.867**	0.127	–	0.835
n2000-k20	**0.588**	**0.588**	**0.588**	**0.588**	**0.588**	**0.588**	0.549	0.038	–	0.589
n2000-k50	0.407	0.407	0.407	0.407	0.407	**0.412**	0.391	0.009	–	0.406
n2000-k100	**0.246**	**0.246**	**0.246**	**0.246**	**0.246**	0.241	0.240	0.005	–	0.246
n5000-k2	0.985	0.985	0.985	0.985	0.985	0.985	**1.000**	0.554	–	0.985
n5000-k5	**0.865**	**0.865**	**0.865**	**0.865**	**0.865**	0.816	**0.865**	0.063	–	0.866
n5000-k10	0.856	0.856	0.856	0.856	0.856	0.859	**0.874**	0.021	–	0.855
n5000-k20	**0.587**	**0.587**	**0.587**	**0.587**	**0.587**	0.572	0.539	0.006	–	0.593
n5000-k50	**0.421**	**0.421**	**0.421**	**0.421**	**0.421**	0.413	0.394	0.002	–	0.421
n5000-k100	**0.248**	**0.248**	**0.248**	**0.248**	**0.248**	0.244	0.238	0.001	–	0.248
Mean	0.641	0.641	0.641	0.641	0.641	0.628	**0.647**	0.276	0.000*	0.642

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

Table W16: Average Adjusted Rand Index (ARI) values of five versions of the PCCC 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 1,800 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.

	5% CS									
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	CSC	DILS	LCC	KMEANS
n500-k2	0.99	0.99	0.99	0.99	0.99	–	0.00	0.95	**1.00**	0.97
n500-k5	**0.91**	**0.91**	0.85	0.85	0.84	0.79	0.00	0.58	0.74	0.77
n500–k10	**0.90**	**0.90**	0.86	0.86	0.85	0.75	0.00	0.24	0.83	0.87
n500-k20	**0.56**	**0.56**	**0.56**	**0.56**	**0.56**	0.52	0.00	0.12	0.52	0.56
n500-k50	0.38	0.38	0.38	0.38	0.38	**0.39**	0.00	0.03	0.37	0.38
n500-k100	0.21	0.21	0.21	0.21	0.21	0.21	0.01	0.02	**0.22**	0.22
n1000-k2	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	0.99	**1.00**	0.98
n1000-k5	**0.93**	**0.93**	**0.93**	**0.93**	**0.93**	–	0.00	0.40	0.84	0.86
n1000-k10	0.89	0.89	**0.90**	**0.90**	**0.90**	0.85	0.00	0.17	0.72	0.80
n1000-k20	**0.61**	**0.61**	**0.61**	**0.61**	**0.61**	0.59	0.00	0.06	0.55	0.57
n1000-k50	**0.42**	**0.42**	**0.42**	**0.42**	**0.42**	0.39	0.00	0.02	**0.42**	0.40
n1000-k100	**0.24**	**0.24**	**0.24**	**0.24**	**0.24**	**0.24**	0.00	0.01	–	0.24
n2000-k2	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	0.51	0.96
n2000-k5	**0.95**	**0.95**	**0.95**	**0.95**	**0.95**	**0.95**	0.01	0.11	0.78	0.77
n2000-k10	0.84	0.84	**0.88**	**0.88**	0.86	**0.88**	0.00	0.05	0.85	0.83
n2000-k20	0.64	0.64	0.64	**0.65**	0.64	0.58	0.00	0.02	0.62	0.59
n2000-k50	0.41	0.41	0.42	0.42	0.42	0.40	0.00	0.01	**0.44**	0.41
n2000-k100	0.25	0.25	0.25	0.25	0.25	0.24	0.00	0.00	**0.26**	0.25
n5000-k2	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	–	**1.00**	0.42	0.93	0.98
n5000-k5	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	0.97	0.32	0.00	0.88	0.87
n5000-k10	**0.98**	**0.98**	**0.98**	**0.98**	**0.98**	–	0.00	0.00	0.48	0.86
n5000-k20	**0.76**	**0.76**	0.71	0.70	0.74	–	0.00	0.00	0.54	0.59
n5000-k50	0.48	0.48	**0.49**	0.48	0.48	0.42	0.00	0.00	0.46	0.42
n5000-k100	0.25	0.25	0.25	0.25	0.25	0.25	0.00	0.00	**0.26**	0.25
Mean	**0.69**	**0.69**	**0.69**	**0.69**	**0.69**	0.48*	0.14	0.22	0.59*	0.64

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

Table W17: Average Adjusted Rand Index (ARI) values of five versions of the PCCC 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.

	10% CS									
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	CSC	DILS	LCC	KMEANS
n500-k2	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	0.53	0.97
n500-k5	**0.97**	**0.97**	**0.97**	**0.97**	**0.97**	–	0.03	0.77	0.92	0.77
n500–k10	0.90	0.90	**0.92**	0.91	0.91	0.81	0.01	0.24	0.77	0.87
n500-k20	0.61	0.61	**0.62**	0.61	0.61	0.54	0.00	0.08	0.52	0.56
n500-k50	0.39	0.39	0.39	0.39	0.39	0.38	0.00	0.03	**0.40**	0.38
n500-k100	**0.22**	**0.22**	**0.22**	**0.22**	**0.22**	**0.22**	0.00	0.01	**0.22**	0.22
n1000-k2	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	0.67	0.98
n1000-k5	**0.99**	**0.99**	0.83	**0.99**	**0.99**	0.96	0.20	0.64	0.88	0.86
n1000-k10	**0.98**	**0.98**	0.94	0.94	**0.98**	–	0.01	0.09	0.77	0.80
n1000-k20	0.68	0.68	0.67	**0.71**	0.70	–	0.00	0.04	0.50	0.57
n1000-k50	**0.43**	**0.43**	**0.43**	**0.43**	**0.43**	0.40	0.00	0.02	0.41	0.40
n1000-k100	**0.26**	**0.26**	**0.26**	**0.26**	**0.26**	0.25	0.00	0.01	0.25	0.24
n2000-k2	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	0.96
n2000-k5	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	0.71	0.20	0.94	0.77
n2000-k10	**0.99**	**0.99**	0.95	0.95	0.95	–	0.03	0.01	0.64	0.83
n2000-k20	**0.90**	**0.90**	0.81	0.82	0.82	–	0.01	0.01	0.51	0.59
n2000-k50	0.49	0.49	**0.51**	0.50	0.49	0.41	0.01	0.01	0.46	0.41
n2000-k100	**0.27**	**0.27**	**0.27**	**0.27**	**0.27**	0.25	0.00	0.00	**0.27**	0.25
n5000-k2	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	–	**1.00**	0.40	–	0.98
n5000-k5	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	–	0.73	0.00	–	0.87
n5000-k10	**1.00**	**1.00**	0.96	**1.00**	**1.00**	–	0.32	0.00	–	0.86
n5000-k20	**0.98**	**0.98**	0.89	0.89	0.94	–	0.03	0.00	–	0.59
n5000-k50	0.56	0.56	0.70	**0.71**	**0.71**	–	0.01	0.00	0.41	0.42
n5000-k100	0.27	0.27	0.34	**0.35**	**0.35**	0.27	0.01	0.00	0.29	0.25
Mean	**0.75**	**0.75**	0.74	**0.75**	**0.75**	0.35*	0.26	0.23	0.47*	0.64

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

Table W18: Average Adjusted Rand Index (ARI) values of five versions of the PCCC algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 10% 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.

	15% CS									
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	CSC	DILS	LCC	KMEANS
n500-k2	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	0.97
n500-k5	**0.99**	**0.99**	0.92	0.91	**0.99**	**0.99**	0.43	0.88	0.92	0.77
n500–k10	**0.98**	**0.98**	0.90	0.90	0.88	–	0.03	0.32	0.94	0.87
n500-k20	**0.71**	**0.71**	**0.71**	0.70	0.70	0.54	0.01	0.08	0.56	0.56
n500-k50	**0.43**	**0.43**	**0.43**	**0.43**	**0.43**	0.40	0.00	0.03	0.41	0.38
n500-k100	0.24	0.24	0.24	0.24	0.24	0.22	0.01	0.02	**0.25**	0.22
n1000-k2	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	–	0.98
n1000-k5	**1.00**	**1.00**	0.85	**1.00**	**1.00**	**1.00**	0.72	0.68	0.99	0.86
n1000-k10	0.99	0.99	0.99	0.99	0.99	**1.00**	0.07	0.09	0.71	0.80
n1000-k20	**0.89**	**0.89**	0.81	0.81	0.82	–	0.01	0.02	0.48	0.57
n1000-k50	0.51	0.51	0.51	0.50	**0.52**	0.41	0.01	0.01	0.46	0.40
n1000-k100	**0.28**	**0.28**	**0.28**	**0.28**	**0.28**	0.27	0.00	0.01	**0.28**	0.24
n2000-k2	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	–	**1.00**	**1.00**	–	0.96
n2000-k5	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	0.73	0.23	**1.00**	0.77
n2000-k10	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	0.40	0.02	–	0.83
n2000-k20	**0.98**	**0.98**	0.90	0.92	**0.98**	0.95	0.03	0.01	0.60	0.59
n2000-k50	0.46	0.46	0.66	**0.68**	**0.68**	–	0.01	0.00	0.44	0.41
n2000-k100	0.04	0.04	**0.34**	0.33	0.33	0.29	0.01	0.00	0.30	0.25
n5000-k2	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	–	**1.00**	0.39	–	0.98
n5000-k5	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	–	0.73	0.01	–	0.87
n5000-k10	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	–	0.74	0.00	–	0.86
n5000-k20	**1.00**	**1.00**	0.92	0.92	**1.00**	**1.00**	0.08	0.00	–	0.59
n5000-k50	0.75	0.75	0.84	0.88	**0.90**	–	0.02	0.00	–	0.42
n5000-k100	0.40	0.40	0.57	0.61	**0.63**	–	0.01	0.00	0.34	0.25
Mean	0.78	0.78	0.79	0.80	**0.81**	0.46*	0.33	0.24	0.40*	0.64

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

Table W19: Average Adjusted Rand Index (ARI) values of five versions of the PCCC algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 15% 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.

	20% CS									
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	CSC	DILS	LCC	KMEANS
n500-k2	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	0.97
n500-k5	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	0.68	0.90	0.99	0.77
n500–k10	**0.99**	**0.99**	**0.99**	**0.99**	**0.99**	0.97	0.07	0.44	0.73	0.87
n500-k20	**0.85**	**0.85**	0.76	0.78	0.80	–	0.02	0.08	0.61	0.56
n500-k50	**0.48**	**0.48**	0.46	**0.48**	**0.48**	0.45	0.01	0.04	0.43	0.38
n500-k100	**0.26**	**0.26**	0.25	0.25	0.25	0.24	0.01	0.02	**0.26**	0.22
n1000-k2	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	–	0.98
n1000-k5	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	0.73	0.67	**1.00**	0.86
n1000-k10	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	0.36	0.15	0.87	0.80
n1000-k20	**0.96**	**0.96**	0.87	0.89	0.93	–	0.03	0.02	0.63	0.57
n1000-k50	**0.67**	**0.67**	0.62	0.66	**0.67**	–	0.01	0.01	0.46	0.40
n1000-k100	**0.32**	**0.32**	**0.32**	**0.32**	**0.32**	0.30	0.01	0.01	0.30	0.24
n2000-k2	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	–	**1.00**	**1.00**	–	0.96
n2000-k5	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	0.73	0.21	–	0.77
n2000-k10	**1.00**	**1.00**	0.93	**1.00**	**1.00**	**1.00**	0.76	0.02	0.93	0.83
n2000-k20	**1.00**	**1.00**	0.89	0.96	**1.00**	**1.00**	0.04	0.00	0.72	0.59
n2000-k50	0.57	0.57	0.77	0.80	**0.82**	–	0.02	0.00	0.53	0.41
n2000-k100	0.35	0.35	0.46	0.48	**0.49**	0.38	0.01	0.00	0.35	0.25
n5000-k2	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	–	**1.00**	0.41	–	0.98
n5000-k5	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	–	0.82	0.01	–	0.87
n5000-k10	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	–	0.75	0.00	–	0.86
n5000-k20	**1.00**	**1.00**	0.95	**1.00**	**1.00**	–	0.24	0.00	–	0.59
n5000-k50	**0.99**	**0.99**	0.93	0.95	**0.99**	**0.99**	0.02	0.00	–	0.42
n5000-k100	–	–	0.75	0.78	**0.81**	–	0.02	0.00	–	0.25
Mean	0.81*	0.81*	0.83	0.85	**0.86**	0.47*	0.39	0.25	0.41*	0.64

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

Table W20: Average Adjusted Rand Index (ARI) values of five versions of the PCCC algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 20% 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.

	0% CS										
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	CSC	DILS	LCC	KMEANS	GT
n500-k2	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	–	0.54	0.54
n500-k5	**0.70**	**0.70**	**0.70**	**0.70**	**0.70**	**0.70**	0.67	0.58	–	0.70	0.61
n500–k10	**0.56**	**0.56**	**0.56**	**0.56**	**0.56**	0.50	0.54	0.10	–	0.56	0.50
n500-k20	**0.39**	**0.39**	**0.39**	**0.39**	**0.39**	0.38	0.36	-0.17	–	0.39	0.21
n500-k50	**0.37**	**0.37**	**0.37**	**0.37**	**0.37**	**0.37**	0.34	-0.45	–	0.37	0.07
n500-k100	**0.37**	**0.37**	**0.37**	**0.37**	**0.37**	0.34	0.33	-0.65	–	0.37	-0.11
n1000-k2	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	–	0.54	0.54
n1000-k5	0.66	0.66	0.66	0.66	0.66	**0.69**	0.66	0.38	–	0.66	0.60
n1000-k10	**0.55**	**0.55**	**0.55**	**0.55**	**0.55**	0.54	**0.55**	-0.01	–	0.55	0.51
n1000-k20	**0.39**	**0.39**	**0.39**	**0.39**	**0.39**	0.38	0.35	-0.19	–	0.39	0.24
n1000-k50	**0.36**	**0.36**	**0.36**	**0.36**	**0.36**	**0.36**	0.34	-0.36	–	0.36	0.10
n1000-k100	**0.37**	**0.37**	**0.37**	**0.37**	**0.37**	0.35	0.34	-0.47	–	0.37	-0.06
n2000-k2	**0.55**	**0.55**	**0.55**	**0.55**	**0.55**	**0.55**	**0.55**	**0.55**	–	0.55	0.55
n2000-k5	**0.70**	**0.70**	**0.70**	**0.70**	**0.70**	0.67	0.67	0.08	–	0.70	0.60
n2000-k10	0.55	0.55	0.55	0.55	0.55	0.54	**0.56**	-0.12	–	0.55	0.51
n2000-k20	**0.39**	**0.39**	**0.39**	**0.39**	**0.39**	0.38	0.35	-0.20	–	0.39	0.24
n2000-k50	0.35	0.35	0.35	0.35	0.35	**0.36**	0.34	-0.29	–	0.35	0.10
n2000-k100	**0.34**	**0.34**	**0.34**	**0.34**	**0.34**	0.33	**0.34**	-0.35	–	0.34	-0.05
n5000-k2	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	0.33	–	0.54	0.54
n5000-k5	0.67	0.67	0.67	0.67	0.67	**0.68**	0.67	-0.10	–	0.67	0.60
n5000-k10	**0.57**	**0.57**	**0.57**	**0.57**	**0.57**	0.54	0.55	-0.13	–	0.57	0.51
n5000-k20	**0.38**	**0.38**	**0.38**	**0.38**	**0.38**	**0.38**	0.34	-0.14	–	0.38	0.23
n5000-k50	**0.35**	**0.35**	**0.35**	**0.35**	**0.35**	0.34	0.32	-0.16	–	0.35	0.10
n5000-k100	**0.34**	**0.34**	**0.34**	**0.34**	**0.34**	0.33	0.32	-0.23	–	0.34	-0.05
Mean	**0.48**	**0.48**	**0.48**	**0.48**	**0.48**	0.47	0.46	-0.04	-1.00*	0.48	0.32

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

Table W21: Average Silhouette coefficients of five versions of the PCCC 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.

	5% CS										
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	CSC	DILS	LCC	KMEANS	GT
n500-k2	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	–	-0.15	0.51	**0.54**	0.54	0.54
n500-k5	0.65	0.65	**0.66**	**0.66**	0.64	0.60	-0.17	0.32	0.49	0.70	0.61
n500–k10	0.53	0.53	**0.56**	**0.56**	0.55	0.45	-0.41	-0.07	0.52	0.56	0.50
n500-k20	**0.39**	**0.39**	**0.39**	**0.39**	**0.39**	0.36	-0.53	-0.21	0.35	0.39	0.21
n500-k50	**0.37**	**0.37**	**0.37**	**0.37**	**0.37**	0.36	-0.72	-0.45	0.35	0.37	0.07
n500-k100	**0.34**	**0.34**	**0.34**	**0.34**	**0.34**	0.32	-0.73	-0.64	0.31	0.37	-0.11
n1000-k2	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	0.53	**0.54**	0.54	0.54
n1000-k5	**0.63**	**0.63**	**0.63**	**0.63**	**0.63**	–	-0.45	0.13	0.59	0.66	0.60
n1000-k10	0.53	0.53	**0.55**	**0.55**	0.54	0.50	-0.34	-0.11	0.44	0.55	0.51
n1000-k20	**0.36**	**0.36**	**0.36**	**0.36**	**0.36**	0.35	-0.37	-0.23	0.33	0.39	0.24
n1000-k50	**0.34**	**0.34**	**0.34**	**0.34**	**0.34**	0.32	-0.70	-0.33	**0.34**	0.36	0.10
n1000-k100	**0.36**	**0.36**	**0.36**	**0.36**	**0.36**	0.34	-0.77	-0.47	–	0.37	-0.06
n2000-k2	**0.55**	**0.55**	**0.55**	**0.55**	**0.55**	**0.55**	**0.55**	**0.55**	0.29	0.55	0.55
n2000-k5	**0.62**	**0.62**	**0.62**	**0.62**	**0.62**	**0.62**	-0.23	-0.09	0.51	0.70	0.60
n2000-k10	0.48	0.48	**0.56**	0.55	0.53	0.49	-0.31	-0.16	0.48	0.55	0.51
n2000-k20	**0.32**	**0.32**	**0.32**	**0.32**	**0.32**	0.29	-0.30	-0.19	**0.32**	0.39	0.24
n2000-k50	0.31	0.31	0.31	0.31	0.31	0.30	-0.57	-0.26	**0.32**	0.35	0.10
n2000-k100	**0.31**	**0.31**	**0.31**	0.30	**0.31**	0.30	-0.78	-0.33	0.24	0.34	-0.05
n5000-k2	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	–	**0.54**	0.25	0.51	0.54	0.54
n5000-k5	**0.61**	**0.61**	**0.61**	**0.61**	**0.61**	0.59	0.14	-0.06	0.54	0.67	0.60
n5000-k10	**0.51**	**0.51**	**0.51**	**0.51**	**0.51**	–	-0.10	-0.06	0.07	0.57	0.51
n5000-k20	0.27	0.27	**0.28**	0.26	0.27	–	-0.13	-0.10	0.18	0.38	0.23
n5000-k50	0.26	0.26	**0.27**	0.26	0.26	0.22	-0.22	-0.14	0.25	0.35	0.10
n5000-k100	**0.26**	**0.26**	**0.26**	**0.26**	**0.26**	0.24	-0.54	-0.20	0.25	0.34	-0.05
Mean	0.44	0.44	**0.45**	**0.45**	0.44	0.11*	-0.28	-0.08	0.32*	0.48	0.32

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

Table W22: Average Silhouette coefficients of five versions of the PCCC 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.

	10% CS										
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	CSC	DILS	LCC	KMEANS	GT
n500-k2	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	0.30	0.54	0.54
n500-k5	**0.62**	**0.62**	**0.62**	**0.62**	**0.62**	–	-0.24	0.42	**0.62**	0.70	0.61
n500–k10	0.50	0.50	**0.53**	**0.53**	**0.53**	0.44	-0.34	-0.06	0.40	0.56	0.50
n500-k20	0.33	0.33	**0.34**	0.33	0.33	0.30	-0.43	-0.26	0.29	0.39	0.21
n500-k50	**0.33**	**0.33**	**0.33**	**0.33**	**0.33**	0.29	-0.67	-0.42	0.27	0.37	0.07
n500-k100	**0.34**	**0.34**	**0.34**	**0.34**	**0.34**	0.30	-0.74	-0.65	0.27	0.37	-0.11
n1000-k2	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	0.33	0.54	0.54
n1000-k5	0.60	0.60	**0.62**	0.60	0.60	0.58	-0.16	0.29	0.53	0.66	0.60
n1000-k10	0.52	0.52	**0.53**	0.52	0.52	–	-0.16	-0.16	0.38	0.55	0.51
n1000-k20	0.28	0.28	**0.29**	**0.29**	0.28	–	-0.33	-0.22	0.20	0.39	0.24
n1000-k50	0.28	0.28	**0.29**	0.28	0.28	0.26	-0.64	-0.33	0.26	0.36	0.10
n1000-k100	0.29	0.29	**0.30**	0.29	0.29	0.27	-0.73	-0.44	0.26	0.37	-0.06
n2000-k2	**0.55**	**0.55**	**0.55**	**0.55**	**0.55**	**0.55**	**0.55**	**0.55**	**0.55**	0.55	0.55
n2000-k5	0.61	0.61	0.61	0.61	0.61	0.61	**0.62**	-0.03	0.57	0.70	0.60
n2000-k10	0.51	0.51	**0.52**	**0.52**	0.51	–	-0.22	-0.12	0.18	0.55	0.51
n2000-k20	**0.27**	**0.27**	0.26	0.25	0.24	–	-0.17	-0.18	0.10	0.39	0.24
n2000-k50	0.21	0.21	**0.24**	0.22	0.22	0.17	-0.32	-0.24	0.21	0.35	0.10
n2000-k100	0.23	0.23	**0.24**	0.23	0.23	0.19	-0.60	-0.32	0.22	0.34	-0.05
n5000-k2	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	–	**0.54**	0.24	–	0.54	0.54
n5000-k5	0.60	0.60	0.60	0.60	0.60	–	**0.63**	-0.04	–	0.67	0.60
n5000-k10	**0.51**	**0.51**	0.50	**0.51**	**0.51**	–	-0.18	-0.05	–	0.57	0.51
n5000-k20	**0.24**	**0.24**	0.23	0.23	0.22	–	-0.18	-0.07	–	0.38	0.23
n5000-k50	0.03	0.03	**0.15**	0.14	0.14	–	-0.24	-0.12	0.02	0.35	0.10
n5000-k100	0.03	0.03	**0.12**	0.10	0.10	0.03	-0.44	-0.18	0.08	0.34	-0.05
Mean	0.40	0.40	**0.41**	0.40	0.40	-0.21*	-0.14	-0.05	0.08*	0.48	0.32

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

Table W23: Average Silhouette coefficients of five versions of the PCCC algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 10% 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.

	15% CS										
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	CSC	DILS	LCC	KMEANS	GT
n500-k2	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	0.54	0.54
n500-k5	0.62	0.62	**0.64**	0.62	0.62	0.62	0.05	0.50	0.56	0.70	0.61
n500–k10	0.50	0.50	**0.53**	**0.53**	0.50	–	-0.22	-0.04	0.49	0.56	0.50
n500-k20	**0.26**	**0.26**	**0.26**	**0.26**	**0.26**	0.18	-0.29	-0.24	0.22	0.39	0.21
n500-k50	0.27	0.27	**0.28**	**0.28**	**0.28**	0.25	-0.64	-0.45	0.25	0.37	0.07
n500-k100	0.28	0.28	**0.29**	0.28	0.28	0.25	-0.72	-0.66	0.25	0.37	-0.11
n1000-k2	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	–	0.54	0.54
n1000-k5	0.60	0.60	0.62	0.60	0.60	0.60	**0.63**	0.31	0.59	0.66	0.60
n1000-k10	**0.51**	**0.51**	**0.51**	**0.51**	**0.51**	**0.51**	-0.23	-0.16	0.29	0.55	0.51
n1000-k20	**0.26**	**0.26**	0.25	0.25	0.24	–	-0.23	-0.21	0.06	0.39	0.24
n1000-k50	0.20	0.20	**0.22**	0.21	0.21	0.12	-0.50	-0.33	0.19	0.36	0.10
n1000-k100	0.24	0.24	**0.25**	0.24	0.24	0.19	-0.69	-0.49	0.22	0.37	-0.06
n2000-k2	**0.55**	**0.55**	**0.55**	**0.55**	**0.55**	–	**0.55**	**0.55**	–	0.55	0.55
n2000-k5	0.60	0.60	0.60	0.60	0.60	0.60	**0.64**	-0.01	0.60	0.70	0.60
n2000-k10	**0.51**	**0.51**	**0.51**	**0.51**	**0.51**	**0.51**	0.02	-0.13	–	0.55	0.51
n2000-k20	**0.25**	**0.25**	**0.25**	0.24	**0.25**	0.23	-0.19	-0.14	0.02	0.39	0.24
n2000-k50	-0.05	-0.05	**0.15**	0.14	0.14	–	-0.34	-0.20	0.06	0.35	0.10
n2000-k100	-0.30	-0.30	**0.14**	**0.14**	0.13	0.07	-0.55	-0.32	0.11	0.34	-0.05
n5000-k2	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	–	**0.54**	0.24	–	0.54	0.54
n5000-k5	0.60	0.60	0.60	0.60	0.60	–	**0.63**	-0.06	–	0.67	0.60
n5000-k10	**0.51**	**0.51**	**0.51**	**0.51**	**0.51**	–	0.25	-0.06	–	0.57	0.51
n5000-k20	**0.23**	**0.23**	0.21	0.21	**0.23**	**0.23**	-0.37	-0.06	–	0.38	0.23
n5000-k50	-0.06	-0.06	**0.11**	0.10	0.10	–	-0.29	-0.12	–	0.35	0.10
n5000-k100	-0.19	-0.19	**0.01**	-0.00	-0.01	–	-0.45	-0.19	-0.08	0.34	-0.05
Mean	0.33	0.33	**0.38**	**0.38**	0.37	-0.15*	-0.06	-0.05	-0.15*	0.48	0.32

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

Table W24: Average Silhouette coefficients of five versions of the PCCC algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 15% 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.

	20% CS										
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	CSC	DILS	LCC	KMEANS	GT
n500-k2	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	0.54	0.54
n500-k5	**0.61**	**0.61**	**0.61**	**0.61**	**0.61**	**0.61**	0.58	0.51	**0.61**	0.70	0.61
n500–k10	**0.50**	**0.50**	**0.50**	**0.50**	**0.50**	**0.50**	-0.21	0.04	0.29	0.56	0.50
n500-k20	**0.26**	**0.26**	**0.26**	**0.26**	0.25	–	-0.34	-0.26	0.15	0.39	0.21
n500-k50	0.22	0.22	**0.23**	**0.23**	0.22	0.16	-0.59	-0.43	0.19	0.37	0.07
n500-k100	0.23	0.23	**0.24**	0.23	0.23	0.18	-0.70	-0.63	0.19	0.37	-0.11
n1000-k2	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	–	0.54	0.54
n1000-k5	0.60	0.60	0.60	0.60	0.60	0.60	**0.64**	0.30	0.60	0.66	0.60
n1000-k10	**0.51**	**0.51**	**0.51**	**0.51**	**0.51**	**0.51**	-0.06	-0.11	0.38	0.55	0.51
n1000-k20	**0.25**	**0.25**	0.24	0.23	0.24	–	-0.24	-0.20	0.08	0.39	0.24
n1000-k50	0.15	0.15	**0.17**	0.16	0.15	–	-0.45	-0.30	0.10	0.36	0.10
n1000-k100	0.16	0.16	**0.18**	0.17	0.16	0.11	-0.64	-0.45	0.13	0.37	-0.06
n2000-k2	**0.55**	**0.55**	**0.55**	**0.55**	**0.55**	–	**0.55**	**0.55**	–	0.55	0.55
n2000-k5	0.60	0.60	0.60	0.60	0.60	0.60	**0.64**	-0.04	–	0.70	0.60
n2000-k10	0.51	0.51	**0.55**	0.51	0.51	0.51	0.33	-0.15	0.44	0.55	0.51
n2000-k20	**0.24**	**0.24**	0.23	0.23	**0.24**	**0.24**	-0.27	-0.13	0.04	0.39	0.24
n2000-k50	-0.18	-0.18	**0.11**	0.10	0.09	–	-0.30	-0.21	-0.01	0.35	0.10
n2000-k100	-0.09	-0.09	**0.06**	0.05	0.04	-0.04	-0.57	-0.30	0.01	0.34	-0.05
n5000-k2	**0.54**	**0.54**	**0.54**	**0.54**	**0.54**	–	**0.54**	0.25	–	0.54	0.54
n5000-k5	0.60	0.60	0.60	0.60	0.60	–	**0.62**	-0.07	–	0.67	0.60
n5000-k10	**0.51**	**0.51**	**0.51**	**0.51**	**0.51**	–	0.26	-0.06	–	0.57	0.51
n5000-k20	**0.23**	**0.23**	**0.23**	**0.23**	**0.23**	–	-0.28	-0.07	–	0.38	0.23
n5000-k50	0.10	0.10	0.10	0.10	**0.11**	0.10	-0.30	-0.12	–	0.35	0.10
n5000-k100	–	–	**-0.03**	-0.04	-0.04	–	-0.43	-0.16	–	0.34	-0.05
Mean	0.30*	0.30*	**0.36**	**0.36**	**0.36**	-0.20*	-0.01	-0.04	-0.22*	0.48	0.32

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

Table W25: Average Silhouette coefficients of five versions of the PCCC algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) obtained with constraint sets of size 20% 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.

	0% CS									
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	CSC	DILS	LCC	KMEANS
n500-k2	0.3	0.6	0.3	0.4	0.4	**0.1**	2.7	2,718.1	–	0.3
n500-k5	0.6	0.5	0.5	0.6	0.7	**0.1**	2.9	2,459.8	–	0.2
n500–k10	1.5	0.5	0.5	0.7	1.0	**0.3**	3.2	2,414.0	–	0.5
n500-k20	4.3	0.8	0.9	1.1	1.6	**0.6**	3.0	2,484.1	–	0.3
n500-k50	7.7	**0.6**	**0.6**	1.0	1.1	2.6	11.0	2,313.2	–	0.2
n500-k100	11.0	1.2	**0.6**	0.7	1.1	8.7	4.2	2,307.5	–	0.5
n1000-k2	0.8	0.7	0.8	0.7	0.8	**0.1**	25.0	3,639.8	–	0.2
n1000-k5	2.0	1.3	1.2	1.7	2.3	**0.2**	27.8	3,614.3	–	0.2
n1000-k10	3.4	0.9	1.1	1.6	2.0	**0.6**	27.1	3,614.5	–	0.2
n1000-k20	8.3	1.7	**1.5**	2.0	2.5	1.7	31.5	3,618.3	–	0.2
n1000-k50	24.4	1.9	**1.8**	2.6	3.6	5.7	32.1	3,614.9	–	0.2
n1000-k100	26.8	1.8	**1.4**	1.6	2.1	18.3	34.1	3,617.5	–	0.6
n2000-k2	1.3	1.5	1.4	1.4	1.3	**0.2**	243.1	3,682.0	–	0.2
n2000-k5	4.0	2.5	2.3	3.0	4.2	**0.4**	258.7	3,675.7	–	0.4
n2000-k10	8.4	2.2	2.4	3.2	4.6	**1.2**	259.6	3,651.8	–	0.4
n2000-k20	18.0	3.2	**2.9**	4.3	5.8	3.8	262.5	3,609.1	–	0.5
n2000-k50	59.4	**3.8**	4.0	5.4	7.6	11.9	268.8	3,663.2	–	0.5
n2000-k100	77.7	**2.6**	2.8	3.8	5.1	39.9	271.6	3,631.1	–	0.6
n5000-k2	3.6	2.7	3.0	3.0	3.0	**0.7**	3,269.0	3,869.5	–	0.5
n5000-k5	9.9	4.3	4.8	6.1	9.2	**1.4**	3,462.1	3,771.3	–	0.5
n5000-k10	14.8	3.7	4.1	5.3	8.0	**3.3**	3,682.9	3,746.6	–	0.4
n5000-k20	81.2	10.9	11.6	17.3	25.4	**9.8**	3,633.0	3,685.8	–	0.9
n5000-k50	200.9	**11.4**	12.2	17.7	25.9	41.3	3,499.3	3,718.3	–	0.9
n5000-k100	458.2	**11.9**	13.1	19.0	28.1	105.8	3,609.3	3,731.3	–	1.1
Sum	1,028.7	**73.2**	75.9	104.2	147.6	258.5	22,924.5	80,851.8	86,400.0*	10.6

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

Table W26: Average running times (in seconds) of five versions of the PCCC 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.

	5% CS									
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	CSC	DILS	LCC	KMEANS
n500-k2	**0.4**	0.5	0.5	0.5	0.7	–	2.9	3,039.7	8.2	0.3
n500-k5	1.4	1.4	0.7	0.9	1.3	**0.1**	2.9	2,506.3	20.2	0.1
n500–k10	3.3	2.0	0.6	0.8	1.1	**0.3**	2.7	2,549.4	28.7	0.1
n500-k20	8.1	2.2	1.1	1.3	1.8	**0.6**	3.0	2,441.9	47.1	0.1
n500-k50	10.3	1.4	**0.7**	0.8	1.3	2.6	3.7	2,507.1	108.4	0.1
n500-k100	17.6	1.1	0.8	**0.7**	1.0	8.6	2.7	2,411.4	210.6	0.2
n1000-k2	0.5	**0.4**	0.8	0.8	0.9	4.2	23.4	3,612.9	165.3	0.1
n1000-k5	2.8	2.2	**1.3**	1.6	2.2	–	22.9	3,617.4	37.3	0.1
n1000-k10	5.6	5.3	1.1	1.5	2.4	**0.5**	24.4	3,606.4	63.3	0.2
n1000-k20	20.9	19.1	2.2	2.5	3.7	**1.8**	22.9	3,620.8	104.2	0.1
n1000-k50	53.2	8.3	**1.9**	2.4	3.6	6.0	24.9	3,611.6	232.5	0.2
n1000-k100	73.1	5.5	**1.5**	1.9	2.7	18.6	25.5	3,630.2	–	0.2
n2000-k2	**0.6**	0.7	0.7	**0.6**	0.7	503.5	263.6	3,716.9	3,669.7	0.3
n2000-k5	5.5	5.3	**1.6**	2.4	4.5	3.0	267.3	3,661.7	403.9	0.2
n2000-k10	12.2	10.7	2.6	3.7	6.5	**1.2**	270.6	3,651.1	136.2	0.4
n2000-k20	109.0	105.6	5.1	6.8	13.2	**3.6**	280.1	3,646.3	254.1	0.2
n2000-k50	182.6	81.7	**3.2**	4.9	7.9	14.3	277.3	3,615.8	537.3	0.7
n2000-k100	414.7	56.3	**3.9**	4.5	7.0	41.4	270.1	3,627.7	1,006.2	0.4
n5000-k2	0.8	0.7	0.7	0.7	**0.5**	–	2,764.0	4,006.1	3,793.6	0.4
n5000-k5	6.3	6.0	**1.7**	2.0	3.9	5,929.3	2,770.6	3,815.8	3,802.6	0.3
n5000-k10	75.5	70.1	**2.7**	4.2	10.2	–	2,696.5	3,860.4	3,863.2	0.5
n5000-k20	443.5	433.5	**10.2**	15.6	36.6	–	2,733.4	3,772.5	2,310.8	0.4
n5000-k50	2,600.7	2,604.5	**14.8**	22.4	33.5	45.0	2,730.1	3,813.6	2,283.4	0.6
n5000-k100	3,607.3	3,318.0	**14.0**	16.9	30.3	116.9	2,639.6	3,759.0	3,608.7	0.6
Sum	7,656.0	6,742.7	**74.3**	100.6	177.4	24,701.6*	18,125.0	82,102.0	30,295.4*	6.9

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

Table W27: Average running times (in seconds) of five versions of the PCCC 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.

	10% CS									
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	CSC	DILS	LCC	KMEANS
n500-k2	**0.3**	0.6	**0.3**	0.5	0.5	7.8	4.2	3,370.1	197.6	0.1
n500-k5	1.3	1.1	**0.8**	1.0	1.7	–	6.0	3,088.7	40.0	0.1
n500–k10	3.4	3.6	**0.6**	1.0	1.7	4.3	4.4	2,884.1	45.9	0.1
n500-k20	14.8	14.1	**1.3**	1.5	2.5	3.0	6.3	3,003.3	79.4	0.1
n500-k50	17.9	6.6	**0.8**	1.0	1.2	2.9	4.6	2,765.2	157.5	0.2
n500-k100	39.7	3.5	**0.8**	1.0	1.4	19.6	3.6	2,892.1	306.4	0.2
n1000-k2	**0.3**	0.5	0.4	0.5	0.4	201.5	24.6	3,649.8	2,158.6	0.2
n1000-k5	1.3	1.3	0.9	**0.8**	1.3	28.9	25.8	3,623.0	1,160.5	0.1
n1000-k10	8.7	8.4	**0.9**	1.5	3.2	–	27.6	3,629.8	299.7	0.2
n1000-k20	67.9	66.2	**2.7**	4.4	7.2	–	27.6	3,638.4	270.8	0.1
n1000-k50	144.7	139.8	**2.4**	3.1	4.6	7.7	27.5	3,645.3	381.8	0.4
n1000-k100	212.4	59.5	**1.9**	**1.9**	2.9	39.0	31.4	3,628.5	708.9	0.2
n2000-k2	0.7	0.4	0.5	0.5	**0.3**	3,742.6	238.8	3,701.4	35.8	0.3
n2000-k5	0.9	0.9	0.6	**0.5**	0.9	870.3	232.5	3,755.0	3,434.3	0.1
n2000-k10	9.7	8.8	**1.1**	1.4	3.1	–	218.2	3,656.9	3,792.7	0.3
n2000-k20	298.7	293.9	**2.9**	4.0	11.2	–	218.8	3,639.1	3,547.9	0.4
n2000-k50	596.2	591.1	6.1	**5.8**	13.3	35.2	222.8	3,661.9	1,238.0	0.3
n2000-k100	1,114.9	1,133.9	**4.7**	4.9	7.9	157.9	219.8	3,651.1	1,916.3	0.5
n5000-k2	1.5	1.3	**0.8**	0.9	1.0	–	2,832.7	3,763.4	–	0.4
n5000-k5	1.1	1.2	**0.9**	**0.9**	1.0	–	2,854.0	3,877.6	–	0.3
n5000-k10	5.1	4.9	**1.1**	1.3	1.9	–	2,682.4	3,888.9	–	0.4
n5000-k20	219.2	212.9	**2.6**	4.5	13.7	–	2,619.7	3,886.3	–	0.5
n5000-k50	3,188.1	3,159.7	**11.4**	20.7	61.8	–	2,663.6	4,056.7	4,121.8	0.5
n5000-k100	3,668.6	3,680.5	**17.5**	20.4	51.5	417.0	2,598.4	3,995.0	3,705.7	0.7
Sum	9,617.4	9,394.7	**63.9**	84.0	196.5	41,537.8*	17,795.1	85,351.6	41,999.4*	6.8

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

Table W28: Average running times (in seconds) of five versions of the PCCC algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) for the constraint sets of size 10% 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.

	15% CS									
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	CSC	DILS	LCC	KMEANS
n500-k2	0.5	**0.3**	0.4	0.5	0.4	27.1	2.9	3,616.4	8.7	0.1
n500-k5	0.8	0.8	**0.5**	**0.5**	0.6	4.3	3.1	3,623.7	256.4	0.1
n500–k10	5.0	5.6	**0.8**	1.2	2.0	–	2.8	3,557.5	95.7	0.3
n500-k20	27.6	28.5	**1.5**	1.6	3.2	9.1	3.5	3,549.5	119.9	0.1
n500-k50	50.7	51.8	**1.2**	1.5	2.1	9.3	4.1	3,530.5	220.3	0.2
n500-k100	94.4	37.3	**1.2**	**1.2**	1.7	10.2	3.5	3,529.4	390.7	0.2
n1000-k2	0.6	0.5	**0.4**	0.5	0.5	538.4	26.3	3,651.7	–	0.2
n1000-k5	0.8	**0.6**	**0.6**	**0.6**	0.7	125.4	23.0	3,648.1	1,564.4	0.1
n1000-k10	3.8	3.7	**0.7**	0.8	1.3	19.7	26.1	3,640.2	3,082.7	0.2
n1000-k20	90.2	90.8	**1.8**	2.4	5.5	–	27.9	3,631.4	1,068.1	0.3
n1000-k50	317.1	314.8	**2.3**	2.8	6.5	37.0	26.0	3,617.4	593.4	0.1
n1000-k100	434.5	432.4	**2.0**	2.2	3.6	40.8	27.6	3,638.6	993.7	0.2
n2000-k2	0.8	0.9	**0.4**	0.6	0.7	–	236.3	3,720.4	–	0.4
n2000-k5	0.9	0.7	0.7	**0.6**	**0.6**	2,432.7	234.7	3,713.4	515.0	0.3
n2000-k10	2.9	2.8	**0.6**	0.8	1.3	561.9	222.1	3,732.1	–	0.5
n2000-k20	51.6	51.8	**1.6**	1.9	3.9	116.6	232.1	3,715.0	4,564.0	0.4
n2000-k50	783.1	787.6	**4.1**	6.0	15.3	–	219.4	3,711.7	3,621.9	0.6
n2000-k100	1,517.3	1,523.4	**6.0**	7.7	14.7	161.0	222.5	3,804.0	3,621.1	0.4
n5000-k2	1.8	1.9	**1.5**	**1.5**	1.8	–	2,930.6	3,888.4	–	0.3
n5000-k5	1.8	1.7	1.5	1.6	**1.2**	–	2,927.7	4,376.8	–	0.3
n5000-k10	1.6	1.5	**1.2**	1.3	1.5	–	2,833.4	4,394.7	–	0.3
n5000-k20	10.7	11.3	**1.7**	2.0	2.8	6,542.6	2,671.3	4,293.2	–	0.3
n5000-k50	1,820.6	1,828.7	**3.8**	9.6	170.7	–	2,656.8	4,159.0	–	0.5
n5000-k100	3,669.2	3,682.6	**23.7**	69.1	299.8	–	2,646.7	4,268.2	4,494.3	0.7
Sum	8,888.4	8,862.0	**60.2**	118.6	542.3	43,036.1*	18,210.3	91,011.3	54,010.3*	7.1

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

Table W29: Average running times (in seconds) of five versions of the PCCC algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) for the constraint sets of size 15% 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.

	20% CS									
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	CSC	DILS	LCC	KMEANS
n500-k2	**0.4**	0.7	**0.4**	**0.4**	**0.4**	54.5	3.5	3,638.6	6.2	0.1
n500-k5	0.6	0.6	**0.4**	0.5	0.5	12.4	3.5	3,621.5	1,076.1	0.1
n500–k10	2.2	2.1	**0.6**	0.8	1.1	7.3	2.8	3,613.8	1,239.7	0.1
n500-k20	21.3	23.9	**0.9**	1.2	2.4	–	4.4	3,622.3	303.5	0.1
n500-k50	103.0	105.6	**1.5**	1.8	2.3	13.1	4.6	3,615.3	325.3	0.1
n500-k100	150.1	150.2	**1.1**	1.3	2.0	40.3	3.2	3,619.9	461.7	0.2
n1000-k2	0.6	0.8	0.6	**0.5**	**0.5**	956.0	27.6	3,691.6	–	0.2
n1000-k5	0.6	0.5	**0.4**	0.5	**0.4**	252.6	25.4	3,696.6	44.8	0.2
n1000-k10	1.5	1.5	**0.6**	0.7	0.9	55.7	24.4	3,659.6	2,649.5	0.1
n1000-k20	43.4	42.4	**1.0**	1.7	3.2	–	24.2	3,646.8	3,670.0	0.2
n1000-k50	859.2	882.2	**2.6**	3.2	5.9	–	27.1	3,671.4	1,929.3	0.3
n1000-k100	1,250.3	1,257.3	**2.1**	3.1	4.1	80.2	28.4	3,655.6	1,585.6	0.5
n2000-k2	0.9	1.0	**0.7**	0.8	0.8	–	264.8	3,941.0	–	0.3
n2000-k5	0.8	0.9	**0.7**	**0.7**	**0.7**	4,395.5	260.7	3,877.4	–	0.4
n2000-k10	0.9	1.1	**0.6**	0.7	0.7	1,207.8	252.8	3,839.2	3,073.3	0.3
n2000-k20	10.7	11.9	**1.0**	1.1	2.2	288.6	250.9	3,768.9	4,291.7	0.3
n2000-k50	561.2	574.9	**2.9**	9.3	37.8	–	255.3	3,715.4	3,875.9	0.3
n2000-k100	3,750.8	3,802.3	**6.3**	7.8	17.3	168.7	248.8	3,696.2	3,666.4	0.6
n5000-k2	3.0	2.7	**2.3**	2.6	2.9	–	2,981.8	5,503.9	–	0.2
n5000-k5	2.0	2.3	2.0	**1.9**	2.1	–	2,939.3	4,871.0	–	0.2
n5000-k10	2.2	2.1	**1.8**	2.0	2.1	–	2,926.3	4,733.6	–	0.3
n5000-k20	2.8	2.9	1.9	**1.8**	2.2	–	2,752.5	4,511.0	–	0.3
n5000-k50	390.3	396.3	**3.0**	4.6	37.3	1,924.0	2,750.3	4,570.2	–	0.4
n5000-k100	3,905.5	3,908.7	**9.1**	47.8	333.6	–	2,649.0	4,514.9	–	0.5
Sum	11,064.1	11,175.0	**44.3**	96.7	463.4	45,456.7*	18,711.7	95,295.8	60,599.0*	6.2

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

Table W30: Average running times (in seconds) of five versions of the PCCC algorithm and the four state-of-the-art algorithms (COPKM, CSC, DILS, LCC) for the constraint sets of size 20% 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.

	0% CS									
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	LCC	CSC	DILS	KMEANS
Banana	0.019	0.019	0.019	0.019	0.019	0.018	–	**0.030**	0.008	0.017
Letter	0.149	0.149	0.149	0.149	0.149	**0.156**	–	–	0.000	0.149
Shuttle	0.193	0.193	0.193	0.193	0.193	**0.429**	–	–	–	0.411
Cifar 10	**0.040**	0.039	0.039	**0.040**	**0.040**	–	–	–	–	0.040
Cifar 100	**0.021**	**0.021**	**0.021**	**0.021**	**0.021**	–	–	–	–	0.021
Mnist	**0.306**	0.304	0.304	**0.306**	**0.306**	0.193	–	–	–	0.312
Mean	0.121	0.121	0.121	0.121	0.121	**0.133***	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 five versions of the PCCC 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 different PCCC versions sometimes devise slightly different assignments for the same instance. This is because the Gurobi solver terminates when the relative MIP optimality gap is less than 0.0001. For some instances the different PCCC versions satisfy this stopping criterion with slightly different assignments. The differences between the results of the PCCC versions 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 versions use the Euclidean distance for parameter d_{il} and not the squared Euclidean distance which can lead to different assignments for some instances.

	0.5% CS									
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	LCC	CSC	DILS	KMEANS
Banana	**0.018**	**0.018**	**0.018**	**0.018**	**0.018**	–	0.006	0.000	0.003	0.017
Letter	0.155	0.155	0.154	0.155	0.155	**0.156**	0.148	–	0.000	0.149
Shuttle	0.502	0.502	**0.503**	0.501	0.502	–	0.312	–	–	0.411
Cifar 10	**0.044**	**0.044**	**0.044**	**0.044**	**0.044**	–	–	–	–	0.040
Cifar 100	0.021	**0.022**	**0.022**	**0.022**	**0.022**	–	–	–	–	0.021
Mnist	**0.391**	**0.391**	0.387	**0.391**	**0.391**	0.217	–	–	–	0.312
Mean	0.188	0.188	0.188	**0.189**	**0.189**	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 five versions of the PCCC 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.

	1% CS									
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	LCC	CSC	DILS	KMEANS
Banana	**0.014**	**0.014**	0.013	0.013	0.013	–	0.011	-0.000	0.004	0.017
Letter	0.150	0.150	0.150	0.151	0.150	0.154	**0.162**	–	0.000	0.149
Shuttle	**0.975**	**0.975**	0.974	0.974	**0.975**	–	–	–	–	0.411
Cifar 10	0.022	0.022	**0.060**	0.047	0.038	–	–	–	–	0.040
Cifar 100	0.000	0.014	**0.021**	**0.021**	**0.021**	–	–	–	–	0.021
Mnist	0.119	0.119	**0.594**	0.374	0.203	–	–	–	–	0.312
Mean	0.213	0.216	**0.302**	0.263	0.233	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 five versions of the PCCC 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.

	5% CS									
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	LCC	CSC	DILS	KMEANS
Banana	**1.000**	**1.000**	**1.000**	**1.000**	**1.000**	–	–	0.996	0.100	0.017
Letter	0.651	0.651	0.588	0.658	**0.667**	–	–	–	0.000	0.149
Shuttle	**1.000**	**1.000**	0.985	**1.000**	**1.000**	–	–	–	–	0.411
Cifar 10	**1.000**	**1.000**	0.570	0.570	0.672	–	–	–	–	0.040
Cifar 100	–	–	**0.303**	0.225	0.229	–	–	–	–	0.021
Mnist	**1.000**	**1.000**	0.745	0.749	0.749	–	–	–	–	0.312
Mean	**0.775***	**0.775***	0.699	0.701	0.719	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 five versions of the PCCC 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.

	0% CS										
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	LCC	CSC	DILS	KMEANS	GT
Banana	**0.389**	**0.389**	**0.389**	**0.389**	**0.389**	**0.389**	–	0.388	0.185	0.389	0.032
Letter	**0.145**	**0.145**	**0.145**	**0.145**	**0.145**	0.141	–	–	-0.020	0.145	0.010
Shuttle	0.356	0.356	0.356	0.356	0.356	**0.459**	–	–	–	0.463	0.300
Cifar 10	**0.051**	0.048	0.048	**0.051**	**0.051**	–	–	–	–	0.051	-0.053
Cifar 100	0.015	0.015	0.015	0.015	**0.016**	–	–	–	–	0.015	-0.114
Mnist	0.004	0.003	0.003	0.004	0.004	**0.012**	–	–	–	0.007	-0.043
Mean	**0.160**	0.159	0.159	**0.160**	**0.160**	-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 five versions of the PCCC 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 different PCCC versions sometimes devise slightly different assignments for the same instance. This is because the Gurobi solver terminates when the relative MIP optimality gap is less than 0.0001. For some instances the different PCCC versions satisfy this stopping criterion with slightly different assignments. The differences between the results of the PCCC versions 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 versions use the Euclidean distance for parameter d_{il} and not the squared Euclidean distance which can lead to different assignments for some instances.

	0.5% CS										
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	LCC	CSC	DILS	KMEANS	GT
Banana	0.353	0.353	**0.358**	**0.358**	**0.358**	–	0.347	0.284	0.143	0.389	0.032
Letter	0.134	0.134	**0.135**	**0.135**	0.134	0.134	0.117	–	-0.020	0.145	0.010
Shuttle	**0.145**	**0.145**	**0.145**	**0.145**	**0.145**	–	0.005	–	–	0.463	0.300
Cifar 10	**0.030**	**0.030**	**0.030**	**0.030**	**0.030**	–	–	–	–	0.051	-0.053
Cifar 100	0.012	**0.014**	**0.014**	**0.014**	**0.014**	–	–	–	–	0.015	-0.114
Mnist	**-0.014**	**-0.014**	-0.015	**-0.014**	**-0.014**	-0.018	–	–	–	0.007	-0.043
Mean	0.110	**0.111**	**0.111**	**0.111**	**0.111**	-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 five versions of the PCCC 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.

	1% CS										
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	LCC	CSC	DILS	KMEANS	GT
Banana	0.261	0.261	**0.280**	**0.280**	**0.280**	–	0.261	-0.118	0.103	0.389	0.032
Letter	0.113	0.113	0.113	**0.114**	0.113	0.111	0.110	–	-0.020	0.145	0.010
Shuttle	0.317	0.317	**0.320**	0.318	0.317	–	–	–	–	0.463	0.300
Cifar 10	-0.029	-0.029	**-0.010**	**-0.010**	-0.015	–	–	–	–	0.051	-0.053
Cifar 100	-0.021	-0.058	0.008	**0.009**	**0.009**	–	–	–	–	0.015	-0.114
Mnist	-0.040	-0.040	**-0.039**	-0.048	-0.048	–	–	–	–	0.007	-0.043
Mean	0.100	0.094	**0.112**	0.110	0.109	-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 five versions of the PCCC 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.

	5% CS										
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	LCC	CSC	DILS	KMEANS	GT
Banana	0.032	0.032	0.032	0.032	0.032	–	–	**0.033**	0.004	0.389	0.032
Letter	-0.027	-0.027	-0.049	-0.033	-0.033	–	–	–	**-0.017**	0.145	0.010
Shuttle	0.309	0.309	**0.350**	0.318	0.309	–	–	–	–	0.463	0.300
Cifar 10	**-0.053**	**-0.053**	-0.203	-0.203	-0.145	–	–	–	–	0.051	-0.053
Cifar 100	–	–	**-0.127**	-0.136	-0.135	–	–	–	–	0.015	-0.114
Mnist	**-0.043**	**-0.043**	-0.116	-0.113	-0.116	–	–	–	–	0.007	-0.043
Mean	-0.130*	-0.130*	-0.019	-0.022	**-0.015**	-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 five versions of the PCCC 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.

	0% CS									
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	LCC	CSC	DILS	KMEANS
Banana	6.8	6.6	6.7	6.5	6.4	**1.0**	–	5,208.4	3,849.2	0.1
Letter	684.8	74.3	**74.1**	111.0	150.3	1,007.8	–	–	4,450.1	0.5
Shuttle	41.6	18.4	**18.3**	24.3	31.7	227.7	–	–	–	0.3
Cifar 10	1,956.3	380.8	**375.6**	1,267.4	1,478.0	–	–	–	–	18.0
Cifar 100	3,658.8	3,547.0	**3,546.9**	3,612.4	3,611.2	–	–	–	–	84.5
Mnist	732.6	**197.5**	199.1	372.9	465.5	3,655.5	–	–	–	4.2
Sum	7,080.9	4,224.6	**4,220.9**	5,394.6	5,743.2	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 five versions of the PCCC 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.

	0.5% CS									
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	LCC	CSC	DILS	KMEANS
Banana	**3.5**	3.6	4.1	4.2	4.1	–	94.1	4,415.0	3,622.2	0.1
Letter	908.5	190.1	**70.9**	103.6	160.8	846.9	3,642.4	–	4,459.9	0.5
Shuttle	148.5	146.7	**25.8**	31.9	50.2	–	4,926.2	–	–	0.3
Cifar 10	1,756.1	1,712.5	**382.5**	587.6	1,057.1	–	–	–	–	18.5
Cifar 100	3,810.7	3,631.2	**3,576.8**	3,624.1	3,612.5	–	–	–	–	82.3
Mnist	1,099.9	1,078.4	**241.9**	321.9	535.5	3,884.6	–	–	–	4.3
Sum	7,727.0	6,762.5	**4,302.1**	4,673.2	5,420.2	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 five versions of the PCCC 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.

	1% CS									
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	LCC	CSC	DILS	KMEANS
Banana	6.7	**6.6**	7.6	7.5	7.4	–	114.5	3,774.8	3,629.6	0.1
Letter	2,038.9	1,051.5	**115.6**	166.6	133.4	841.7	3,785.3	–	4,568.9	0.5
Shuttle	43.8	43.3	**10.0**	12.3	19.7	–	–	–	–	0.4
Cifar 10	3,935.5	3,957.2	**3,085.1**	3,742.0	3,803.6	–	–	–	–	16.7
Cifar 100	3,820.8	3,838.7	3,575.2	**1,837.6**	3,628.8	–	–	–	–	87.1
Mnist	3,785.2	3,775.2	**3,342.5**	3,728.4	3,666.3	–	–	–	–	4.3
Sum	13,630.9	12,672.4	10,136.0	**9,494.4**	11,259.2	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 five versions of the PCCC 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.

	5% CS									
Dataset	PCCC	PCCC-N2	PCCC-N2-S	PCCC-N3-S	PCCC-N5-S	COPKM	LCC	CSC	DILS	KMEANS
Banana	**0.4**	**0.4**	**0.4**	**0.4**	**0.4**	–	–	4,386.9	4,283.3	0.1
Letter	1,820.1	1,813.6	**229.5**	2,365.4	2,874.9	–	–	–	4,109.1	0.5
Shuttle	21.2	21.4	**21.0**	21.4	22.4	–	–	–	–	0.3
Cifar 10	**18.1**	**18.1**	21.8	22.3	51.6	–	–	–	–	17.5
Cifar 100	–	–	3,759.6	**3,631.8**	3,700.6	–	–	–	–	85.2
Mnist	18.2	**18.1**	20.7	21.2	22.1	–	–	–	–	4.3
Sum	5,477.9*	5,471.6*	**4,053.1**	6,062.4	6,672.0	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 five versions of the PCCC 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.

	5% NCS				
Lower bound l	PCCC	PCCC-S	PCCC-W	CSC-W	KMEANS
0.5	0.44	0.49	**0.53**	-0.01	0.53
0.6	0.43	0.49	**0.52**	-0.01	0.53
0.7	0.44	0.50	**0.52**	-0.01	0.53
0.8	0.49	**0.57**	0.55	-0.01	0.53
0.9	0.49	**0.56**	**0.56**	0.00	0.53
1.0	0.52	**0.58**	**0.58**	-0.01	0.53
Mean	0.47	0.53	**0.54**	-0.01	0.53

Table W43: Average Adjusted Rand Index (ARI) values of three versions of the PCCC algorithm and the state-of-the-art algorithm CSC-W obtained with noisy constraint sets of size 5% NCS. 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.

	10% NCS				
	PCCC	PCCC-S	PCCC-W	CSC-W	KMEANS
Lower bound l					
0.5	0.34	0.48	**0.52**	0.01	0.53
0.6	0.43	**0.62**	0.60	0.05	0.53
0.7	0.49	**0.67**	0.64	0.13	0.53
0.8	0.55	**0.70**	0.69	0.30	0.53
0.9	0.46	0.71	**0.73**	0.32	0.53
1.0	0.78	**0.81**	**0.81**	0.33	0.53
Mean	0.51	0.66	**0.67**	0.19	0.53

Table W44: Average Adjusted Rand Index (ARI) values of three versions of the PCCC algorithm and the state-of-the-art algorithm CSC-W obtained with noisy constraint sets of size 10% NCS. 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.

	15% NCS				
	PCCC	PCCC-S	PCCC-W	CSC-W	KMEANS
Lower bound l					
0.5	–	0.42	**0.68**	0.31	0.53
0.6	–	0.52	**0.68**	0.33	0.53
0.7	–	0.70	**0.77**	0.32	0.53
0.8	0.54	0.73	**0.77**	0.46	0.53
0.9	0.58	0.84	**0.85**	0.55	0.53
1.0	**0.92**	0.90	0.90	0.69	0.53
Mean	0.34*	0.68	**0.77**	0.44	0.53

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

Table W45: Average Adjusted Rand Index (ARI) values of three versions of the PCCC algorithm and the state-of-the-art algorithm CSC-W obtained with noisy constraint sets of size 15% NCS. 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.

	20% NCS				
Lower bound l	PCCC	PCCC-S	PCCC-W	CSC-W	KMEANS
0.5	–	0.52	**0.72**	0.35	0.53
0.6	–	0.64	**0.75**	0.44	0.53
0.7	–	0.72	**0.79**	0.73	0.53
0.8	–	0.80	**0.84**	0.76	0.53
0.9	–	0.89	**0.90**	0.79	0.53
1.0	**0.97**	0.96	0.96	0.81	0.53
Mean	0.16*	0.76	**0.83**	0.65	0.53

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

Table W46: Average Adjusted Rand Index (ARI) values of three versions of the PCCC algorithm and the state-of-the-art algorithm CSC-W obtained with noisy constraint sets of size 20% NCS. 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.