UNIVERSITY OF
EASTERN FINLAND

Generalized centroid index

Cluster level quality measure

Pasi Fränti and Mohammad Rezaei

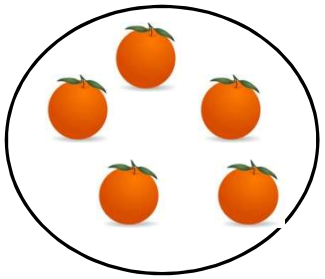
30.11.2016

Clustering accuracy

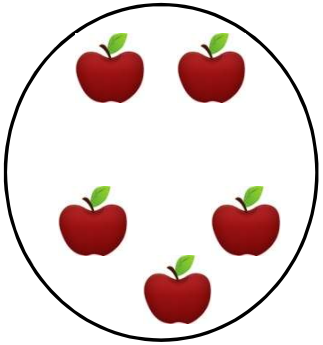
Classification accuracy

Known class labels

Solution A:

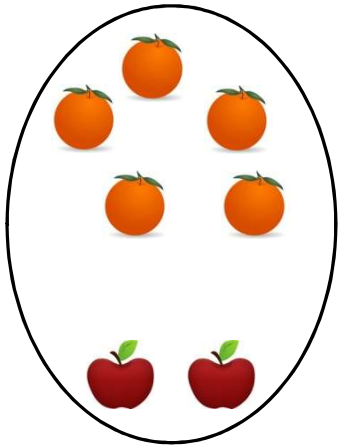


Oranges
100 %

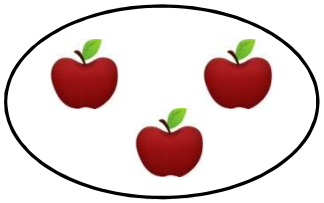


Apples
100 %

Solution B:



Oranges
Precision = 5/7 = 71%
Recall = 5/5 = 100%

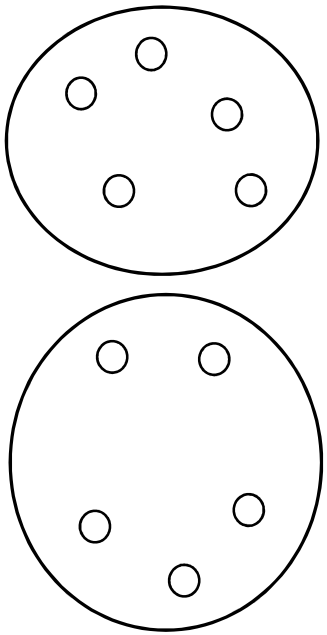


Apples
Precision = 3/3 = 100%
Recall = 3/5 = 60%

Clustering accuracy

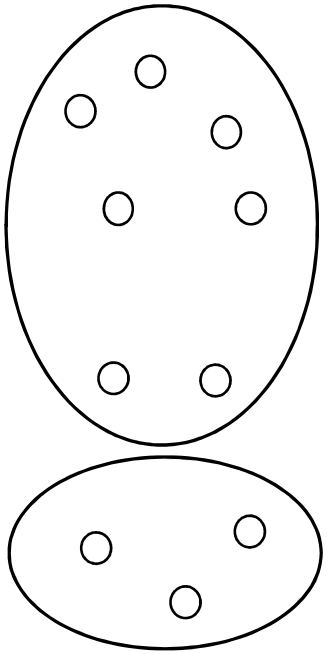
No class labels!

Solution A:



???

Solution B:

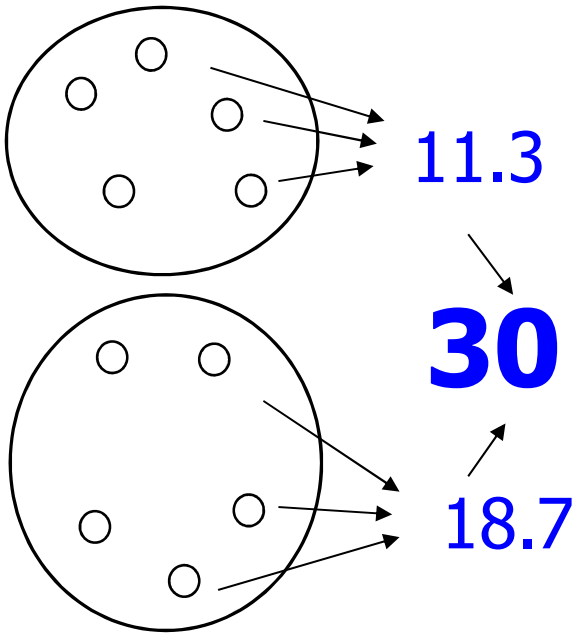


Internal index

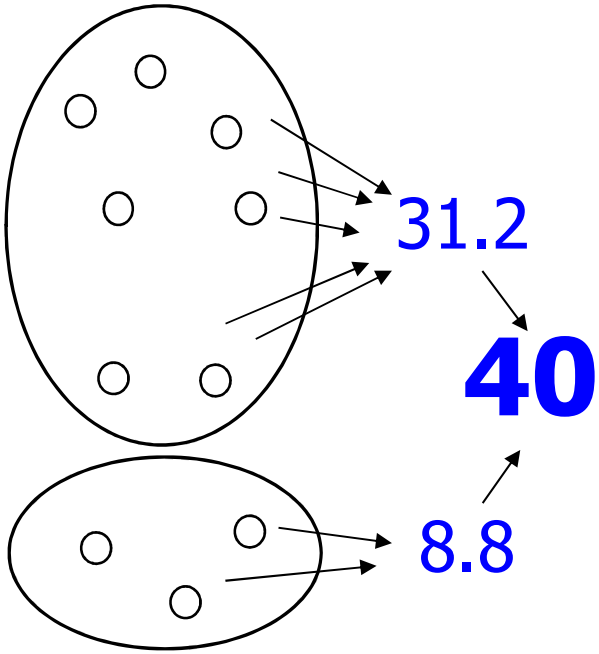
Sum-of-squared error (MSE)

$$f = \frac{1}{N}\sum_{i=1}^{N}\sum_{x_i \in c_k} \| x_i - c_k \|^2$$

Solution A:



Solution B:

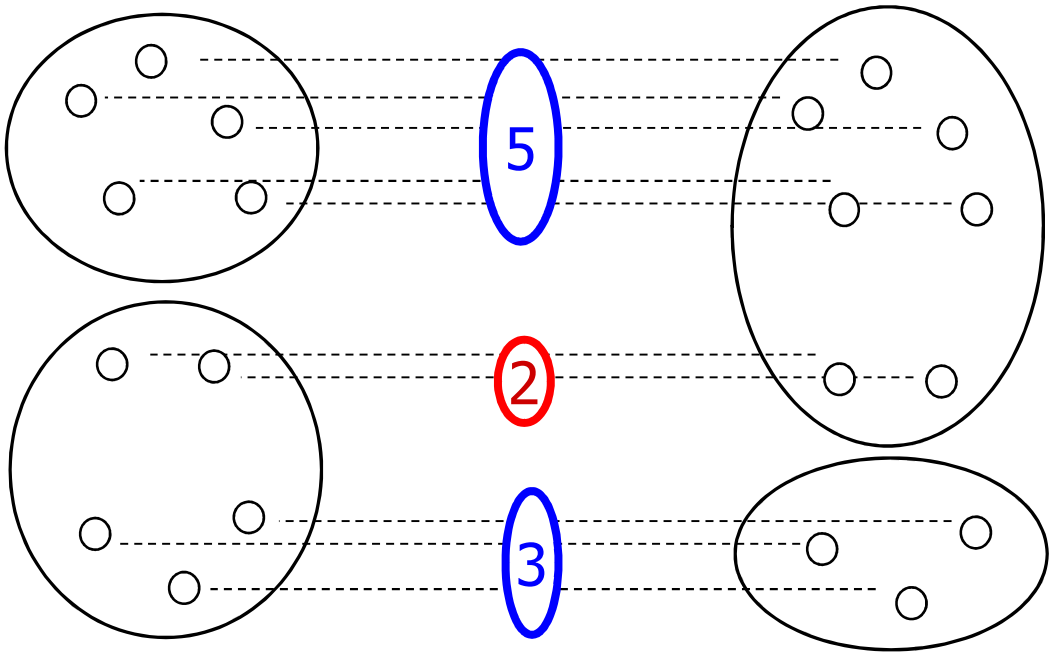


External index

Compare two solutions

Solution A:

Solution B:



5/7 = 71%

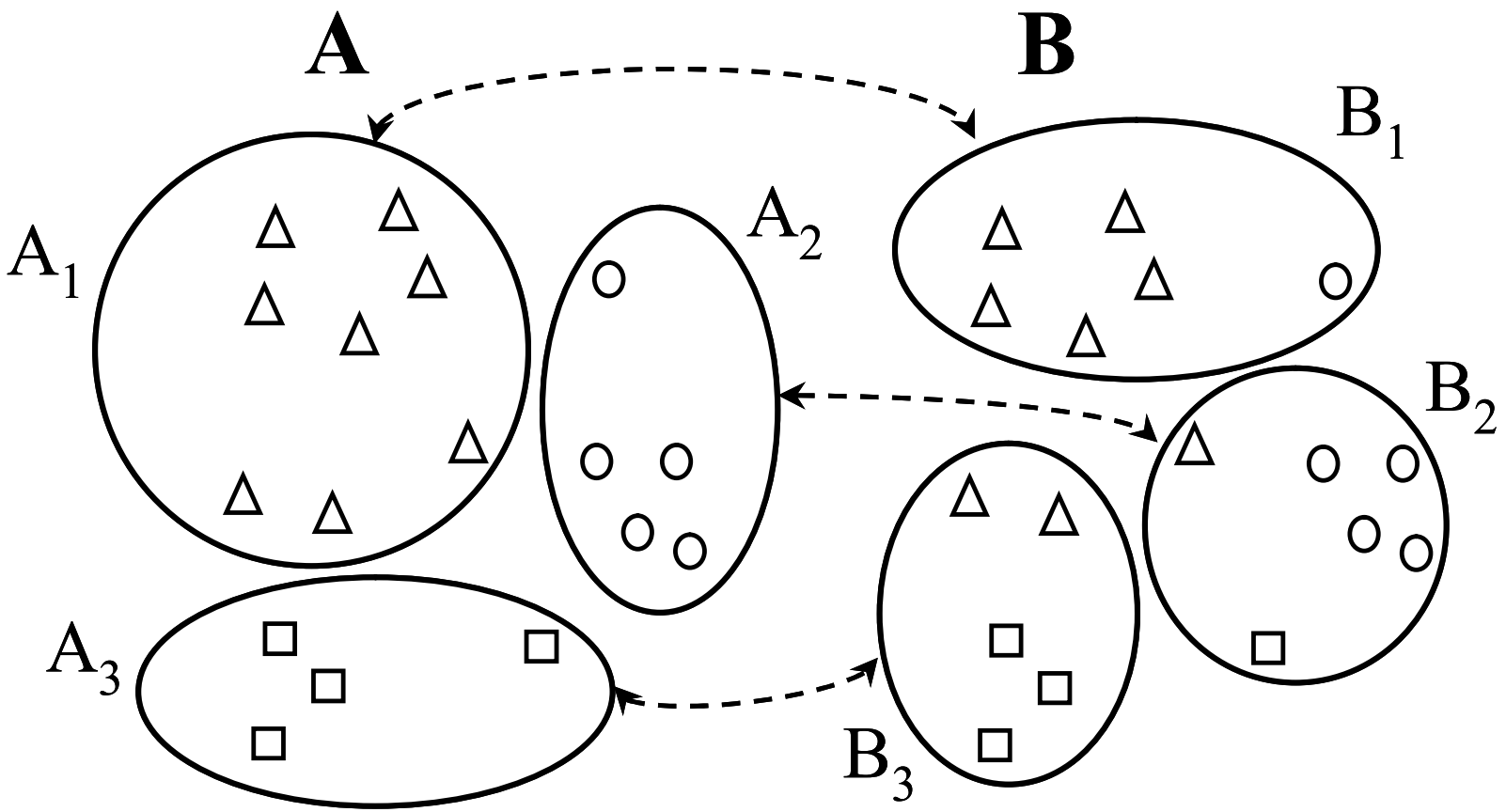
2/5 = 40%

3/5 = 60%

- Two clustering (A and B)
- Clustering against ground truth

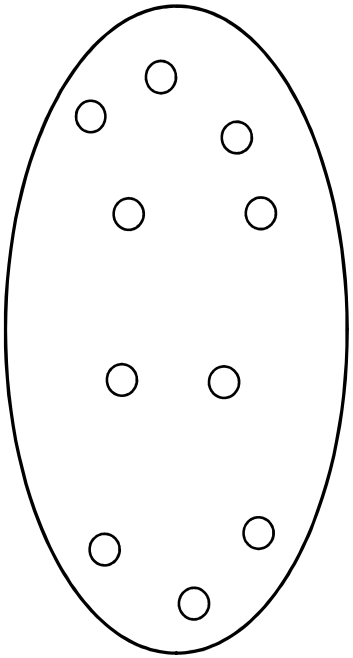
Set-matching based methods

M. Rezaei and P. Fränti, "Set-matching methods for external cluster validity", *IEEE Trans. on Knowledge and Data Engineering*, 28 (8), 2173-2186, August 2016.



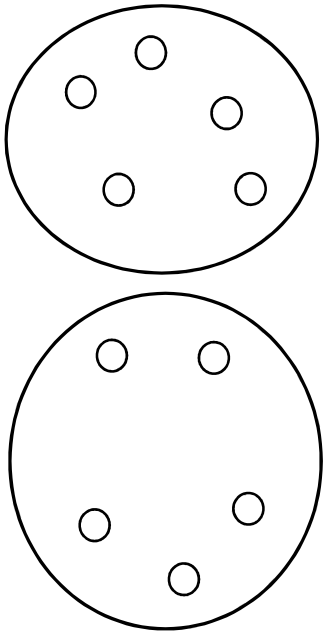
What about this…?

Solution 1:



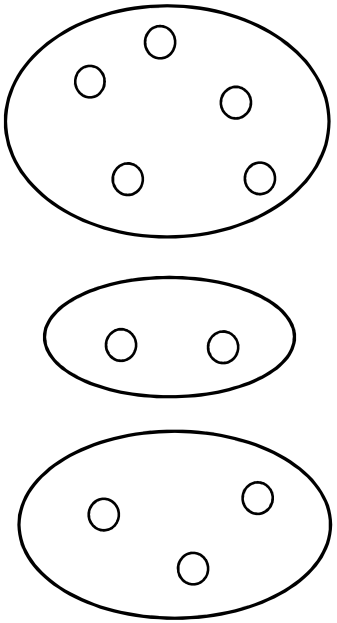
?

Solution 2:



?

Solution 3:



External index

Selection of existed methods

Pair-counting measures

- Rand index (RI) [Rand, 1971]
- Adjusted Rand index (ARI) [Hubert & Arabie, 1985]

Information-theoretic measures

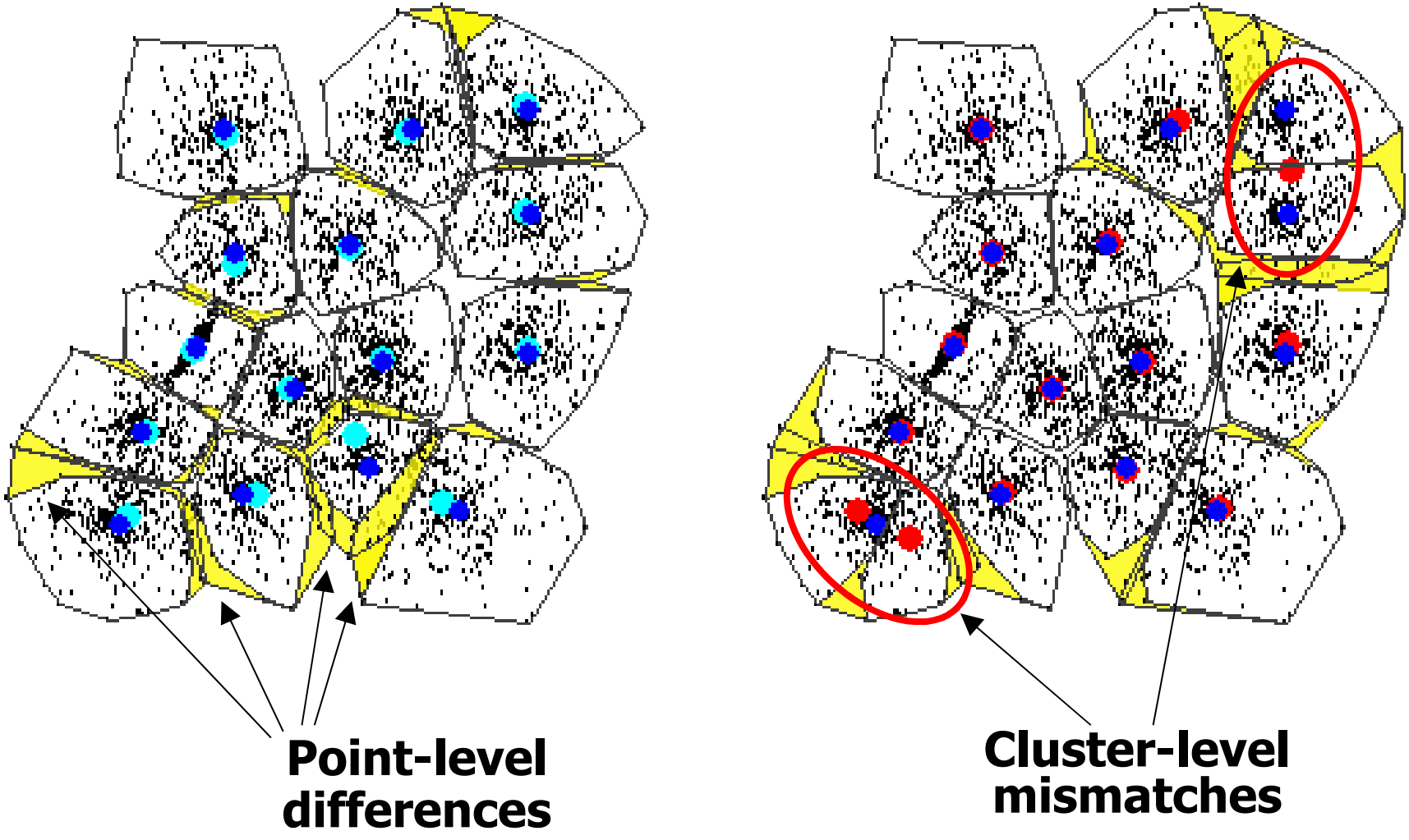
- Mutual information (MI) [Vinh, Epps, Bailey, 2010]
- Normalized Mutual information (NMI) [Kvalseth, 1987]

Set-matching based measures

- Normalized van Dongen (NVD) [Kvalseth, 1987]
- Criterion H (CH) [Meila & Heckerman, 2001]
- Purity [Rendon et al, 2011]
- Centroid index (CI) [Fränti, Rezaei & Zhao, 2014]

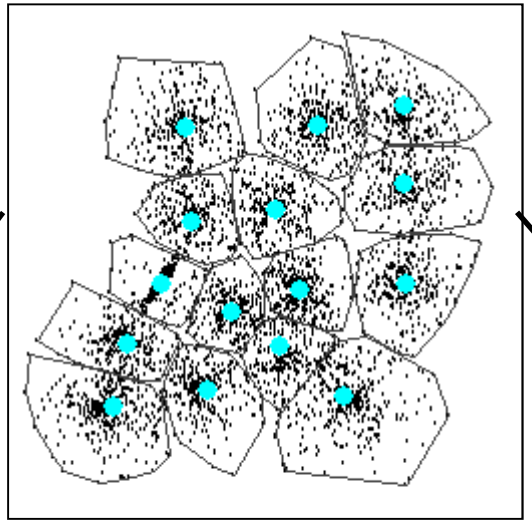
Cluster level measure

Point level vs. cluster level



Point level vs. cluster level

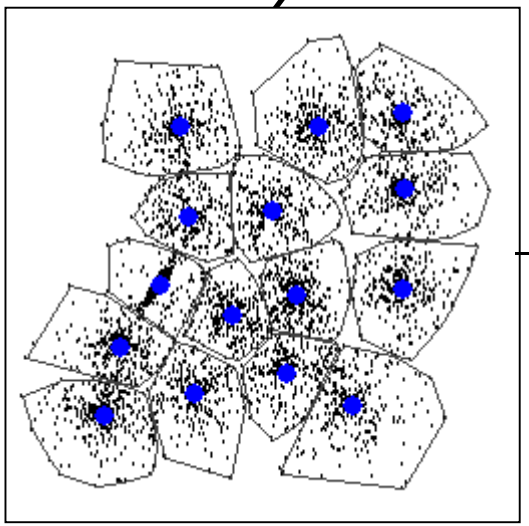
Agglomerative (AC)



ARI=0.91

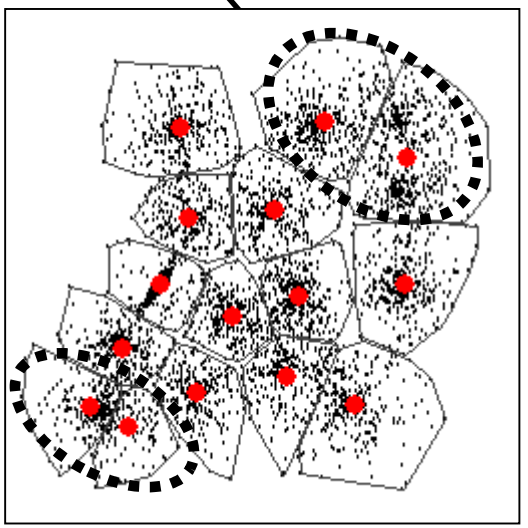
ARI=0.82

Random Swap (RS)

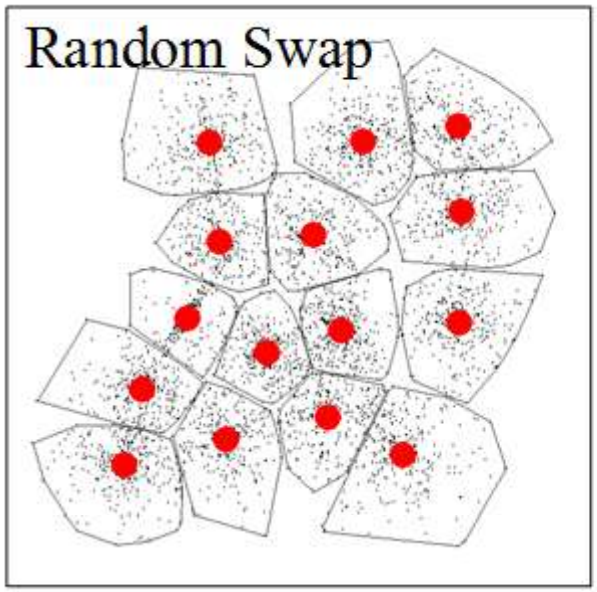


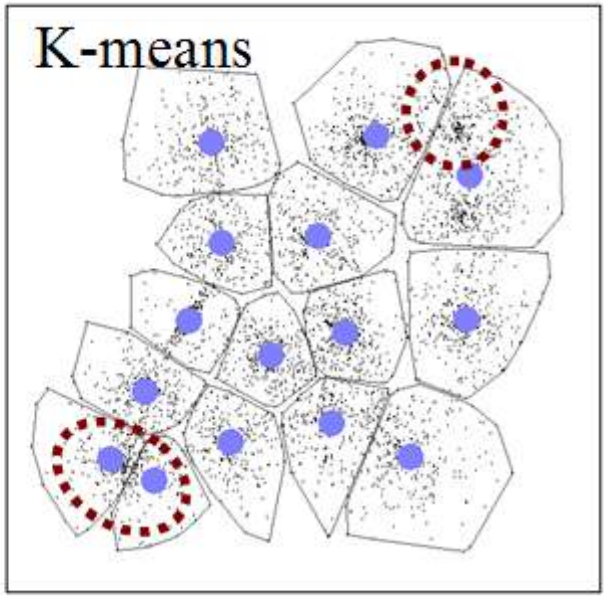
ARI=0.88

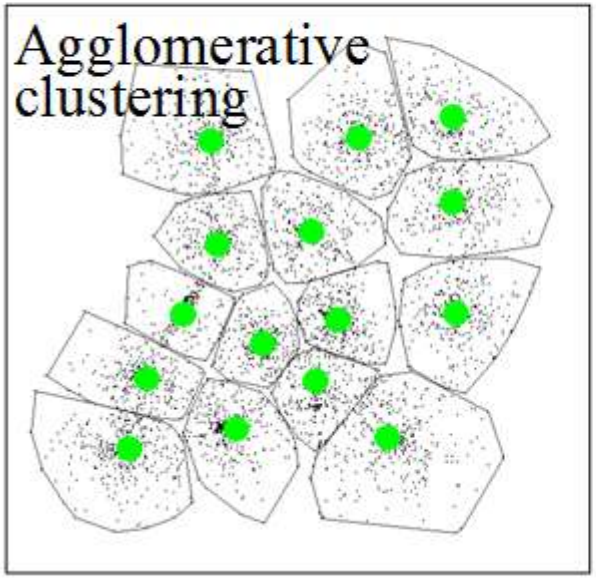
K-means



Point level vs. cluster level





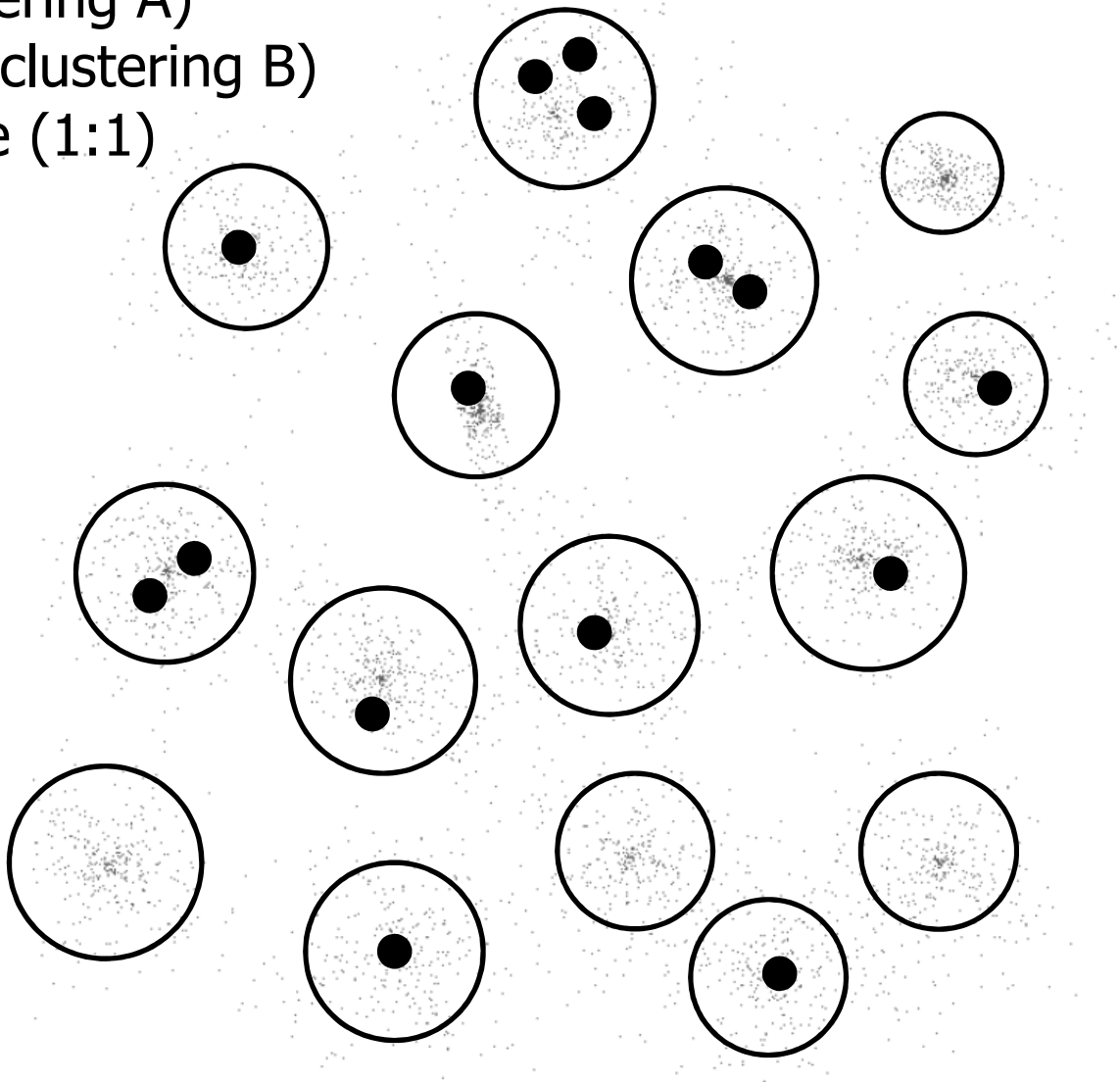


	RS AC	RS KM	AC KM
RI	0.99	0.99	0.98
ARI	0.91	0.88	0.82
MI	3.64	3.64	3.48
NMI	0.93	0.94	0.90
NVD	0.05	0.07	0.10
CH	0.05	0.10	0.14
CI	0	1	1

Centroid index

Pigeon hole principle

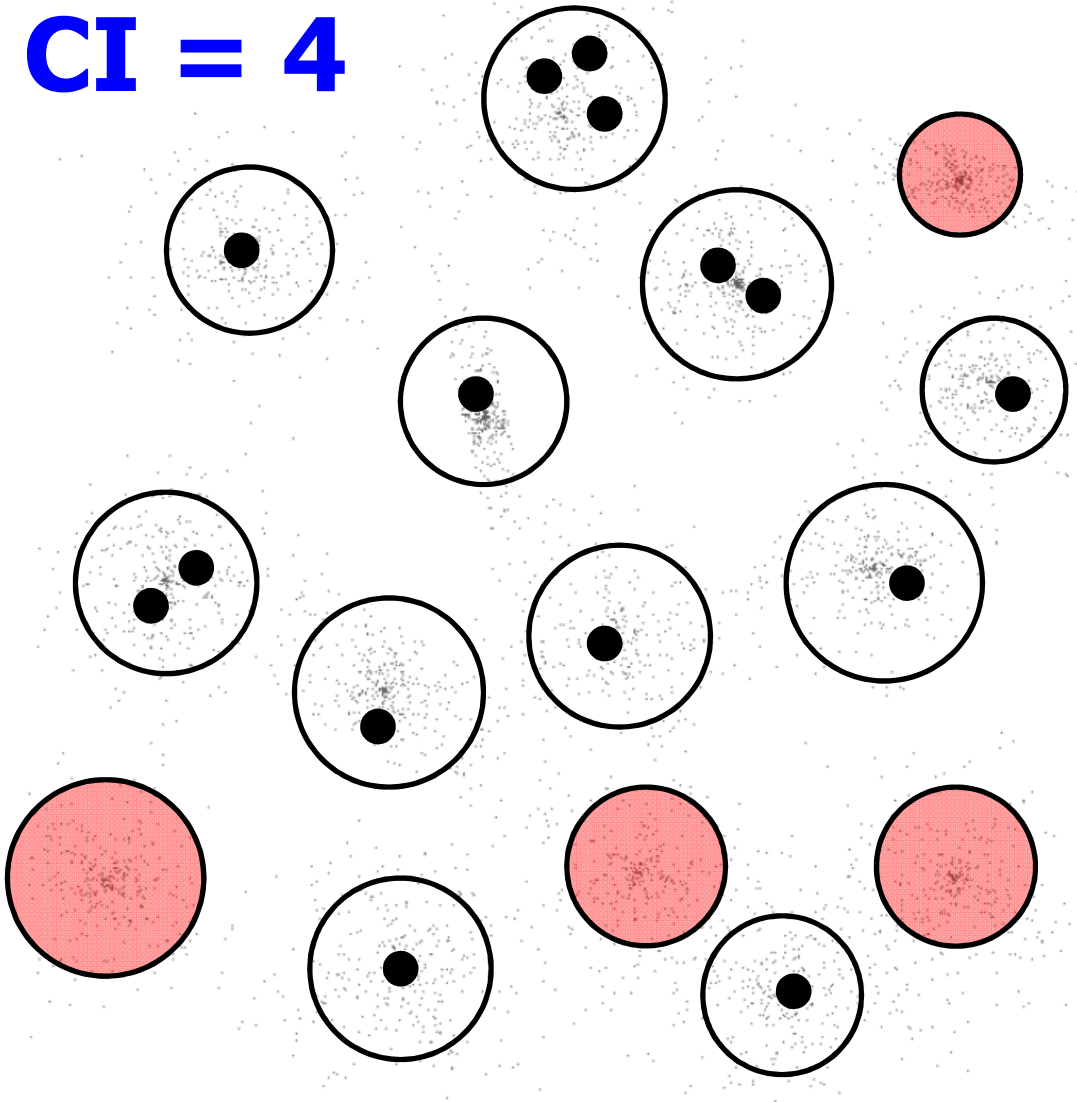
- 15 pigeons (clustering A)
- 15 pigeon holes (clustering B)
- Only one bijective (1:1) mapping exists



Centroid index (CI)

[Fränti, Rezaei, Zhao, *Pattern Recognition* 2014]

CI = 4



Definitions

Find nearest centroids ($A \rightarrow B$):

$$NN(A_i) = \arg\min_{1 \le j \le k} \left\| c[A_i] - c[B_j] \right\|$$

Detect prototypes with no mapping:

$$Orphan(B) = \begin{cases} 1 & InDegree(A) = 0 \\ 0 & InDegree(A) > 0 \end{cases}$$

Number of orphans:

$$CI_1(A \rightarrow B) = \sum_{j=1}^{k} Orphan(B_j)$$

Number of zero mappings!

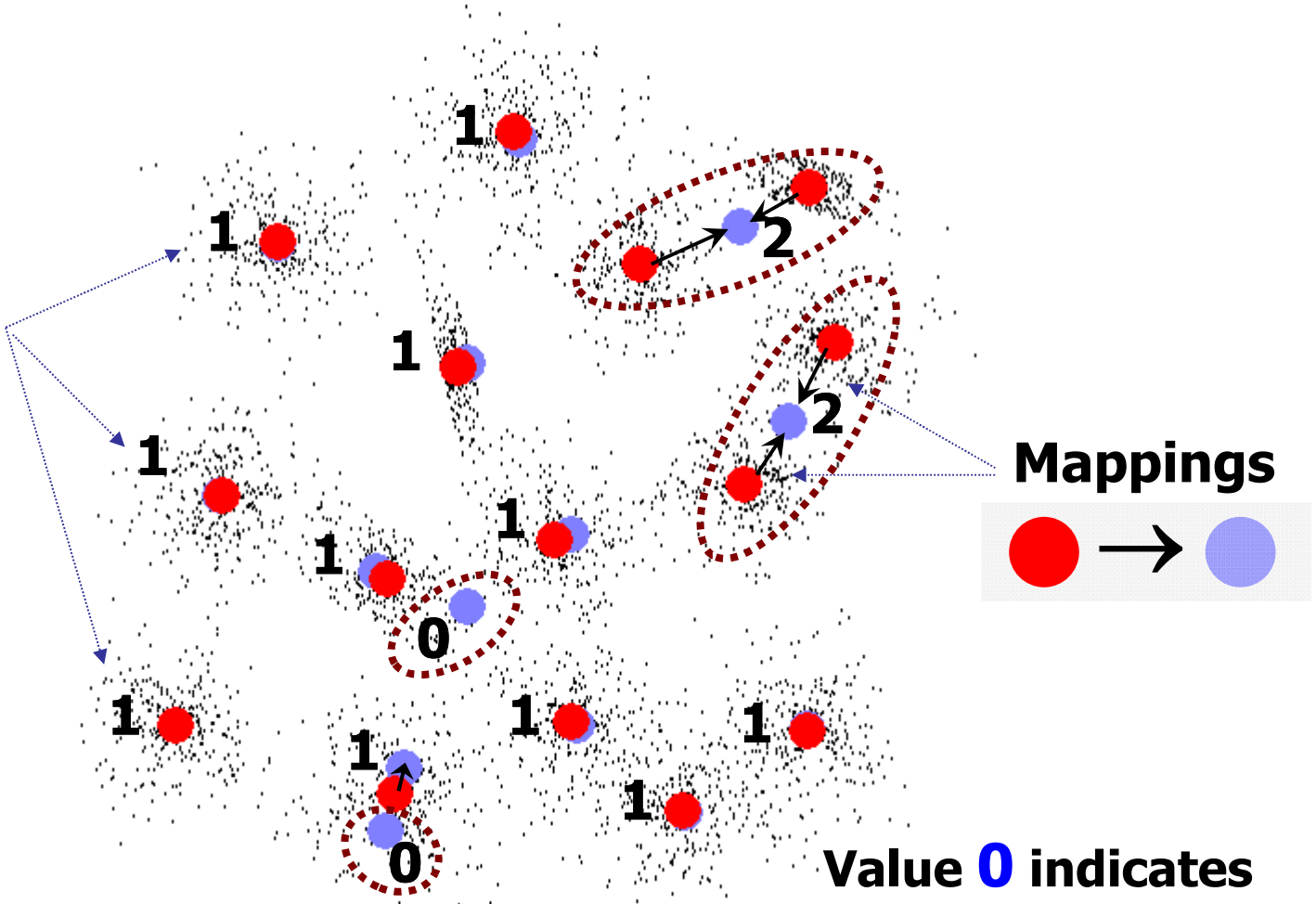
Centroid index:

Mapping both ways

$$CI(A, B) = \max\{CI_1(A \rightarrow B), CI_1(B \rightarrow A)\}$$

Example

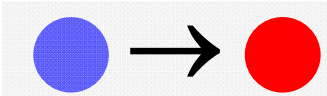
S_2

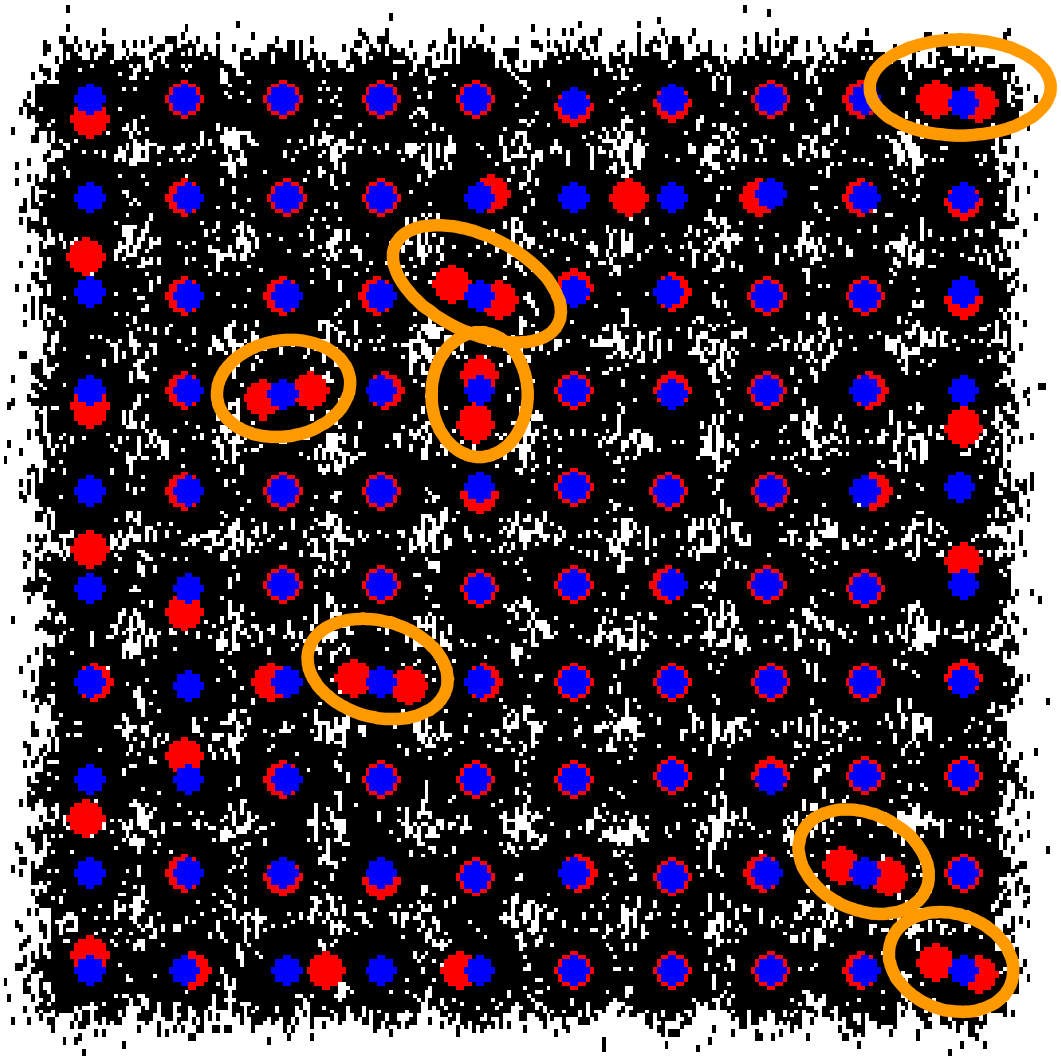

Indegree Counts
Mappings
Value 0 indicates an orphan cluster
CI = 2

Example

Birch1

Mappings

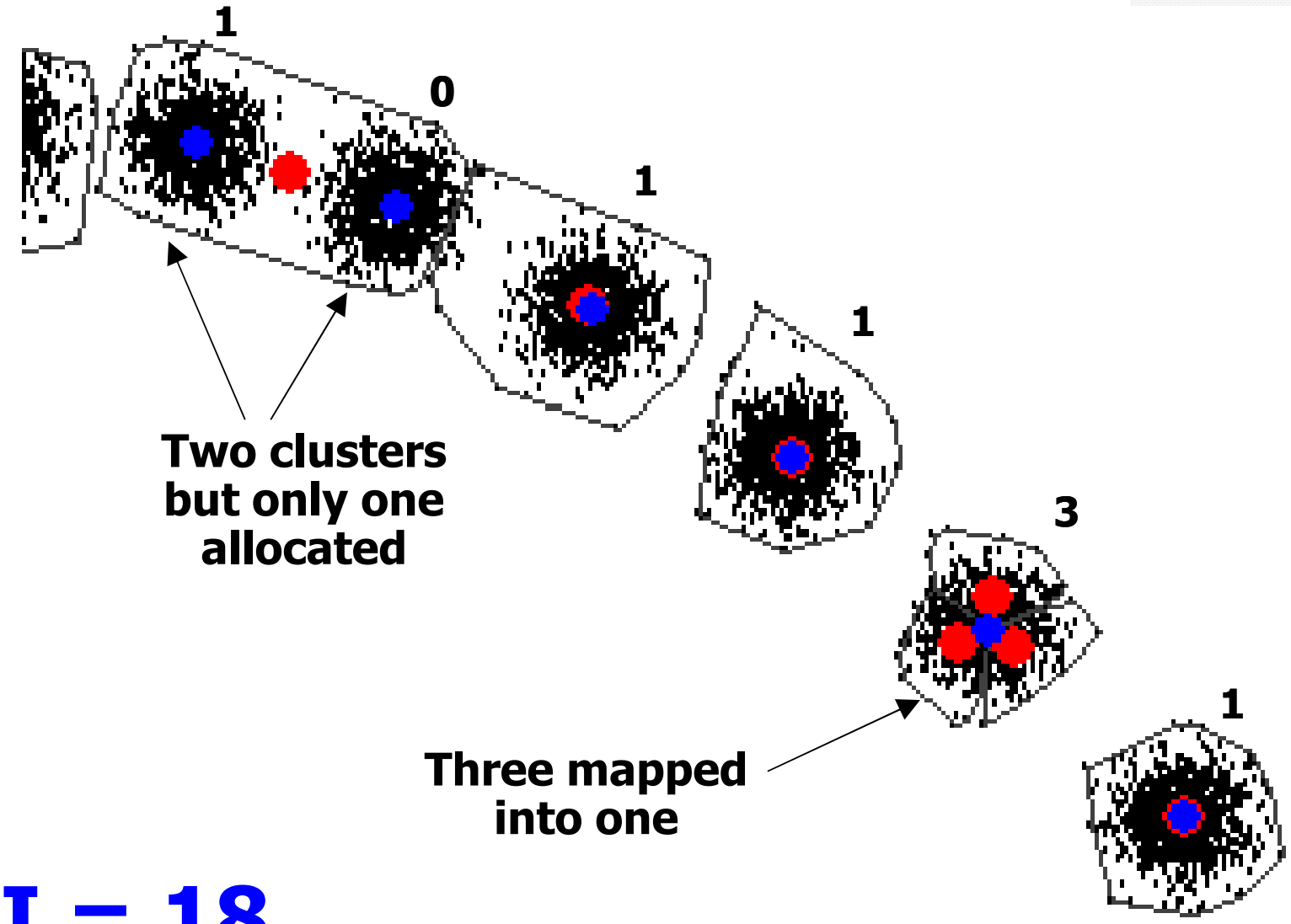




CI = 7

Example

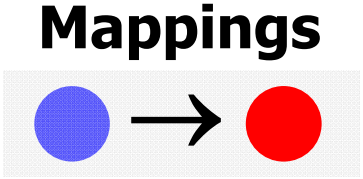
Birch2

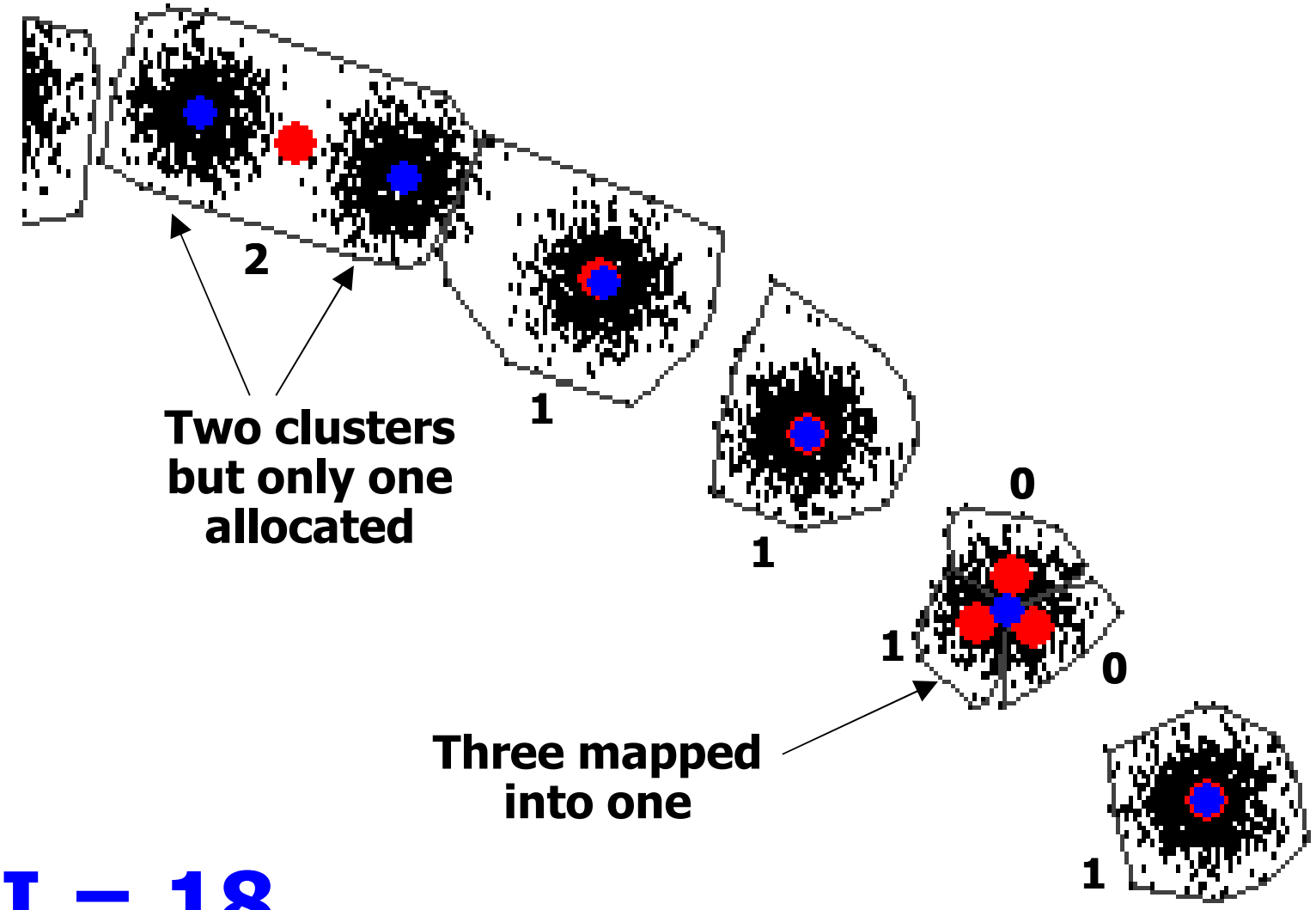


CI = 18

Example

Birch2





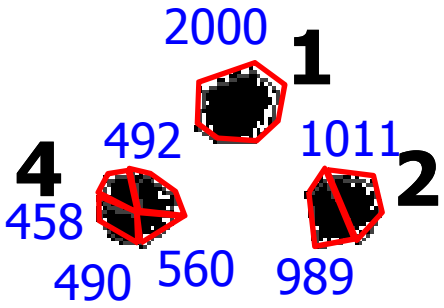
CI = 18

Unbalanced example

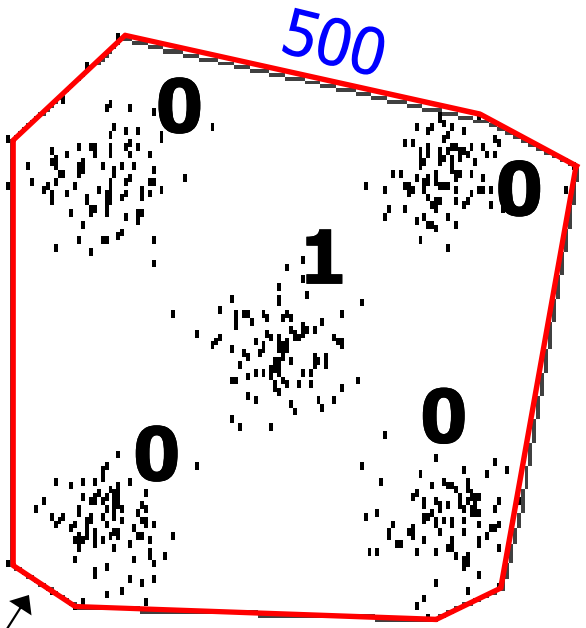
K-means result

KM→GT

CI = 4



K-means tend to put too many clusters here …



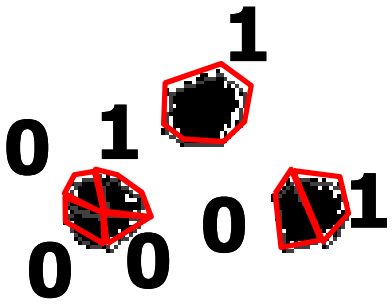
… and too few here

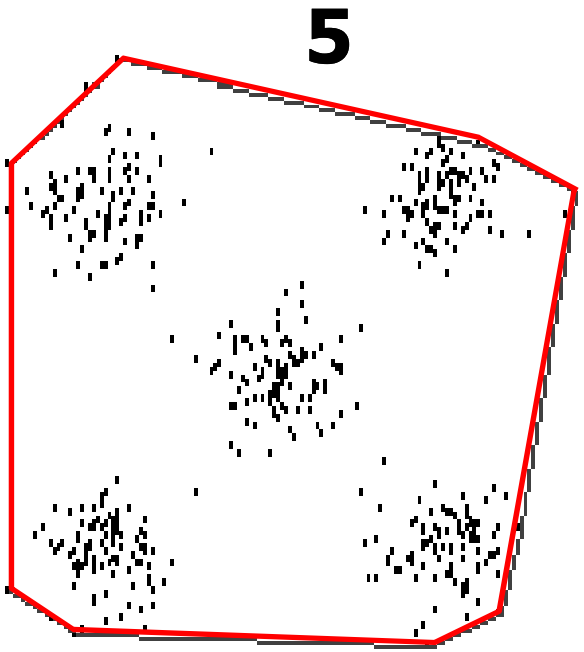
Unbalanced example

K-means result

GT→KM

CI = 4





Experiments

Mean Squared Errors

Green = Correct clustering structure

Data set	Clustering quality (MSE)							
	KM	RKM	KM++	XM	AC	RS	GKM	GA
Bridge	179.76	176.92	173.64	179.73	168.92	164.64	164.78	161.47
House	6.67	6.43	6.28	6.20	6.27	5.96	5.91	5.87
Miss America	5.95	5.83	5.52	5.92	5.36	5.28	5.21	5.10
House	3.61	3.28	2.50	3.57	2.62	2.83	-	2.44
$Birch_1$	5.47	5.01	4.88	5.12	4.73	4.64	-	4.64
$Birch_2$	7.47	5.65	3.07	6.29	2.28	2.28	-	2.28
$Birch_3$	2.51	2.07	1.92	2.07	1.96	1.86	-	1.86
S_1	19.71	8.92	8.92	8.92	8.93	8.92	8.92	8.92
S_2	20.58	13.28	13.28	15.87	13.44	13.28	13.28	13.28
S_3	19.57	16.89	16.89	16.89	17.70	16.89	16.89	16.89
S_4	17.73	15.70	15.70	15.71	17.52	15.70	15.71	15.70

Raw numbers don't tell much

Adjusted Rand Index

[Hubert & Arabie, 1985]

Data set	Adjusted Rand Index (ARI)							
	KM	RKM	KM++	XM	AC	RS	GKM	GA
Bridge	0.38	0.40	0.39	0.37	0.43	0.52	0.50	1
House	0.40	0.40	0.44	0.47	0.43	0.53	0.53	1
Miss America	0.19	0.19	0.18	0.20	0.20	0.20	0.23	1
House	0.46	0.49	0.52	0.46	0.49	0.49	-	1
Birch $_1$	0.85	0.93	0.98	0.91	0.96	1.00	-	1
Birch $_2$	0.81	0.86	0.95	0.86	1	1	-	1
Birch $_3$	0.74	0.82	0.87	0.82	0.86	1.00	1.00	1
S_1	**0.83**	1.00	1.00	1.00	1.00	1.00	1.00	1.00
S_2	**0.80**	0.99	0.99	**0.89**	0.98	0.99	0.99	0.99
S_3	**0.86**	0.96	0.96	0.96	0.92	0.96	0.96	0.96
S_4	**0.82**	0.93	0.93	0.94	**0.77**	0.93	0.93	0.93

How high is good?

Normalized Mutual information

[Kvalseth, 1987]

Data set	Normalized Mutual Information (NMI)							
	KM	RKM	KM++	XM	AC	RS	GKM	GA
Bridge	0.77	0.78	0.78	0.77	0.80	0.83	0.82	1.00
House	0.80	0.80	0.81	0.82	0.81	0.83	0.84	1.00
Miss America	0.64	0.64	0.63	0.64	0.64	0.66	0.66	1.00
House	0.81	0.81	0.82	0.81	0.81	0.82	-	1.00
Birch $_1$	0.95	0.97	0.99	0.96	0.98	1.00	-	1.00
Birch $_2$	0.96	0.97	0.99	0.97	1.00	1.00	-	1.00
Birch $_3$	0.90	0.94	0.94	0.93	0.93	0.96	-	1.00
S_1	**0.93**	1.00	1.00	1.00	1.00	1.00	1.00	1.00
S_2	**0.90**	0.99	0.99	**0.95**	0.99	0.93	0.99	0.99
S_3	**0.92**	0.97	0.97	0.97	0.94	0.97	0.97	0.97
S_4	**0.88**	0.94	0.94	0.95	**0.85**	0.94	0.94	0.94

Normalized Van Dongen

[Kvalseth, 1987]

Data set	Normalized Van Dongen (NVD)							
	KM	RKM	KM++	XM	AC	RS	GKM	GA
Bridge	0.45	0.42	0.43	0.46	0.38	0.32	0.33	0.00
House	0.44	0.43	0.40	0.37	0.40	0.33	0.31	0.00
Miss America	0.60	0.60	0.61	0.59	0.57	0.55	0.53	0.00
House	0.40	0.37	0.34	0.39	0.39	0.34	-	0.00
Birch $_1$	0.09	0.04	0.01	0.06	0.02	0.00	-	0.00
Birch $_2$	0.12	0.08	0.03	0.09	0.00	0.00	-	0.00
Birch $_3$	0.19	0.12	0.10	0.13	0.13	0.00	-	0.00
S_1	**0.09**	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S_2	**0.11**	0.00	0.00	**0.06**	0.01	0.04	0.00	0.00
S_3	**0.08**	0.02	0.02	0.02	0.05	0.00	0.00	0.02
S_4	**0.11**	0.04	0.04	0.03	**0.13**	0.04	0.04	0.04

Lower is better

Centroid Similarity Index

[Fränti, Rezaei, Zhao, 2014]

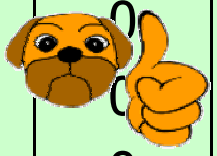
Data set	Centroid Similarity Index (CSI)							
	KM	RKM	KM++	XM	AC	RS	GKM	GA
Bridge	0.47	0.51	0.49	0.45	0.57	0.62	0.63	1.00
House	0.49	0.50	0.54	0.57	0.55	0.63	0.66	1.00
Miss America	0.32	0.32	0.32	0.33	0.38	0.40	0.42	1.00
House	0.54	0.57	0.63	0.54	0.57	0.62	---	1.00
Birch $_1$	0.87	0.94	0.98	0.93	0.99	1.00	---	1.00
Birch $_2$	0.76	0.84	0.94	0.83	1.00	1.00	---	1.00
Birch $_3$	0.71	0.82	0.87	0.81	0.86	0.99	---	1.00
S_1	**0.83**	1.00	1.00	1.00	1.00	1.00	1.00	1.00
S_2	**0.82**	1.00	1.00	**0.91**	1.00	1.00	1.00	1.00
S_3	**0.89**	0.99	0.99	0.99	0.98	0.99	0.99	0.99
S_4	**0.87**	0.98	0.98	0.99	**0.85**	0.98	0.98	0.98

Ok but lacks threshold

Centroid Index

[Fränti, Rezaei, Zhao, 2014]

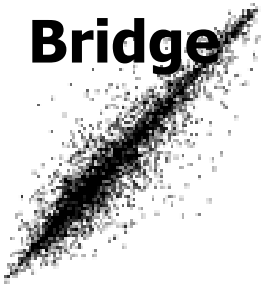
Data set	C-Index (CI_2)							
	KM	RKM	KM++	XM	AC	RS	GKM	GA
Bridge	74	63	58	81	33	33	35	0
House	56	45	40	37	31	22	20	0
Miss America	88	91	67	88	38	43	36	0
House	43	39	22	47	26	23	---	0
Birch $_1$	7	3	1	4	0	0	---	0
Birch $_2$	18	11	4	12	0	0	---	0
Birch $_3$	23	11	7	10	7	2	---	0
S_1	**2**	0	0	0	0	0	0	0
S_2	**2**	0	0	**1**	0	0	0	0
S_3	**1**	0	0	0	0	0	0	0
S_4	**1**	0	0	0	**1**	0	0	0



Going deeper…

Accurate clustering

GAIS-2002 similar to GAIS-2012 ?



	Method	MSE
GKM	Global K-means	164.78
RS	Random swap (5k)	164.64
GA	Genetic algorithm	161.47
RS_{8M}	Random swap (8M)	161.02
GAIS-2002	GAIS	160.72
+ RS_{1M}	GAIS + RS (1M)	160.49
+ RS_{8M}	GAIS + RS (8M)	160.43
GAIS-2012	GAIS	160.68
+ RS_{1M}	GAIS + RS (1M)	160.45
+ RS_{8M}	GAIS + RS (8M)	160.39
+ PRS	GAIS + PRS	160.33
+ RS_{8M} +	GAIS + RS (8M) + PRS	160.28

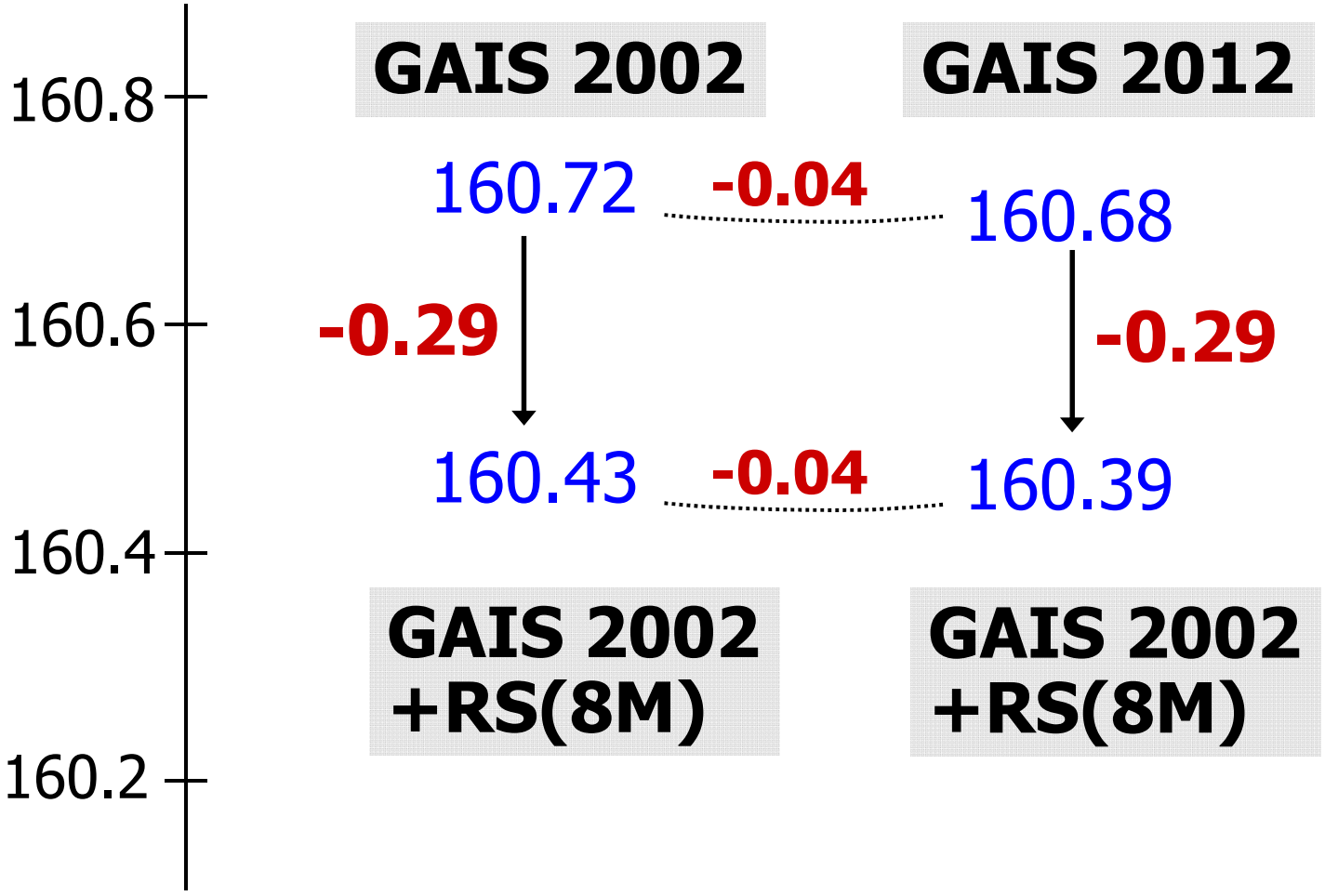
-0.04

-0.29

-0.29

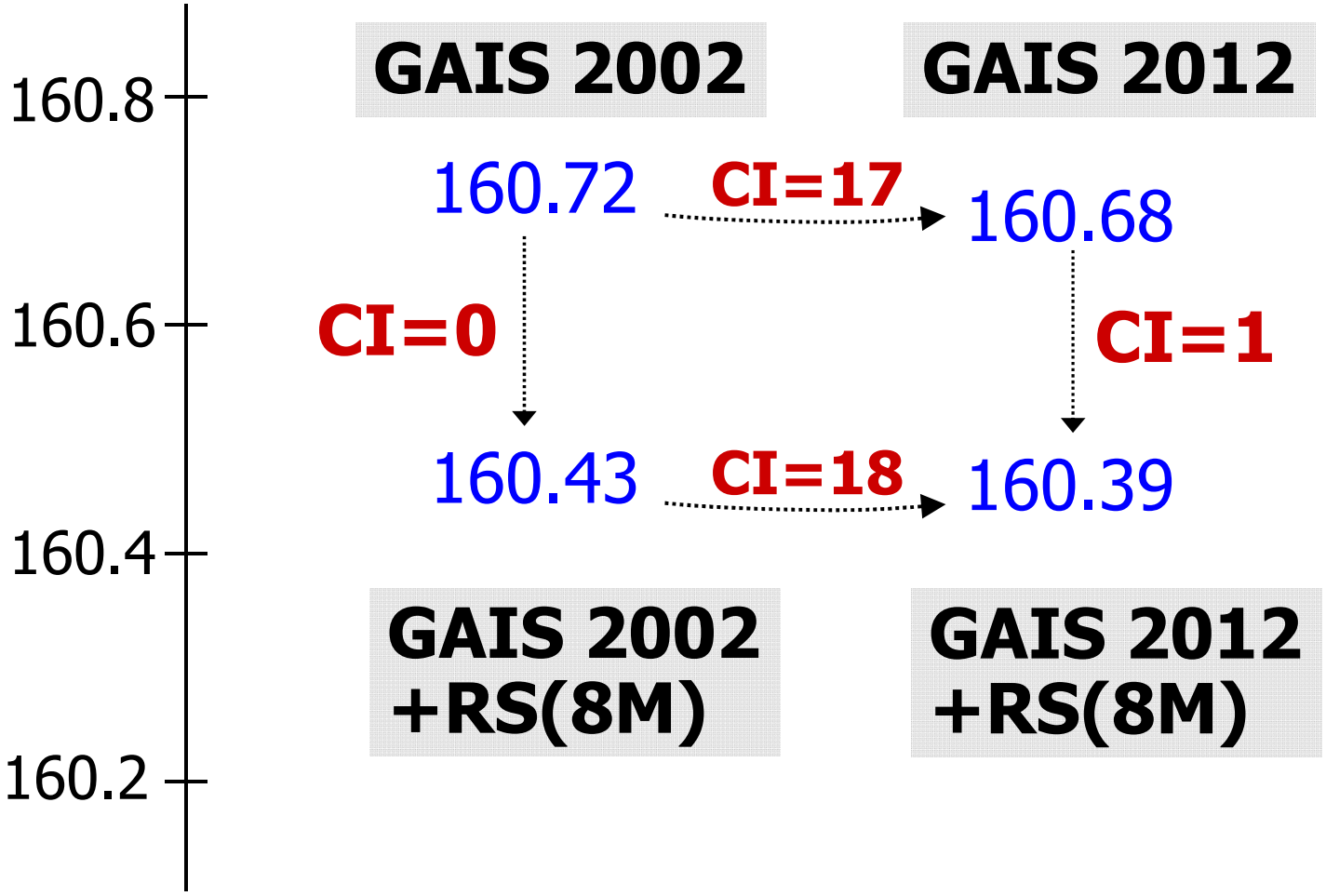
GAIS'02 and GAIS'12 the same?

Virtually the same MSE-values



GAIS'02 and GAIS'12 the same?

But different structure!



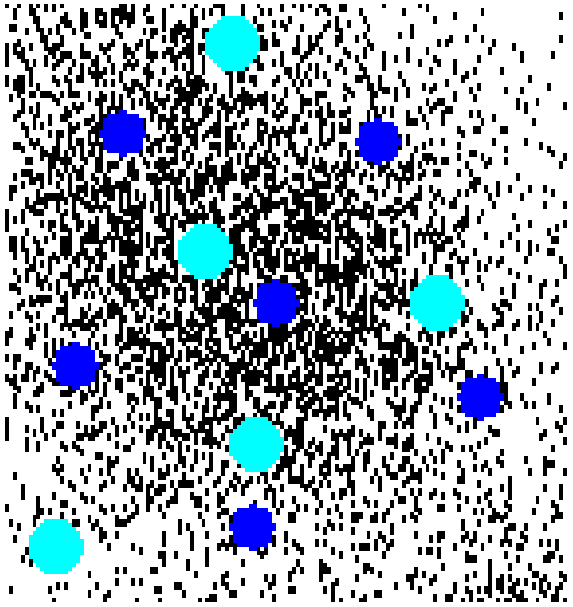
Seemingly the same solutions

Same structure
"same family"

Main algorithm:	RS_{8M}	**GAIS 2002**			**GAIS 2012**				
+ Tuning 1	×	×	RS_{1M}	RS_{8M}	×	RS_{1M}	RS_{8M}		RS_{8M}
+ Tuning 2	×	×	×	×	×	×	×	×	
RS_{8M}	---	19	19	19	23	24	24	23	22
GAIS (2002)	23	---	0	0	14	15	15	14	16
+ RS_{1M}	23	0	---	0	14	15	15	14	13
+ RS_{8M}	23	0	0	---	14	15	15	14	13
GAIS (2012)	25	17	18	18	---	1	1	1	1
+ RS_{1M}	25	17	18	18	1	---	0	0	1
+ RS_{8M}	25	17	18	18	1	0	---	0	1
+ PRS	25	17	18	18	1	0	0	---	1
+ RS_{8M} + PRS	24	17	18	18	1	1	1	1	---

But why?

- Real cluster structure missing
- Clusters allocated like well optimized “grid”
- Several grids results different allocation
- Overall clustering quality can still be the same

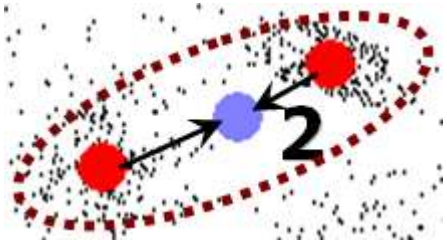


Generalization

Three alternatives

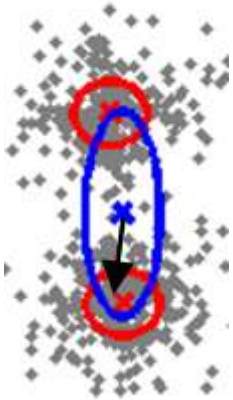
1. Prototype similarity

Prototype must exist

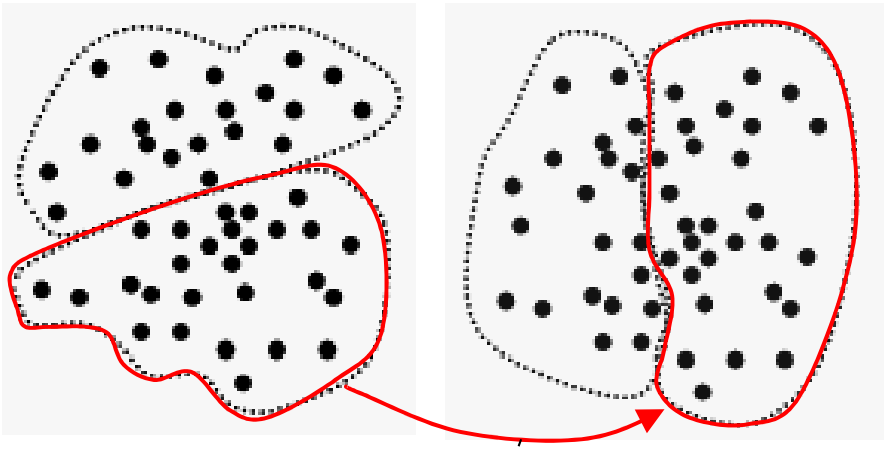


2. Model similarity

Derived from model



3. Partition similarity

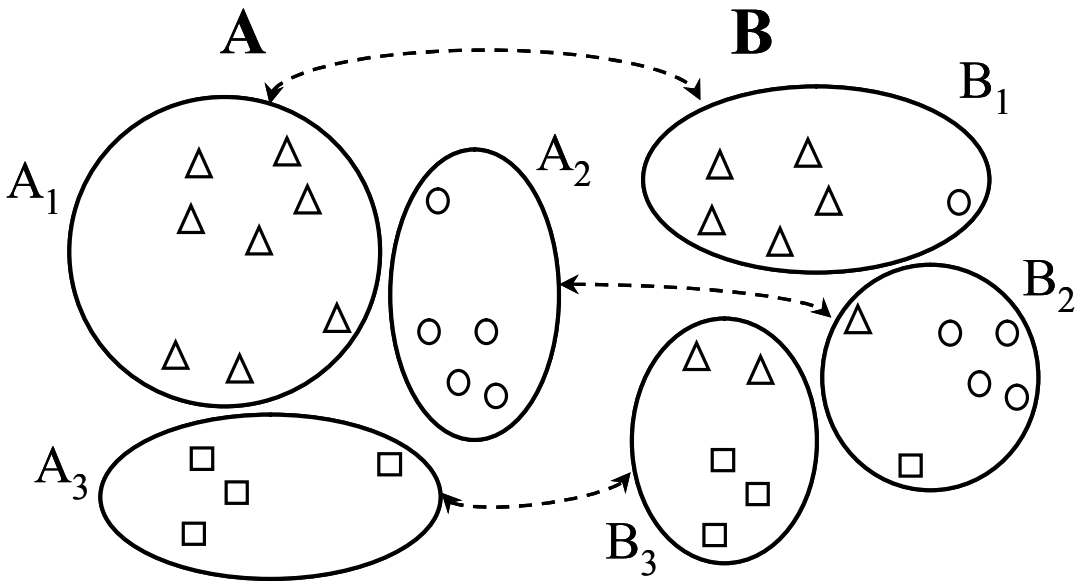


$$J = \frac{|P_i \cap G_j|}{|P_i \cup G_j|}$$

Partition similarity

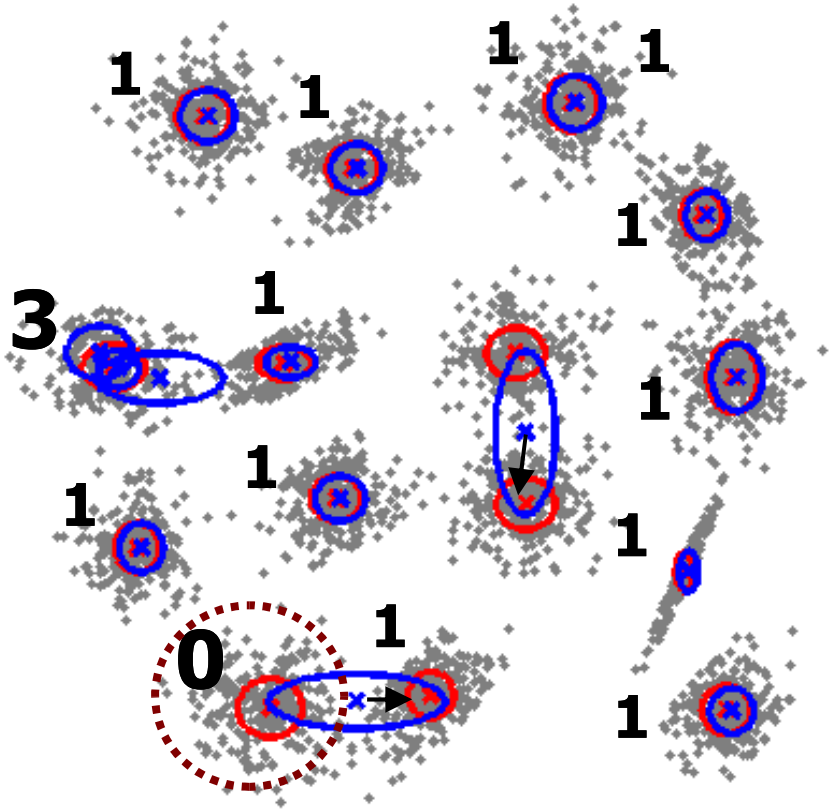
- Cluster similarity using Jaccard
- Calculated from contigency table

	B_1	B_2	B_3	$\sum$
A_1	5	1	2	8
A_2	1	4	0	5
A_3	0	1	3	4
$\sum$	6	6	5	17



Gaussian mixture model

$$S_{BC} = \frac{1}{8}\left(c[A_i] - c[B_j]\right)^T \Sigma^{-1}\left(c[A_i] - c[B_j]\right) + \frac{1}{2}\ln\left(\frac{|\Sigma|}{\sqrt{|\Sigma_1||\Sigma_2|}}\right)$$



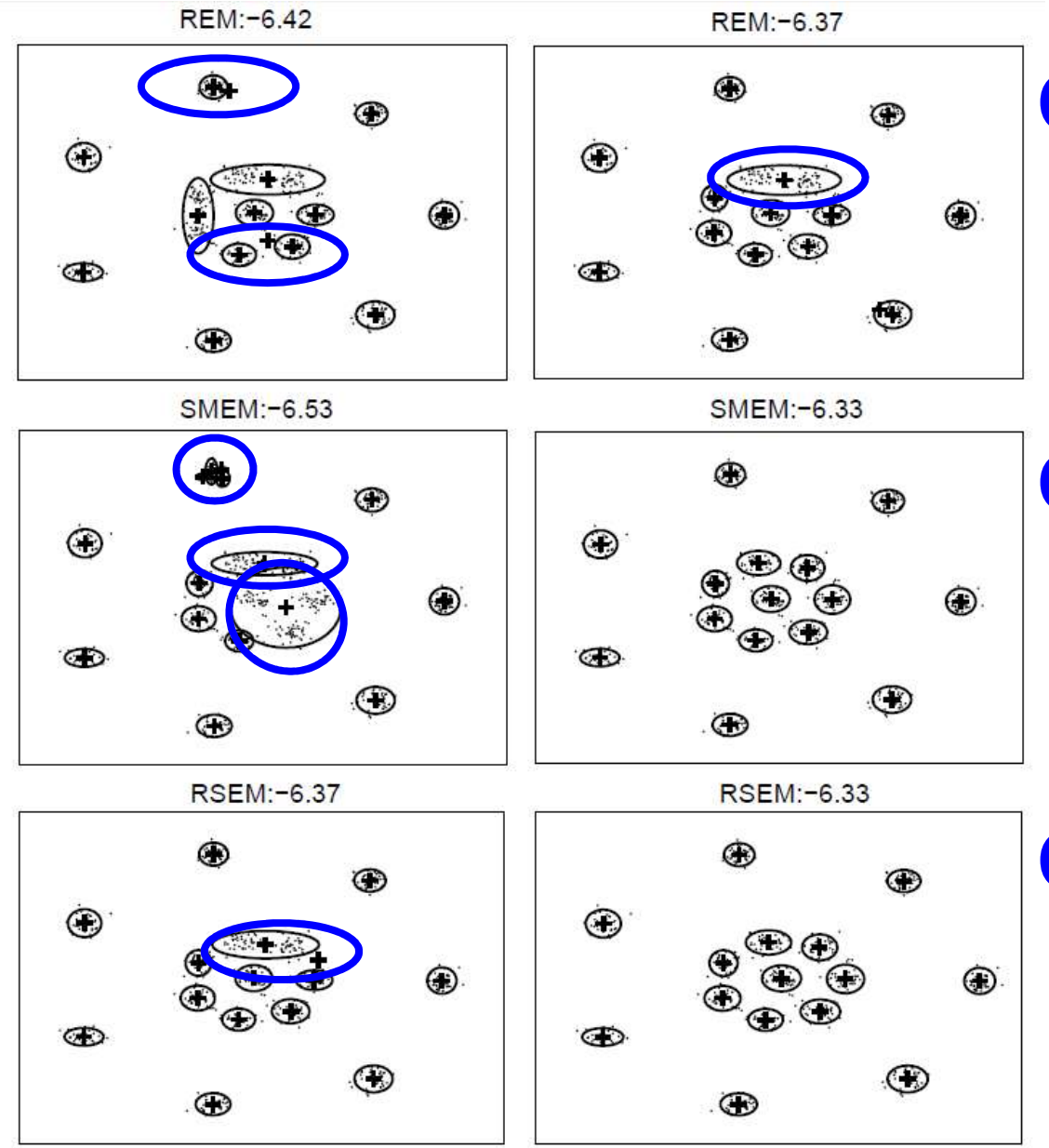
RI	0.98
ARI	0.84
MI	3.60
NMI	0.94
NVD	0.08
CH	0.16

CI=2

Split-and-Merge EM

Random Swap EM

Gaussian mixture model



CI=2

CI=1

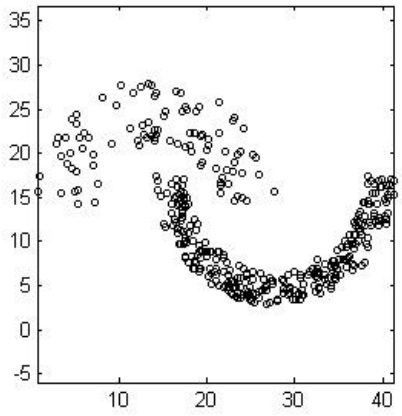
CI=3

CI=0

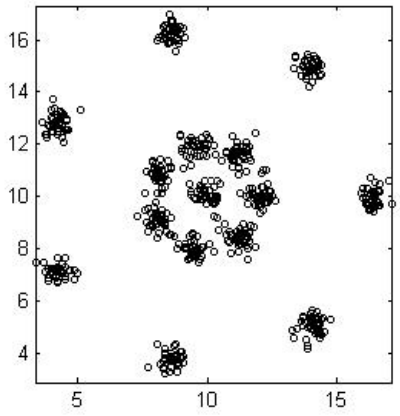
CI=1

CI=0

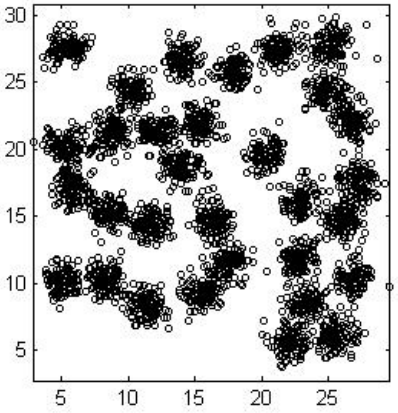
Arbitrary-shape data



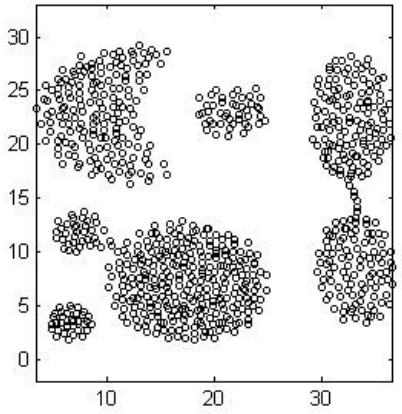
A.K. Jain's Toy problem



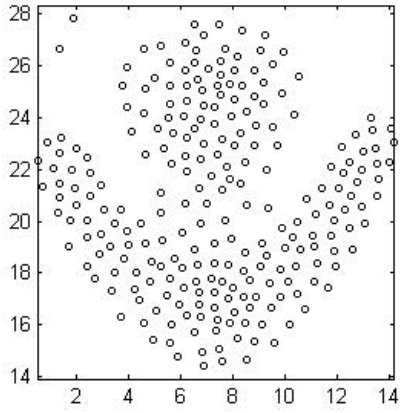
R15



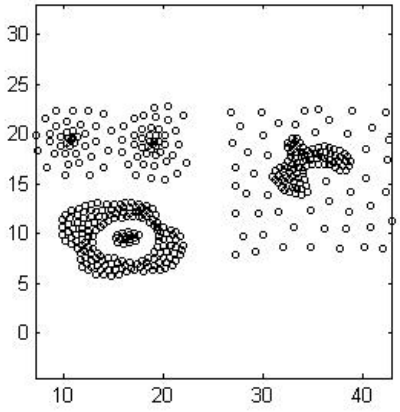
D31



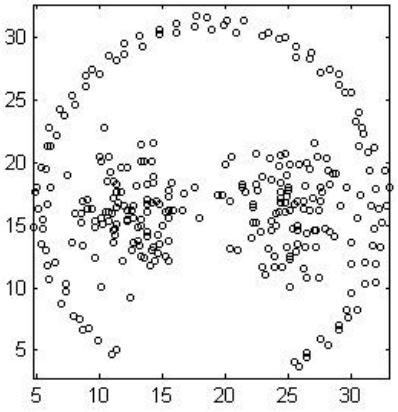
Aggregation



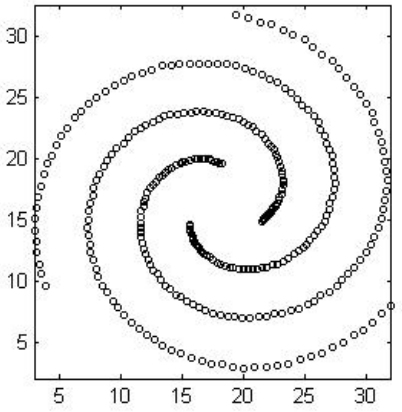
Flame



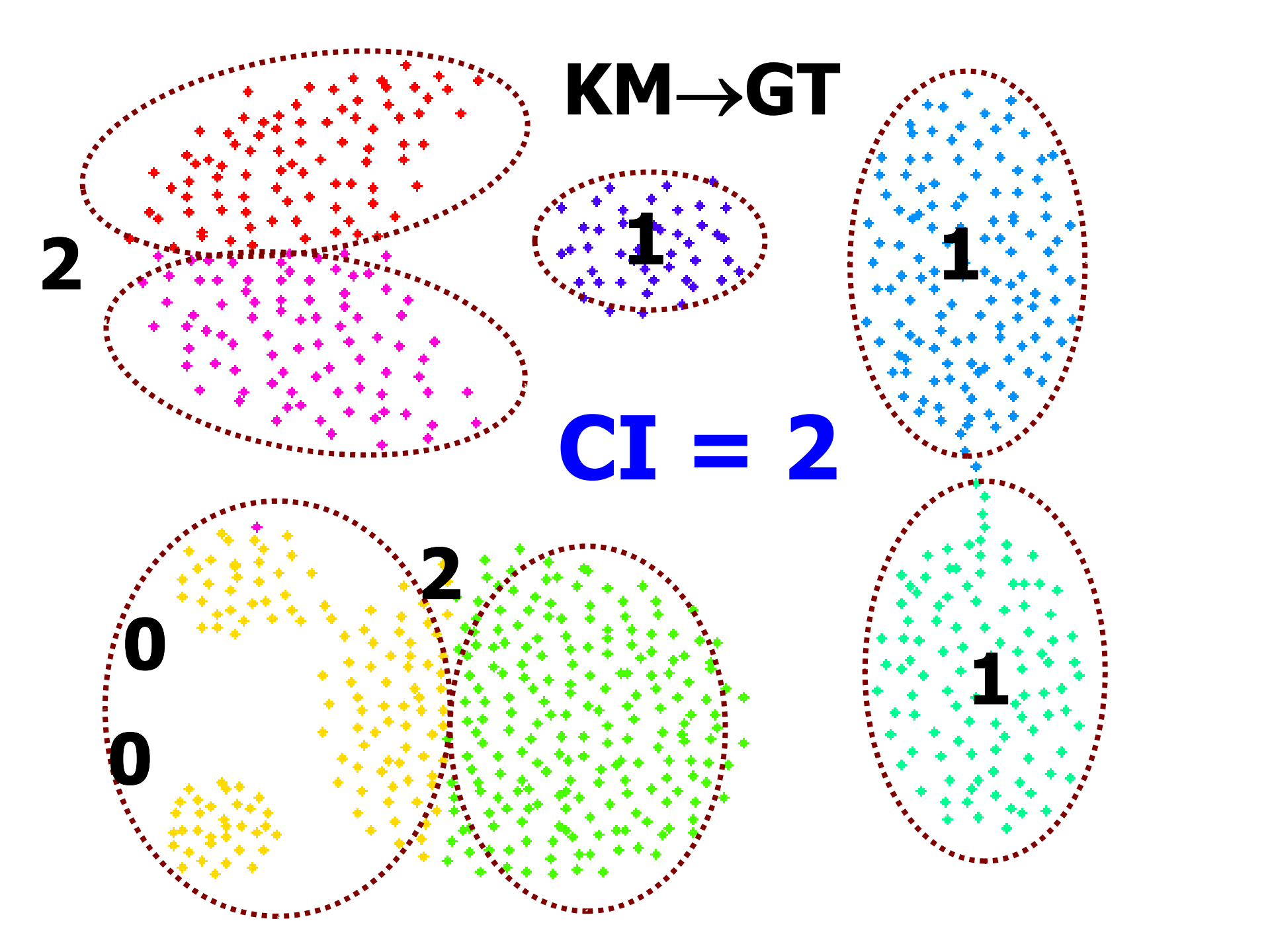
Zahn's Compound

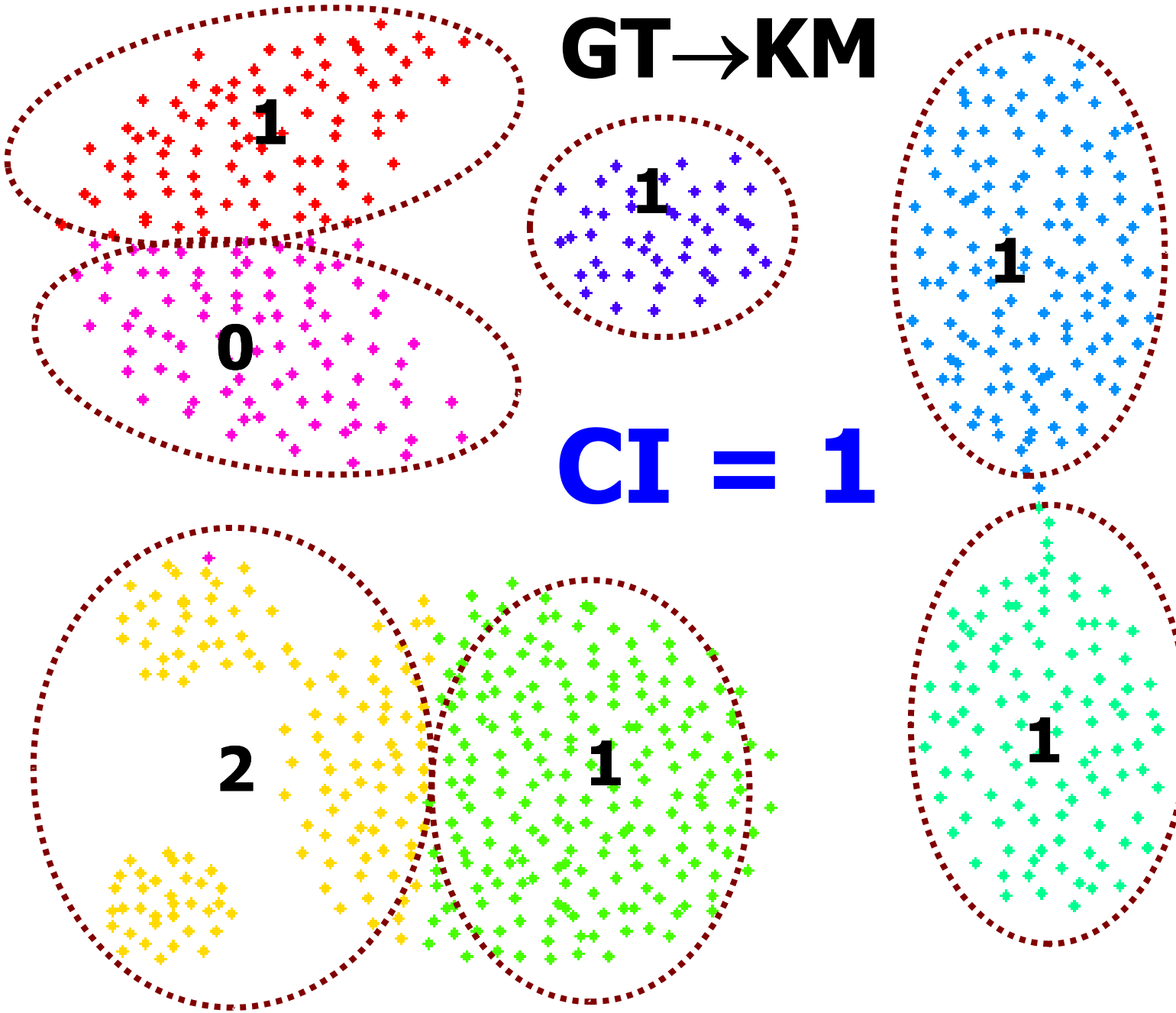


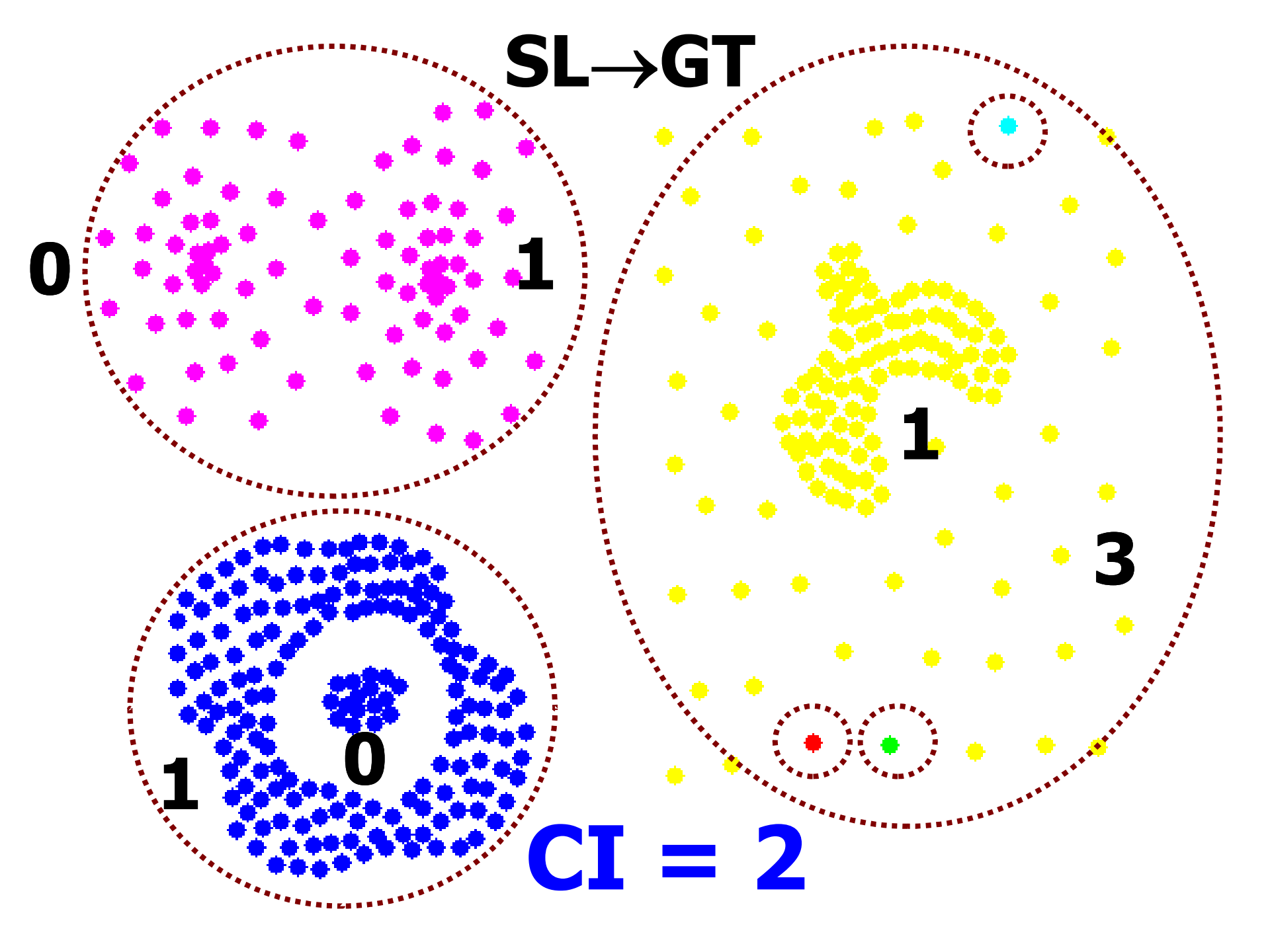
Path-based1

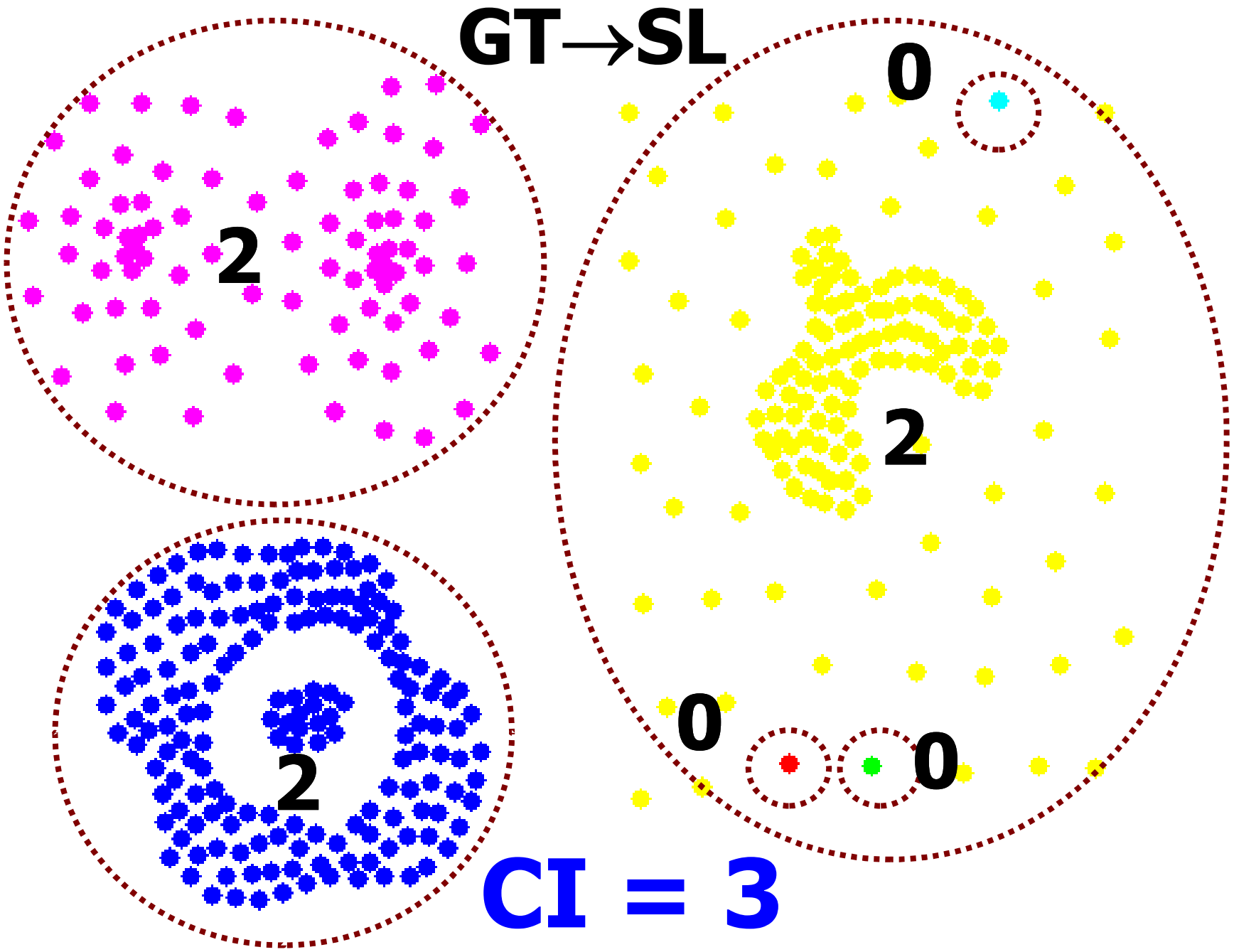


path-based2: spiral


KM→GT
2
1
1
CI = 2
0
0
2
1


GT→KM
1
0
1
1
1
CI = 1
2
1
1


SL→GT
0
1
1
3
1
0
CI = 2


GT→SL
2
0
2
2
0
0
CI = 3

Summary of experiments

prototype similarity

	RI	ARI	MI	NMI	NVD	CH	CSI	CI
Birch2								
KM	1.00	0.81	6.26	0.96	0.12	0.24	0.88	18
KM++	1.00	0.95	6.54	0.99	0.03	0.06	0.97	4
RS	1.00	1.00	6.64	1.00	0.00	0.00	1.00	0
GA	1.00	1.00	6.64	1.00	0.00	0.00	1.00	0
S1								
KM	0.98	0.82	3.57	0.93	0.09	0.17	0.83	2
KM++	1.00	1.00	3.90	0.98	0.00	0.00	1.00	0
RS	1.00	1.00	3.90	0.98	0.00	0.00	1.00	0
GA	1.00	1.00	3.90	0.98	0.00	0.00	1.00	0
S2								
KM	0.97	0.80	3.46	0.90	0.11	0.18	0.82	2
KM++	1.00	0.99	3.87	0.99	0.00	0.00	1.00	0
RS	1.00	0.99	3.87	0.99	0.00	0.00	1.00	0
GA	1.00	0.99	3.87	0.99	0.00	0.00	1.00	0

Summary of experiments

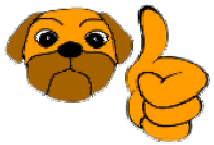
partition similarity

	RI	ARI	MI	NMI	NVD	CH	CSI	CI
Unbalanced								
KM	0.92	0.79	1.85	0.81	0.14	0.29	0.86	4
KM++	1.00	1.00	2.03	1.00	0.00	0.00	1.00	0
RS	1.00	1.00	2.03	1.00	0.00	0.00	1.00	0
GA	1.00	1.00	2.03	1.00	0.00	0.00	1.00	0
SL	1.00	0.99	1.91	0.97	0.02	0.05	0.98	3
DBSCAN	1.00	1.00	2.02	0.99	0.00	0.00	1.00	0
SAM	0.93	0.81	1.85	0.82	0.12	0.25	0.88	4
Aggregate								
KM	0.91	0.71	2.16	0.84	0.14	0.24	0.86	2
SL	0.93	0.80	1.96	0.88	0.09	0.18	0.91	2
DBSCAN	0.99	0.98	2.41	0.98	0.01	0.01	0.99	0
SAM	1.00	1.00	2.45	1.00	0.00	0.00	1.00	0
Compound								
KM	0.84	0.54	1.71	0.72	0.25	0.34	0.75	2
SL	0.89	0.74	1.54	0.80	0.13	0.26	0.87	3
DBSCAN	0.95	0.88	1.90	0.87	0.10	0.12	0.90	2
SAM	0.83	0.53	1.78	0.76	0.19	0.34	0.81	2

Conclusions

- Simple is cluster level measure
- Generalized to GMM and arbitrary-shaped data
- Value has clear interpretation:

CI=0 **CI>0**



Correct

Number of wrong clusters