Supplement 1:

Divisive hierarchical maximum likelihood clustering

Illustration using 4 cluster case

Synthetic data topology

4 cluster case

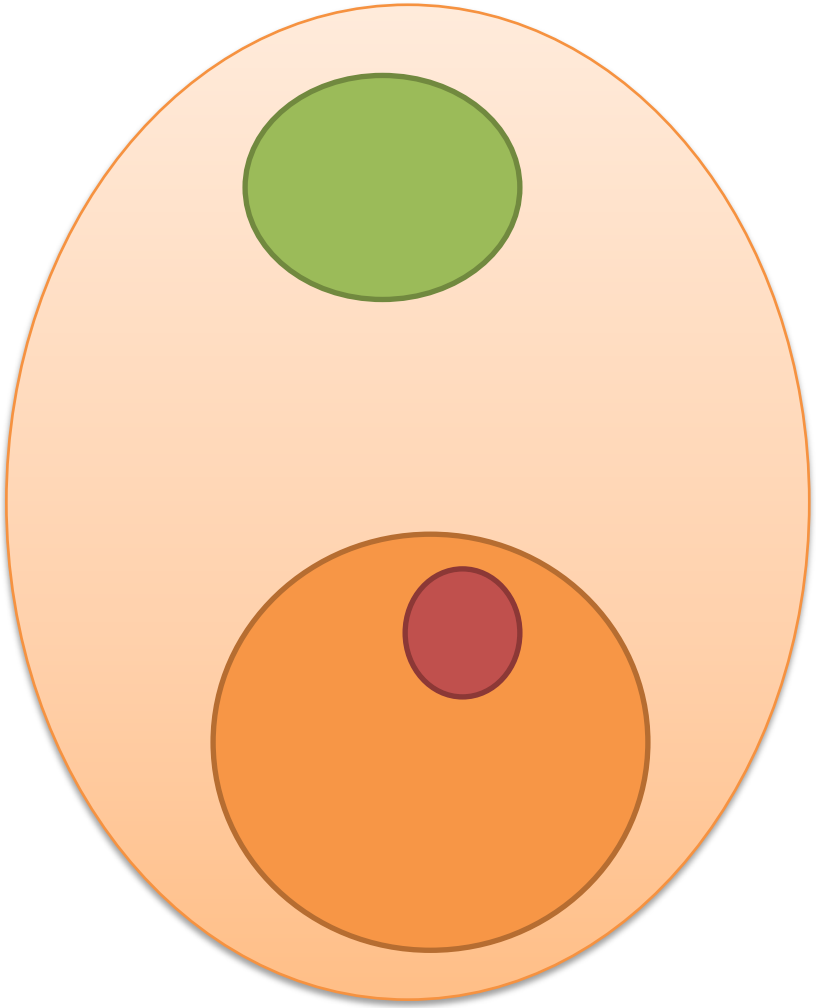
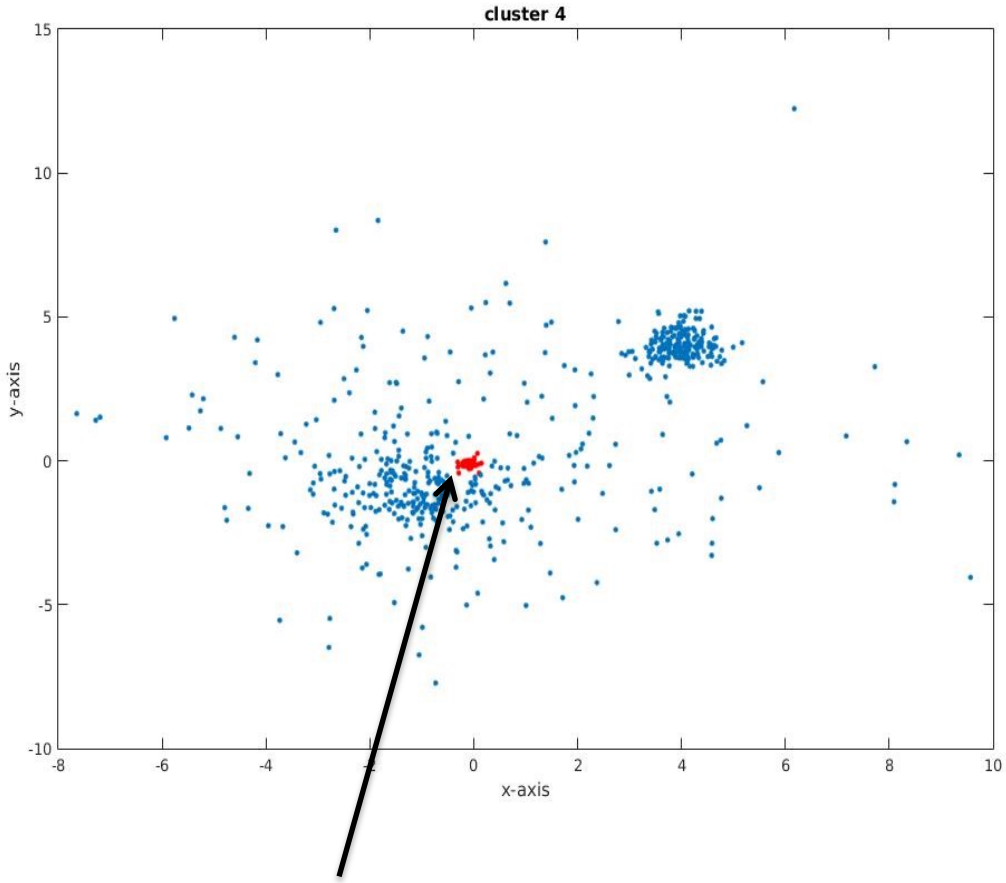


Fig. S1a

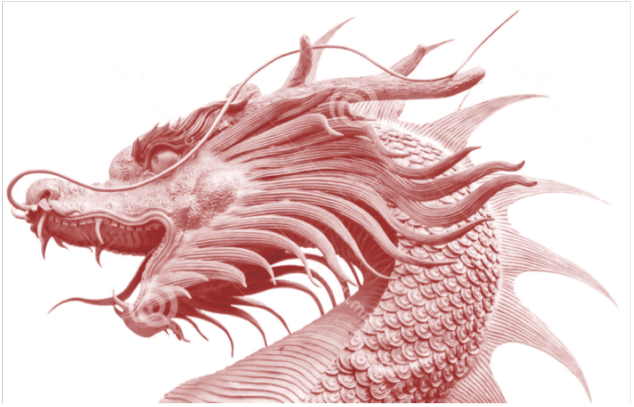
Description in 2D-plane

Determine location (mean μ)



Densest cluster

Fig. S1b



Dragon method: an illustration

- Two steps
  1. Finding location.
  2. Tuning cluster.

STEP 1: Finding Location

Take out only 1 sample at a time such that Likelihood is increased

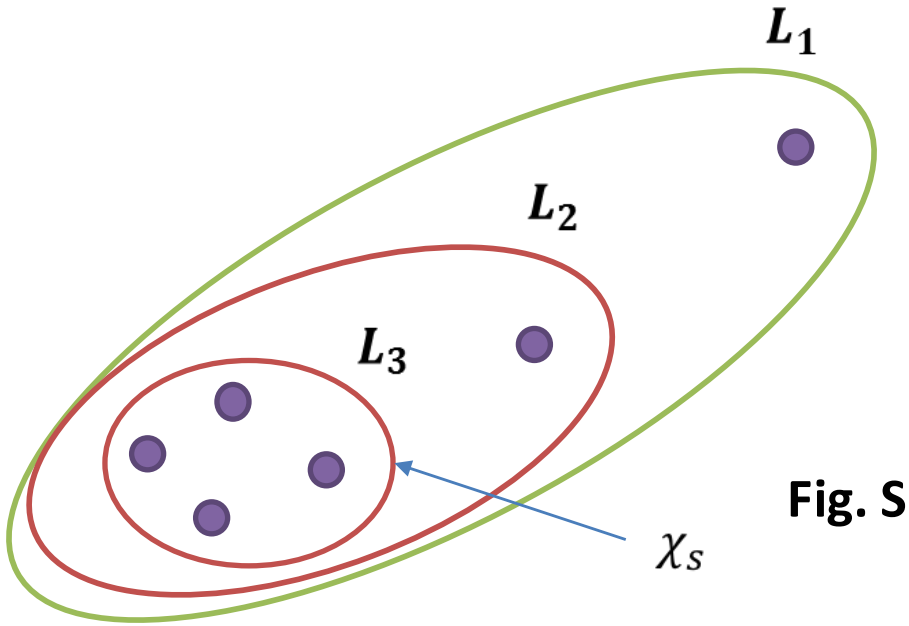


Fig. S2

Maximize distance P

$$\hat{x} = \arg\max_{x \in \not{x}} P \qquad (1)$$

where $P = (x - \mu)^T \Sigma^{-1} (x - \mu)$ (2)

Remove $\hat{x} \in \not{x}$ such that $L^* > L$ (i.e., new L > old L)

This procedure gives a cluster χ_s

Step 2: Tuning cluster

- From the mean of χ_s, find distance (or dot product) to all the samples.
- Perform k-means in this inner product space.

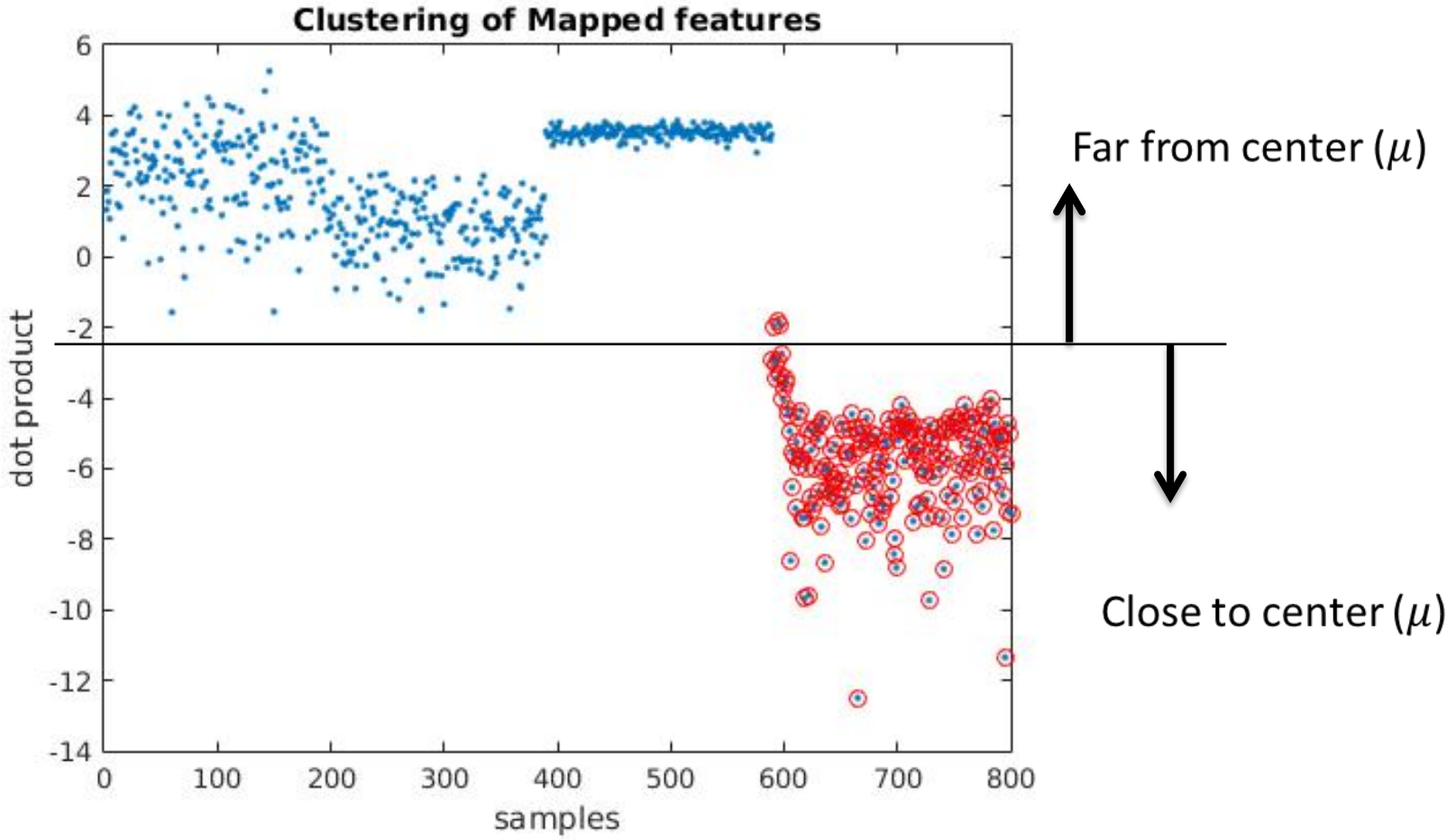


Fig. S3

- Conducting the same 2-step procedure to all the remaining clusters one-by-one (assuming 4-clusters), we get Fig. S4.

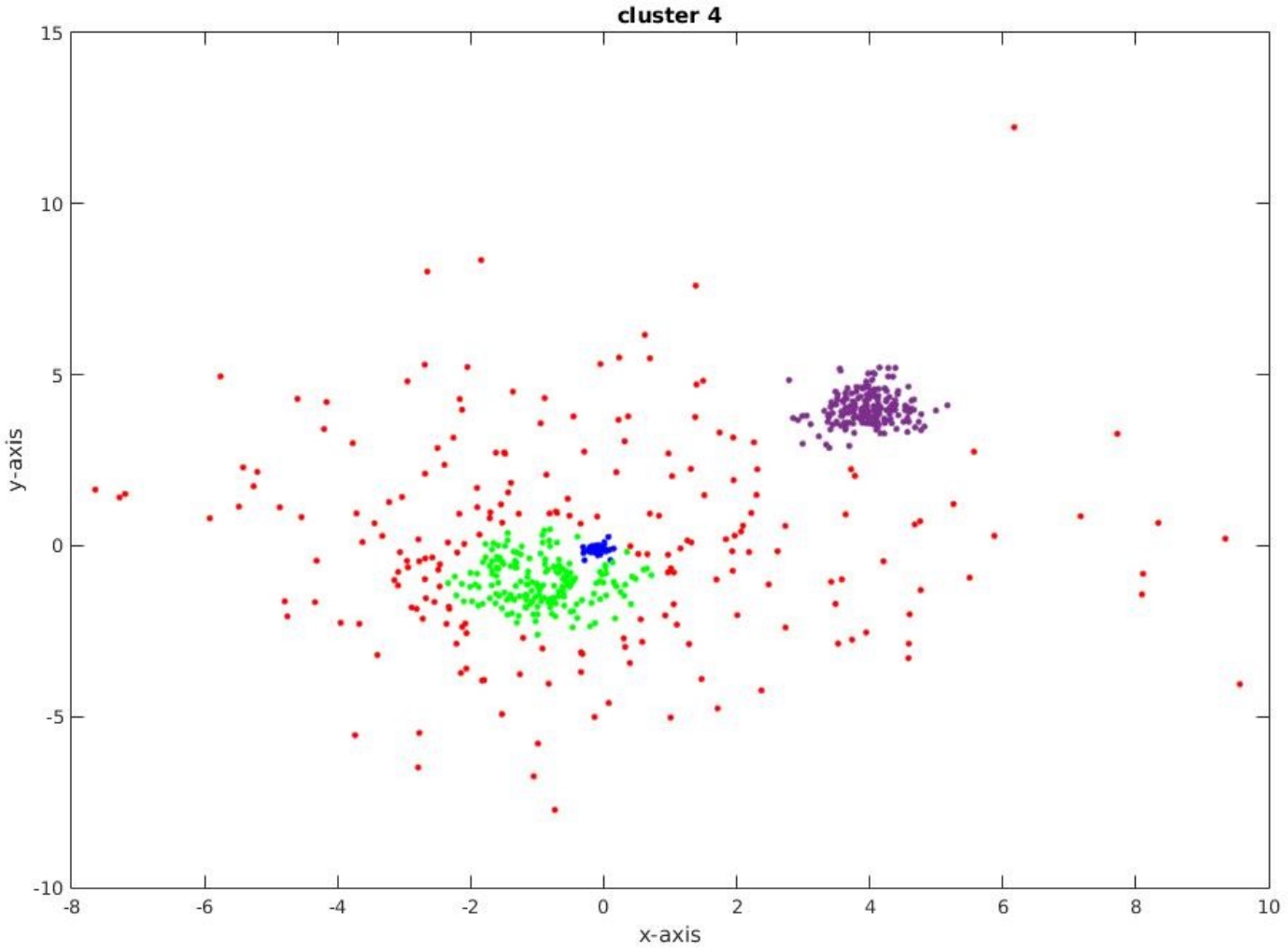


Fig. S4

Ltot and δLtot plots

(to identify number of clusters)

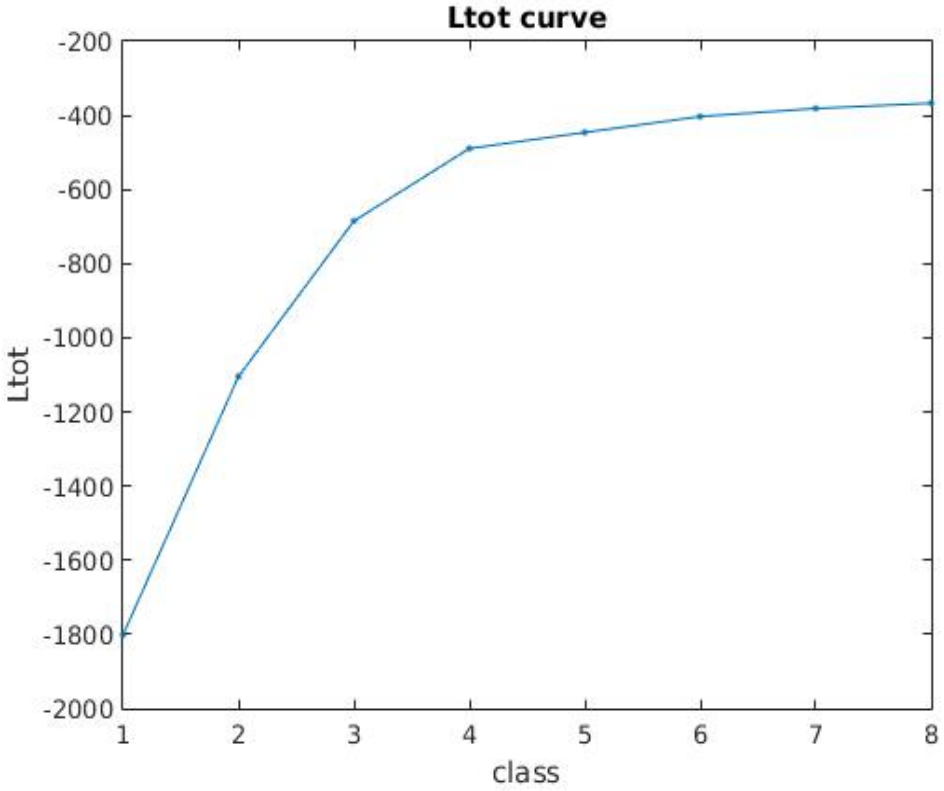


Fig. S5a

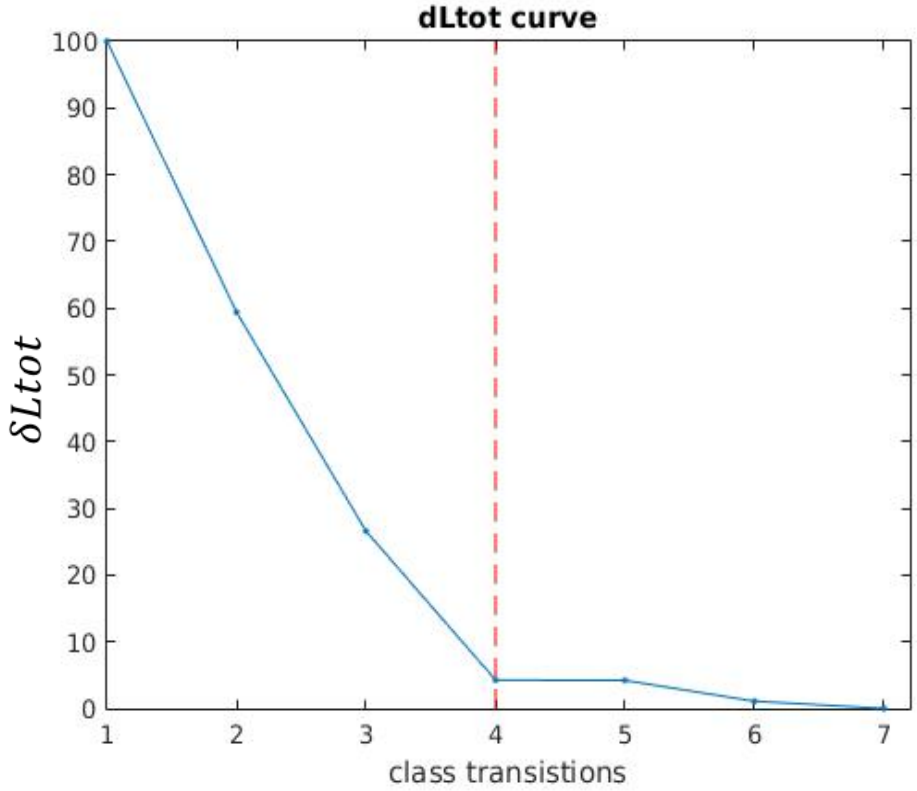


Fig. S5b

Computation of $\delta Ltot$ curve

$\delta Ltot \leftarrow diff(Ltot)$

$\delta Ltot \leftarrow \delta Ltot - \min(\delta Ltot)$

$\delta Ltot \leftarrow \frac{\delta Ltot}{\max(\delta Ltot)}$ (to have a ranged between [0,1] or [0,100] if mult. By 100)

Synthetic data: Flame

Flame data was provided by Fu and Medico, 2007

Table S1.1

Methods	Rand Score
SLINK	0.54
CLINK	0.50
ALINK	0.72
Wa-LINK	0.60
Wt-LINK	0.70
MLINK	0.68
SLINK (Div)	0.54
CLINK (Div)	0.50
ALINK (Div)	0.54
Dunn's original (Div)	0.54
Dunn's variant (Div)	0.50
Macnaughton-Smith et al. (Div)	0.51
Principal Direction (Div)	0.56
Kmeans	0.73
DRAGON	0.95

Flame: N=240, nClusters=2, nDimensions=2: L. Fu and E. Medico, FLAME, a novel fuzzy clustering method for the analysis of DNA microarray data. *BMC bioinformatics*, 2007. 8(1): p. 3.

Synthetic data: Pathbased

Pathbased data was provided by Chang and Yeung, 2008

Table S1.2

Methods	Rand Score
SLINK	0.34
CLINK	0.69
ALINK	0.74
Wa-LINK	0.76
Wt-LINK	0.71
MLINK	0.75
SLINK (Div)	0.34
CLINK (Div)	0.63
ALINK (Div)	0.73
Dunn's original (Div)	0.72
Dunn's variant (Div)	0.70
Macnaughton-Smith et al. (Div)	0.72
Principal Direction (Div)	0.68
Kmeans	0.75
DRAGON	0.93

Pathbased: N=300, nClusters=3, nDimensions=2: H. Chang and D.Y. Yeung, Robust path-based spectral clustering. *Pattern Recognition*, 2008. 41(1): p. 191-203.

Synthetic data: Aggregation

Aggregation data was provided by Gionis et al., 2007

Table S1.3

Methods	Rand Score
SLINK	0.93
CLINK	0.93
ALINK	1.00
Wa-LINK	0.94
Wt-LINK	0.92
MLINK	0.98
SLINK (Div)	0.75
CLINK (Div)	-
ALINK (Div)	0.72
Dunn's original (Div)	0.77
Dunn's variant (Div)	0.77
Macnaughton-Smith et al. (Div)	0.83
Principal Direction (Div)	0.84
Kmeans	0.92
DRAGON	0.98

Pathbased: N=788, nClusters=7, nDimensions=2: A. Gionis, H. Mannila, and P. Tsaparas, Clustering aggregation. *ACM Transactions on Knowledge Discovery from Data (TKDD)*, 2007. 1(1): p. 1-30.