On Spectral Bipartite Clustering Algorithm and Automatic Determination of the Number of Clusters

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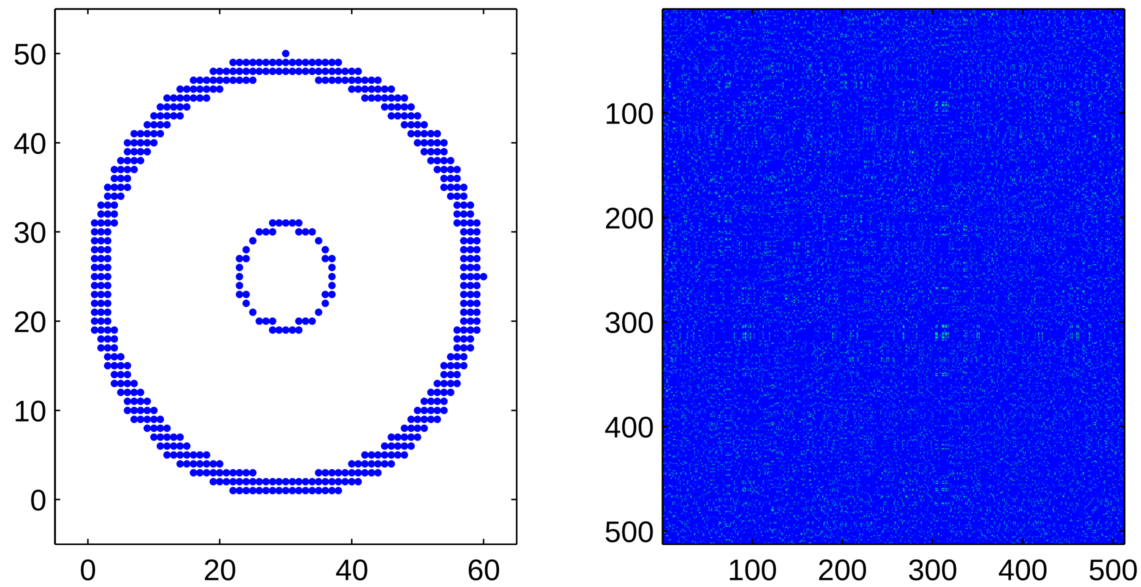
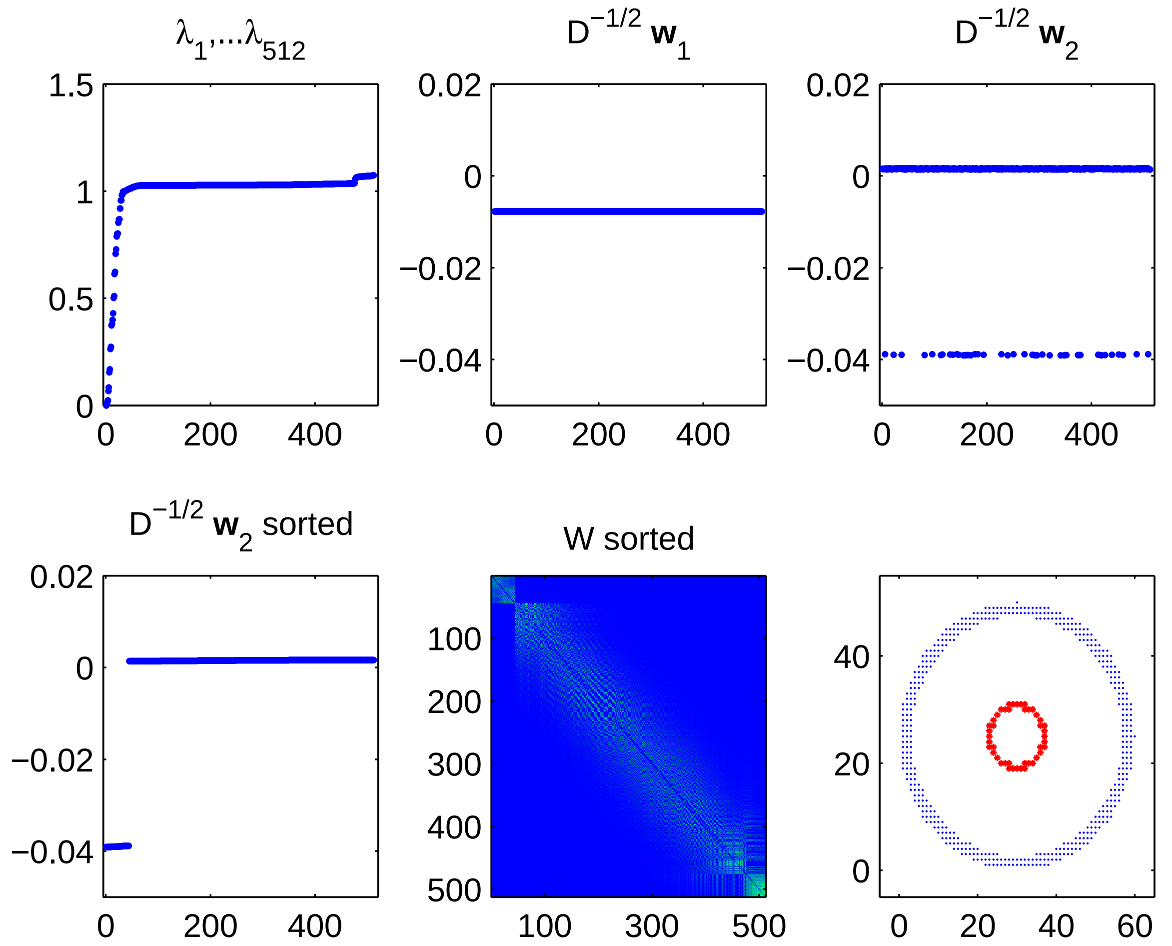
The clustering problem



Recovering the structure



Graph notation

$G = (V, E)$ is a simple, finite, undirected, weighted graph where:

$V = \{1, 2, 3, ..., n\}$ is a set of vertices and

E is a set of edges $\{i, j\}$, $i, j \in V$, with weights $w_{ij} \in \mathbb{R}^+$.

The weighted adjacency matrix of G is a $n \times n$ matrix

$$W = [w_{ij}].$$

$w_{ij} = 0$ means vertices i and j are not connected by an edge.

Graph cut

Let $V_1, V_2 \subset V$, $V_1, V_2 \neq \emptyset$. We define

$$\mathrm{cut}(V_1, V_2) = \sum_{i \in V_1, j \in V_2} w_{ij},$$

$$d_i = \sum_{j=1}^{n} w_{ij},$$

$$\mathrm{vol}(V_l) = \sum_{i \in V_l} d_i = \sum_{i \in V_l} \sum_{j \in V} w_{ij} = \mathrm{cut}(V_l, V \setminus V_l) + \mathrm{within}(V_l).$$

Partitioning functions

Let $\pi = \{V_1, V_2\}$ be the partition of V.

Ratio cut*

$$R(V_1, V_2) = \frac{\operatorname{cut}(V_1, V_2)}{|V_1|} + \frac{\operatorname{cut}(V_1, V_2)}{|V_2|}$$

favors partitions into sets with equal number of vertices.

Normalized cut**

$$N(V_1, V_2) = \frac{\operatorname{cut}(V_1, V_2)}{\operatorname{vol}(V_1)} + \frac{\operatorname{cut}(V_1, V_2)}{\operatorname{vol}(V_2)}$$

favors partitions into sets with equal weights of edges within subsets.

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* Hagen and Kahng, 1992
** Shi and Malik, 2000

Graph Laplacian

$L = [l_{ij}]$ is a real $n \times n$ matrix, s.t.

$$l_{ij} = \begin{cases} \sum_{k=1}^{n} w_{ik} & , \quad i = j \\ -w_{ij} & , \quad i \neq j \end{cases}.$$

The matrix L satisfies the following properties:

- → $L = D - W$, where D is a degree matrix (diagonal matrix with degrees $d_1, d_2, \cdots, d_n$ on its diagonal);
- → L is symmetric and positive semi-definite;
- → $L\mathbf{1} = 0$ for $\mathbf{1} = [1, ..., 1]^T$;
- → The multiplicity k of the eigenvalue 0 equals the number of connected components in the graph;
- → L has n real-valued eigenvalues $0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$.

Normalized graph Laplacian

$L_n = [l_{n_{ij}}]$ is a $n \times n$ matrix, s.t.

$$(l_n)_{ij} = \begin{cases} 1 \quad , & i = j \\ -\frac{w_{ij}}{\sqrt{d_i}\sqrt{d_j}} \quad , & i \neq j \end{cases}.$$

In other words,

$$L_n = D^{-1/2}(D - W)D^{-1/2}.$$

L_n is symmetric and positive semi-definite matrix with the smallest eigenvalue 0 and corresponding eigenvector $D^{\frac{1}{2}}\mathbf{1}$.

Relaxation of the discrete problem

The partition $\pi = \{V_1, V_2\}$ of V is determined by a vector $\mathbf{y}$ s.t.

$$y_i = \begin{cases} \frac{1}{2} & \text{za } i \in V_1 \\ -\frac{1}{2} & \text{za } i \in V_2 \end{cases}$$

The Ratio cut problem:

$$\min_{\substack{y_i \in \{-\frac{1}{2}, \frac{1}{2}\} \\ |\mathbf{y}^T \mathbf{1}| \leq \beta}} \frac{1}{2} \sum_{i,j} \left(y_i - y_j\right)^2 w_{ij}$$

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The Theorem

Theorem 1 *Let $A \in \mathbb{R}^{n\times n}$ be a symmetric matrix with eigenvalues $\lambda_1 < \lambda_2 < \lambda_3 \leq \cdots \leq \lambda_n$ and eigenvectors $\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_n$. For a fixed $0 \leq \alpha < 1$, the problem*

$$\min_{\substack{\mathbf{y}\in\mathbb{R}^n \\ |\mathbf{y}^T\mathbf{v}^{[1]}|\leq\alpha \\ \mathbf{y}^T\mathbf{y}=1}} \mathbf{y}^T A \mathbf{y}$$

has the solution $y = \pm\alpha\mathbf{v}_1 \pm \sqrt{1-\alpha^2}\mathbf{v}_2$.

The solution (1)

Corollary 1 *For* $0 \leq \beta < \frac{n}{2}$ *the relaxed Ratio Cut problem*

$$\min_{\substack{y \in \mathbb{R}^n \\ |\mathbf{y}^T \mathbf{1}| \leq \frac{2\beta}{\sqrt{n}} \\ \mathbf{y}^T \mathbf{y} = 1}} \mathbf{y}^T L \mathbf{y}$$

has the solution

$$\mathbf{y} = \pm \frac{2\beta}{\sqrt{n}} \mathbf{1} \pm \sqrt{1 - 4\frac{\beta^2}{n^2}} \mathbf{v}_2.$$

$\mathbf{v}_2$ is the Fiedler vector of the Laplacian L.

The solution (2)

Corollary 2 *For* $0 \leq \beta < \sqrt{\theta n} \left\| D^{\frac{1}{2}} \mathbf{1} \right\|_2$ *the relaxed normalized cut problem*

$$\min_{\substack{y \in \mathbb{R}^n \\ |\mathbf{y}^T D \mathbf{1}| \leq \frac{\beta}{\sqrt{\theta n}} \\ \mathbf{y}^T D \mathbf{y} = 1}} \quad \mathbf{y}^T L \mathbf{y}$$

has the solution

$$\mathbf{y} = \pm \frac{\beta}{\sqrt{\theta n} \left\| D^{\frac{1}{2}} \mathbf{1} \right\|_2^2} \mathbf{1} \pm \sqrt{1 - \frac{\beta^2}{\theta n \left\| D^{\frac{1}{2}} \mathbf{1} \right\|_2^2}} D^{-\frac{1}{2}} \mathbf{w}_2,$$

$D^{-\frac{1}{2}} \mathbf{w}_2$ is the normalized Fiedler vector (of the normalized Laplacian).

Constructing the partition

According to the definition, the sets V_1 and V_2 are determined by

$$V_1 = \{i : \mathbf{v}_2(i) < 0\}, \quad V_2 = \{i : \mathbf{v}_2(i) \geq 0\},$$

for the Ratio Cut, and

$$V_1 = \{i : D^{-\frac{1}{2}}\mathbf{w}_2(i) < 0\}, \quad V_2 = \{i : D^{-\frac{1}{2}}\mathbf{w}_2(i) \geq 0\}$$

for the Normalized Cut.

Recursive bipartitioning - the algorithm

Input: Adjacency matrix W, number of clusters k to construct.
Output: Cluster indicator vector $\mathbf{y}$.

1. Bipartition V. Set counter $k_c = 2$.
2. **If** $k_c < k$ **then**
3. For each subset of V compute the optimal bipartition.
4. Within all $(k_c + 1)$-partitions, choose the one with the smallest value of the partitioning function.
5. Set $k_c = k_c + 1$ and proceed recursively with step 2.
6. Stop.

Bipartite graph

Undirected bipartite graph G is a triplet $G = (T, D, E)$.
$T = \{t_1, \cdots, t_m\}$ and $D = \{d_1, ..., d_n\}$ are two sets of vertices and

$$E = \{\{t_i, d_j\} : t_i \in T, d_j \in D\}$$

is a set of edges.

For example, D is a set of documents, T is a set of terms and edge $\{t_i, d_j\}$ exists if document d_j contains term t_i.

The adjacency matrix has the form

$$W = \begin{bmatrix} 0 & A \\ A^T & 0 \end{bmatrix},$$

where A is the *term* × *document* matrix.

Connection to SVD*

Let

$$D = \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix}, \quad L = \begin{bmatrix} D_1 & -A \\ -A^T & D_2 \end{bmatrix}.$$

Then

$$L_n = D^{-\frac{1}{2}} \begin{bmatrix} D_1 & -A \\ -A^T & D_2 \end{bmatrix} D^{-\frac{1}{2}} = \begin{bmatrix} I & -D_1^{-\frac{1}{2}} A D_2^{-\frac{1}{2}} \\ -D_2^{-\frac{1}{2}} A D_1^{-\frac{1}{2}} & I \end{bmatrix}.$$

*Inderjit Dhillon, 2001

Connection to SVD (2)

Let

$$\mathbf{w} = \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix}, \quad \mathbf{u} \in \mathbb{R}^m, \quad \mathbf{v} \in \mathbb{R}^n,$$

be an eigenvector of the <u>normalized</u> Laplacian,

$$D^{-\frac{1}{2}} L D^{-\frac{1}{2}} \mathbf{w} = \lambda \mathbf{w}.$$

Then

$$\begin{aligned} D_1^{-\frac{1}{2}} A D_2^{-\frac{1}{2}} \mathbf{v} &= (1-\lambda)\mathbf{u}, \\ D_2^{-\frac{1}{2}} A^T D_1^{-\frac{1}{2}} \mathbf{u} &= (1-\lambda)\mathbf{v}. \end{aligned}$$

Connection to SVD (3)

Instead of computing the Fiedler vector of L_n, we compute the left and right singular vector of the normalized matrix

$$A_n = D_1^{-\frac{1}{2}} A D_2^{-\frac{1}{2}}$$

which correspond to the second largest singular value,

$$A_n \mathbf{v}_2 = \sigma_2 \mathbf{u}_2,$$

where $\sigma_2 = 1 - \lambda_2$

This is more stable!

$D_1^{-\frac{1}{2}} \mathbf{u}_2$ partitions terms and $D_2^{-\frac{1}{2}} \mathbf{v}_2$ partitions documents!

Advantages and disadvantages of SC

- Does not make assumptions on the form of the clusters (k-means can recognize only convex sets);
- Possible to implement efficiently for large data sets as long as the similarity graph is sparse;
- There are no issues of getting stuck in local minima or restarting the algorithm for several times with different initializations;
- Only two singular vectors need to be calculated.

But

- The number of clusters has to be predefined;
- The choice of similarity function and its parameters can affect the results of clustering a lot;
- Cannot serve as a "black box algorithm" which automatically detects the correct clusters in any given set.

The coupling matrix

In [1] the authors introduce a spectral clustering algorithm for calculating the number of metastable states of Markov chains based on a concept of block diagonal dominance.

Definition 1 *Let* $\pi = \{V_1, \cdots, V_k\}$ *be the partition of* V. *Let* $W_{ml} = W(V_m, V_l)$, $m, l \in \{1 \cdots, k\}$, *be blocks of the corresponding block decomposition of stochastic matrix W. The coupling matrix of the decomposition is matrix* B *defined by*

$$B_{ml} = \|W_{ml}\|_{\mathbf{1}} = \frac{1}{|V_m|} \sum_{i \in V_m, j \in V_l} |w_{ij}|.$$

[1] An SVD Approach to Identifying Metastable States of Markov Chains, D. Fritzsche, V. Mehrmann, D. Szyld, E. Virnik

Identification of nearly decoupled bloks - the INDB algorithm

Input: Stochastic matrix W, treshold *thr* $(= 1 - \delta)$.

Output: Number k and sizes n_i, $i = 1, \cdots, k$, of identified blocks in W, a permutation matrix P such that PWP^T is bd-dominant.

1. Compute the second left and right singular vectors of W, $\mathbf{u}_2$ and $\mathbf{v}_2$.
2. Sort it and use the resulting permutation P to permute the matrix W.
3. Identify two potential blocks W_{11} and W_{22} by using the change in sign in $\mathbf{u}_2$ and $\mathbf{v}_2$.
4. The hight of the first (second) block is the number of negative (positive) values in $\mathbf{u}_2$, the width of the first (second) block is the number of negative (positive) values in $\mathbf{v}_2$.
5. **if** *The norm of the diagonal blocks is larger than thr* **then**
6. Separate two found blocks.
7. Proceed recursively with step 1. applied to each of the blocks.
8. **else** The current block cannot be further reduced.

Automatization

If the noise is not too large, a block diagonally dominant structure can be successfully recovered by proposed algorithm.

But, there is still a parametar *thr* to be predetermined. Variation of the idea would be to stop with recursive normalized spectral bipartitioning when the corresponding coupling matrix fails to be diagonally dominant.

Definition 2 *The matrix B is (strictly) diagonally dominant if*

$$|b_{ii}| > \sum_{j, j \neq i} |b_{ij}|$$

for all i.

Where to stop?

In examples with very small between-cluster similarity we needed even stronger criteria - we stopped when the matrix failed to satisfy

$$|b_{ii}| > \sum_{\substack{j,k \\ j \neq k}} |b_{jk}|.$$

We also observed diagonal dominance of the scaled coupling matrices

$$B_r = D^{-1}B,$$

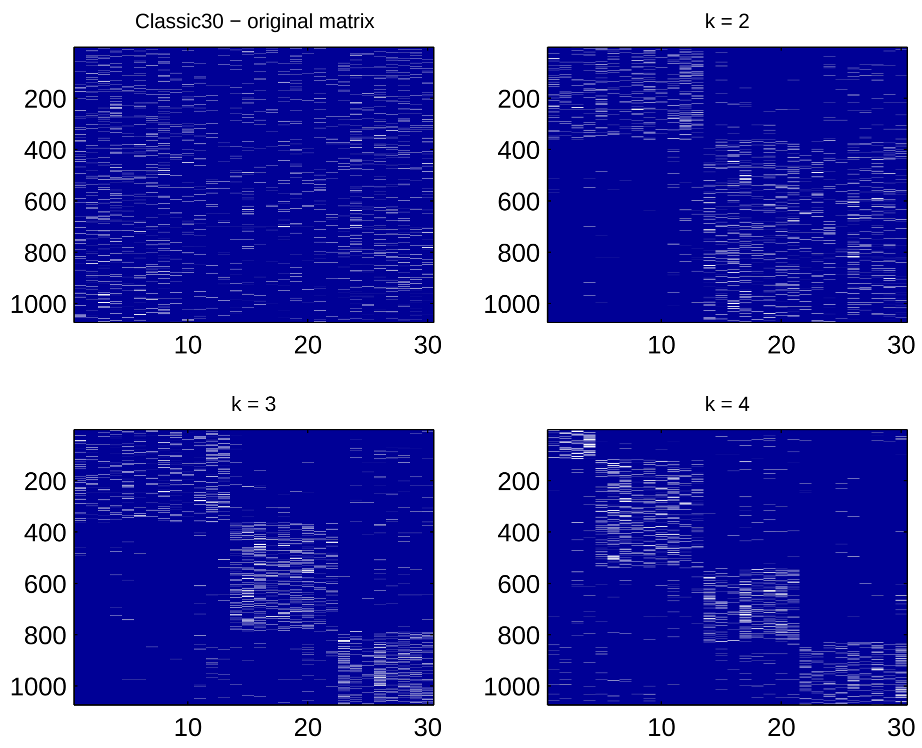
$$B_c = BD^{-1},$$

$$B_a = D^{-1/2}BD^{-1/2},$$

where $D = \operatorname{diag} B$.

Example - full matrices

The *Classic** collection of abstracts (Medline - 1033 medical abstracts, Cranfield - 1400 aeronautical systems abstracts and Cisi - 1460 information retrieval abstracts) is naturally divided in three clusters. The data is clustered by the recursive normalized spectral clustering algorithm for $k = 2$, $k = 3$ and $k = 4$.



Example - full matrices (2)

In the following table we give a number of clusters found by different criteria:

	B		B_{scal} (dds)			B (thr)				
	dd	dds	r	c	a	0.5	0.6	0.7	0.8	0.9
$Classic30$ (1073×30)	18	3	5	5	5	21	21	21	17	2
$Classic150$ (3652×150)	10	3	4	4	4	105	103	73	5	1
$Classic300$ (5577×300)	7	3	3	3	3	200	98	29	1	1
$Random4$ (770×795)	7	4	4	4	4	6	4	3	3	1
$Random8$ (930×880)	10	8	8	8	8	8	6	6	5	2
$Mat1$ (3213×146)	6	1	1	3	2	2	1	1	1	1

dd - diagonal dominance

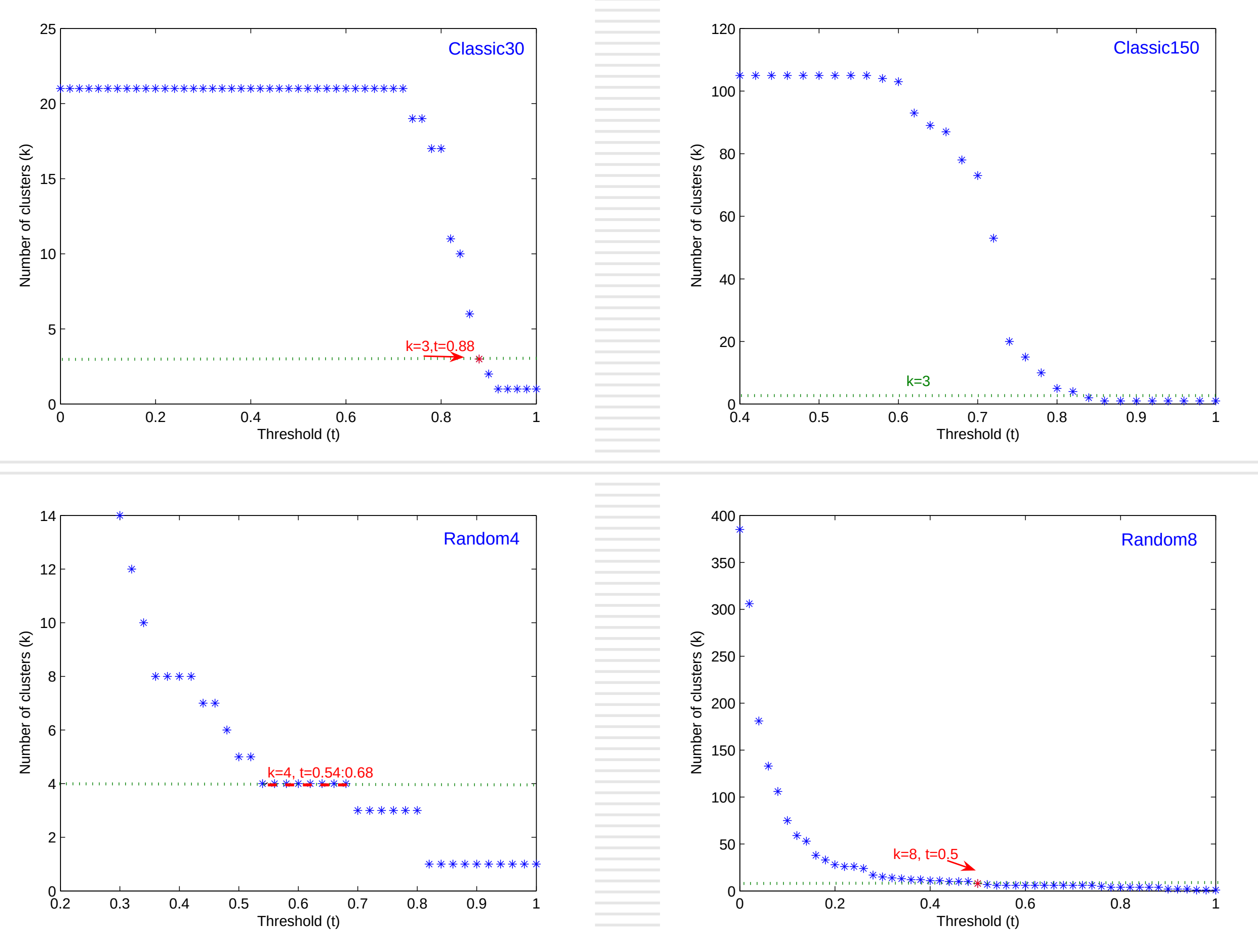
dds - diagonal dominance (stronger criteria)

B_{scal} - scaled matrix (r - row, c - column, a - all)

thr - threshold as a measure of diagonal dominance (INDB algorithm)

Example - full matrices(3)

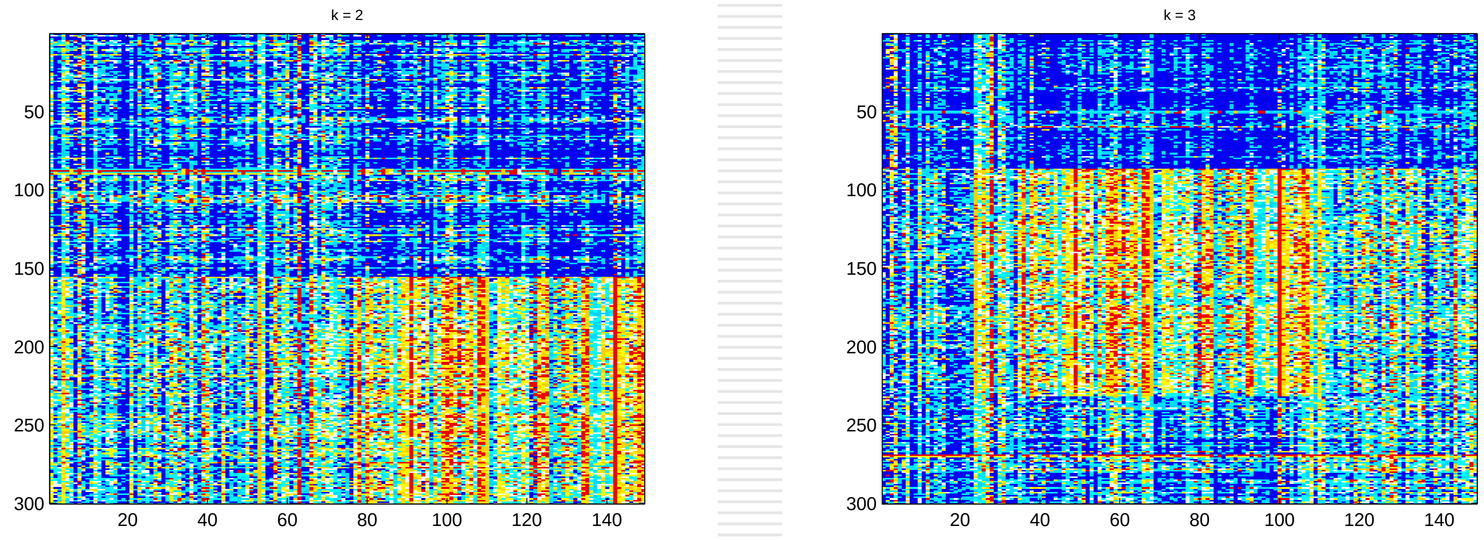
Number of clusters as a result of different thresholds.



Example Imaginable

An example* of 300 words graded by 149 people on how imaginable these words are. Grades are scaled from 1 to 7.

The data is clustered by the recursive normalized spectral clustering algorithm for $k = 2$ and $k = 3$.



* The data was provided by Fekete Istvan, BME, Department of Cognitive Science

Example Imaginable (2)

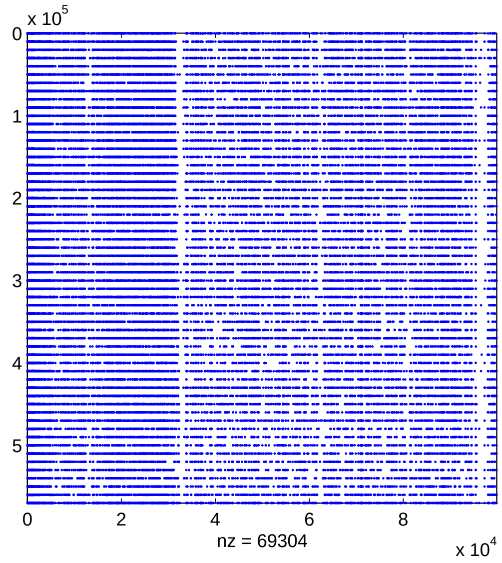
The result of 3-clustering (representative words):

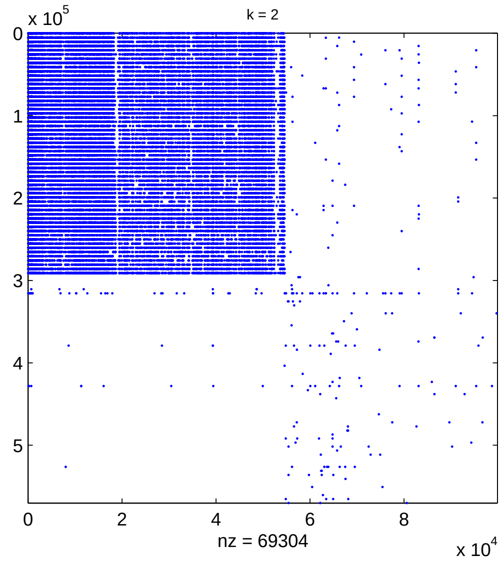
cluster 1 (146)	**cluster 2** (69)	**cluster 3** (85)
coffee	*dance*	*faith*
apple	*dream*	*fate*
table	*cinema*	*love*
dog	*clothes*	*hope*
computer	*congressman*	*freedom*
bird	*coastline*	*time*
honey	*night*	*responsibility*
tea	*decrease*	*beauty*
book	*proposal*	*friendship*
bed	*line*	*culture*
⋮	⋮	⋮

	B		B_{scal} (dds)			B (thr)			
	dd	dds	r	c	a	0.1	0.2	0.3	0.6
$Imaginable(300 \times 149)$	2	1	1	1	1	9	5	2	1

Example - sparse matrix

Matrix (570166×99899) represents big store receipts registered during one month.





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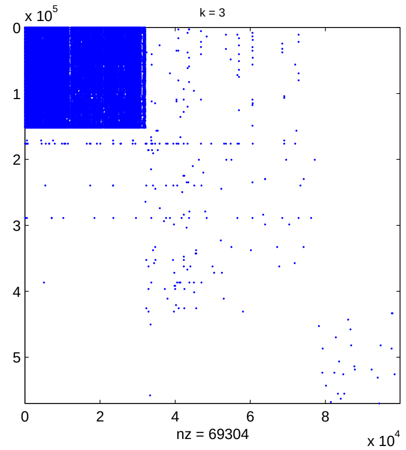

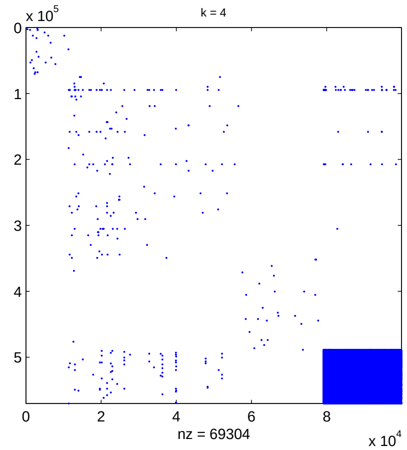

	B		$B_{scal}\ (dds)$			$B(thr)$	
	dd	dds	r	c	a	0.01	0.005
(570166×99899)	> 8	3	> 8	> 8	> 8	1	1

Conclusion

- Clustering according to normalized singular vectors of normalized similarity matrix outperforms the unnormalized version of spectral clustering.
- It can be hard to predict the treshold value in INDB algorithm that will result with good number of clusters.
- Diagonal dominance as a stoping criteria in recursive normalised spectral clustering works if the perturbation is not too large.
- In examples with very small between-cluster similarity we needed stronger criteria.
- Scaling the coupling matrix showed no effect on determination of the number of clusters.