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

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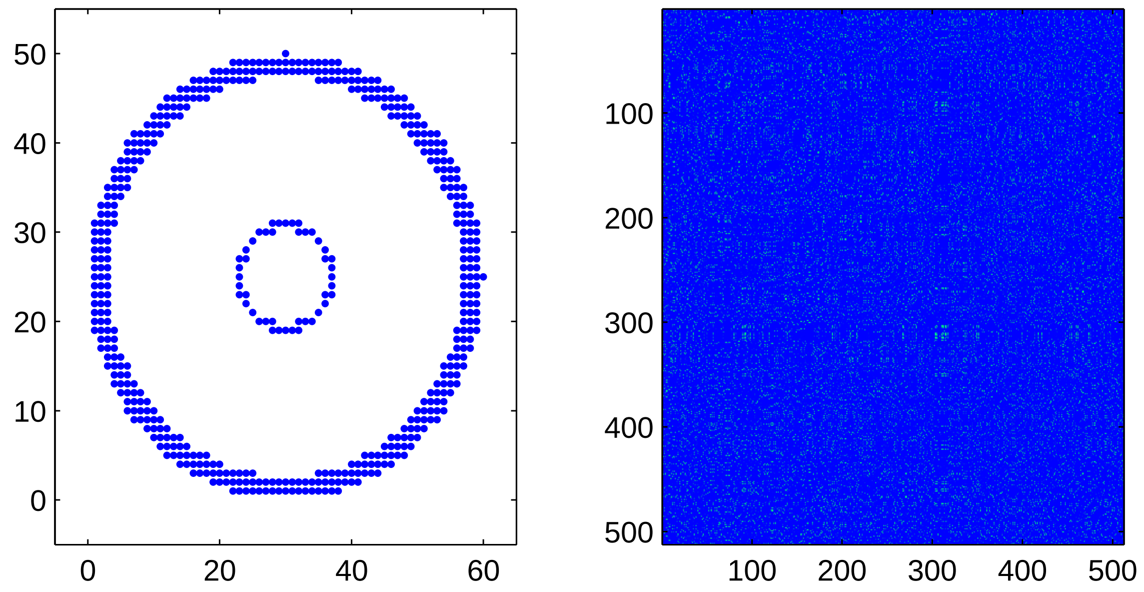
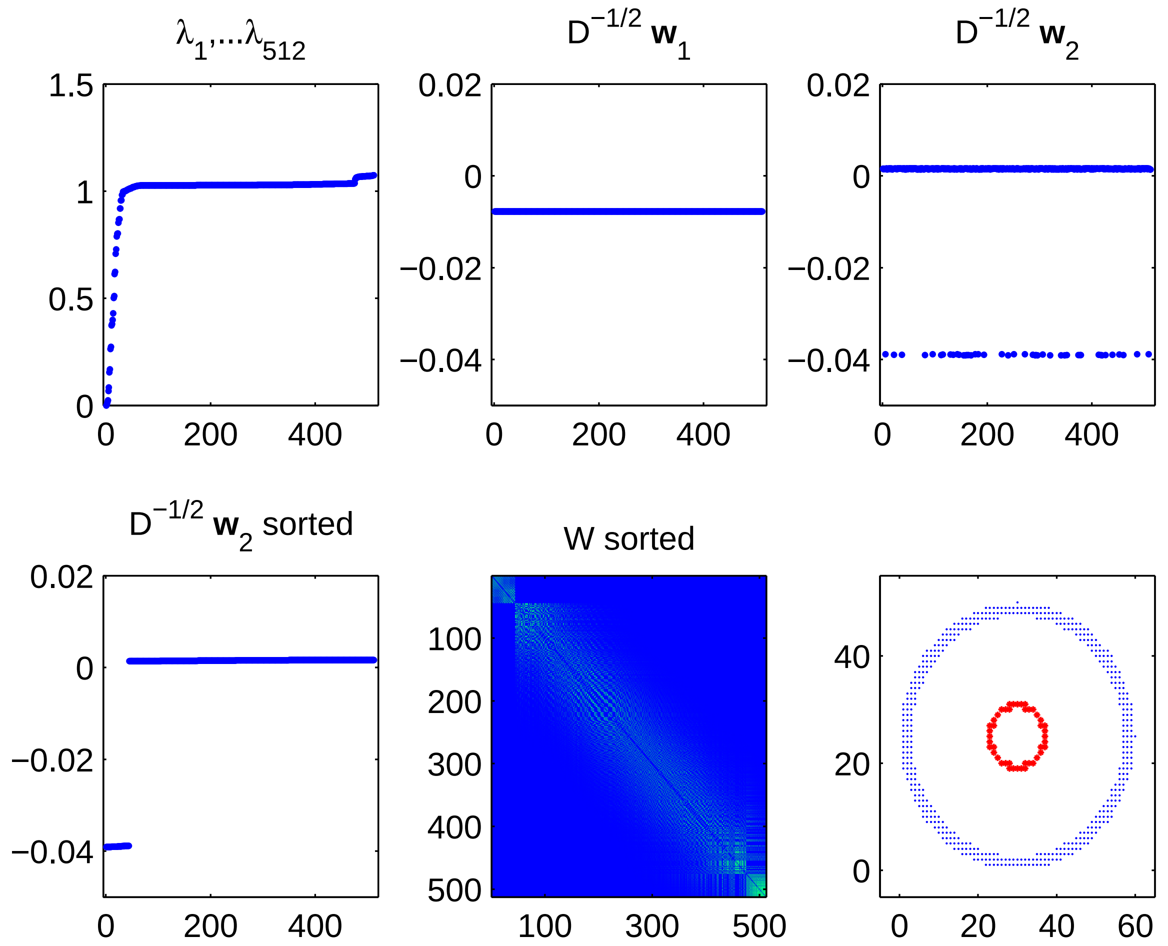
# The clustering problem





# 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*

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

favors partitions into sets with equal number of vertices.

Normalized cut**

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

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 $\quad 0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$.

# 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:

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

The Normalized cut problem:

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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*

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

*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* $\times$ *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 normalized 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

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

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

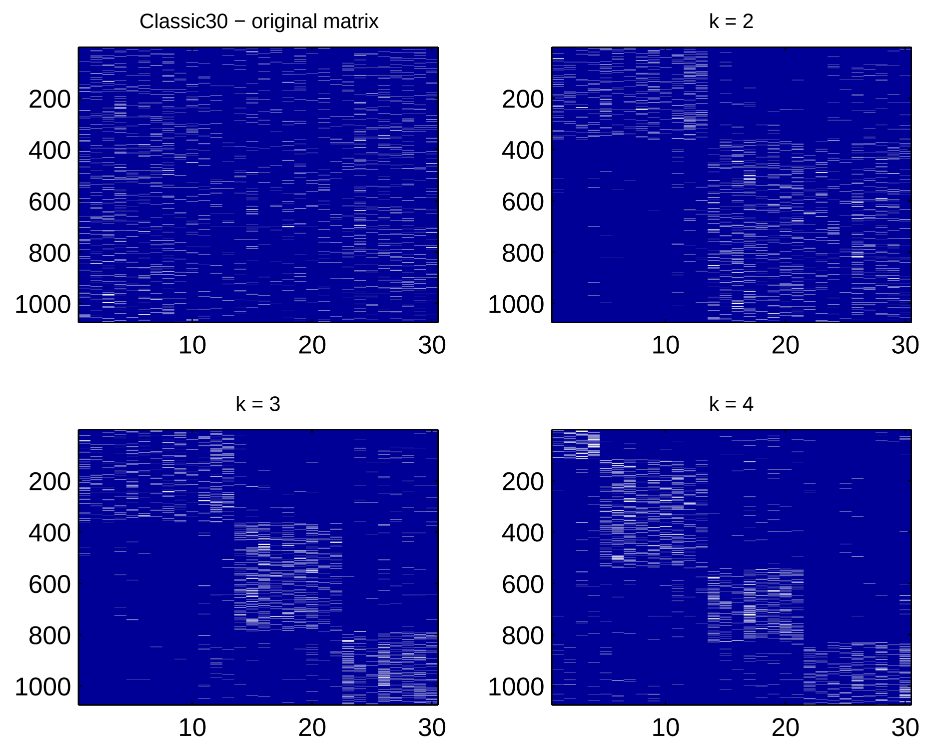
$$B_a = D^{-1/2}BD^{-1/2},$$

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 |
| $Classic30$ $(1073 \times 30)$ | 18 | $\boxed{3}$ | 5 | 5 | 5 | 21 | 21 | 21 | 17 | 2 |
| $Classic150$ $(3652 \times 150)$ | 10 | $\boxed{3}$ | 4 | 4 | 4 | 105 | 103 | 73 | 5 | 1 |
| $Classic300$ $(5577 \times 300)$ | 7 | $\boxed{3}$ | $\boxed{3}$ | $\boxed{3}$ | $\boxed{3}$ | 200 | 98 | 29 | 1 | 1 |
| $Random4$ $(770 \times 795)$ | 7 | $\boxed{4}$ | $\boxed{4}$ | $\boxed{4}$ | $\boxed{4}$ | 6 | $\boxed{4}$ | 3 | 3 | 1 |
| $Random8$ $(930 \times 880)$ | 10 | $\boxed{8}$ | $\boxed{8}$ | $\boxed{8}$ | $\boxed{8}$ | $\boxed{8}$ | 6 | 6 | 5 | 2 |
| $Mat1$ $(3213 \times 146)$ | $\boxed{6}$ | 1 | 1 | 3 | 2 | 2 | 1 | 1 | 1 | 1 |

dd - diagonal dominance

dds - diagonal dominance (stronger criteria)

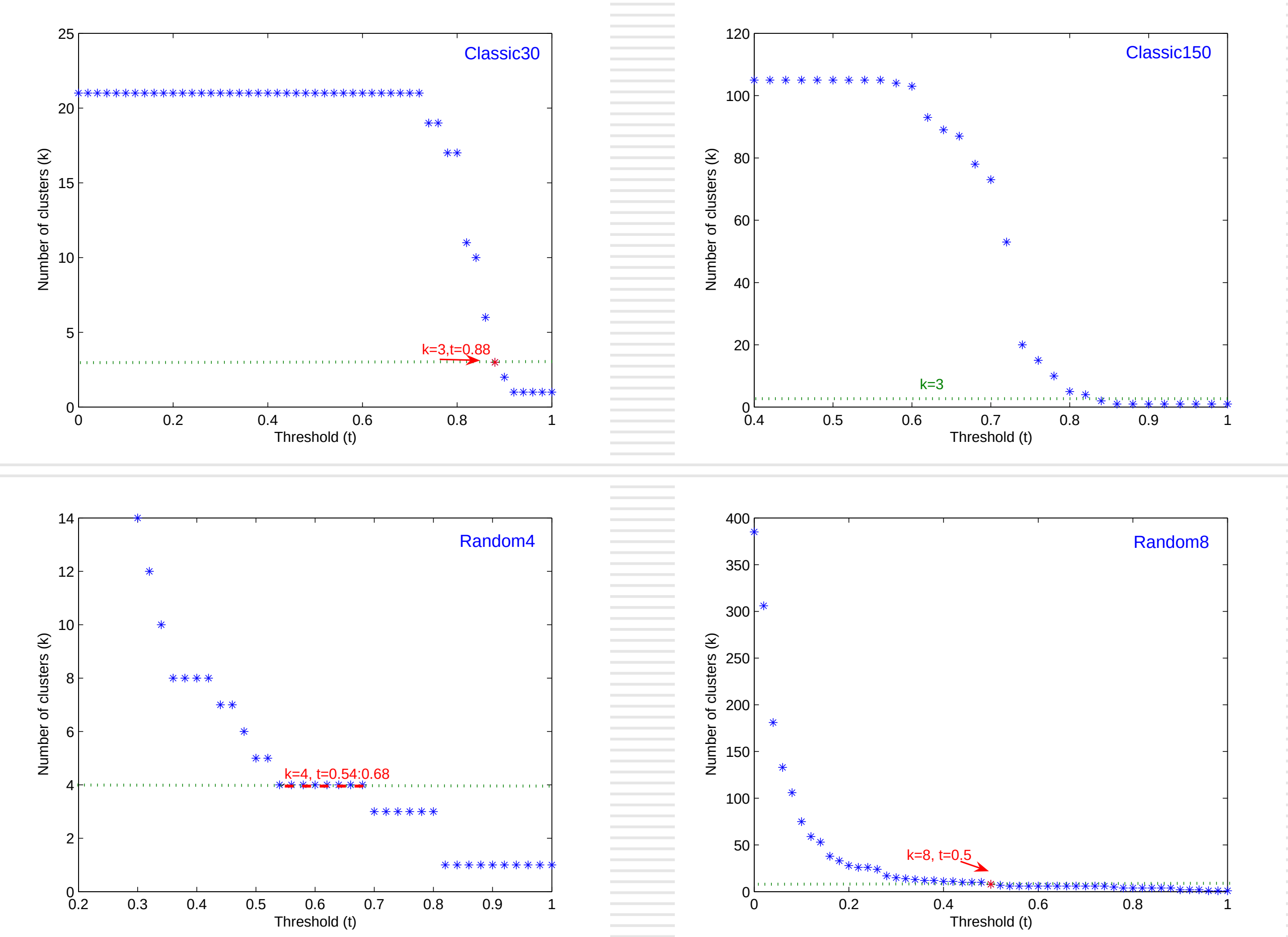
$B_{scal}$ - scaled matrix (r - row, c - column, a - all)

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

# Example - full matrices(3)



Number of clusters as a result of different thresholds.

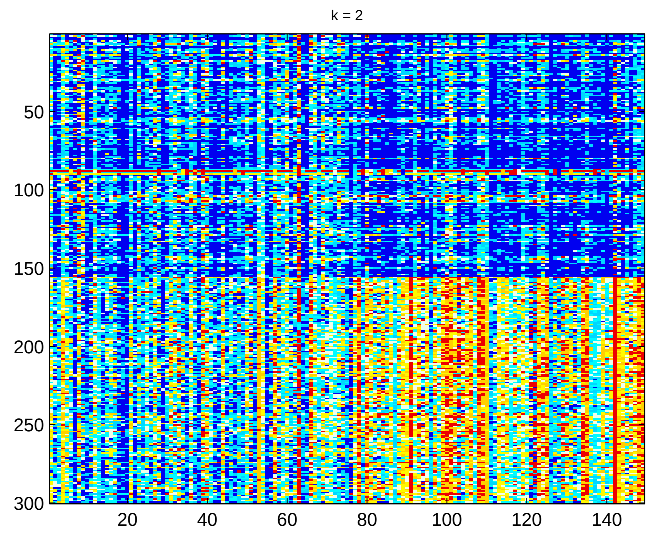


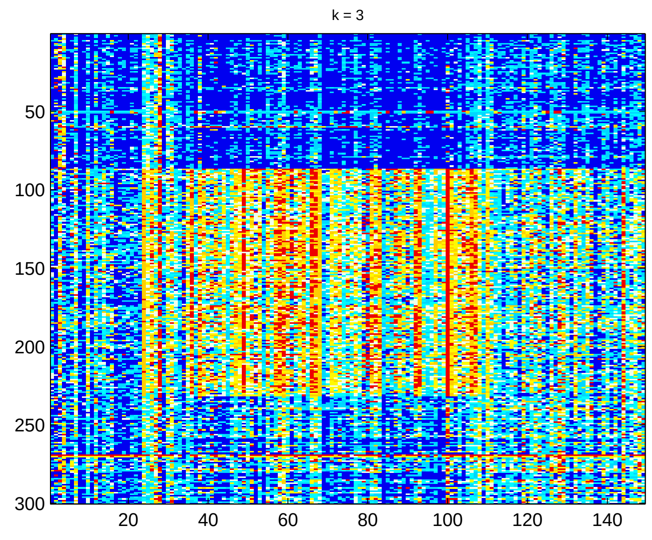
# Example Imaginable



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):

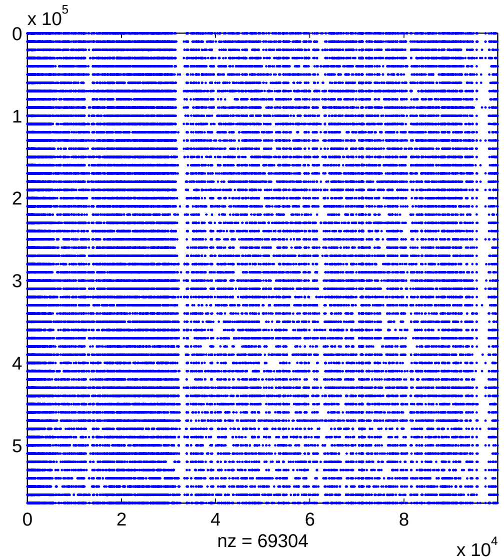
| **cluster 1** (146) | **cluster 2** (69) | **cluster 3** (85) |
|---|---|---|
| *coffee* | *dance* | *faith* |
| *apple* | *dream* | *fate* |
| *table* | *cinema* | *love* |
| *dog* | *clothes* | *hope* |
| *computer* | *congressman* | *freedom* |
| *bird* | *coastline* | *time* |
| *honey* | *night*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

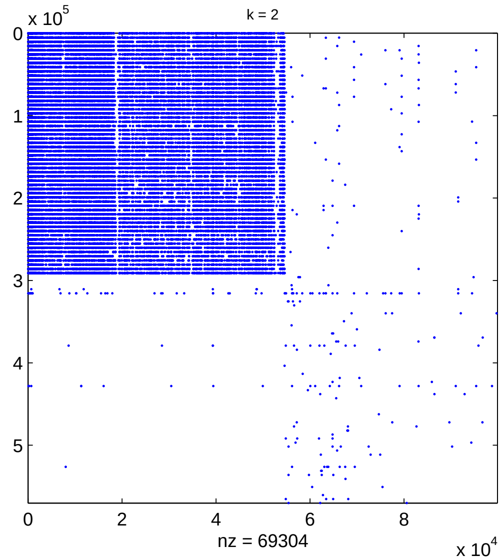
| | $B$ | | $B_{scal}$ $(dds)$ | | | $B$ $(thr)$ | | | |
|---|---|---|---|---|---|---|---|---|---|
| | $dd$ | $dds$ | $r$ | $c$ | $a$ | 0.1 | 0.2 | 0.3 | 0.6 |
| $Imaginable(300 \times 149)$ | 2 | 1 | 1 | 1 | 1 | 9 | 5 | 2 | 1 |

# Example - sparse matrix



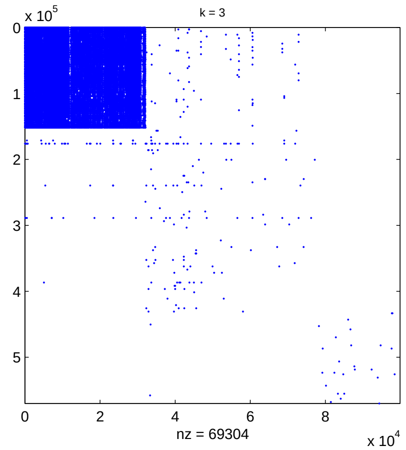
Matrix $(570166 \times 99899)$ represents big store receipts registered during one month.

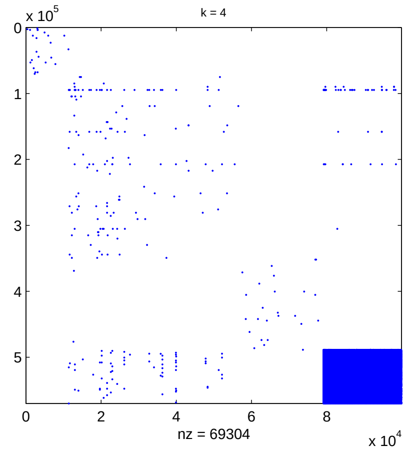


# Example - sparse matrix (2)






| | $B$ | | $B_{scal}\ (dds)$ | | | $B(thr)$ | |
|---|---|---|---|---|---|---|---|
| | $dd$ | $dds$ | $r$ | $c$ | $a$ | 0.01 | 0.005 |
| $(570166 \times 99899)$ | $> 8$ | 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.