







Sparsity-sensitive Diagonal Co-clustering Algorithms for the Effective Handling of Text Data

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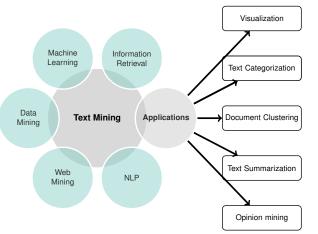
Context Co-clustering Motivations

- Exponential growth of textual documents on the web, e.g. the PUBMED database contains more than 20 millions of biomedical articles
- · It is become more laborious to access what we are looking for
- We need automated Text Mining tools to help us understand, interpret and organize this vast amount of information



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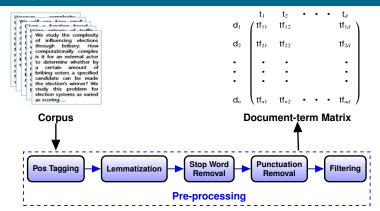




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Context Co-clustering Motivations

Data Representation



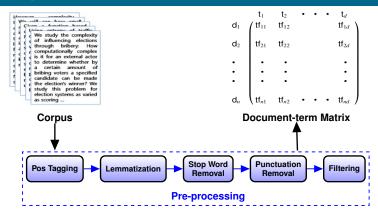
Document Representation

- Vector space model
- tf_{ij}=Frequency of term j in document i

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Weighting scheme

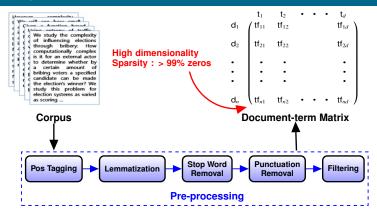
· TF-IDF weighting scheme

$$w_{ij} = tf_{ij} \times \log \frac{N}{d_i}$$

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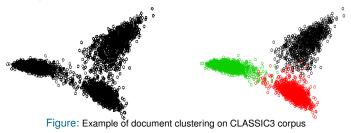
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Context Co-clustering Motivations

Document Clustering :

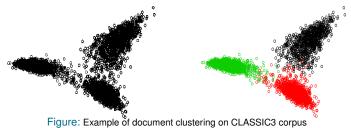
- A widely used unsupervised learning technique, to group together similar documents based on their content
- Documents within a cluster are semantically coherent or deal with the same topics



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Document Clustering :

- A widely used unsupervised learning technique, to group together similar documents based on their content
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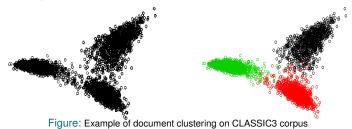
Advantages :

• Organization of documents, efficient browsing and navigation of huge text corpora, speed up search engines, etc.

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Advantages :

 Organization of documents, efficient browsing and navigation of huge text corpora, speed up search engines, etc.

Challenges :

- High dimensionality
- Sparsity

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Co-clustering

 It is an important extension of traditional one-sided clustering, that addresses the problem of simultaneous clustering of both dimensions of data matrices Hartigan, 1972

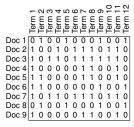
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(a) Original Data

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Doc 9 1 0 0 0 0 0 1 1 0 0	0 1 0 Doc 5	110000110	010

(a) Original Data

(b) Clustering

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Why Co-clustering?

- · Exploit the duality between object space and attribute space
- Cluster Characterization
- Technique for dimensionality reduction
- Reduce Computation time

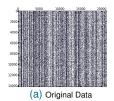
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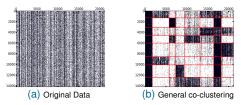
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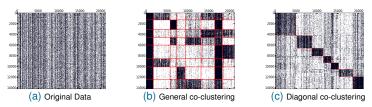
Context Co-clustering Motivations



Motivations

- When dealing with high dimensional sparse data, several co-clusters are primarily composed of zeros.
- Seeking homogeneous blocks is not sufficient to produce meaningful results.

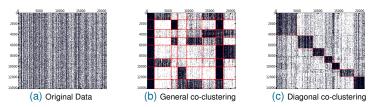
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- When dealing with high dimensional sparse data, several co-clusters are primarily composed of zeros.
- · Seeking homogeneous blocks is not sufficient to produce meaningful results.
- · Seeking diagonal structure turns out to be more beneficial.
 - · In good agreement with sparsity
 - · Produces directly the most relevant co-clusters and ignore noisy ones
 - Cluster hypothesis
 - · Allows a direct interpretation of co-clusters
 - Parsimonious

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Contributions

- Graph-based block diagonal clustering
- Model-based block diagonal clustering

Graph Modularity Modularity for Co-clustering Experiments

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Graph Modularity Modularity for Co-clustering Experiments

Contributions

Motivations

- Existing graph-based Co-clustering approaches use a spectral relaxation of the discrete optimization problem
 - Find minimum cut using spectral relaxation (Dhillon, 2001)
 - Find maximum Modularity using spectral relaxation (Labiod and Nadif, 2011)
- Eigen vector computation may be prohibitive when dealing with high dimensional matrices

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Contributions

- We propose a new block-diagonal clustering algorithm (Coclus) (Ailem, Role, and Nadif, 2015; Ailem, Role, and Nadif, 2016)
- · Coclus is based on the direct maximization of graph modularity
- Use an iterative alternating optimization procedure

M. Ailem, F. Role, and M. Nadif (2015). "Co-clustering Document-term Matrices by Direct Maximization of Graph Modularity". In: *CIKM*'2015. ACM, pp. 1807–1810.

M. Ailem, F. Role, and M. Nadif (2016). "Graph modularity maximization as an effective method for co-clustering text data". In: *Knowledge-Based Systems Journal* 109, pp. 160–173.

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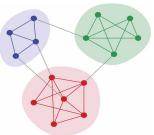
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Graph Modularity Modularity for Co-clustering Experiments

Graph Modularity



- Introduced by Newman and Girvan (2004)
- · Identify community structure in graphs
- · Measure the strength of the community structure of a graph
- Maximize the difference between the original graph and its corresponding random version
- *Q*=(number of intra-cluster edges) (expected number of edges)

Given the graph G(V, E) and its corresponding adjacency matrix A :

$$Q(\mathbf{A}, \mathbf{C}) = \frac{1}{2|E|} \sum_{i=1}^{n} \sum_{i'=1}^{n} (a_{ii'} - \frac{a_{i.}a_{i'.}}{2|E|}) c_{ii'},$$
(1)

- where |E| represents the number of edges
- a_{ii} = 1 if there is an edge between nodes i and i'
- a_i and $a_{i'}$ the degree of nodes *i* and *i'* respectively, and $\frac{a_i, a_{i'}}{2|E|}$ represents the expected number of edges between nodes *i* and *i'*
- $c_{ii'} = \sum_k z_{ik} z_{i'k}$ is equal to 1 if *i* and *i'* belong to the same community *k*

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Graph Modularity Modularity for Co-clustering Experiments

Modularity for Co-clustering

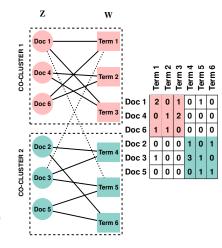
Given a rectangular positive matrix **A**, modularity can be reformulated as follows in the co-clustering context:

$$Q(\mathbf{A}, \mathbf{C}) = \frac{1}{a_{..}} \sum_{i=1}^{n} \sum_{j=1}^{d} (a_{ij} - \frac{a_{i.}a_{.j}}{a_{..}}) c_{ij}, \qquad (2)$$

$$Q(\mathbf{A}, \mathbf{ZW}^{t}) = \frac{1}{a_{\cdots}} \sum_{i=1}^{n} \sum_{j=1}^{d} \sum_{k=1}^{g} (a_{ij} - \frac{a_{i,a,j}}{a_{\cdots}}) z_{ik} w_{jk}, \quad (3)$$

where $a_{..} = \sum_{i,j} a_{ij} = |E|$ is the number of edges (or edge weights for weighted graphs) and $c_{ij} = \sum_k z_{ik} w_{jk} = 1$ if nodes *i* and *j* belong to the same co-cluster *k* and 0 otherwise

$$Q(\mathbf{A}, \mathbf{C}) = \frac{1}{a_{..}} Trace[(\mathbf{A} - \boldsymbol{\delta})^{t} \mathbf{Z} \mathbf{W}^{t}] = Q(\mathbf{A}, \mathbf{Z} \mathbf{W}^{t}).$$
(4)



Graph Modularity Modularity for Co-clustering Experiments

Alternated Maximization of Modularity

Proposition

Let A be a $(n \times d)$ positive data matrix and C be a $(n \times d)$ matrix defining a block seriation, the modularity measure Q(A, C) can be rewritten as

1)
$$Q(\mathbf{A}, \mathbf{C}) = \frac{1}{a_{\cdots}} \sum_{i=1}^{n} \sum_{k=1}^{g} (a_{ik}^{\mathbf{W}} - \frac{a_{i.}a_{.k}^{\mathbf{W}}}{a_{\cdots}}) z_{ik} = \frac{1}{a_{\cdots}} Trace[(\mathbf{A}^{\mathbf{W}} - \boldsymbol{\delta}^{\mathbf{W}})^{t} \mathbf{Z}] = Q(\mathbf{A}^{\mathbf{W}}, \mathbf{Z})$$

where $\delta^{\mathbf{W}} := \{\delta_{ik}^{\mathbf{W}} := \frac{a_{i,a_{.k}}^{\mathbf{W}}}{a_{..}}; i = 1, ..., n; k = 1, ..., g\}$ with $a_{.k}^{\mathbf{W}} = \sum_{j=1}^{d} w_{jk} a_{.j}$

2)
$$Q(\mathbf{A}, \mathbf{C}) = \frac{1}{a_{..}} \sum_{j=1}^{d} \sum_{k=1}^{g} (a_{kj}^{\mathbf{Z}} - \frac{a_{.j} a_{k.}^{\mathbf{Z}}}{a_{..}}) w_{jk} = \frac{1}{a_{..}} Trace[(\mathbf{A}^{\mathbf{Z}} - \boldsymbol{\delta}^{\mathbf{Z}})W] = Q(\mathbf{A}^{\mathbf{Z}}, \mathbf{W})$$

where $\delta^{\mathbf{Z}} := \{ \delta^{\mathbf{Z}}_{kj} = \frac{a_{,j}a_{k}^{\mathbf{Z}}}{a_{..}}; j = 1, ..., d; k = 1, ..., g \}$ with $a_{k.}^{\mathbf{Z}} = \sum_{i=1}^{n} z_{ik}a_{i.}$

Graph Modularity Modularity for Co-clustering Experiments

Coclus Algorithm

Algorithm 1: Coclus

Input : positive data matrix A, number of co-clusters gStep 1. Initialization of W repeat Step 2. Compute $A^W = AW$

Step 3. Compute Z maximizing $Q(A^W, Z)$ by

$$z_{ik} = \arg\max_{1 \le \ell \le g} \left(a_{i\ell}^{\mathbf{W}} - \frac{a_{i.}a_{.\ell}^{\mathbf{W}}}{a_{..}} \right) \forall i = 1, \dots, n; k = 1, \dots, g$$

Step 4. Compute $A^Z = Z^t A$ **Step 5.** Compute W maximizing $Q(A^Z, W)$ by

$$w_{jk} = \operatorname*{arg\,max}_{1 \le \ell \le g} \left(a_{\ell j}^{\mathbf{Z}} - \frac{a_{\ell}^{\mathbf{Z}} a_{.j}}{a_{..}} \right) \forall j = 1, \dots, d; k = 1, \dots, g$$

Step 6. Compute $Q(\mathbf{A}, \mathbf{ZW}^t)$

until Convergence;

Output : partition matrices Z and W, and modularity value Q

Complexity : $O(nz \cdot it \cdot g)$

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Datasets	Characteristics											
	#Documents	#Documents #Words #Clusters Sparsity (%) Bala										
CLASSIC4	7095	5896	4	99.41	0.323							
NG20	19949	43586	20	99.99	0.991							
SPORTS	8580	14870	7	99.99	0.036							
REVIEWS	4069	18483	5	99.99	0.098							

- Evaluation measure : Accuracy (Acc) and Normalized mutual information (NMI) (Strehl and Ghosh, 2003)
- Data Types : binary, contingency and TF-IDF

Method	Data Type	References	Co-clustering	Type of implementation
Spec	Positive data	(I. Dhillon, 2001)	Diagonal	Scickit Learn
Block	Binary	(Li, 2005)	Diagonal	Our python implementation
ITCC	Positive data	(I. S. Dhillon, Mallela, and D. S. Modha, 2003)	Non-diagonal	C++ implementation
SpecCo	Positive data	(Labiod and Nadif, 2011)	Diagonal	Our python implementation
χ -Sim	Positive data	(Bisson and Hussain, 2008)	Non-diagonal	MATLAB implementation of the authors
FNMTF	Positive data	(Wang et al., 2011)	Non-diagonal	MATLAB implementation of the authors

Graph Modularity Modularity for Co-clustering Experiments

Datasets	Characteristics											
	#Documents	#Documents #Words #Clusters Sparsity (%) Balan										
CLASSIC4	7095	5896	4	99.41	0.323							
NG20	19949	43586	20	99.99	0.991							
SPORTS	8580	14870	7	99.99	0.036							
REVIEWS	4069	18483	5	99.99	0.098							

- Evaluation measure : Accuracy (Acc) and Normalized mutual information (NMI) (Strehl and Ghosh, 2003)
- Data Types : binary, contingency and TF-IDF

Method	Data Type	References	Co-clustering	Type of implementation
Spec	Positive data	(I. Dhillon, 2001)	Diagonal	Scickit Learn
Block	Binary	(Li, 2005)	Diagonal	Our python implementation
ITCC	Positive data	(I. S. Dhillon, Mallela, and D. S. Modha, 2003)	Non-diagonal	C++ implementation
SpecCo	Positive data	(Labiod and Nadif, 2011)	Diagonal	Our python implementation
χ -Sim	Positive data	(Bisson and Hussain, 2008)	Non-diagonal	MATLAB implementation of the authors
FNMTF	Positive data	(Wang et al., 2011)	Non-diagonal	MATLAB implementation of the authors

		Binary							Contingency					TF-IDF						
datasets	per.	Spec	ITCC	Block	SpecCo	χ -Sim	FNMTF	CoClus	Spec	ITCC	SpecCo	$\chi ext{-Sim}$	FNMTF	CoClus	Spec	ITCC	SpecCo	χ -Sim	FNMTF	CoClus
CLASSIC4	Acc	0.34	0.65	0.52	0.45	0.31	0.50	0.90	0.53	0.87	0.58	0.31	0.56	0.90	0.44	0.60	0.45	0.35	0.76	0.88
	NMI	0.14	0.51	0.16	0.02	0.15	0.30	0.72	0.45	0.67	0.48	0.15	0.30	0.73	0.02	0.55	0.009	0.13	0.58	0.70
NG20	Acc	0.14	0.43	0.20	0.19	0.26	0.13	0.40	0.05	0.45	0.30	0.30	0.09	0.37	0.19	0.41	0.15	0.29	0.40	0.37
	NMI	0.29	0.55	0.22	0.42	0.33	0.03	0.55	0.02	0.52	0.49	0.37	0.07	0.52	0.32	0.44	0.38	0.41	0.40	0.52
SPORTS	Acc	0.56	0.45	0.47	0.59	0.57	0.28	0.70	0.44	0.56	0.68	0.53	0.36	0.75	0.45	0.54	0.61	0.67	0.57	0.68
	NMI	0.47	0.49	0.38	0.45	0.48	0.15	0.54	0.38	0.58	0.59	0.48	0.19	0.62	0.43	0.58	0.45	0.55	0.54	0.59
REVIEWS	Acc	0.56	0.58	0.53	0.59	0.46	0.34	0.65	0.50	0.71	0.45	0.41	0.38	0.72	0.35	0.63	0.46	0.44	0.43	0.65
	NMI	0.36	0.46	0.42	0.39	0.31	0.18	0.54	0.40	0.57	0.34	0.23	0.17	0.58	0.03	0.51	0.35	0.28	0.27	0.52

Results obtained after running each algorithm 100 times with random initialization

We retained the solution optimizing the associated criterion (maximizing the modularity for CoClus)

Superiority of Coclus in almost all situations

Robustness w.r.t the type of data (binary tables, contingency tables and TF-IDF weighted tables)

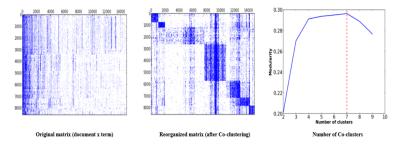
Graph Modularity Modularity for Co-clustering Experiments

Assessing the Number of Co-clusters

- Most previous co-clustering algorithms require the number of co-clusters as an input parameter
- The modularity measure can be used to predict the right number of co-clusters
- Run Coclus algorithm with different values of g (number of co-clusters)
- · For each number of co-cluster the modularity is computed
- Retain the number of co-clusters for which the modularity measure reaches it's maximum value

Graph Modularity Modularity for Co-clustering Experiments

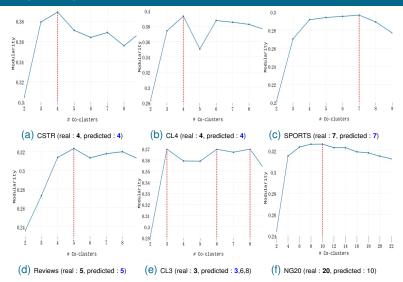
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Graph Modularity Modularity for Co-clustering Experiments

Assessing the right number of co-clusters



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Motivation

- Investigate probabilistic mixture models allowing to make precise assumptions about the anatomy of diagonal co-clusters
- Flexibility
- · Give rise to both soft and hard co-clustering

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Motivation

- Investigate probabilistic mixture models allowing to make precise assumptions about the anatomy of diagonal co-clusters
- Flexibility
- · Give rise to both soft and hard co-clustering

Contribution

- We present a sparse generative mixture model for co-clustering text data
- This model is based on the Poisson distribution, which arises naturally for contingency tables, such as document-term matrices
- The proposed model takes into account the sparsity in its formulation

Sparse Poisson Latent Block Model (SPLBM) Soft SPLBM-based Co-clustering Algorithm Hard SPLBM-based Co-clustering Algorithm Experiments

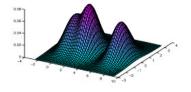
Model-based clustering - Finite mixture model

The matrix is assumed to be an i.i.d sample $\mathbf{X} = (\mathbf{x}_1, ..., \mathbf{x}_n)$ where $\mathbf{x}_i = (x_{i1}, ..., x_{id}) \in \mathbb{R}^d$ is generated from a probability density function (pdf) with density :

$$f(\mathbf{x}_i,\theta) = \sum_{k=1}^g \pi_k f_k(\mathbf{x}_i,\alpha_k),$$

The likelihood of data X can be written as :

$$f(\mathbf{X}, \boldsymbol{\theta}) = \prod_{i} \sum_{k=1}^{g} \pi_{k} f_{k}(\mathbf{x}_{i}, \alpha_{k}),$$



where

- $f_k(., \alpha_k)$ is the density of an observation \mathbf{x}_i from the *k*-th component
- $\alpha'_k s$ are the corresponding class parameters
- π_k represents the proportions of each cluster.
- Each component *k* of the mixture represents a cluster.

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Model-based co-clustering - Latent block model (LBM)

For each block $k\ell$, the values x_{ij} are generated according to a probability density function (pdf) $f(x_{ij}; \alpha_{k\ell})$ (Govaert and Nadif, 2003)



Likelihood function

Denoting by Z and W the sets of all possible partitions, the likelihood function of a data matrix **X** of size $n \times d$ can be written

$$f(\mathbf{X}; \boldsymbol{\theta}) = \sum_{(\mathbf{Z}, \mathbf{W}) \in \mathcal{Z} \times \mathcal{W}} \prod_{i,k} \pi_k^{z_{ik}} \prod_{j,\ell} \rho_{\ell}^{w_{j\ell}} \prod_{i,j,k,\ell} f(x_{ij}; \alpha_{k\ell})^{z_{ik}w_{j\ell}}$$

Where

- $\theta = (\pi, \rho, \alpha)$, is the parameters of the latent block model.
- π and ρ are the mixing proportions.
- $\alpha = (\alpha_{k\ell}; k = 1, \dots, g, \ell = 1, \dots, m)$ is the matrix of parameters of each block (k, ℓ) .
- g (resp. m) represents the number of row (resp. column) clusters.

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Latent block model (LBM)

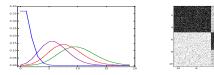
Algorithm 2: Generative Process of LBM **Input** : $n, d, g, m, \theta = (\pi, \rho, \alpha)$ **Output:** data matrix **X**, vector of row labellings $\mathbf{z} = (z_1, \ldots, z_n)$ and vector of column labellings $\mathbf{w} = (w_1, \ldots, w_d)$ for i = 1 to n do - Generate the row label z_i according to the multinomial distribution $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_g)$ end **for** *i* = 1 **to** *d* **do** - Generate the column label w_i according to the multinomial distribution $\boldsymbol{\rho} = (\rho_1, \ldots, \rho_p)$ end for i = 1 to n do for i = 1 to d do - Generate a value x_{ii} according to the distribution $f(.; \alpha_{z_i, w_i})$ end end

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Intuition

• For each diagonal block *kk* the values x_{ij} are distributed according to the Poisson distribution $\mathcal{P}(\lambda_{ij})$ where the parameter λ_{ij} takes the following form :

$$\lambda_{ij} = x_{i,x,j} \sum_k z_{ik} w_{jk} \gamma_{kk},$$

For each off-diagonal block kℓ with k ≠ ℓ the values x_{ij} are distributed according to the Poisson distribution P(λ_{ij}) where the parameter λ_{ij} takes the following form :

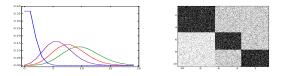
$$\lambda_{ij} = x_{i,} x_{,j} \sum_{k,\ell \neq k} z_{ik} w_{j\ell} \gamma.$$

• Assuming $\forall \ell \neq k \quad \gamma_{k\ell} = \gamma$ leads to suppose that all blocks outside the diagonal share the same parameter.

Likelihood function

$$\begin{split} \mathbf{X}; \boldsymbol{\theta}) &= \sum_{(\mathbf{z}, \mathbf{w}) \in \mathcal{Z} \times \mathcal{W}} \prod_{i, k} \pi_k^{\neg k} \prod_{j, k} \rho_\ell^{\neg k} \\ &\times \prod_{i, j, k} (f(x_{ij}; \boldsymbol{\alpha}_{kk}))^{z_{ik} w_{jk}} \times \prod_{i, j, k, \ell \neq k} (f(x_{ij}; \boldsymbol{\alpha}_{k\ell}))^{z_{ik} w_{j\ell}} \end{split}$$

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$$\lambda_{ij} = x_{i,} x_{,j} \sum_{k} z_{ik} w_{jk} \gamma_{kk}.$$

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 Assuming ∀ℓ ≠ k γ_{kℓ} = γ leads to suppose that all blocks outside the diagonal share the same parameter.

Likelihood function

$$f(\mathbf{X}; \boldsymbol{\theta}) = \sum_{(\mathbf{z}, \mathbf{w}) \in \mathcal{Z} \times \mathcal{W}} \prod_{i,k} \pi_k^{z_{ik}} \prod_{j,k} \rho_\ell^{w_{jk}}$$
$$\times \prod_{i,j,k} (f(x_{ij}; \alpha_{kk}))^{z_{ik}w_{jk}} \times \prod_{i,j,k,\ell \neq k} (f(x_{ij}; \alpha_{k\ell}))^{z_{ik}w_{j\ell}}$$

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Sparse Poisson Latent Block Model (SPLBM)

Complete Data Likelihood

$$\begin{aligned} f(\mathbf{X}, \mathbf{Z}, \mathbf{W}; \boldsymbol{\theta}) &= \prod_{i,k} \pi_k^{z_{ik}} \prod_{j,k} \rho_k^{w_{jk}} & \times \prod_{i,j,k} \left(\frac{e^{-x_i, x_j \gamma_{kk}} (x_{i,x,j} \gamma_{kk})^{x_{ij}}}{x_{ij}!} \right)^{z_{ik} w_{jk}} \\ & \times \prod_{i,j,k,\ell \neq k} \left(\frac{e^{-x_i, x_j \gamma} (x_i, x_j \gamma)^{x_{ij}}}{x_{ij}!} \right)^{z_{ik} w_{j\ell}} \end{aligned}$$

Complete Data Log-likelihood

$$L_{C}(\mathbf{Z}, \mathbf{W}, \boldsymbol{\theta}) = \log f(\mathbf{X}, \mathbf{Z}, \mathbf{W}; \boldsymbol{\theta}) = \sum_{k=1}^{k} \mathcal{L}_{C}^{k}$$
$$\mathcal{L}_{C}^{k} = z_{.k} \log \pi_{k} + w_{.k} \log \rho_{k} + x_{kk}^{\mathbf{ZW}} \log(\frac{\gamma_{kk}}{\gamma}) - x_{k.}^{\mathbf{Z}} x_{.k}^{\mathbf{W}} (\gamma_{kk} - \gamma) + \frac{N}{g} (\log(\gamma) - \gamma N)$$
where $x_{kk}^{\mathbf{ZW}} = \sum_{ij} z_{ik} w_{jk} x_{ij}, z_{.k} = \sum_{i} z_{ik}$ and $w_{.k} = \sum_{j} w_{jk}, x_{k.}^{\mathbf{Z}} = \sum_{i} z_{ik} x_{i.}$ and $x_{.k}^{\mathbf{W}} = \sum_{j} w_{jk} x_{.j}$

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Complete Data Log-likelihood

$$\begin{split} \mathbf{L}_{\mathbf{C}}(\mathbf{Z},\mathbf{W},\boldsymbol{\theta}) &= \log f(\mathbf{X},\mathbf{Z},\mathbf{W};\boldsymbol{\theta}) = \sum_{k=1}^{s} \mathcal{L}_{\mathbf{C}}^{k} \\ \mathcal{L}_{\mathbf{C}}^{k} &= z_{.k} \log \pi_{k} + w_{.k} \log \rho_{k} + x_{kk}^{\mathbf{ZW}} \log(\frac{\gamma_{kk}}{\gamma}) - x_{k.}^{\mathbf{Z}} x_{.k}^{\mathbf{W}}(\gamma_{kk} - \gamma) + \frac{N}{g} (\log(\gamma) - \gamma N) \\ \text{where } x_{kk}^{\mathbf{ZW}} &= \sum_{ij} z_{ik} w_{jk} x_{ij}, z_{.k} = \sum_{i} z_{ik} \text{ and } w_{.k} = \sum_{j} w_{jk}, x_{.k}^{\mathbf{Z}} = \sum_{i} z_{ik} x_{i.} \text{ and } x_{.k}^{\mathbf{W}} = \sum_{j} w_{jk} x_{.j} \end{split}$$

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Sparse Poisson Latent Block Model (SPLBM)

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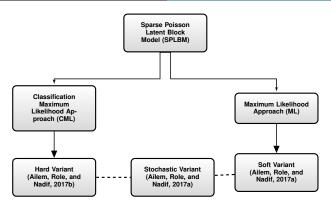


Figure: SPLBM-based co-clustering algorithms

 M. Ailem, F. Role, and M. Nadif (2017b). "Sparse Poisson Latent Block Model for Document Clustering". In: *IEEE TKDE journal* 29.7, p. 1563.
 M. Ailem, F. Role, and M. Nadif (2017a). "Model-based co-clustering for the effective handling of sparse data". In: *Pattern Recognition* 72, pp. 108–122.

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Soft SPLBM-based Co-clustering Algorithm

- Estimate the model's parameters $\boldsymbol{\theta}, \widetilde{\mathbf{Z}}$ and $\widetilde{\mathbf{W}}$
- We rely on the Expectation-Maximization (EM) algorithm that consists in maximizing the expectation of the complete data likelihood $L_C(\mathbf{Z}, \mathbf{W}, \theta)$ given by :

$$\mathbb{E}\left(\mathbf{L}_{\mathbf{C}}(\mathbf{Z}, \mathbf{W}, \boldsymbol{\theta}) | \boldsymbol{\theta}^{(t)}, \mathbf{X}\right) = \sum_{i,k} \tilde{z}_{ik}^{(t)} \log \pi_k + \sum_{j,k} \tilde{w}_{jk}^{(t)} \log \rho_k \\ + \sum_{i,j,k} \tilde{e}_{ijk}^{(t)} \left(x_{ij} \log(\gamma_{kk}) - x_{i.} x_{.j} \gamma_{kk}\right) \\ + \sum_{i,j,k,\ell \neq k} \tilde{e}_{ikj\ell}^{(t)} \left(x_{ij} \log(\gamma) - x_{i.} x_{.j} \gamma\right),$$

where $\tilde{z}_{ik}^{(t)} = \mathbb{E}(z_{ik} = 1 | \mathbf{X}, \boldsymbol{\theta}^{(t)}), \tilde{w}_{j\ell} = \mathbb{E}(w_{j\ell}^{(t)} = 1 | \mathbf{X}, \boldsymbol{\theta}^{(t)}),$ $\tilde{e}_{ikj\ell}^{(t)} = \mathbb{E}(e_{ikj\ell} = 1 | \mathbf{X}, \boldsymbol{\theta}^{(t)}) = \mathbb{E}(z_{ik}w_{j\ell} = 1 | \mathbf{X}, \boldsymbol{\theta}^{(t)}) \text{ and } \tilde{e}_{ijk}^{(t)} = \mathbb{E}(z_{ik}w_{jk} = 1 | \mathbf{X}, \boldsymbol{\theta}^{(t)}).$

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where $\tilde{z}_{ik}^{(t)} = \mathbb{E}(z_{ik} = 1 | \mathbf{X}, \boldsymbol{\theta}^{(t)}), \tilde{w}_{j\ell} = \mathbb{E}(w_{j\ell}^{(t)} = 1 | \mathbf{X}, \boldsymbol{\theta}^{(t)}),$ $\tilde{e}_{ikj\ell}^{(t)} = \mathbb{E}(e_{ikj\ell} = 1 | \mathbf{X}, \boldsymbol{\theta}^{(t)}) = \mathbb{E}(z_{ik}w_{j\ell} = 1 | \mathbf{X}, \boldsymbol{\theta}^{(t)}) \text{ and } \tilde{e}_{ijk}^{(t)} = \mathbb{E}(z_{ik}w_{jk} = 1 | \mathbf{X}, \boldsymbol{\theta}^{(t)}).$ The coupling of **Z** and **W** in *e* makes the direct application of the EM algorithm difficult, due to the determination of \tilde{e}_{ijk} and $\tilde{e}_{ikj\ell}$

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Model Fitting Using the Variational EM Algorithm

- Solution : Use a mean-field variational EM (VEM) algorithm for inferences
- The VEM algorithm is equivalent to maximizing the following soft co-clustering criteria:

$$F_{C}(\widetilde{\mathbf{Z}}, \widetilde{\mathbf{W}}, \boldsymbol{\theta}) = L_{C}(\widetilde{\mathbf{Z}}, \widetilde{\mathbf{W}}, \boldsymbol{\theta}) + H(\widetilde{\mathbf{Z}}) + H(\widetilde{\mathbf{W}}),$$

- where $H(\widetilde{\mathbf{Z}}) = -\sum_{i,k} \widetilde{z}_{ik} \log \widetilde{z}_{ik}$ and $H(\widetilde{\mathbf{W}}) = -\sum_{j,k} \widetilde{w}_{jk} \log \widetilde{w}_{jk}$ are respectively the entropy of the missing variables $\widetilde{\mathbf{Z}}$ and $\widetilde{\mathbf{W}}$
- $L_{C}(\widetilde{\mathbf{Z}}, \widetilde{\mathbf{W}}, \boldsymbol{\theta})$ is the soft complete data likelihood defined as follows :

$$L_{C}(\widetilde{\mathbf{Z}}, \widetilde{\mathbf{W}}, \boldsymbol{\theta}) = \sum_{i,k} \widetilde{z}_{ik} \log \pi_{k} + \sum_{j,k} \widetilde{w}_{jk} \log \rho_{k} + \sum_{i,j,k} \widetilde{z}_{ik} \widetilde{w}_{jk} x_{ij} \log(\frac{\gamma_{kk}}{\gamma}) \\ - \sum_{k} x_{k.}^{\widetilde{\mathbf{Z}}} x_{.k}^{\widetilde{\mathbf{W}}} \gamma_{kk} + \gamma \sum_{k} x_{k.}^{\widetilde{\mathbf{Z}}} x_{.k}^{\widetilde{\mathbf{W}}} + N(\log(\gamma) - \gamma N)$$

The SPLBvem algorithm consists of the expectation and maximization steps

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Model Fitting Using the Variational EM Algorithm

M-step

Computation of γ̂_{kk} for all k. It is easy to show that ∀k the γ̂_{kk}'s maximizing F_C can be computed separately for each k.

$$\hat{\gamma}_{kk} = \frac{x_{kk}^{\widetilde{\mathbf{Z}}\widetilde{\mathbf{W}}}}{x_{k.}^{\widetilde{\mathbf{Z}}} x_{.k}^{\widetilde{\mathbf{W}}}}$$

• Computation of $\hat{\gamma}$ maximizing F_{C} . It is easy to show that $\hat{\gamma}$ is given by:

$$\hat{\gamma} = \frac{N - \sum_{k} x_{kk}^{\widetilde{\mathbf{Z}}\widetilde{\mathbf{W}}}}{N^2 - \sum_{k} x_{k.}^{\widetilde{\mathbf{Z}}} x_{.k}^{\widetilde{\mathbf{W}}}}.$$

• **Computation of** $\hat{\pi}_k$, $\hat{\rho}_k$ **for all k**. Under the constraints $\sum_k \pi_k = \sum_k \rho_k = 1$, it is easy to show that each $\hat{\pi}_k$ and $\hat{\rho}_k$ maximizing F_C are respectively given by $\pi_k = \frac{\widetilde{Z}_{kk}}{n}$ and $\rho_k = \frac{\widetilde{W}_k}{d}$.

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Model Fitting Using the Variational EM Algorithm

E-step

- The E-step consists in computing the posterior probabilities \widetilde{z}_{ik} and \widetilde{w}_{jk} maximizing F_C
- Plugging the estimation of γ_{kk} 's and γ (explicitly in some terms of F_C) we obtain

$$\begin{aligned} F_{\mathrm{C}}(\widetilde{\mathbf{Z}},\widetilde{\mathbf{W}},\widehat{\boldsymbol{\theta}}) &= \sum_{i,k} \widetilde{z}_{ik} \log \hat{\pi}_k + \sum_{j,k} \widetilde{w}_{jk} \log \hat{\rho}_k + \sum_{i,j,k} \widetilde{z}_{ik} \widetilde{w}_{jk} x_{ij} \log(\frac{\hat{\gamma}_{kk}}{\hat{\gamma}}) \\ &+ N(\log(\hat{\gamma}) - 1) - \sum_{i,k} \widetilde{z}_{ik} \log \widetilde{z}_{ik} - \sum_{j,k} \widetilde{w}_{jk} \log \widetilde{w}_{jk}. \end{aligned}$$

Taking x_{ik}^W = ∑_j w_{jk}x_{ij} and x_{kj}^Z = ∑_i z_{ik}x_{ij} it is easy to show that under the constraints:

• $\sum_k \tilde{z}_{ik} = 1$ • $\sum_k \tilde{w}_{ik} = 1$

$$\begin{split} \widetilde{z}_{ik} &\propto \pi_k \exp(x_{ik}^{\widetilde{\mathbf{W}}} \log \frac{\gamma_{kk}}{\gamma}). \\ \widetilde{w}_{jk} &\propto \rho_k \exp(x_{kj}^{\widetilde{\mathbf{Z}}} \log \frac{\gamma_{kk}}{\gamma}). \end{split}$$

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The SPLBvem Algorithm

Algorithm 3: SPLBvem

Input: X, g Initialization : $\widetilde{\mathbf{Z}}, \widetilde{\mathbf{W}}, \pi_k, \rho_k, \gamma_{kk}, \gamma$ repeat $x_{ik}^{\mathbf{W}} = \sum_{i} \widetilde{\mathbf{W}}_{ik} x_{ii}$ step 1. $\widetilde{z}_{ik} \propto \pi_k \exp(x_{ik}^{\widetilde{\mathbf{W}}} \log \frac{\gamma_{kk}}{\gamma})$ step 2. $\pi_k = \frac{\widetilde{z}_{i,k}}{n}, \ \gamma_{kk} = \frac{\sum_i \widetilde{z}_{ik} x_{ik}}{\sqrt{2} \sqrt{w}} = \frac{x_{ik}^{\widetilde{Z}\widetilde{W}}}{\sqrt{2} \sqrt{w}}, \ \gamma = \frac{N - \sum_k x_{ik}^{\widetilde{Z}\widetilde{W}}}{N^2 - \sum_k \sqrt{2} \sqrt{w}}$ $x_{li}^{\widetilde{\mathbf{Z}}} = \sum_{i} \widetilde{z}_{ik} x_{ij}$ step 3. $\widetilde{\mathbf{w}}_{jk} \propto \rho_k \exp(x \widetilde{\mathbf{z}}_{kj} \log \frac{\gamma_{kk}}{\gamma})$ step 4. $\rho_k = \frac{\widetilde{w}_{,k}}{d}, \ \gamma_{kk} = \frac{\sum_j \widetilde{w}_{jk} x_{kj}^Z}{\sqrt{2} \sqrt{\widetilde{w}}} = \frac{x_{kk}^Z \widetilde{w}}{\sqrt{2} \sqrt{\widetilde{w}}}, \ \gamma = \frac{N - \sum_k x_{kk}^Z \widetilde{w}}{N^2 - \sum_k \sqrt{2} \sqrt{\widetilde{w}}}$ until Convergence; **Output :** \mathbf{Z} , \mathbf{W} , π_k , ρ_k , γ_{kk} , γ

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The hard SPLBM-based co-clustering algorithm (SPLBcem)

Intuition

- · It consists in maximizing the classification likelihood instead of its expectation
- This is done by incorporating a classification step (C-step) between the E and M steps of the SPLBvem

Algorithm 4: SPLBcem

$$\begin{split} & \text{initialization : } X, g \\ & \text{initialization : } Z, W, \pi_k, \rho_k, \gamma_{kk}, \gamma \\ & \text{repeat} \\ & x_{ik}^{\widetilde{W}} = \Sigma_j \widetilde{w}_{jk} x_{ij} \\ & \text{step 1: } \overline{z_{ik}} \propto \pi_k \exp(x_{ik}^{\widetilde{W}} \log \frac{\gamma_{kk}}{\gamma}) \\ & \text{step 1: } \overline{z_{ik}} \approx \pi_k \exp(x_{ik}^{\widetilde{W}} \log \frac{\gamma_{kk}}{\gamma}) \\ & \text{step 2: } \pi_k = \frac{\overline{z_k}}{n}, \gamma_{kk} = \frac{\sum_i \overline{z_{ik}} x_{ik}^{\widetilde{W}}}{x_k^{\widetilde{L}} x_k^{\widetilde{W}}} = \frac{\overline{X_k^{\widetilde{W}}}}{x_{k}^{\widetilde{L}} x_k^{\widetilde{W}}} , \gamma = \frac{N - \sum_k \overline{X_k^{\widetilde{W}}}}{N^2 - \sum_k x_k^{\widetilde{L}} x_k^{\widetilde{W}}} \\ & \overline{X_{kj}^{\widetilde{Z}}} = \sum_i \overline{z_{ik}} x_{ij} \\ & \text{step 3: } w_{jk} = \arg \max_k \overline{w}_{jk} \\ & \text{step 4. } \rho_k = \frac{\overline{w}_{k}}{x_k}, \gamma_{kk} = \frac{\sum_j \overline{w}_{jk} x_{kj}^{\widetilde{Z}}}{x_k^{\widetilde{L}} x_k^{\widetilde{W}}} = \frac{x_{kk}^{\widetilde{W}}}{x_k^{\widetilde{L}} x_k^{\widetilde{W}}} , \gamma = \frac{N - \sum_k x_{kk}^{\widetilde{Z}} \overline{x}_k^{\widetilde{W}}}{N^2 - \sum_k x_k^{\widetilde{L}} x_k^{\widetilde{K}}} \\ & \text{unif} Convergence: \end{split}$$

until Convergence; Output : Z, W, π_k , ρ_k , γ_{kk} , γ

Advantages

- SPLBcem is considerably faster and scalable than SPLBvem
- It allows us to avoid numerical difficulties, related to the computation of the posterior probabilities \tilde{z}_{ik} and \tilde{w}_{jk}

Sparse Poisson Latent Block Model (SPLBM) Soft SPLBM-based Co-clustering Algorithm Hard SPLBM-based Co-clustering Algorithm Experiments

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$$\begin{split} & \text{intuition: } \mathbf{X}, g \\ & \text{initialization: } \mathbf{Z}, \mathbf{W}, \pi_k, \rho_k, \gamma_{kk}, \gamma \\ & \text{repeat} \\ & \mathbf{x}_{ik}^{\widetilde{\mathbf{X}}} = \Sigma_j \widetilde{\mathbf{w}}_{jk} \mathbf{x}_{ij} \\ & \text{step 1: } \overline{z}_{ik} \propto \pi_k \exp(\mathbf{x}_{ik}^{\widetilde{\mathbf{W}}} \log \frac{\gamma_{kk}}{\gamma}) \\ & \text{step 1: } \overline{z}_{ik} \approx \pi_k \exp(\mathbf{x}_{ik}^{\widetilde{\mathbf{W}}} \log \frac{\gamma_{kk}}{\gamma}) \\ & \text{step 2: } \pi_k = \frac{\overline{z}_{.k}}{n}, \gamma_{kk} = \frac{\sum_i \overline{z}_{ik} \mathbf{x}_{ik}^{\widetilde{\mathbf{W}}}}{\overline{x}_k^{\widetilde{\mathbf{X}}, \mathbf{X}_k^{\widetilde{\mathbf{W}}}}} = \frac{\overline{X}_{ik}^{\widetilde{\mathbf{W}}}}{x_k^{\widetilde{\mathbf{X}}, \mathbf{X}_k^{\widetilde{\mathbf{W}}}}} , \gamma = \frac{N - \sum_k \overline{X}_{ik}^{\widetilde{\mathbf{X}}} \overline{x}_{ik}^{\widetilde{\mathbf{X}}}}{N^2 - \sum_k x_k^{\widetilde{\mathbf{X}}, \mathbf{X}_k^{\widetilde{\mathbf{X}}}}} \\ & \overline{x}_{kj}^{\widetilde{\mathbf{Z}}} = \sum_i \overline{z}_{ik} \mathbf{x}_{ij} \\ & \text{step 3: } \overline{w}_{jk} \approx \alpha_k \exp(\mathbf{x}_{k}^{\widetilde{\mathbf{Z}}} \log \frac{\gamma_{kk}}{\gamma}) \\ & \text{step 4: } \rho_k = \frac{\overline{w}_{.k}}{n}, \gamma_{kk} = \frac{\sum_j \widetilde{w}_{jk} \mathbf{x}_{ij}^{\widetilde{\mathbf{Z}}}}{x_k^{\widetilde{\mathbf{X}}, \mathbf{x}_k^{\widetilde{\mathbf{X}}}}} = \frac{\overline{x}_{kk}^{\widetilde{\mathbf{X}}} \overline{x}_{k}^{\widetilde{\mathbf{X}}}}{x_k^{\widetilde{\mathbf{X}}, \mathbf{x}_k^{\widetilde{\mathbf{X}}}}}, \gamma = \frac{N - \sum_k x_{kk}^{\widetilde{\mathbf{X}}} \overline{x}_{k}^{\widetilde{\mathbf{X}}}}{N^2 - \sum_k x_{kk}^{\widetilde{\mathbf{X}}} x_{k}^{\widetilde{\mathbf{X}}}}} \\ & \text{step 4: } \rho_k = \frac{\overline{w}_{.k}}{n}, \gamma_{kk} = \frac{\sum_j \widetilde{w}_{jk} \mathbf{x}_{ij}^{\widetilde{\mathbf{X}}}}{x_k^{\widetilde{\mathbf{X}}, \mathbf{x}_k^{\widetilde{\mathbf{X}}}}} = \frac{\overline{x}_{kk}^{\widetilde{\mathbf{X}}} \overline{x}_{k}^{\widetilde{\mathbf{X}}}}{x_k^{\widetilde{\mathbf{X}}, \mathbf{x}_k^{\widetilde{\mathbf{X}}}}}, \gamma = \frac{N - \sum_k x_{kk}^{\widetilde{\mathbf{X}}} \overline{x}_{k}^{\widetilde{\mathbf{X}}}}{N^2 - \sum_k x_{kk}^{\widetilde{\mathbf{X}}} \overline{x}_{k}^{\widetilde{\mathbf{X}}}}} \end{aligned}$$

until Convergence; Output : Z, W, π_k , ρ_k , γ_{kk} , γ

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- SPLBcem is considerably faster and scalable than SPLBvem
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 *z*_{ik} and
 *w*_{jk}

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The stochastic SPLBM-based co-clustering algorithm (SPLBsem)

SPLBvem and SPLBcem are very dependant on their starting points!

Algorithm 5: SPLBsem

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Algorithm 5: SPLBsem

Output : Z, W, π_k , ρ_k , γ_{kk} , γ

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Algorithm 5: SPLBsem

Input: X, g Initialization : $\widetilde{\mathbf{Z}}$, $\widetilde{\mathbf{W}}$, π_k , ρ_k , γ_{kk} , γ repeat $x_{ik}^{\widetilde{\mathbf{W}}} = \sum_{i} \widetilde{\mathbf{w}}_{ik} x_{ii}$ step 1. $\widetilde{z}_{ik} \propto \pi_k \exp(x_{ik}^{\widetilde{\mathbf{W}}} \log \frac{\gamma_{kk}}{\gamma})$ **step 1'.** simulation of z_i according to $\mathcal{M}(\tilde{z}_{i1}, \ldots, \tilde{z}_{ip})$ step 2. $\pi_k = \frac{\widetilde{z}_{,k}}{n}, \gamma_{kk} = \frac{\sum_i \widetilde{z}_{ik} x_{jk}^{\widetilde{\mathbf{W}}}}{\widetilde{x}_{,k}^{\widetilde{\mathbf{Z}}} x_{,k}^{\widetilde{\mathbf{W}}}} = \frac{\widetilde{x}_{kk}^{\widetilde{\mathbf{Z}}}}{\widetilde{x}_{,k}^{\widetilde{\mathbf{Z}}} x_{,k}^{\widetilde{\mathbf{W}}}}, \gamma = \frac{N - \sum_k x_{kk}^{\widetilde{\mathbf{Z}}} x_{kk}^{\widetilde{\mathbf{W}}}}{N^2 - \sum_k x_{kk}^{\widetilde{\mathbf{Z}}} x_{,k}^{\widetilde{\mathbf{W}}}}$ $\widetilde{X}_{ki} = \sum_{i} \widetilde{z}_{ik} x_{ii}$ step 3. $\widetilde{w}_{ik} \propto \rho_k \exp(x_{ki}^{\widetilde{\mathbf{Z}}} \log \frac{\gamma_{kk}}{\gamma_{ki}})$ **step 3'.** simulation of w_i according to $\mathcal{M}(\widetilde{w}_{i1}, \ldots, \widetilde{w}_{ig})$ step 4. $\rho_k = \frac{\widetilde{w}_{,k}}{d}, \gamma_{kk} = \frac{\sum_j \widetilde{w}_{jk} \chi_{kj}^{\widetilde{Z}}}{\chi_{kj}^{\widetilde{Z}} \chi_{kj}^{\widetilde{W}}} = \frac{\chi_{kk}^{\widetilde{Z}}}{\chi_{kj}^{\widetilde{Z}} \chi_{kj}^{\widetilde{W}}}, \gamma = \frac{N - \sum_k \chi_{kk}^{\widetilde{Z}}}{N^2 - \sum_k \chi_{kk}^{\widetilde{Z}} \chi_{kj}^{\widetilde{W}}}$ until Convergence; **Output :** Z, W, π_k , ρ_k , γ_{kk} , γ

Advantages : It does not stop at the first stationary point of the likelihood function, which makes it possible to avoid bad local maxima due to the initial position

Sparse Poisson Latent Block Model (SPLBM) Soft SPLBM-based Co-clustering Algorithm Hard SPLBM-based Co-clustering Algorithm Experiments

The stochastic SPLBM-based co-clustering algorithm (SPLBsem)

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Input: X, g Initialization : $\widetilde{\mathbf{Z}}$, $\widetilde{\mathbf{W}}$, π_k , ρ_k , γ_{kk} , γ repeat $x_{ik}^{\widetilde{\mathbf{W}}} = \sum_{i} \widetilde{\mathbf{W}}_{ik} x_{ii}$ step 1. $\widetilde{z}_{ik} \propto \pi_k \exp(x_{ik}^{\widetilde{\mathbf{W}}} \log \frac{\gamma_{kk}}{\gamma})$ **step 1'.** simulation of z_i according to $\mathcal{M}(\tilde{z}_{i1}, \ldots, \tilde{z}_{ip})$ step 2. $\pi_k = \frac{\widetilde{z}_{,k}}{n}, \gamma_{kk} = \frac{\sum_i \widetilde{z}_{ik} x_{jk}^{\widetilde{\mathbf{W}}}}{\widetilde{x}_{,k}^{\widetilde{\mathbf{Z}}} x_{,k}^{\widetilde{\mathbf{W}}}} = \frac{\widetilde{x}_{kk}^{\widetilde{\mathbf{Z}}}}{\widetilde{x}_{,k}^{\widetilde{\mathbf{Z}}} x_{,k}^{\widetilde{\mathbf{W}}}}, \gamma = \frac{N - \sum_k x_{kk}^{\widetilde{\mathbf{Z}}} x_{kk}^{\widetilde{\mathbf{W}}}}{N^2 - \sum_k x_{kk}^{\widetilde{\mathbf{Z}}} x_{,k}^{\widetilde{\mathbf{W}}}}$ $\widetilde{X}_{ki} = \sum_{i} \widetilde{z}_{ik} x_{ii}$ step 3. $\widetilde{w}_{ik} \propto \rho_k \exp(x_{ki}^{\widetilde{\mathbf{Z}}} \log \frac{\gamma_{kk}}{\gamma_{ki}})$ **step 3'.** simulation of w_i according to $\mathcal{M}(\widetilde{w}_{i1}, \ldots, \widetilde{w}_{ig})$ step 4. $\rho_k = \frac{\widetilde{w}_{,k}}{d}, \gamma_{kk} = \frac{\sum_j \widetilde{w}_{jk} \chi_{kj}^{\widetilde{Z}}}{\sqrt{\Sigma} \chi \widetilde{W}} = \frac{\chi_{kk}^{\widetilde{Z}}}{\sqrt{\Sigma} \chi \widetilde{W}}, \gamma = \frac{N - \sum_k \chi_{kk}^{\widetilde{Z}} \widetilde{W}}{N^2 - \sum_k \chi^2 \chi \widetilde{W}}$ until Convergence: **Output :** Z, W, π_k , ρ_k , γ_{kk} , γ

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Weakness : SPLBsem does not share the convergence properties of SPLBvem and SPLBcem and may require a large number of iterations to reach a steady state

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The stochastic SPLBM-based co-clustering algorithm (SPLBsem)

Algorithm 5: SPLBsem

Input: X, g Initialization : $\widetilde{\mathbf{Z}}$, $\widetilde{\mathbf{W}}$, π_k , ρ_k , γ_{kk} , γ repeat $x_{ik}^{\widetilde{\mathbf{W}}} = \sum_{i} \widetilde{\mathbf{W}}_{ik} x_{ii}$ step 1. $\widetilde{z}_{ik} \propto \pi_k \exp(x_{ik}^{\widetilde{\mathbf{W}}} \log \frac{\gamma_{kk}}{\gamma})$ **step 1'.** simulation of z_i according to $\mathcal{M}(\tilde{z}_{i1},\ldots,\tilde{z}_{ip})$ step 2. $\pi_k = \frac{\widetilde{z}_{,k}}{n}, \gamma_{kk} = \frac{\sum_i \widetilde{z}_{ik} x_{jk}^{\widetilde{\mathbf{W}}}}{\widetilde{x}_{,k}^{\widetilde{\mathbf{Z}}} x_{,k}^{\widetilde{\mathbf{W}}}} = \frac{\widetilde{x}_{kk}^{\widetilde{\mathbf{Z}}}}{\widetilde{x}_{,k}^{\widetilde{\mathbf{Z}}} x_{,k}^{\widetilde{\mathbf{W}}}}, \gamma = \frac{N - \sum_k x_{kk}^{\widetilde{\mathbf{Z}}} x_{kk}^{\widetilde{\mathbf{W}}}}{N^2 - \sum_k x_{kk}^{\widetilde{\mathbf{Z}}} x_{,k}^{\widetilde{\mathbf{W}}}}$ $\widetilde{X}_{ki} = \sum_{i} \widetilde{z}_{ik} x_{ii}$ step 3. $\widetilde{w}_{ik} \propto \rho_k \exp(x_{ki}^{\widetilde{\mathbf{Z}}} \log \frac{\gamma_{kk}}{\gamma})$ **step 3'.** simulation of w_i according to $\mathcal{M}(\widetilde{w}_{i1}, \ldots, \widetilde{w}_{ig})$ step 4. $\rho_k = \frac{\widetilde{\mathbf{w}}_{,k}}{d}, \gamma_{kk} = \frac{\sum_j \widetilde{\mathbf{w}}_{jk} \widetilde{\mathbf{X}}_{kj}^{\widetilde{\mathbf{Z}}}}{\sqrt{\Sigma} \sqrt{W}} = \frac{x_{kk}^{\widetilde{\mathbf{Z}}}}{x_{kk}^{\widetilde{\mathbf{Z}}} \sqrt{W}}, \gamma = \frac{N - \sum_k x_{kk}^{\widetilde{\mathbf{Z}}} \widetilde{\mathbf{X}}}{N^2 - \sum_k x_{kk}^{\widetilde{\mathbf{Z}}} \sqrt{W}}$ until Convergence: **Output :** Z, W, π_k , ρ_k , γ_{kk} , γ

Advantages : It does not stop at the first stationary point of the likelihood function, which makes it possible to avoid bad local maxima due to the initial position

Weakness : SPLBsem does not share the convergence properties of SPLBvem and SPLBcem and may require a large number of iterations to reach a steady state

• Solution ⇒ initialize SPLBvem with the parameters resulting from SPLBsem ⇒ SPLBsvem

Sparse Poisson Latent Block Model (SPLBM) Soft SPLBM-based Co-clustering Algorithm Hard SPLBM-based Co-clustering Algorithm Experiments

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Global Performance Comparison - Document Clustering

Datasets	Characteristics								
	#Documents	#Words	#Clusters	Sparsity (%)	Balance				
SPORTS	8580	14870	7	99.14	0.036				
TDT2	9394	36771	30	99.64	0.028				
Yahoo_K1B	2340	21839	6	99.41	0.043				
Reuters40	8203	18914	40	99.75	0.003				

Data : contingency tables

 Evaluation measures : Acc, NMI (Strehl and Ghosh, 2003) and ARI (Rand, 1971)

Comparative study

- Proposed diagonal co-clustering : Coclus, SPLBcem, SPLBvem, SPLBsem, SPLBsvem
- Non-diagonal co-clustering : ITČC (I. S. Dhillon, Mallela, and D. S. Modha, 2003), PLBvem (Govaert and Nadif, 2010) and LDA (Blei, Ng, and Jordan, 2003)
- Clustering : Spherical kmeans (I. Dhillon and D. Modha, 2001)

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- Clustering : Spherical kmeans (I. Dhillon and D. Modha, 2001)

datasets	per.	Skmeans	ITCC	LDA	PLBvem	C oClus	S PLBcem	SPLBvem	SPLBsem	SPLBsvem
SPORTS	Acc	0.49	0.53	0.53	0.47	0.75	0.85	0.85	0.86	0.81
	NMI	0.50	0.60	0.54	0.64	0.62	0.69	0.70	0.71	0.67
	ARI	0.30	0.44	0.33	0.49	0.55	0.76	0.75	0.77	0.69
TDT2	Acc	0.57	0.59	0.60	0.59	0.87	0.83	0.84	0.84	0.85
	NMI	0.76	0.78	0.73	0.76	0.84	0.81	0.82	0.84	0.84
	ARI	0.46	0.52	0.49	0.51	0.85	0.81	0.80	0.85	0.85
Yahoo_K1B	Acc	0.57	0.61	0.62	0.58	0.60	0.79	0.84	0.86	0.88
_	NMI	0.64	0.58	0.58	0.62	0.54	0.66	0.69	0.72	0.75
	ARI	0.39	0.40	0.37	0.38	0.31	0.60	0.72	0.76	0.79
REUTERS40	Acc	0.26	0.27	0.47	0.25	0.61	0.73	0.74	0.73	0.77
	NMI	0.50	0.52	0.51	0.52	0.54	0.57	0.58	0.57	0.62
	ARI	0.11	0.18	0.42	0.15	0.51	0.71	0.75	0.73	0.76

- Diagonal co-clustering are better in almost all situations
- . In particular the SPLBsvem which leverages the benefits of both soft and stochastic variants

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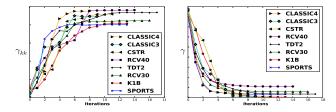
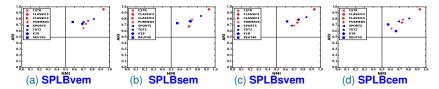


Figure: Behaviour of the γ_{kk} 's (left) and γ (right) parameters at each iteration.

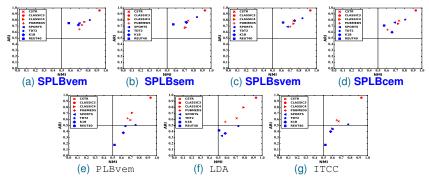
Sparse Poisson Latent Block Model (SPLBM) Soft SPLBM-based Co-clustering Algorithm Hard SPLBM-based Co-clustering Algorithm Experiments

· The proposed diagonal approaches deal well with unbalanced datasets

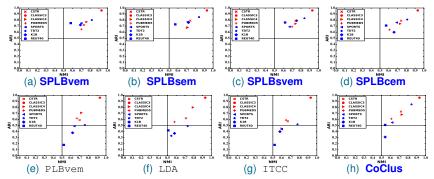
- The proposed diagonal approaches deal well with unbalanced datasets
- The diagonal approaches reach good performance in both NMI and ARI on unbalanced datasets
- · ARI, unlike NMI, is more sensitive to cluster merging/splitting



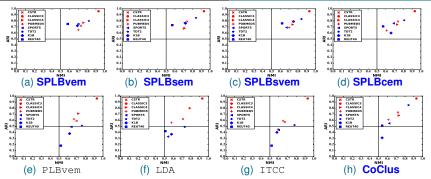
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- The proposed diagonal approaches deal well with unbalanced datasets
- The diagonal approaches reach good performance in both NMI and ARI on unbalanced datasets
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Sparse Poisson Latent Block Model (SPLBM) Soft SPLBM-based Co-clustering Algorithm Hard SPLBM-based Co-clustering Algorithm Experiments



- Comparison of the standard deviation in cluster size (SDCS) of clusters obtained by each method SDCS = $\left(\frac{1}{k-1}\sum_{k=1}^{g}(z_k - \frac{n}{g})^2\right)^{0.5}$
- . The SDCS values of the clusters obtained with SPLBcem are the closest to the real SDCS of the datasets

	Clustering	Co-clustering				
Data		Non-diagonal			Diagonal	Real SDCS
	Skmeans	ITCC	LDA	PLBcem	SPLBcem	
REUTERS40	112.638	144.195	362.102	201.162	642.839	654.556
REUTERS30	161.797	238.353	414.568	261.291	752.129	747.879
K1B	154.3684	198.828	261.765	189.849	336.555	513.303
TDT2	154.143	216.152	189.609	235.698	516.685	481.830
SPORTS	760.099	346.066	482.714	393.510	1359.321	1253.011

Sparse Poisson Latent Block Model (SPLBM) Soft SPLBM-based Co-clustering Algorithm Hard SPLBM-based Co-clustering Algorithm Experiments

Assessing the Quality of Term Clusters

- Lack of benchmark datasets providing the true cluster labels of both the objects and attributes.
- Most studies evaluate the co-clustering algorithms based on the object (document) clustering only.
- · We propose two different approaches to evaluate term clusters :
 - · Visual assessment of term cluster coherence
 - · Quantitative evaluation of term cluster quality
- We use a biomedical document-term matrix, namely the PUBMED5 dataset.
- PUBMED5 dataset is a document-term matrix of size 12648 × 19518 that contains documents about 5 different diseases.

Disease	Number of documents
Migraine	
Age-related Macular Degeneration	
	2596
Kidney Calculi	1549
Hay Fever	1517

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Disease	Number of documents	
Migraine	3703	
Age-related Macular Degeneration	3283	
Otitis	2596	
Kidney Calculi	1549	
Hay Fever	1517	

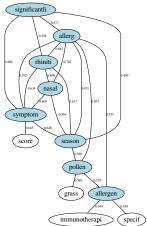
Sparse Poisson Latent Block Model (SPLBM) Soft SPLBM-based Co-clustering Algorithm Hard SPLBM-based Co-clustering Algorithm Experiments

Visual assessment of term cluster coherence

Assess if the top terms present in a co-cluster are densely interconnected and form a semantically coherent set.

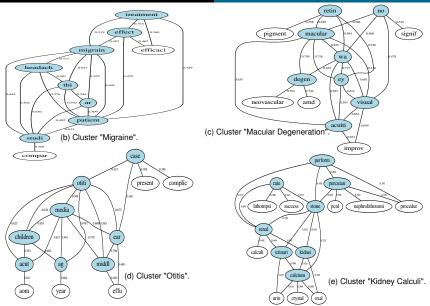
Principle

- Co-clustering with SPLBcem on the PUBMED5 dataset into g = 5 blocks
- Por each diagonal block c, we extract the corresponding matrix X_c
- **3** Build a term-term cosine similarity matrix $S_c = X_c^{norm'} X_c^{norm}$ for each diagonal block
- 4 Place the n = 8 top terms of c in a graph
- Connect each top word their k = 5 most similar neighbors according to the cosine similarity recorded in S_c



(a) Cluster "Hay fever".

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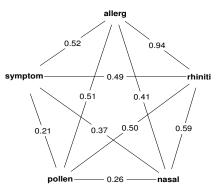
Quantitative evaluation of term cluster quality

Principle

 Use the Point-wise Mutual Information (PMI) to measure the degree of association between word pairs

$$\mathsf{PMI}(w_i, w_j) = \log \frac{p(w_i, w_j)}{p(w_i)p(w_j)}$$

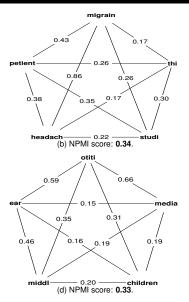
- PMI can be estimated using an external corpus
- Use the whole English WIKIPEDIA corpus that consists of approximately 4 millions of documents and 2 billions of words
- The NPMI(w_i, w_j) = $\frac{PMI(w_i, w_j)}{-\log(p(w_i, w_j))}$ ranges between -1 and +1, the higher the NPMI, the greater the correlation between words w_i and w_j

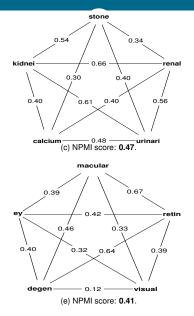


(a) NPMI score: 0.48.

Introduction

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- From this model, three co-clustering algorithms have been inferred
 - A hard variant SPLBcem
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 - A stochastic variant SPLBsem
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 - · Reduce the computational time
 - · Robust against highly unbalanced datasets
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Context

- Exponential growth of biomedical text data (PUBMED, GO, ...)
- There is a genuine need for text mining techniques to analyse and interpret these large amounts of information
- Help researchers to characterize relationships between biomedical entities (genes, diseases, ...) quickly and efficiently

Motivations

- Genome-wide association studies (GWAS) : examination of many genetic variants (SNPs) in different individuals to study their correlations with phenotypic traits
- · GWAS allow to identify groups of genes associated with a common phenotype
- · GWAS do not provide information about associations in these gene groups

Contributions

- A biomedical text mining framework (Ailem et al., 2016) to augment the results of GWAS
- · Benefits of co-clustering in biomedical text mining application
- Illustration on GWAS of asthma disease (Moffatt et al., 2010), which reported 10 genes associated with asthma
- Assess the strength of association between these genes and infer new candidate genes likely associated with asthma

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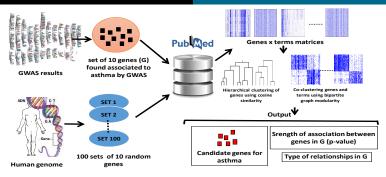
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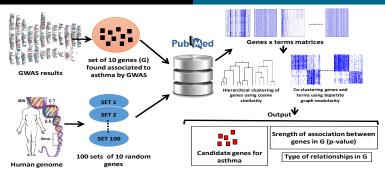
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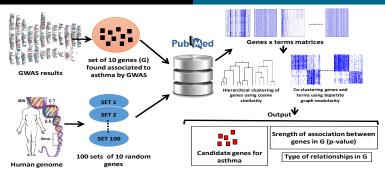
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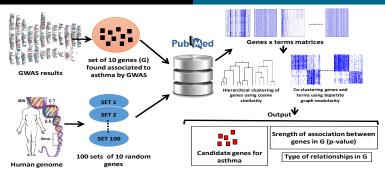
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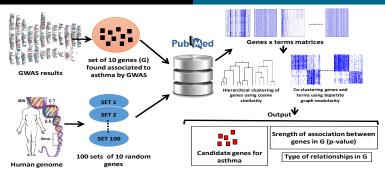


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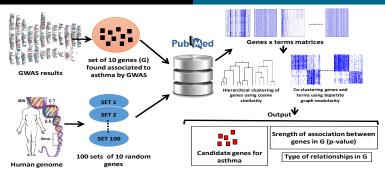
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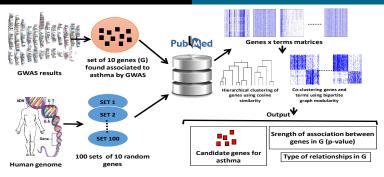
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New candidate genes for asthma

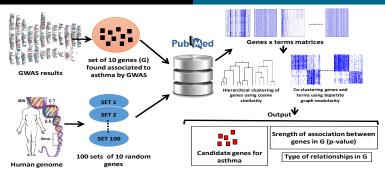
The Biomedical Framework Results and Discussions



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The Biomedical Framework Results and Discussions

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- Introduction
 - Context
 - Co-clustering
 - Motivations
- 2 Graph-based Co-clustering
 - Graph Modularity
 - Modularity for Co-clustering
 - Experiments
- 3 Model-based Co-clustering
 - Sparse Poisson Latent Block Model (SPLBM)
 - Soft SPLBM-based Co-clustering Algorithm
 - Hard SPLBM-based Co-clustering Algorithm
 - Experiments

Using Co-clustering in Biomedical Text Mining Framework

- The Biomedical Framework
- Results and Discussions

Conclusion and Perspectives

The Biomedical Framework Results and Discussions

Results and Discussions

- The mean cosine similarities of asthma gene vectors is greater than would be expected by chance (empirical p-value < 1%)
- Application of clustering and co-clustering to 100 sets of 20 genes that each included the 10 asthma genes plus 10 random genes, returned an average purity of 89%
- 20 Top terms of asthma genes co-cluster

Smoking immune-mediated child immunohistochemistry drug

diabetes chronic microenvironment childhood inflammation th2 enterotoxin cytokine influenza crohn environmental proinflammatory autoimmune asthma necrosis

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The Biomedical Framework Results and Discussions

Candidate genes for asthma

- Moreover, 104 random genes were grouped with the 10 asthma associated-genes and, therefore, might be new candidates for asthma
- We ranked these candidate genes according to their cosine similarity with the group of asthma genes (G)
- Study the Top 20 genes
- · Use the biomedical literature and experts to validate the results

IL1RL1	RAG1	CLEC1B	IL23R
STAT6	EFNA3	S1PR5	TGFBR1
FCMR		CHRNB4	NFKB1
TNFRSF1A	TMED1	NOD2	TSLP
NLRP10	POMP	SPINK1	

- Reported associated with asthma or allergy
- · Reported associated with auto-immune diseases
- · Encode proteins that are involved in immune-related mechanisms

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Main contributions

Three main contributions

- Graph-based Diagonal co-clustering approach
 Model-based Diagonal co-clustering approach
 Using Co-clustering for Biomedical Text Mining
- · Assessing the right number of co-clusters
- Methods for assessing term clusters
- · Soft, hard and stochastic assignments
- · Extensive experiments on real world text datasets
- Availability : Coclust python module (https://pypi.python.org/pypi/coclust)

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Toward Semantic (co)-clustering

Motivation

 Existing (co)-clustering methods ignore the semantic relationships between words, which may result in a significant loss of semantics since documents that are about the same topic may not necessarily use exactly the same vocabulary.

Contribution

- We propose a new (co)-clustering models which goes beyond the bag of word representation so as to preserve more semantics.
- We achieve our objective by successfully integrating word2vec into a (co)-clustering framework.
- The proposed models substantially outperforms existing (co)-clustering models in terms of document clustering, cluster interpretability as well as document/word embedding.

M. Ailem, A. Salah, and M. Nadif (2017). "Non-negative Matrix Factorization Meets Word Embedding". In: *SIGIR*. ACM, pp. 1081–1084.

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A. Salah, M. Ailem, and M. Nadif (2018). "Word Co-occurrence Regularized Non-Negative MatrixTri-Factorization for Text Data Co-clustering". In: AAAI'2018.



- Investigate an overlapping version of the Coclus algorithm
- Study the theoretical link between graph-based and model-based approaches
- Assessing the number of (co-)clusters for model-based approaches using information criteria such as BIC, AIC, ICL ...
- Investigate Bayesian non-parametric formulations of SPLBM, which would allows us to overcome the problem of the number of clusters as well as handle evolving data

Thank you for your attention!

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