Modèles de graphes aléatoires pour l'analyse des réseaux

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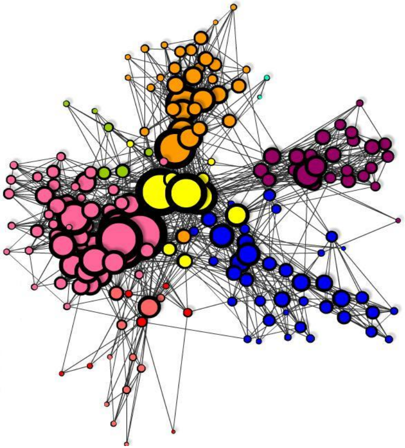
Contents

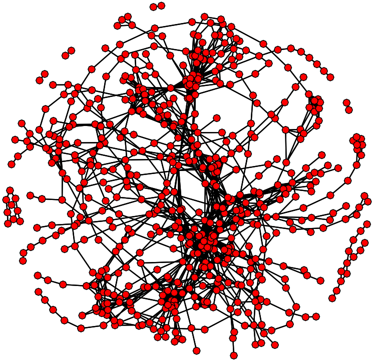
Real networks

- **Many scientific fields** :
  - World Wide Web
  - Biology, sociology, physics
- **Nature of data under study**:
  - Interactions between N objects
  - $\mathcal{O}(N^2)$ possible interactions
- **Network topology** :
  - Describes the way nodes interact, structure/function relationship



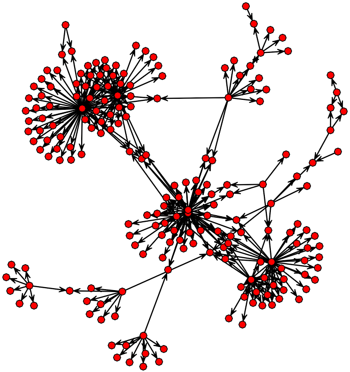
Sample of 250 blogs (nodes) with their links (edges) of the French political Blogosphere.

In Biology



The metabolic network of bacteria *Escherichia coli* (Lacroix et al., 2006).

In Biology



Subset of the yeast transcriptional regulatory network (Milo et al., 2002).

Real networks

- **Properties** :
  - Sparsity : $m = \mathrm{O}(N)$
  - Existence of a giant component
  - Heterogeneity
  - Preferential attachment
  - Small world

$\hookrightarrow$ Topological structure (groups of vertices)

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Graph clustering

- **Existing methods look for** :
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  - Disassortative mixing
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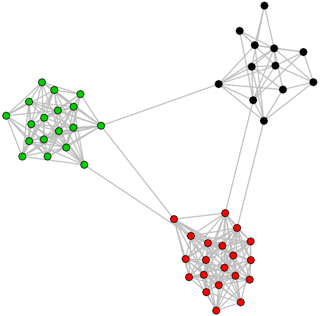

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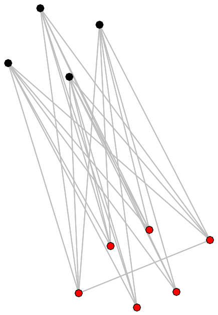

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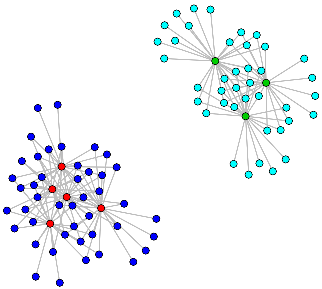


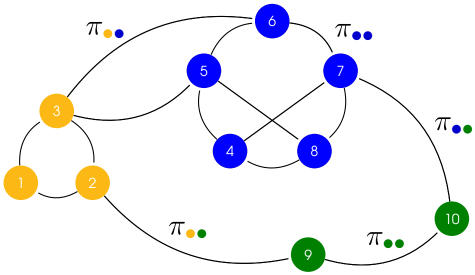
Stochastic Block Model (SBM)

- Nowicki and Snijders (2001)
  - Earlier work : Govaert et al. (1977)
- $\mathbf{Z}_i$ independent hidden variables :
  - $\mathbf{Z}_i \sim \mathcal{M}\Big(1,\ \boldsymbol{\alpha} = (\alpha_1, \alpha_2, \dots, \alpha_K)\Big)$
  - $Z_{ik} = 1$: vertex i belongs to class k
- $\mathbf{X} \,|\, \mathbf{Z}$ edges drawn independently :

$$X_{ij} | \{Z_{ik} Z_{jl} = 1\} \sim \mathcal{B}(\pi_{kl})$$

- A mixture model for graphs :

$$X_{ij} \sim \sum_{k=1}^{K} \sum_{l=1}^{K} \alpha_k \alpha_l \mathcal{B}(\pi_{kl})$$



$\pi_{\bullet\bullet}$
6
$\pi_{\bullet\bullet}$
5
7
3
$\pi_{\bullet\bullet}$
4
8
1
2
10
$\pi_{\bullet\bullet}$
$\pi_{\bullet\bullet}$
9

Maximum likelihood estimation

- **Log-likelihoods of the model** :
  - Observed-data : $\log p(\mathbf{X} \mid \boldsymbol{\alpha}, \boldsymbol{\Pi}) = \log \left\{\sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\alpha}, \boldsymbol{\Pi})\right\}$
    $\hookrightarrow$ K^N terms
- Expectation Maximization (EM) algorithm requires the knowledge of $p(\mathbf{Z} \mid \mathbf{X}, \boldsymbol{\alpha}, \boldsymbol{\Pi})$

Problem

$p(\mathbf{Z} \mid \mathbf{X}, \boldsymbol{\alpha}, \boldsymbol{\Pi})$ is not tractable (no conditional independence)

Variational EM

Daudin et al. (2008)

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Criteria

Since $\log p(\mathbf{X} \,|\, \boldsymbol{\alpha}, \boldsymbol{\Pi})$ is not tractable, we *cannot* rely on:

- $AIC = \log p(\mathbf{X} \,|\hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\Pi}}) - C$
- $BIC = \log p(\mathbf{X} \,|\hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\Pi}}) - \frac{C}{2} \log \frac{N(N-1)}{2}$

ICL

Biernacki et al. (2000) $\hookrightarrow$ Daudin et al. (2008)

Variational Bayes EM $\hookrightarrow$ $ILvb$

Latouche et al. (2012)

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Bayesian framework

- **Conjugate prior distributions** :
  - $p\Big(\boldsymbol{\alpha} \,|\, \mathbf{n}^0 = \{n_1^0, \dots, n_K^0\}\Big) = \mathrm{Dir}(\boldsymbol{\alpha};\ \mathbf{n}^0)$
  - $p\Big(\boldsymbol{\Pi} \,|\, \boldsymbol{\eta}^0 = (\eta_{kl}^0), \boldsymbol{\zeta}^0 = (\zeta_{kl}^0)\Big) = \prod_{k \leq l} \mathrm{Beta}(\pi_{kl};\ \eta_{kl}^0, \zeta_{kl}^0)$
- **Non informative Jeffreys prior** :
  - $n_k^0 = 1/2$
  - $\eta_{kl}^0 = \zeta_{kl}^0 = 1/2$

- $p(\mathbf{Z}, \boldsymbol{\alpha}, \boldsymbol{\Pi} \,|\, \mathbf{X})$ not tractable

Decomposition

$$\log p(\mathbf{X}) = \mathcal{L}\,(q) + \mathrm{KL}\,(q(\cdot) \,||\, p(\cdot \,|\, \mathbf{X}))$$

where

$$\mathcal{L}(q) = \sum_{\mathbf{Z}} \int \int q(\mathbf{Z}, \boldsymbol{\alpha}, \boldsymbol{\Pi}) \log \left\{ \frac{p(\mathbf{X}, \mathbf{Z}, \boldsymbol{\alpha}, \boldsymbol{\Pi})}{q(\mathbf{Z}, \boldsymbol{\alpha}, \boldsymbol{\Pi})} \right\} d\,\boldsymbol{\alpha}\, d\,\boldsymbol{\Pi}$$

Factorization

$$q(\mathbf{Z}, \boldsymbol{\alpha}, \boldsymbol{\Pi}) = q(\boldsymbol{\alpha})q(\boldsymbol{\Pi})q(\mathbf{Z}) = q(\boldsymbol{\alpha})q(\boldsymbol{\Pi}) \prod_{i=1}^{N} q(\mathbf{Z}_i)$$

Variational Bayes EM
Latouche et al. (2009)

E-step

- $q(\mathbf{Z}_i) = \mathcal{M}(\mathbf{Z}_i;\ 1, \boldsymbol{\tau_i} = \{\tau_{i1}, \dots, \tau_{iK}\})$

M-step

- $q(\boldsymbol{\alpha}) = \text{Dir}(\alpha;\ \mathbf{n})$
- $q(\mathbf{\Pi}) = \prod_{k \leq l}^{K} \text{Beta}(\pi_{kl};\ \eta_{kl}, \zeta_{kl})$

A new model selection criterion : ILvb
Latouche et al. (2012)

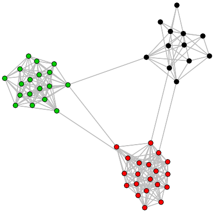
- $\log p(\mathbf{X}\,|K) = \mathcal{L}\,(q) + \mathrm{KL}(...)$
- After convergence, use $\mathcal{L}\,(q)$ as an approximation of $\log p(\mathbf{X}\,|K)$

ILvb

$$IL_{vb} = \log\left\{\frac{\Gamma(\sum_{k=1}^{K} n_k^0)\prod_{k=1}^{K}\Gamma(n_k)}{\Gamma(\sum_{k=1}^{K} n_k)\prod_{k=1}^{K}\Gamma(n_k^0)}\right\} + \sum_{k\leq l}^{K}\log\left\{\frac{\Gamma(\eta_{kl}^0+\zeta_{kl}^0)\Gamma(\eta_{kl})\Gamma(\zeta_{kl})}{\Gamma(\eta_{kl}+\zeta_{kl})\Gamma(\eta_{kl}^0)\Gamma(\zeta_{kl}^0)}\right\} - \sum_{i=1}^{N}\sum_{k=1}^{K}\tau_{ik}\log\tau_{ik}$$

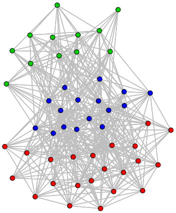
- **Two topological structures** :
  - Affiliation :

$$\mathbf{\Pi} = \begin{pmatrix} \lambda & \epsilon & \dots & \epsilon \\ \epsilon & \lambda & & \vdots \\ \vdots & & \ddots & \epsilon \\ \epsilon & \dots & \epsilon & \lambda \end{pmatrix}$$



  - Affiliation and a class of hubs :

$$\mathbf{\Pi} = \begin{pmatrix} \lambda & \epsilon & \dots & \epsilon & \lambda \\ \epsilon & \lambda & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \lambda & \dots & \dots & \dots & \lambda \end{pmatrix}$$



Affiliation networks

(a) $Q_{True} \backslash Q_{VBMOD}$

	2	3	4	5	6	7
3	0	100	0	0	0	0
4	0	0	100	0	0	0
5	0	0	0	**100**	0	0
6	0	0	0	0	**97**	3
7	0	0	0	2	14	**84**

(b) $Q_{True} \backslash Q_{ILvb}$

	2	3	4	5	6	7
3	0	100	0	0	0	0
4	0	0	100	0	0	0
5	0	0	0	**99**	1	0
6	0	0	4	23	**73**	0
7	0	2	14	44	27	**13**

Affiliation networks and a class of hubs

(c) $Q_{True} \backslash Q_{VBMOD}$

	2	3	4	5	6	7
3	95	**0**	3	0	0	2
4	1	95	**4**	0	0	0
5	0	0	94	**6**	0	0
6	0	0	1	83	**16**	0
7	0	0	2	15	78	**5**

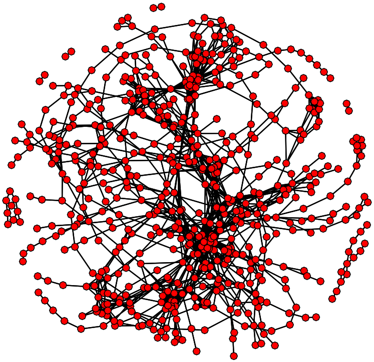
(d) $Q_{True} \backslash Q_{ILvb}$

	2	3	4	5	6	7
3	0	**100**	0	0	0	0
4	0	0	**100**	0	0	0
5	0	0	2	**98**	0	0
6	0	0	1	29	**70**	0
7	0	0	3	34	45	**18**

Experiments on the metabolic network of ecoli

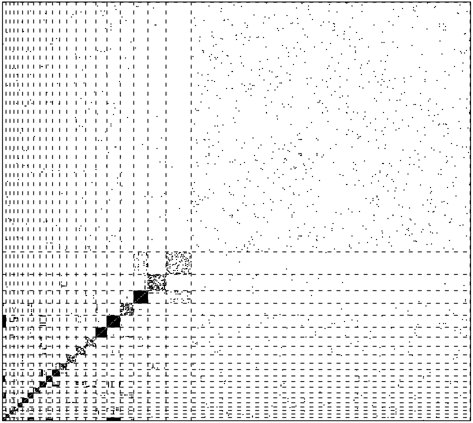
- Lacroix et al. (2006)
- Lab : Biométrie et Biologie Évolutive (Lyon 1)
- Represents pathways of biochemical reactions
- 605 vertices, 1782 edges

The metabolic network of ecoli



The metabolic network of bacteria *Escherichia coli* (Lacroix et al., 2006).

Results (1)



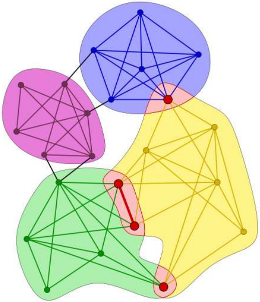
Dot plot representation of the metabolic network after classification of the vertices into $Q_{VB} = 22$ classes.

Results (2)

- Among the classes, eight are cliques
- Six have within probability connectivity greater than 0.5
- Cliques and pseudo-cliques gather reactions involving a same compound
  - Responsible for cliques : chorismate, pyruvate, L-aspartate, L-glutamate, D-glyceraldehyde-3-phosphate and ATP
- Classes 1 and 17 both associated to pyruvate

Contents

Overlaps in networks



Palla et al. (2006)

Problem

The stochastic block model (SBM) and most existing methods assume that each vertex belongs to a single class

Stochastic Block Model (SBM)

- Nowicki and Snijders (2001)
- $\mathbf{Z}_i$ independent hidden variables :

$$\mathbf{Z}_i \sim \mathcal{M}\Big(1,\ \boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_K)\Big)$$

Overlapping Stochastic Block model (OSBM)

- Latouche et al. (2011)
- Z_{ik} independent hidden variables :

$$\mathbf{Z}_i \sim \prod_{k=1}^{K} \mathcal{B}(Z_{ik};\ \alpha_k) = \prod_{k=1}^{K} \alpha_k^{Z_{ik}} (1 - \alpha_k)^{1 - Z_{ik}}$$

Overlapping Stochastic Block model (OSBM)

- Latouche et al. (2011)
- $\mathbf{X} \mid \mathbf{Z}$ edges drawn independently :

$$X_{ij} \mid \mathbf{Z}_i, \mathbf{Z}_j \sim \mathcal{B}\big(X_{ij};\, \mathbf{\Pi}_{\mathbf{Z}_i,\mathbf{Z}_j}\big)\big)$$

- $\mathbf{\Pi}_{\mathbf{Z}_i,\mathbf{Z}_j} = g\big(a_{\mathbf{Z}_i,\mathbf{Z}_j}\big)$
- $a_{\mathbf{Z}_i,\mathbf{Z}_j} = \underbrace{\mathbf{Z}_i^{\intercal}\, \mathbf{W}\, \mathbf{Z}_j}_{i \leftrightarrow j} + \underbrace{\mathbf{Z}_i^{\intercal}\, \mathbf{U}}_{i \rightarrow ?} + \underbrace{\mathbf{V}^{\intercal}\, \mathbf{Z}_j}_{? \rightarrow j} + \underbrace{W^*}_{\text{bias}}$
- $g(t) = 1/\left(1 + \exp(-t)\right)$ is the logistic function

Experiments on simulated data

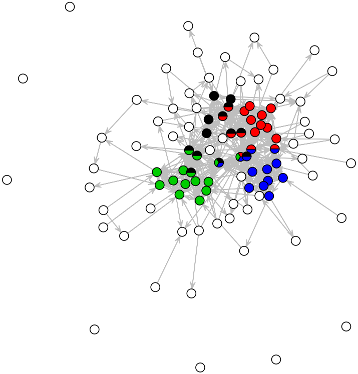
- **Two topological structures** :
  - Community structures (affiliation) :

$$\mathbf{W} = \begin{pmatrix} \boldsymbol{\lambda} & -\epsilon & \dots & -\epsilon \\ -\epsilon & \boldsymbol{\lambda} & & \vdots \\ \vdots & & \ddots & -\epsilon \\ -\epsilon & \dots & -\epsilon & \boldsymbol{\lambda} \end{pmatrix}$$

  - Community structures and stars :

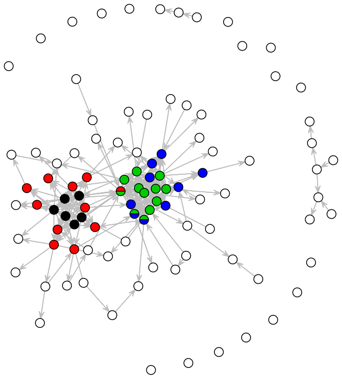
$$\mathbf{W} = \begin{pmatrix} \boldsymbol{\lambda} & \boldsymbol{\lambda} & -\epsilon & \dots & \dots & \dots & -\epsilon \\ \boldsymbol{-\epsilon} & \boldsymbol{-\lambda} & -\epsilon & \dots & \dots & \dots & \vdots \\ \vdots & -\epsilon & \boldsymbol{\lambda} & \boldsymbol{\lambda} & -\epsilon & \dots & \vdots \\ \vdots & \vdots & \boldsymbol{-\epsilon} & \boldsymbol{-\lambda} & -\epsilon & \dots & \vdots \\ \vdots & \vdots & \vdots & -\epsilon & \ddots & -\epsilon & -\epsilon \\ \vdots & \vdots & \vdots & \vdots & -\epsilon & \boldsymbol{\lambda} & \boldsymbol{\lambda} \\ -\epsilon & \dots & \dots & \dots & \dots & \boldsymbol{-\epsilon} & \boldsymbol{-\lambda} \end{pmatrix}$$

Community structures



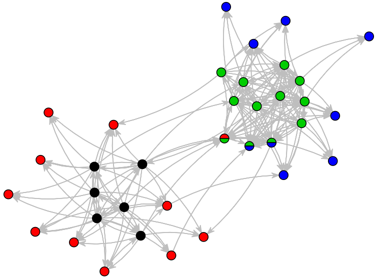
Example of an overlapping stochastic block model (OSBM) network with community structures.

Community structures and stars



Example of an overlapping stochastic block model (OSBM) network with community structures and stars.

Community structures and stars



Example of an overlapping stochastic block model (OSBM) network with community structures and stars.

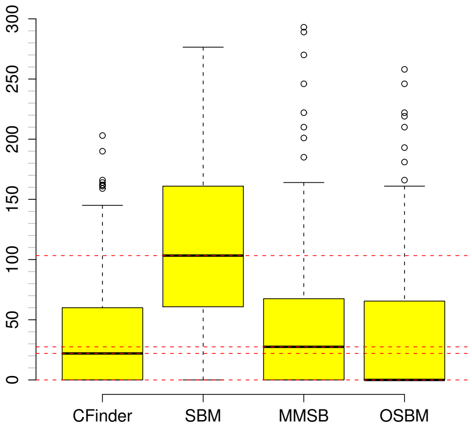
Experiments on simulated data

- $N = 100$
- $\lambda = 4$
- $\epsilon = 1$
- $W^* = -5.5$
- $\mathbf{U} = \mathbf{V} = \begin{pmatrix} \epsilon & \dots & \epsilon \end{pmatrix}$
- $\alpha_k = 0.25$
- $K = 4$
- 100 simulations
- 4 graph clustering methods :
  - CFinder (Palla et al. 2006)
  - Stochastic Block Model (SBM)
  - Mixed Membership Stochastic Block Model (MMSB) (Airoldi et al. 2008)
  - Overlapping Stochastic Block Model (OSBM)

How to compare the methods ?

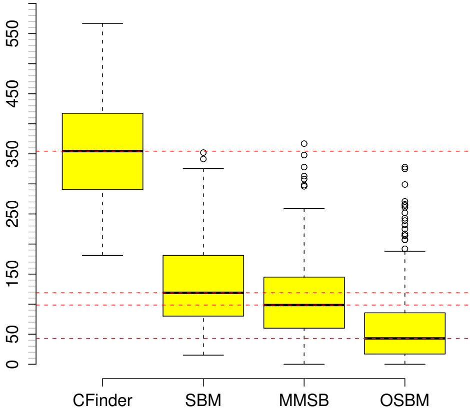
- CFinder and OSBM can deal with outliers ($\mathbf{Z}_i = \mathbf{0}$)
- SBM and MMSB are run with $K+1$ classes
  $\hookrightarrow$ identify the class of outliers
- Compute $\mathbf{P} = \mathbf{Z}\,\mathbf{Z}^\intercal$ and $\hat{\mathbf{P}} = \hat{\mathbf{Z}}\hat{\mathbf{Z}}^\intercal$:
  - invariant to column permutations of $\mathbf{Z}$ and $\hat{\mathbf{Z}}$
  - number of shared clusters between each pair of vertices
- Compute L_2 distance $d(\mathbf{P}, \hat{\mathbf{P}})$

Community structures



L_2 distance $d(\mathbf{P}, \hat{\mathbf{P}})$ over the 100 samples of networks with community structures for CFinder, SBM, MMSB and OSBM.

Community structures and stars



L_2 distance $d(\mathbf{P}, \hat{\mathbf{P}})$ over the 100 samples of networks with community structures for CFinder, SBM, MMSB and OSBM.

Model selection

- Community structure
- $N = 100$
- $\epsilon = 1$
- $W^* = -5.5$
- $\alpha_k = 1/K$
- $K_{True} \in \{3, \ldots, 7\}$
- $K \in \{2, \ldots, 8\}$
- 100 simulations

Results

Table: $K_{True} \backslash K_{IL_{osbm}} (p_{intra} \approx 0.92)$

	2	3	4	5	6	7	8
3	0	**99**	1	0	0	0	0
4	0	0	**99**	1	0	0	0
5	0	0	0	**93**	5	2	0
6	0	0	0	7	**64**	22	7
7	0	0	0	0	16	**47**	37

Results

Table: $K_{True} \backslash K_{IL_{osbm}} (p_{intra} \approx 0.62)$

	2	3	4	5	6	7	8
3	0	**99**	1	0	0	0	0
4	0	0	**85**	9	5	0	1
5	0	0	4	**53**	26	9	8
6	0	0	0	18	**34**	27	21
7	0	0	0	4	18	**30**	48

The French blogosphere network

	UMP	UDF	liberal	PS	analysts	others
cluster 1	30 + 3	0 + 1	0	0	0 + 1	0
cluster 2	2 + 3	29 + 1	0	0	1 + 3	0
cluster 3	0	0	24	0	1 + 1	0
cluster 4	0	0 + 2	0	40	0 + 4	1
outliers	5	1	1	17	5	30

Classification of the blogs into $K = 4$ clusters using OSBM. 196 vertices, 2864 edges.

Conclusion

- Computational cost : $O(K^4N^2) \neq O(K^2N^2)$
- New model selection criterion : ILosbm
- R package **OSBM** soon available on the CRAN
- Can be used to analyze SBM networks

References

- K. Nowicki and T.A.B. Snijders (2001), Estimation and prediction for stochastic blockstructures. 96, 1077-1087
- E.M. Airoldi, D.M. Blei, S.E. Fienberg, E.P. Xing (2008), Mixed membership stochastic blockmodels. Journal of Machine Learning Research, 9, 1981-2014
- J-J. Daudin, F. Picard et S. Robin (2008), A mixture model for random graphs. Statistics and Computing, 18, 2, 151-171
- P. Latouche, E. Birmelé, C. Ambroise (2011), Overlapping stochastic block models with application to the French political blogosphere network. Annals of Applied Statistics, 5, 1, 309-336
- P. Latouche, E. Birmelé, C. Ambroise (2012), Variational Bayesian inference and complexity control for stochastic block models. Statistical Modelling, 12, 1, 93-115