

# Some statistical approaches in random graph modeling

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# Outline

Molecular interactions networks

Some statistical networks models

- Exponential random graphs

- (Overlapping) Stochastic block models

- Latent space models

Analyzing networks: (probabilistic) node clustering

# Outline

## Molecular interactions networks

### Some statistical networks models

Exponential random graphs

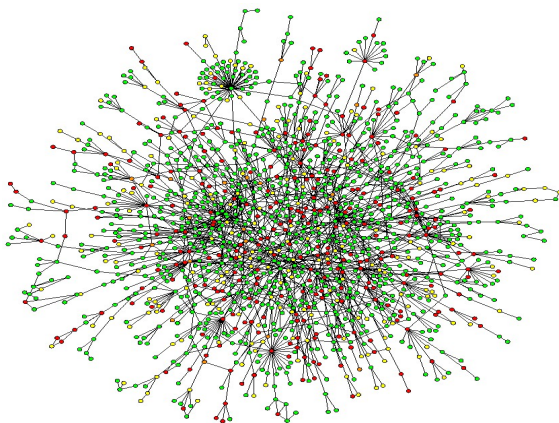
(Overlapping) Stochastic block models

Latent space models

### Analyzing networks: (probabilistic) node clustering

# What kind of networks? (1/3)

## Protein interactions networks (PIN)



**Figure:** Yeast Protein Interaction Network. Source:  
<http://www.bordalierinstitute.com/images/yeastProteinInteractionNetwork.jpg>

# What kind of networks? (1/3)

## Protein interactions networks (PIN)

- ▶ Describe possible **physical interactions** between proteins (formation of protein complex, phosphorylation cascade).
- ▶ Public databases store interactions known from the literature.
- ▶ Many interactions are based on yeast two-hybrid experiments, inducing **many false positive**.

# What kind of networks? (2/3)

## Metabolic networks

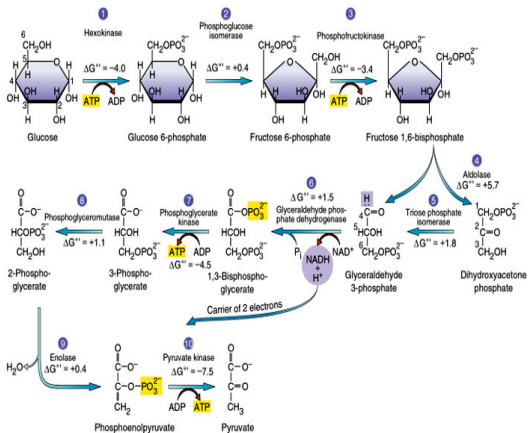


Figure: Glycolysis pathway.

# What kind of networks? (2/3)

## Metabolic networks

- ▶ Describe **chemical reactions** between metabolites (small molecules) transforming a substrate to a product.
- ▶ Most reactions need to be catalyzed by enzymes and are considered to be reversible.
- ▶ The metabolic networks are mostly inferred using comparative genomics techniques, inducing **many false negatives**.
- ▶ Modeled using oriented hypergraphs.

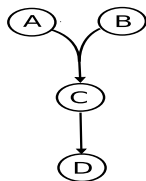


Figure: Oriented hypergraph modeling a metabolic network. Source: V. Lacroix.

# What kind of networks? (3/3)

## Gene regulatory networks

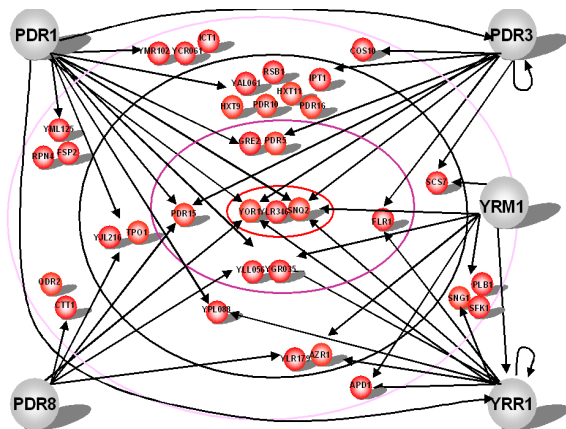


Figure: PDR network in *S. cerevisiae*. Source: Lab. Génomique de la levure, ENS.



# What kind of networks? (3/3)

## Gene regulatory networks

- ▶ Describe regulations (inhibitions or activations) of gene expressions, by other genes.
- ▶ Oriented graph, with positive or negative label.
- ▶ Either static or dynamic (in time).
- ▶ Mostly **statistically inferred** from transcription data sets.

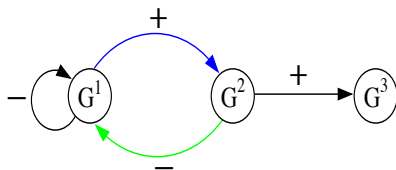


Figure: Example of a regulatory motif. Source: S. Lèbre.

# Challenges

## Main issues

- ▶ Analyzing large data sets (thousands of nodes and edges), with many **noise**.
- ▶ Identifying **structures** (motifs, groups, etc).
- ▶ Observed networks are **sampled** from existing ones.

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Some statistical networks models

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- (Overlapping) Stochastic block models

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Analyzing networks: (probabilistic) node clustering

# Some models

## Some famous models

- ▶ Erdős Rényi random graph
- ▶ Degree distribution (power law, fixed degree sequence, etc)
- ▶ Preferential attachment (dynamic model)
- ▶ ...

Here, we are going to focus on (static) 'statistical' models,

- ▶ Exponential random graph model (ERGM) [Frank & Strauss 86].
- ▶ Stochastic block model or MixNet [Frank & Harary 82, Holland *et al.* 83, Snijders & Nowicki 97, Daudin *et al.* 08].
- ▶ Overlapping stochastic block models (OSBM) [Latouche *et al.* 11a] or mixed membership SBM [Airoldi *et al.* 08].
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We refer to [Goldenberg *et al.* 10] for a recent overview.

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# Exponential random graphs (1/2)

## Notations

- ▶  $X = (X_{ij})_{1 \leq i, j \leq n}$  the (binary) adjacency matrix of the graph
- ▶  $S(X)$  a known vector of graph statistics on  $X$
- ▶  $\theta$  a vector of parameters

$$\mathbb{P}_{\theta}(X = x) = \frac{1}{c(\theta)} \exp(\theta^{\top} S(x)), \quad c(\theta) = \sum_{\text{graphs } y} \exp(\theta^{\top} S(y))$$

## Examples

- ▶  $S(X)$  may contain the number of edges, triangles,  $k$ -stars, ...
- ▶  $S$  may also contain **covariates**.

## Remarks

- ▶  $S(X)$  becomes a vector of **sufficient statistics**
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# Exponential random graphs (2/2)

## Issues on parameter estimation

- ▶ Maximum likelihood estimation is difficult
- ▶ Maximum pseudo-likelihood estimators may be used [Frank & Strauss 86]. **Quality of approximation ?**
- ▶ MCMC approaches [Hunter *et al.* 11]: may be slow to converge
- ▶ Very different values of  $\theta$  can give rise to essentially the same distribution
- ▶ [Chatterjee & Diaconis 11] established a 'degeneracy' of these models, which are 'ill-posed'

## Other issues

- ▶ What about clustering the nodes ?

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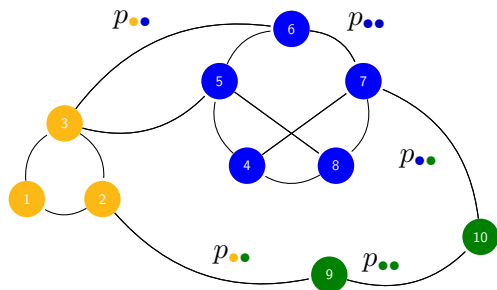
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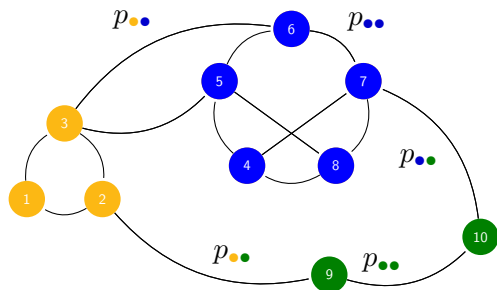


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$$X_{12} = 1, X_{15} = 0$$

## Binary case

- ▶  $Q$  groups (=colors  $\bullet\bullet\bullet$ ).
- ▶  $\{Z_i\}_{1 \leq i \leq n}$  i.i.d. vectors  $Z_i = (Z_{i1}, \dots, Z_{iQ}) \sim \mathcal{M}(1, \pi)$ , where  $\pi = (\pi_1, \dots, \pi_Q)$  group proportions.  $Z_i$  is not observed,
- ▶ Observations: edges indicator  $X_{ij}$ ,  $1 \leq i < j \leq n$ ,
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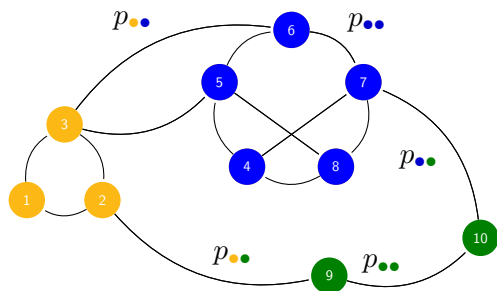
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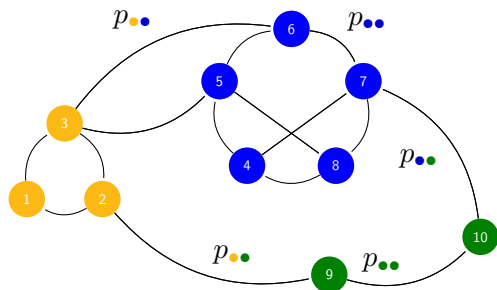


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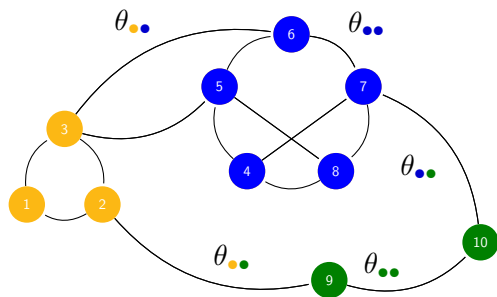
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# Stochastic block model (weighted graphs)



$$n = 10, Z_{5\bullet} = 1$$
$$X_{12} \in \mathbb{R}, X_{15} = 0$$

## Weighted case

- ▶ Observations: weights  $X_{ij}$ , where  $X_{ij} = 0$  or  $X_{ij} \in \mathbb{R}^s \setminus \{0\}$ ,
- ▶ Conditional on the  $\{Z_i\}$ 's, the random variables  $X_{ij}$  are independent with distribution

$$\mu_{Z_i Z_j}(\cdot) = p_{Z_i Z_j} f(\cdot, \theta_{Z_i Z_j}) + (1 - p_{Z_i Z_j}) \delta_0(\cdot)$$

(Assumption:  $f$  has continuous cdf at zero).

# SBM properties

## Results

- ▶ **Identifiability** of parameters [Allman *et al.* 09, Allman *et al.* 11].
- ▶ **Parameter estimation / node clustering** procedures:  
**exact EM** approach is not possible

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## Remaining challenges

- ▶ Behavior of the nodes posterior dist. / Quality of variational approx. ?
- ▶ Consistency of the MLE ?  
(ongoing works of Céliste, Daudin & Pierre and Mariadassou & Matias)

# Overlapping SBM / Mixed membership SBM

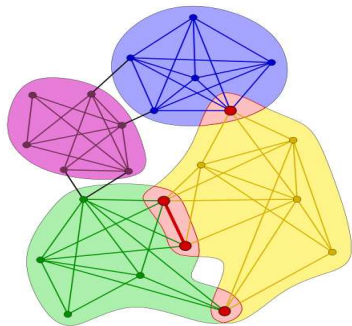


Figure: Overlapping mixture model. Source: Palla *et al.*, Nature, 2005.

Nodes may belong to many classes  
[Latouche *et al.* 11a, Airoldi *et al.* 08].

# OSBM [Latouche et al. 11a]

## Model

- ▶  $Z_i = (Z_{i1}, \dots, Z_{iQ}) \sim \prod_{q=1}^Q \mathcal{B}(\pi_q)$
- ▶  $X_{ij} | Z_i, Z_j \sim \mathcal{B}(g(p_{Z_i Z_j}))$  where  $g(x) = (1 + e^{-x})^{-1}$  (logistic function) and

$$p_{Z_i Z_j} = Z_i^\top W Z_j + Z_i^\top U + V^\top Z_j + \omega$$

$W$  is a  $Q \times Q$  real matrix while  $U$  and  $V$  are  $Q$ -dimensional real vectors and  $\omega$  real number.

## Results [Latouche et al. 11a]

- ▶ Parameter's identifiability
- ▶ Variational Bayes approach + variational logistic Bayes
- ▶ Model selection criterion

## Issues

- ▶ Quality of (double) variational approximation ?

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- ▶  $Z_i$  i.i.d. vectors in a *latent space*  $\mathbb{R}^d$ .
- ▶ Conditional on  $\{Z_i\}$ , the  $\{X_{ij}\}$  are independent Bernoulli r.v.  
 $\log\text{-odds}(X_{ij} = 1 | Z_i, Z_j, U_{ij}, \theta) = \theta_0 + \theta_1^T U_{ij} - \|Z_i - Z_j\|$ ,  
where  $\log\text{-odds}(A) = \log \mathbb{P}(A) / (1 - \mathbb{P}(A))$ ;  $\{U_{ij}\}$  set of covariate vectors and  $\theta$  parameters vector.
- ▶ This may be extended to weighted networks

## Results [Handcock *et al.* 07]

- ▶ Two-stage maximum likelihood or MCMC procedures are used to infer the model's parameters
- ▶ Assuming  $Z_i$  sampled from mixture of multivariate normal, one may obtain a clustering of the nodes.

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# Clustering the nodes of a network

## Probabilistic approach

- ▶ Using either mixture or overlapping mixture models, one may recover nodes groups.
- ▶ These groups reflect a common 'connectivity behaviour'.

## Non probabilistic approach = community detection

- ▶ Many clustering methods try to group the nodes that belong to the same **clique**.
- ▶ Here the nodes in the same groups tend to be connected with each other.

# Clustering the nodes of a network

## Probabilistic approach

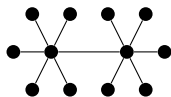
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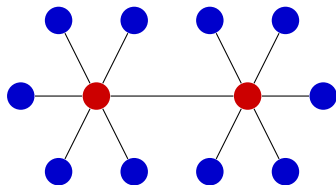
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# Major difference between probabilistic/non probabilistic approach

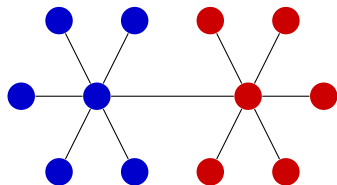
Observation of



may lead to either



MixNet model



Clustering based on cliques





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