

# The Exchangeable Graph Model

Edoardo Airoldi

*Department of Computer Science  
Lewis-Sigler Institute for Integrative Genomics  
Princeton University, USA*

Santa Fe Institute, December 4<sup>th</sup> 2008, Santa Fe, NM

## Overview

- Statistical elements of graph data analysis
- Data is collection of measurements on pairs
  - Binary case: a graph, denoted  $G = (N, Y)$
  - General case: square matrices, same  $N$  units
- This talk
  - A model that resolves measurements on pairs into node-specific binary strings via exchangeability

Santa Fe Institute

2

## Agenda

- Background
- The exchangeable graph model
- Applications

## Background: $p^*$ or ERG models

$$\Pr(Y=y|\Theta=\theta) = \exp\{ \sum_k \theta_k S_k(y) + A(\theta) \}$$

where  $S_k(y)$  counts specific structure  $k$ , such as

- edges  $S_1(y) = \sum_{1 \leq i < j \leq n} Y_{ij}$
- triangles  $S_3(y) = \sum_{1 \leq i < j < h \leq n} Y_{ij} Y_{ih} Y_{jh}$ .

*Frank & Strauss (JASA, 1986), Snijders et al. (Soc. Met., 2004), Hanneke & Xing (LNCS, 2007)*

## Background: latent space models

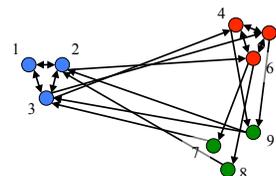
$$\log\text{-odds}(Y_{ij}=1|\theta_i, \theta_j, \alpha) = \alpha - |\theta_i - \theta_j|$$

where  $\theta_i$  is a point in  $\mathbb{R}^k$ , for all nodes  $i$  in  $N$ .

Close points in  $\mathbb{R}^k$  are likely to be connected.

*Hoff et al. (JASA, 2002), Sarkar & Moore (NIPS, 2006),  
Handcock et al. (JRSS/A, 2007, with disc.)*

## Background: blockmodels



$\theta_i \sim \text{Dirichlet}(\alpha)$ , for all nodes  $i$  in  $N$

$y_{ij}|\theta_i, \theta_j \sim \text{Bernoulli}(\theta_i \cdot B \theta_j)$ , for all pairs  $(i, j)$

where  $\theta_i$  is a point in the  $K$ -simplex, and  $B$  is  $K \times K$ .

Nodes in the same block share similar connectivity.

*Lorraine & White (J. Math. Soc., 1971), Nowicki & Snijders (JASA, 2001), Airoldi et al. (Link-KDD 2005, JMLR, 2008), Newman & Leicht (PNAS 2007), Hofman & Wiggins (Phys. Rev Lett. 2008)*

## Remarks

ERG summarizes  $G$  using exp model on motif counts. Cannot offer node-specific predictions.

LSM projects  $Y$  onto a  $\mathbb{R}^k$ . MCMC does not scale, hard identifiability problem, no clustering effect.

MMB fractionally, sparsely maps nodes to blocks with similar connectivity, as per B. nVEM scales.

Desiderata: node attributes, sparsity, tractability

## Agenda

- Background
- The exchangeable graph model
- Applications

## The exchangeable graph model

$b_i \sim \text{Uniform}$  (vertex set of hypercube), for all nodes  $i$

$y_{ij}|b_i, b_j \sim \text{Bernoulli}(q(b_i, b_j))$ , for all pairs  $(i, j)$

where  $b_i$  is a binary string,  $K$ -bit long.

A step-up in complexity from,

$y_{ij} \sim \text{Bernoulli}(p)$ , for all pairs  $(i, j)$

*Erdos & Renyi (1959), Gilbert (1959)*

## Specifications

- Number of bits captures complexity,  $K < |N|$
- Function  $q(b_i, b_j)$  is asymmetric in the arguments, e.g., consider  $q = b_i \cdot b_j / |b_i|$ , where  $|b_i| \neq |b_j|$
- How to control sparsity of the bit-strings?

Concentrate density in the corners of the hypercube,  $h_i$ , then sample IID bits  $b_i|h_i$ . Write  $\text{Bit}^K(\alpha)$

## Some results

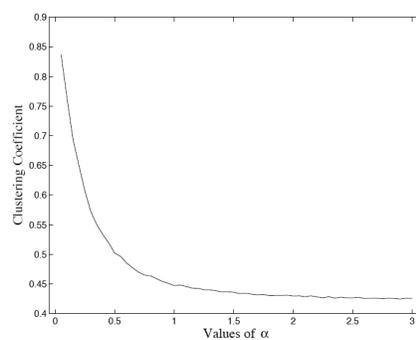
- Two sources of variability:
  - Pr (edge) decreases with  $K$   
*More complexity reduces chances of an edge*
  - Pr (edge) increases with  $1/\alpha$   
*Concentration of density improve chances of an edge*
- Emergence of the giant component in  $(K, \alpha)$ 
  - (i) phase transition, (ii) structure in the giant comp.

Santa Fe Institute

11

## Structure in the giant component

- As negative correlation among bits in node-specific strings increases, clear structure emerges



Santa Fe Institute

Edo Airoldi

## Inference on the bit-strings

- Model

$$b_i \sim \text{Bit}^K(\alpha), \text{ for all nodes } i$$

$$y_{ij}|b_i, b_j \sim \text{Bernoulli} ( q(b_i, b_j) ), \text{ for all pairs } (i, j)$$

- Likelihood

$$\mathbb{L}(Y=y|\alpha) = \int db_{1:N} \left( \prod_{ij} \text{Bern} (y_{ij}|b_i, b_j) \prod_i \text{Bit}^K(b_i|\alpha) \right)$$

- Variational EM algorithm; approximate E-Step

## Agenda

- Background
- The exchangeable graph model
- Applications

## Assessing graph complexity

Make inference on bit strings

- How many bits to explain observed connectivity with high probability?
- How much information is retained at different bit-lengths? For instance, compute information profile for  $K \leq N$ , or entropy histogram for a given  $k$ .

## Performing model comparison

Consider statistical models of paired measurements

- Degree distribution, suite of properties, likelihood
- Alternative:
  1. given graph  $G$ , fit models  $p_{1:M}(G|\Theta)$
  2. sample  $B$  graphs from  $p_{1:M}(G|\Theta_{EST})$
  3. compute  $M$  distributions on EHs and IPs
  4. compare models:
    - complexity of models' supports
    - similarity of graph and model complexity

## P-value of size of modules' overlap

### In general

- Distribution  $H^K(\alpha)$  specifies multiple membership
- EGM gives model-based probability of overlap size, e.g. via empirical null (*Efron, JASA, 2003*)

### Genomics example

- Size of common neighborhood is used to infer gene duplication and loss, given evolutionary tree

## Concluding remarks

### 1. In theory

New tool to explore variability of graph connectivity

### 2. In practice

- i. Likelihood-based approach to size of neighborhoods
- ii. Information-based approach to goodness-of-fit and model comparison for models of paired measurements