Uncovering Latent Structure in Valued Graphs

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ECCS07, October 2007

Outline

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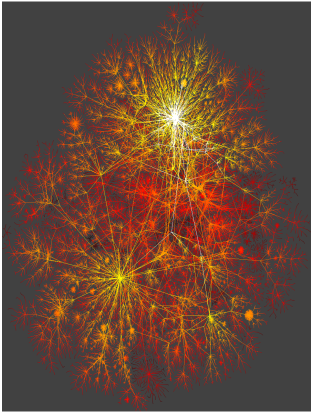
Motivations for the study of networks

Networks...

- Arise in many fields:
  - → Biology, Chemistry
  - → Physics, Internet.
- Represent an interaction pattern:
  - → $\mathcal{O}(n^2)$ interactions
  - → between n elements.
- Have a topology which:
  - → reflects the structure/function relationship



From Barabási website

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Some Notations

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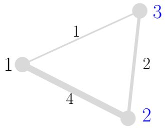
  - → V a set of vertices in $\{1, \ldots, n\}$;
  - → E a set of edges in $\{1, \ldots, n\}^2$;
  - → $\mathbf{X} = (X_{ij})$ the adjacency matrix, with X_{ij} the value of the edge between i and j.
- **Random graph definition:**
  - → The joint distribution of the X_{ij} describes the topology of the network.
- **Example:**



$V = \{1, 2, 3\}$
$E = \{\{1, 2\}, \{2, 3\}, \{3, 1\}\}$

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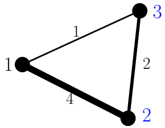

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ERMG Probabilistic Model (vertices)

- **Vertices heterogeneity**
  - → Hypothesis: the vertices are distributed among Q classes with different connectivity;
  - → $\mathbf{Z} = (\mathbf{Z}_i)_i$; $Z_{iq} = \mathbb{1}\{i \in q\}$ are indep. hidden variables;
  - → $\alpha = \{\alpha_q\}$, the *prior* proportions of groups;
  - → $(\mathbf{Z}_i) \sim \mathcal{M}(1, \alpha)$.
- **Example:**
  - → Example for 8 nodes and 3 classes with $\alpha = (0.25, 0.25, 0.5)$

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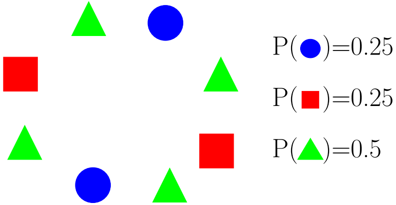

ERMG Probabilistic Model (edges)

- **$\mathbf{X}$ distribution**
  - → conditional distribution : $X_{ij}|\{i \in q, j \in l\} \sim f_{\theta_{ql}}$;
  - → $\boldsymbol{\theta} = (\theta_{ql})$ is the connectivity paramater matrix;
  - → ERMG : "Erdös-Rényi Mixture for Graphs".
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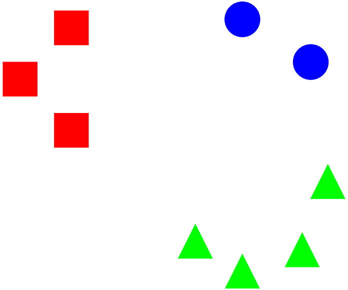

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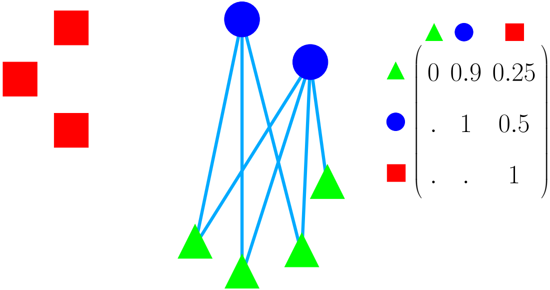

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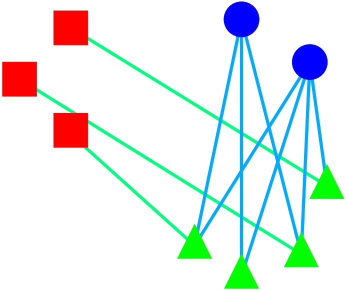

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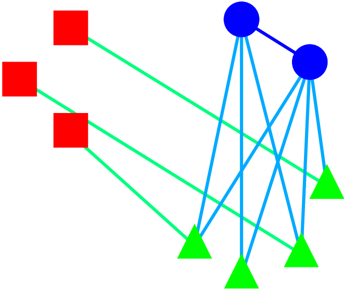

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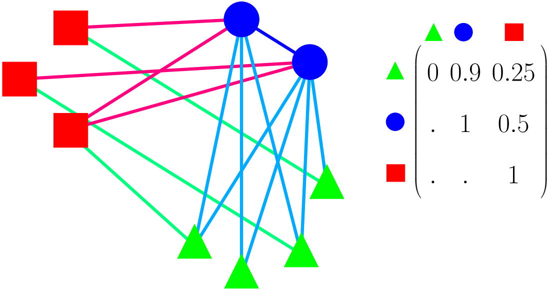

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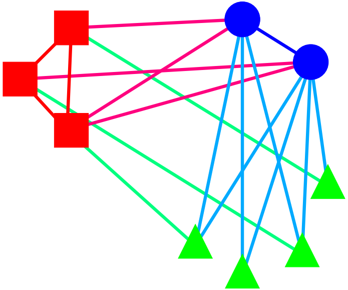

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ERMG edge values

- **Classical Distributions:**

→ f_θ can be any probability distribution;

→ Bernoulli: presence/absence of an edge;

→ Multinomial: nature of the connection (friend, lover, colleague);

→ Poisson: in coauthorship networks, number of copublished papers;

→ Gaussian: intensity of the connection (airport network);

→ Bivariate Gaussian: directed networks where forward and backward edges are correlated;

→ Etc.

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Log-Likelihood of the model

First Idea: Use maximum likelihood estimators

- **Complete data likelihood**

$$\mathcal{L}(\mathbf{X}, \mathbf{Z}) = \sum_i \sum_q Z_{iq} \ln \alpha_q + \sum_{i<j} \sum_{q,l} Z_{iq} Z_{jl} \ln f_{\theta_{ql}}(X_{ij})$$

  with $f_{\theta_{ql}}(X_{ij})$ likelihood of edge value X_{ij} under $i \sim q$ and $j \sim l$.

- **Observed data likelihood**

$$\mathcal{L}(\mathbf{X}) = \ln \sum_{\mathbf{Z}} \exp \mathcal{L}(\mathbf{X}, \mathbf{Z})$$

- The observed data likelihood requires a sum over Q^n terms, and is thus untractable;
- EM-like strategies require the knowledge of $\Pr(\mathbf{Z}|\mathbf{X})$, also untractable (no conditional independence) and thus also fail.

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Variational Inference: Pseudo Likelihood

Main Idea: Replace complicated $\Pr(\mathbf{Z}|\mathbf{X})$ by a simple $\mathcal{R}_{\mathbf{X}}[\mathbf{Z}]$ such that $KL(\mathcal{R}_{\mathbf{X}}[\mathbf{Z}], \Pr(\mathbf{Z}|\mathbf{X}))$ is minimal.

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- For simple $\mathcal{R}_{\mathbf{X}}$, $\mathcal{J}(\mathcal{R}_{\mathbf{X}}[\mathbf{Z}])$ is tractable,
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2 Steps Iterative Algorithm

- Step 1 **Optimize** $\mathcal{J}(\mathcal{R}_{\mathbf{X}}[\mathbf{Z}])$ **w.r.t.** $\mathcal{R}_{\mathbf{X}}[\mathbf{Z}]$:
  - → Restriction to a "comfortable" class of functions;
  - → $\mathcal{R}_{\mathbf{X}}[\mathbf{Z}] = \prod_i h(\mathbf{Z}_i; \boldsymbol{\tau}_i)$, with $h(.; \boldsymbol{\tau}_i)$ the multinomial distribution;
  - → τ_{iq} is a variational parameter to be optimized using a fixed point algorithm:

$$\tilde{\tau}_{iq} \propto \alpha_q \prod_{j \neq i} \prod_{l=1}^{Q} f_{\theta_{ql}}(X_{ij})^{\tilde{\tau}_{jl}}$$

- Step 2 **Optimize** $\mathcal{J}(\mathcal{R}_{\mathbf{X}}[\mathbf{Z}])$ **w.r.t.** (α, θ):
  - → Constraint: $\sum_q \alpha_q = 1$

$$\begin{aligned} \tilde{\alpha}_q &= \sum_i \tilde{\tau}_{iq}/n \\ \tilde{\theta}_{ql} &= arg \max_{\theta} \sum_{ij} \tilde{\tau}_{iq}\tilde{\tau}_{jl} \log f_{\theta}(X_{ij}) \end{aligned}$$

  - → Closed expression of $\tilde{\theta}_{ql}$ for classical distributions.

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Model Selection Criterion

- We derive a statistical BIC-like criterion to select the number of classes:
- The likelihood can be split: $\mathcal{L}(\mathbf{X}, \mathbf{Z}|Q) = \mathcal{L}(\mathbf{X}|\mathbf{Z}, Q) + \mathcal{L}(\mathbf{Z}|Q)$.
- These terms can be penalized separately:

$$\begin{aligned} \mathcal{L}(\mathbf{X}|\mathbf{Z}, Q) &\rightarrow \text{pen}_{\mathbf{X}|\mathbf{Z}} = \frac{Q(Q+1)}{2} \log \frac{n(n-1)}{2} \\ \mathcal{L}(\mathbf{Z}|Q) &\rightarrow \text{pen}_{\mathbf{Z}} = (Q-1)\log(n) \end{aligned}$$

$$ICL(Q) = \max_{\theta} \mathcal{L}(\mathbf{X}, \tilde{\mathbf{Z}}|\theta, m_Q) - \frac{1}{2}\left(\frac{Q(Q+1)}{2} \log \frac{n(n-1)}{2} - (Q-1)\log(n)\right)$$

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Quality of the Estimates: Simulation Setup

→ Undirected graph with $Q = 3$ classes;

→ Poisson-valued edges;

→ $n = 100,\ 500$ vertices;

→ $\alpha_q \propto a^q$ for $a = 1,\ 0.5,\ 0.2$;
- $a = 1$: balanced classes;
- $a = 0.2$: unbalanced classes $(80.6\%,\ 16.1\%,\ 3.3\%)$

→ Connectivity matrix of the form $\begin{pmatrix} \lambda & \gamma\lambda & \gamma\lambda \\ \gamma\lambda & \lambda & \gamma\lambda \\ \gamma\lambda & \gamma\lambda & \lambda \end{pmatrix}$ for $\gamma = 0.1,\ 0.5,\ 0.9,\ 1.5$ and $\lambda = 2,\ 5$.
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- $a = 0.2$: unbalanced classes $(80.6\%,\ 16.1\%,\ 3.3\%)$

→ Connectivity matrix of the form $\begin{pmatrix} \lambda & \gamma\lambda & \gamma\lambda \\ \gamma\lambda & \lambda & \gamma\lambda \\ \gamma\lambda & \gamma\lambda & \lambda \end{pmatrix}$ for $\gamma = 0.1,\ 0.5,\ 0.9,\ 1.5$ and $\lambda = 2,\ 5$.

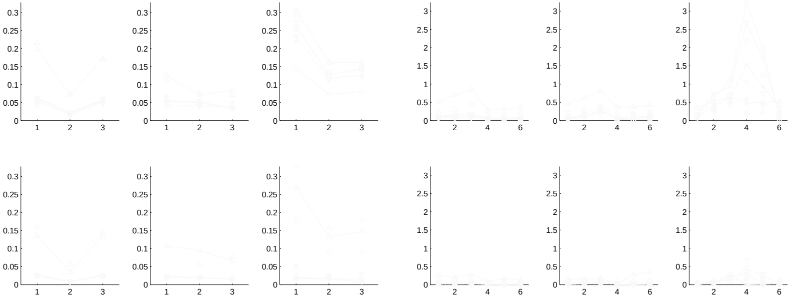
- $\gamma = 1$: all classes equivalent (same connectivity pattern);
- $\gamma <> 1$: classes are different;
- λ: mean value of an edge;

→ 100 repeats for each setup.

Quality of the Estimates: Results

- Root Mean Square Error (RMSE) = $\sqrt{Bias^2 + Variance}$

RMSE for the α_q | RMSE for the λ_{ql}



x-axis: $\alpha_1, \alpha_2, \alpha_3$ | x-axis: $\lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{12}, \lambda_{13}, \lambda_{23}$

Top: $n = 100$, Bottom: $n = 500$

Left to right: $a = 1, 0.5, 0.2$

Solid line: $\lambda = 5$, dashed line: $\lambda = 2$

Symbols depend on γ: $\circ = 0.1$, $\triangledown = 0.5$, $\triangle = 0.9$, $* = 1.5$

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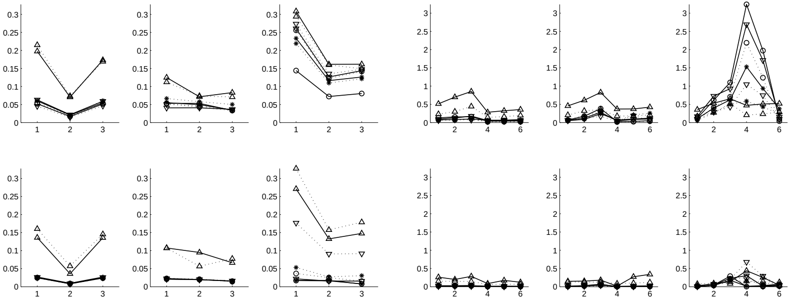

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Number of Classes: Simulation Setup

- → Undirected graph with $Q^\star = 3$ classes;
- → Poisson-valued edges;
- → $n = 50,\ 100,\ 500,\ 1000$ vertices;
- → $\alpha_q = (57.1\%, 28, 6\%, 14, 3\%)$ (or $a = 0.5$);
- → $\lambda = 2, \gamma = 0.5$;
- → Retrieve Q that maximizes ICL;
- → 100 repeats for each value of n;

Number of Classes: Results

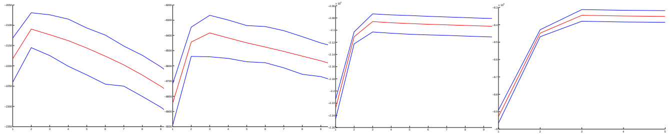
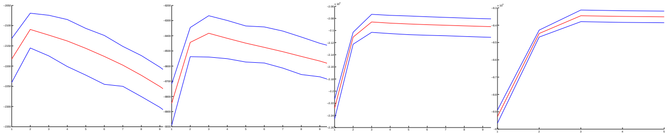


Figure: Mean ICL and 90% confidence interval as a function of $Q = 1..10$. From left to right: $n = 50, n = 100, n = 500, n = 1000$.

	Q		
n	2	3	4
50	82	**17**	1
100	7	**90**	3
500	0	**100**	0
1000	0	**100**	0

Table: Frequency (in %) at which Q is selected for various n

Number of Classes: Results



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Summary

Flexibility of ERMG

- Probabilistic model which captures features of real-networks,
- Models various network topologies,
- A promising alternative to existing methods.

Estimation and Model selection

- Variational approaches to compute approximate MLE when dependencies are complex,
- A statistical criterion to choose the number of classes (ICL).

Extensions

- Network motifs