Lectures 2: Random Graphs

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The Erdös-Rényi class $\mathcal{G}_{n,p}$

Today we discuss about random graphs. The *Erdös-Rényi class* $\mathcal{G}_{n,p}$ of random graphs is defined as follows.

Simulations

The Erdös-Rényi class $\mathcal{G}_{n,p}$

Today we discuss about random graphs. The *Erdös-Rényi class* $\mathcal{G}_{n,p}$ of random graphs is defined as follows.

Let \mathcal{V} denote the set of *n* vertices, $\mathcal{V} = \{1, 2, \cdots, n\}$, and let \mathcal{G} denote the

set of all graphs with vertices \mathcal{V} . There are exactly $2^{\binom{n}{2}}$ such graphs. The probability mass function on \mathcal{G} , $P : \mathcal{G} \to [0, 1]$, is obtained by assuming that, as random variables, edges are independent from one another, and each edge occurs with probability $p \in [0, 1]$. Thus a graph $G \in \mathcal{G}$ with *m* edges will have probability P(G) given by

$$P(G) = p^m(1-p) \binom{n}{2}^{-m}.$$

(explain why)

The Erdös-Rényi class $\mathcal{G}_{n,p}$

Probability space

Formally, $\mathcal{G}_{n,p}$ stands for the the probability space (\mathcal{G}, P) composed of the set \mathcal{G} of all graphs with *n* vertices, and the probability mass function *P* defined above.

The Erdös-Rényi class $\mathcal{G}_{n,p}$

Probability space

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A reformulation of *P*: Let $G = (\mathcal{V}, \mathcal{E})$ be a graph with *n* vertices and *m* edges and let *A* be its adjacency matrix. Then:

$$P(G) = \prod_{(i,j)\in\mathcal{E}} Prob((i,j) \text{ is an edge}) \prod_{(i,j)\notin\mathcal{E}} Prob((i,j) \text{ is not an edge}) =$$
$$= \prod_{1\leq i< j\leq n} p^{A_{i,j}} (1-p)^{1-A_{i,j}}$$

where the product is over all ordered pairs (i, j) with $1 \le i < j \le n$. Note:

$$|\{(i,j), 1 \le i < j \le n\}| = \binom{n}{2} \& |\{(i,j) \in \mathcal{E}\}| = |\mathcal{E}| = m = \sum_{1 \le i < j \le n} A_{i,j}.$$

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The Erdös-Rényi class $\mathcal{G}_{n,p}$

Computations in $\mathcal{G}_{n,p}$

How to compute the expected number of edges of a graph in $\mathcal{G}_{n,p}$?

The Erdös-Rényi class $\mathcal{G}_{n,p}$

Computations in $\mathcal{G}_{n,p}$

How to compute the expected number of edges of a graph in $\mathcal{G}_{n,p}$? Let $X_2 : \mathcal{G} \to \{0, 1, \cdots, \binom{n}{2}\}$ be the random variable of *number of* edges of a graph G.

$$X_2 = \sum_{1 \leq i < j \leq n} \mathbb{1}_{(i,j)}$$
, $\mathbb{1}_{(i,j)}(G) = \left\{ egin{array}{ccc} 1 & \textit{if} & (i,j) \ \textit{is edge in } G \\ 0 & \textit{if} & \textit{otherwise} \end{array}
ight.$

Use linearity and the fact that $\mathbb{E}[1_{(i,j)}] = Prob((i,j) \in \mathcal{E}) = p$ to obtain:

$$\mathbb{E}[\textit{Number of Edges}] = \left(egin{array}{c} n \\ 2 \end{array}
ight) p = rac{n(n-1)}{2}p$$

The Erdös-Rényi class $\mathcal{G}_{n,p}$ MLE of p

Given a realization G of a graph with n vertices and m edges, how to estimate the most likely p that explains the graph. Concept: The Maximum Likelihood Estimator (MLE). In statistics: The MLE of a parameter θ given an observation x of a random variable $X \sim p_X(x; \theta)$ is the value θ that maximizes the probability $P_X(x; \theta)$:

$$\theta_{MLE} = argmax_{\theta}P_X(x;\theta).$$

In our case: our observation G has m edges. We know

$$P(G;p) = p^{m}(1-p) \binom{n}{2}^{-m}$$

The Erdös-Rényi class $\mathcal{G}_{n,p}$ MLE of p

Lemma

Given a random graph with n vertices and m edges, the MLE estimator of p is

$$p_{MLE} = \frac{m}{\binom{n}{2}} = \frac{2m}{n(n-1)}.$$

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The Erdös-Rényi class $\mathcal{G}_{n,p}$ MLE of p

Lemma

Given a random graph with n vertices and m edges, the MLE estimator of p is

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Why

Note
$$log(P(G; p)) = mlog(p) + (\binom{n}{2} - m)log(1-p)$$
 and solve for p:

$$\frac{dlog(P)}{dp} = \frac{m}{p} - \frac{\binom{n}{2} - m}{1 - p} = 0.$$

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The Erdös-Rényi class $\mathcal{G}_{n,p}$ Method of Moments Estimator for p

An alternative parameter estimation method is the moment matching method. Given a likelihood function for observed data $p(x; \theta)$ and a sequence of observations (x_1, x_2, \dots, x_N) , the moment matching method computes the parameters $\theta \in \mathbb{R}^d$ by solving the system of equations:

$$\mathbb{E}[X] = \frac{1}{N} \sum_{t=1}^{N} x_t \cdots \mathbb{E}[X^d] = \frac{1}{N} \sum_{t=1}^{N} x_t^d$$

(or unbiased estimates of the moments). In particular, for the Erdös-Rényi class, we match the first moment with the observation: $\frac{n(n-1)}{2}p = m$. Hence

$$p_{MM}=\frac{2m}{n(n-1)},$$

same as the MLE estimator.

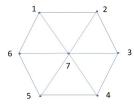
Cliques

Definition

Given a graph $G = (\mathcal{V}, \mathcal{E})$, a subset of q vertices $S \subset \mathcal{V}$ is called a q-clique if the subgraph $(S, \mathcal{E}|_{S \times S})$ is complete.

In other words, S is a q-clique if for every $i \neq j \in S$, $(i, j) \in \mathcal{E}$ (or $(j, i) \in \mathcal{E}$), that is, (i, j) is an edge in G.

• Each edge is a 2-clique.

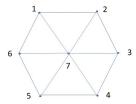


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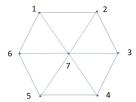
- Each edge is a 2-clique.
- $\{1,2,7\}$ is a 3-clique. And so are $\{2,3,7\},\{3,4,7\},\{4,5,7\},\{5,6,7\},\{1,6,7\}$

Cliques

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- Each edge is a 2-clique.
- $\{1, 2, 7\}$ is a 3-clique. And so are $\{2, 3, 7\}, \{3, 4, 7\}, \{4, 5, 7\}, \{5, 6, 7\}, \{1, 6, 7\}$
- There is no k-clique, with $k \ge 4$.

Finding the largest clique is a NP-hard problem, see for instance: *https*://en.wikipedia.org/wiki/Clique_problem

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The Erdös-Rényi class $\mathcal{G}_{n,p}$

Computations in $\mathcal{G}_{n,p}$: q-cliques

How to compute the expected number of *q*-cliques?

The Erdös-Rényi class $\mathcal{G}_{n,p}$

Computations in $\mathcal{G}_{n,p}$: *q*-cliques

How to compute the expected number of *q*-cliques?

For k = 2 we computed earlier the number of edges, which is also the number of 2-cliques.

We shall compute now the number of 3-cliques: triangles, or 3-cycles.

Let $X_3 : \mathcal{G} \to \mathbb{N}$ be the random variable of number of 3-cliques. Note the

maximum number of 3-cliques is $\begin{pmatrix} n \\ 3 \end{pmatrix}$.

Let S_3 denote the set of all distinct 3-cliques of the complete graph with n vertices, $S_3 = \{(i, j, k), 1 \le i < j < k \le n\}$. Let

$$1_{(i,j,k)}(G) = \begin{cases} 1 & if \quad (i,j,k) \text{ is a } 3-\text{clique in } G\\ 0 & if \quad \text{otherwise} \end{cases}$$

The Erdös-Rényi class $\mathcal{G}_{n,p}$

Expectation of the number of 3-cliques

Note:
$$X_3 = \sum_{(i,j,k) \in S_3} 1_{(i,j,k)}$$
. Thus
 $\mathbb{E}[X_3] = \sum_{(i,j,k) \in S_3} \mathbb{E}[1_{(i,j,k)}] = \sum_{(i,j,k) \in S_3} Prob((i,j,k) \text{ is a clique}).$

Since $Prob((i, j, k) \text{ is a clique}) = p^3$ we obtain:

$$\mathbb{E}[\text{Number of } 3-\text{cliques}] = \binom{n}{3}p^3 = \frac{n(n-1)(n-2)}{6}p^3.$$

The Erdös-Rényi class $\mathcal{G}_{n,p}$ Number of 3 cliques

Assume we observe a graph G with n vertices and m edges. What would be the expected number N_3 of 3-cliques?

$$\mathbb{E}[X_3|X_2 = m] = \frac{1}{L} \sum_{k=1}^{L} X_3(G_k)$$

where *L* denotes the numbe of graphs with *m* edges and *n* vertices, and G_1, \dots, G_L is an enumeration of these graphs.

The Erdös-Rényi class $\mathcal{G}_{n,p}$ Number of 3 cliques

Assume we observe a graph G with n vertices and m edges. What would be the expected number N_3 of 3-cliques?

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where *L* denotes the numbe of graphs with *m* edges and *n* vertices, and G_1, \dots, G_L is an enumeration of these graphs. We approximate:

$$\mathbb{E}[X_3|X_2=m] \approx \mathbb{E}[X_3; p = p_{MLE}(m)]$$

and obtain:

$$E[X_3|X_2=m] \approx \frac{4(n-2)}{3n^2(n-1)^2}m^3.$$

The Erdös-Rényi class $\mathcal{G}_{n,p}$

Expectation of the number of q-cliques

Let $X_q : \mathcal{G} \to \mathbb{N}$ be the random variable of number of *q*-cliques. Note the maximum number of *q*-cliques is $\binom{n}{q}$. Let S_q denote the set of all distinct *q*-cliques of the complete graph with *n* vertices, $S_q = \{(i_1, i_2, \cdots, i_q) , 1 \leq i_1 < i_2 < \cdots < i_q \leq n\}$. Note $|S_q| = \binom{n}{q}$. Let

$$1_{(i_1,i_2,\cdots,i_q)}(G) = \begin{cases} 1 & if \quad (i_1,i_2,\cdots,i_q) \text{ is a } q-clique \text{ in } G \\ 0 & if \quad otherwise \end{cases}$$

Simulations

The Erdös-Rényi class $\mathcal{G}_{n,p}$

Expectation of the number of q-cliques

Since
$$X_q = \sum_{(i_1, \dots, i_q) \in S_q} 1_{i_1, \dots, i_q}$$
 and
 $Prob((i_1, \dots, i_q) \text{ is a clique}) = p \begin{pmatrix} q \\ 2 \end{pmatrix}$ we obtain:

$$\mathbb{E}[\textit{Number of } q-\textit{cliques}] = \left(egin{array}{c} n \ q \end{array}
ight) p^{q(q-1)/2}.$$

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The Erdös-Rényi class $\mathcal{G}_{n,p}$

Expectation of the number of *q*-cliques

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$$X_q = \sum_{(i_1, \dots, i_q) \in S_q} 1_{i_1, \dots, i_q}$$
 and
 $Prob((i_1, \dots, i_q) \text{ is a clique}) = p^{\begin{pmatrix} q \\ 2 \end{pmatrix}}$ we obtain:

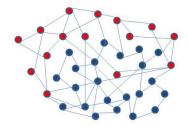
$$\mathbb{E}[\mathsf{Number of } q-\mathsf{cliques}] = \left(egin{array}{c} n \ q \end{array}
ight) p^{q(q-1)/2}.$$

Using a similar argument as before, if G has m edges, then

$$\mathbb{E}[X_q|X_2=m] \approx \binom{n}{q} \left(\frac{2m}{n(n-1)}\right)^{q(q-1)/2}$$

The Stochastic Block Model

The *Stochastic Block Model* (SBM), a.k.a. *Planted Partition Model*, was introduced in mathematial sociology by Holland, Laskey and Leinhardt in 1983 and by Wang and Wong in 1987. Here we follow Abbe (2017).



A Stochastic Block Model with k =2 classes ('red' and 'blue') over n =15+22 = 37 nodes. Number of edges: $m_{rr} = 21, m_{rb} = 6, m_{bb} = 35.$

Figure: Example of a SBM

The Stochastic Block Model The general SBM

Data. Let *n* be a positive integer (the number of vertices), *k* be a positive integer (the number of communities), $\mathfrak{p} = (p_1, p_2, \dots, p_k)$ be a probability vector on $[k] := \{1, 2, \dots, k\}$ (the prior on the *k* communities), and *Q* be a $k \times k$ symmetric matrix with entries in [0, 1] (the connectivity probabilities).

Definition

The pair (Z, G) is drawn under SBM(n, p, Q) if Z is an n-dimensional random vector with i.i.d. components distributed under p, and G is an n-vertex graph where vertices i and j are connected with probability Q_{Z_i,Z_j} , independently of other pairs of vertices.

The *community sets* are defined by $\Omega_i = \Omega_i(Z) = \{v \in [n], Z_v = i\}, 1 \le i \le k.$

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The Stochastic Block Model

The Symmetric SBM (SSBM)

Definition

The pair (Z, G) is drawn under SSBM(n, k, a, b) if Z is an n-dimensional random vector with i.i.d. components uniformly distributed over $[k] = \{1, 2, \dots, k\}$, and G is an n-vertex graph where distinct vertices i and j are connected with probability a if $Z_i = Z_j$ and probability b if $Z_i \neq Z_j$, independently of other pairs of vertices.

Data:

• the number of vertices: *n*; • the number of communities: *k*; • prior on *k* communities: $\mathfrak{p} = Q = \begin{bmatrix} a & b & \cdots & b \\ b & a & \cdots & b \\ \vdots & \vdots & \ddots & \vdots \\ b & b & \cdots & a \end{bmatrix}$. • connectivity probabilities: *Q*

The Erdös-Rényi random graph is obtained when $a = b = p_{\pm}$, $a = b_{\pm}$

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The Binary Symmetric Stochastic Block Model Distributions (1)

Consider a realization (Z, G) drawn randomly under SSBM(n, 2, a, b) that models two communities. This means every node belongs with equal probability to either community, 1 or 2: $Z = (Z_1, Z_2, \dots, Z_n)$, where $Z_i \in \{1, 2\}, P(Z_i = 1) = P(Z_i = 2) = \frac{1}{2}$. The graph G of n nodes has adjacency matrix A. The conditional probability of realization A given the vector Z:

$$P(A|Z) = \prod_{1 \le u < v \le n} Q_{Z_u, Z_v}^{A_{u,v}} (1 - Q_{Z_u, Z_v})^{1 - A_{u,v}} =$$

= $a^{m_{11} + m_{22}} b^{m_{12}} (1 - a)^{m_{11}^c + m_{22}^c} (1 - b)^{m_{12}^c}$

where
$$m_{11}$$
, m_{22} are the number of edges inside community 1, respectively 2, m_{12} is the number of edges between the two communities, and m_{11}^c , m_{22}^c , m_{12}^c are the number of missing edges inside each community/between the two communities.

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The Binary Symmetric Stochastic Block Model Distributions (2)

Explicitely these numbers are given by:

$$m_{11} = \#$$
Edges inside community $1 = \sum_{\substack{i < j \\ i, j \in \Omega_1}} A_{i,j}$

$$m_{11}^c = \left(\begin{array}{c} n_1 \\ 2 \end{array} \right) - m_{11} \quad n_1 = |\Omega_1|$$

 $m_{22} = \#$ Edges inside community $2 = \sum_{\substack{i < j \\ i, j \in \Omega_2}} A_{i,j}$

$$m_{22}^{c} = \begin{pmatrix} n_2 \\ 2 \end{pmatrix} - m_{22} \quad n_2 = |\Omega_2|$$

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The Binary Symmetric Stochastic Block Model Distributions (3)

$$m_{12} = \# \text{Edges between community 1 and } 2 = \sum_{\substack{i \in \Omega_1 \\ j \in \Omega_2}} A_{i,j}$$

$$m_{12}^c = n_1 n_2 - m_{12} \qquad j \in \Omega_2$$
Example:
$$n = 9, \ \Omega_1 = \{1, 2, 3, 4, 5\}, \ \Omega_2 = \{6, 7, 8, 9\}.$$

$$m_{11} = 5, \ m_{11}^c = 5$$

$$m_{22} = 4, \ m_{22}^c = 2$$

$$m_{12} = 3, \ m_{11}^c = 17$$

The Stochastic Block Model

Community Detection

The main problem: Community Detection.

This means a partition of the set of vertices $\mathcal{V} = \{1, 2, \dots, n\}$ compatible with the observed graph *G* for a given connectivity probability matrix *W*. To formulate mathematically we need to define the *agreement* between two community vectors.

Definition

The agreement between two community vectors $x, y \in [k]^n$ is obtained by maximizing the number of common components of these two vectors over all possible relabelling (i.e., permutations):

$$Agr(x,y) = \max_{\pi \in S_k} \frac{1}{n} \sum_{i=1}^n \mathbf{1}(x_i = \pi(y_i))$$

where S_k denotes the group of permutations.

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Simulations

The Binary Symmetric Stochastic Block Model Model Calibration: Supervised Learning

How to estimate parameters a, b in the 2-community symmetric stochastic block model SSBM(n, 2, a, b). Use the Maximum Likelihood Estimator (MLE):

$$(a_{MLE}, b_{MLE}) = argmax_{a,b}Prob(G|Z, a, b)$$

Setup: Assume we have access to a training (i.e., labelled) data set (Z, G). Then for parameters a, b maximize:

$$a^{m_{11}+m_{22}}(1-a)^{m_{11}^c+m_{22}^c}b^{m_{12}}(1-b)^{m_{12}^c}$$

Take the logarithm and obtain:

$$a_{MLE} = \frac{m_{11} + m_{22}}{\binom{n_1}{2} + \binom{n_2}{2}} = \frac{2(m_{11} + m_{22})}{n_1(n_1 - 1) + n_2(n_2 - 1)}$$

$$b_{MLE} = \frac{m_{12}}{n_1 n_2}$$
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The Binary Symmetric Stochastic Block Model Model Calibration: Unsupervised Learning

Assume we have access to only one realization $G = (\mathcal{V}, A)$ of the random graph drawn from a binary symmetric SBM SSBM(n, 2, a, b). The MLE is hard to solve. Instead we use the Method of Moment Matching. Since there are two parameters to estimate, a and b, we need to equations. We choose to match the numbers of 2-cliques (edges) and the number of 3-cliques. The expectations are computed by conditioning first on $n_1 = |\Omega_1|$ the size of partition, with $n_2 = n - n_1$:

$$\mathbb{E}[X_2|n_1] = \begin{pmatrix} n_1 \\ 2 \end{pmatrix} a + n_1 n_2 b + \begin{pmatrix} n_2 \\ 2 \end{pmatrix} a$$
$$\mathbb{E}[X_3|n_1] = \begin{pmatrix} n_1 \\ 3 \end{pmatrix} a^3 + \left[\begin{pmatrix} n_1 \\ 2 \end{pmatrix} n_2 + n_1 \begin{pmatrix} n_2 \\ 2 \end{pmatrix} \right] ab^2 + \begin{pmatrix} n_2 \\ 3 \end{pmatrix} a^3$$

Simulations

$$\mathbb{E}[X_2|n_1] = \begin{pmatrix} n_1 \\ 2 \end{pmatrix} a + n_1 n_2 b + \begin{pmatrix} n_2 \\ 2 \end{pmatrix} a =$$

$$= \frac{n_1(n_1 - 1) + (n - n_1)(n - n_1 - 1)}{2} a + n_1(n - n_1) b$$

$$= \frac{n_1^2 - n_1 + n^2 - 2nn_1 + n_1^2 - n + n_1}{2} a + (nn_1 - n_1^2) b$$

$$= \begin{pmatrix} n_1^2 - nn_1 + \frac{n(n - 1)}{2} \end{pmatrix} a + (nn_1 - n_1^2) b$$

Next compute the expectation of the number of edges by double expectation. To do so we need

$$\mathbb{E}[n_1] = \mathbb{E}\left[\sum_{\nu=1}^n \mathbf{1}_{Z_{\nu}=1}\right] = \frac{n}{2}$$
$$\mathbb{E}[n_1^2] = \mathbb{E}\left[\left(\sum_{\nu=1}^n \mathbf{1}_{Z_{\nu}=1}\right)^2\right] = n\frac{1}{2} + 2\frac{n(n-1)}{2}\frac{1}{4} = \frac{n(n+1)}{4}$$
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Thus

$$\mathbb{E}[X_2] = \mathbb{E}[\mathbb{E}[X_2|n_1]] = \left(\frac{n^2 + n}{4} - \frac{n^2}{2} + \frac{n^2 - n}{2}\right)a + \left(\frac{n^2}{2} - \frac{n^2 + n}{4}\right)b =$$
$$= \frac{n^2 - n}{4}(a + b)$$

Similarly,

$$\mathbb{E}[X_3|n_1] = \binom{n_1}{3} a^3 + \left[\binom{n_1}{2}n_2 + n_1\binom{n_2}{2}\right] ab^2 + \binom{n_2}{3} a^3$$
$$= \frac{n_1(n_1-1)(n_1-2) + n_2(n_2-1)(n_2-2)}{6} a^3 + \frac{n_1n_2(n_1-1+n_2-1)}{2} ab^2$$
$$= \frac{n_1^3 + n_2^3 - 3(n_1^2 + n_2^2) + 2(n_1 + n_2)}{6} a^3 + \frac{(n_1 - n_1^2)(n-2)}{2} ab^2$$
$$= \frac{(n_1 + n_2)(n_1^2 - n_1n_2 + n_2^2) - 3(n_1^2 + n_2^2) + 2n}{6} a^3 + \frac{(n_1 - n_1^2)(n-2)}{2} ab^2$$

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$$=\frac{(n-3)(n^2-2nn_1+2n_1^2)-nn_1(n-n_1)+2n}{6}a^3+\frac{(nn_1-n_1^2)(n-2)}{2}ab^2$$
$$=\frac{n^3-3n^2+2n+(3n-6)n_1^2-(3n^2-6n)n_1}{6}a^3+\frac{(nn_1-n_1^2)(n-2)}{2}ab^2$$

Substitute $\mathbb{E}[n_1] = \frac{n}{2}$ and $\mathbb{E}[n_1^2] = \frac{n^2+n}{4}$:

$$\mathbb{E}[X_3] = \frac{n(n-2)}{6}(n-1+\frac{3}{4}(n+1)-\frac{3}{2}n)a^3 + \frac{n(n-2)(\frac{n}{2}-\frac{n+1}{4})}{2}ab^2$$
$$= \frac{n(n-1)(n-2)}{24}a^3 + \frac{n(n-1)(n-2)}{8}ab^2 = \frac{n(n-1)(n-2)}{24}(a^3+3ab^2)$$

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The Binary Symmetric Stochastic Block Model Model Calibration: Unsupervised Learning (2)

Assuming the graph has m 2-cliques (=edges) and t 3-cliques (=triangles) then by the moment matching method:

$$m = \frac{n(n-1)}{4}(a+b)$$
, $t = \frac{n(n-1)(n-2)}{24}(a^3+3ab^2)$

Note: the SSBM(n, 2, a, b) class reduces to the Erdös-Renyi class $\mathcal{G}_{n,p}$ if a = b = p.

From where we solve for *a* and *b* in terms of *n*, *m* and *t*: Let $c_1 = \frac{4m}{n(n-1)}$ and $c_2 = \frac{24t}{n(n-1)(n-2)}$. Thus $b = c_1 - a$ and $4a^3 - 6c_1a^2 + 3c_1^2a - c_2 = 0 \Rightarrow (2a - c_1)^3 + c_1^3 - 2c_2 = 0$

Thus:

The Binary Symmetric Stochastic Block Model Model Calibration: Unsupervised Learning. Modified Estimator

The closed form expression deduced earlier using the moment matching method may produce un-feasible solutions. Specifically, the estimates a_{MM} , b_{MM} may not remain in the range [0, 1]. Now we derive a modifed estimator that satisfies the feasibility constraints $a, b \in [0, 1]$. Our designing principle was to satisfy *exactly*:

$$m = \mathbb{E}[X_2]$$
, $t = \mathbb{E}[X_3]$

Instead the modified estimator will satisfy the first constraint exactly, but will strive to satisfy the second constraint as much as possible, Specifically, it solves the following optimization problem:

$$\begin{array}{ll} \textit{minimize} & |\mathbb{E}[X_3] - t| \\ \text{subject to :} \\ m = \mathbb{E}[X_2] \\ 0 \leq a, b \leq 1 \end{array}$$

Simulations

The Binary Symmetric Stochastic Block Model Model Calibration: Unsupervised Learning. Modified Estimator (2)

Substituting $a + b = 2p = \frac{4m}{n(n-1)}$ into the objective function, after a bit of algebra we obtain:

$$\frac{6}{n(n-1)(n-2)}|t - \mathbb{E}[X_3]| = |(a-p)^3 - \delta|$$

where $p = \frac{2m}{n(n-1)}$, $\delta = \frac{6t}{n(n-1)(n-2)} - p^3$. Let $P(x) = (x-p)^3 - \delta$. Note $P'(x) = 3(x-p)^2 \ge 0$. Hence $x \mapsto P(x)$ is monotone increasing (in fact, strictly increasing).

On the other hand, b = 2p - a and the constraint $b \in [0, 1]$ imply $0 \le 2p - a \le 1$. Since $a \in [0, 1]$ we obtain:

$$\textit{max}(0,2p-1) \leq a \leq \textit{min}(1,2p)$$

With $A_1 = max(0, 2p - 1)$ and $A_2 = min(1, 2p)$ we obtain: minimize |P(a)|

$$A_1 \leq a \leq A_2$$

The Binary Symmetric Stochastic Block Model Calibration Algorithm 1

The last optimization probem can be solved exactly. The solutions is as follows:

Algorithm (1)

Input: n, m, t.

Compute:

$$p = \frac{2m}{n(n-1)}, \delta = \frac{6t}{n(n-1)(n-2)} - p^3$$
$$A_1 = max(0, 2p - 1), A_2 = min(1, 2p)$$
$$P(A_1) = (A_1) - p)^3 - \delta, P(A_2) = (A_2 - p)^3 - \delta.$$

The Binary Symmetric Stochastic Block Model Calibration Algorithm 1 - cont'ed

Algorithm (1 continued)

Q Test and compute the Constrained Moment Matching estimates:
 If P(A₁) ≤ 0 ≤ P(A₂) then

$$a_{CMM} = p + \sqrt[3]{\delta}$$
, $b_{CMM} = p - \sqrt[3]{\delta}$

$$a_{CMM} = A_2 \quad , \quad b_{CMM} = 2p - A_2$$

• If $P(A_1) > 0$ then

$$a_{CMM} = A_1$$
 , $b_{CMM} = 2p - A_1$

Output: a cmm and b cmm.

The Binary Symmetric Stochastic Block Model Calibration Algorithm 2

While the Algorithm 1 produces estimates a_{CMM} , $b_{CMM} \in [0, 1]$ it is often the case that one would like to obtain a, b > 0. The following algorithm provides such an "engineering fix":

Algorithm (2) Input: n, m, t. Compute: $p = \frac{2m}{n(n-1)}, \delta = \frac{6t}{n(n-1)(n-2)} - p^{3}$ $A_{1} = max(0, 2p - 1), A_{2} = min(1, 2p)$ $P(A_{1}) = (A_{1}) - p)^{3} - \delta, P(A_{2}) = (A_{2} - p)^{3} - \delta.$

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The Binary Symmetric Stochastic Block Model Calibration Algorithm 2 - cont'ed

Algorithm (2 continued)

2 Test and compute:

• If $P(A_1) \leq 0 \leq P(A_2)$ then

$$a_{CMM}=p+\sqrt[3]{\delta}$$
 , $b_{CMM}=p-\sqrt[3]{\delta}$

• If $P(A_2) < 0$ then

$$a_{CMM} = A_2$$
, $b_{CMM} = 2p - A_2$

• If $P(A_1) > 0$ then

$$a_{CMM} = A_1$$
 , $b_{CMM} = 2p - A_1$

The Binary Symmetric Stochastic Block Model Calibration Algorithm 2 - cont'ed

Algorithm (2 continued)

- Adjust to produce the Modified Constrained Moment Matching estimates
 - If $0 < a_{CMM}, b_{CMM}$ then

$$a_{MCMM} = a_{CMM}$$
 , $b_{MCMM} = b_{CMM}$

• If $b_{CMM} = 0$ then

$$a_{MCMM}=0.99a_{CMM}~,~~b_{MCMM}=0.01a_{CMM}$$

• If $a_{CMM} = 0$ then

$$a_{MCMM} = 0.01 b_{CMM}$$
 , $b_{MCMM} = 0.99 b_{CMM}$

Output: and b_{MCMM}.

The Stochastic Block Model

Types of Community Detection Algorithms

Types of algorithm:

Let $(Z, G) \sim SBM(n, p, Q)$. Then the following recovery requirements are solved if there exists an algorithm that takes G as input and outputs $\hat{Z} = \hat{Z}(G)$ such that:

- Exact recovery: $P\{Agr(Z, \hat{Z}) = 1\} = 1 o(1)$
- Almost exact recovery: $P\{Agr(Z, \hat{Z}) = 1 o(1)\} = 1 o(1)$
- Partial recovery: $P\{Agr(Z, \hat{Z}) \ge \alpha\} = 1 o(1), \ \alpha \in (0, 1).$

Note these definitions apply to an algorithm, where probabilities are computed over all realizations of SBM(n, p, Q) model.

The Symmetric Stochastic Block Model SSBM(n, 2, a, b)Expectation of number of 4-cliques (1)

Under SSBM(n, 2, a, b) the conditional expectation of X_4 given the size n_1 of the first community, is given by the following formula:

$$\mathbb{E}[X_4|n_1] = \begin{pmatrix} n_1 \\ 4 \end{pmatrix} a^6 + \begin{pmatrix} n_1 \\ 3 \end{pmatrix} n_2 a^3 b^3 + \begin{pmatrix} n_1 \\ 2 \end{pmatrix} \begin{pmatrix} n_2 \\ 2 \end{pmatrix} a^2 b^4 + n_1 \begin{pmatrix} n_2 \\ 3 \end{pmatrix} a^3 b^3 + \begin{pmatrix} n_2 \\ 4 \end{pmatrix} a^6$$

where the terms represent the cases when all four vertices are in community 1, three vertices in community 1 and one vertex in community 2, two vertices in each community, one vertex in community 1 and three in community 2, and finally, all four vertices are in community 2. Next, the expectation of the number of 4-cliques given parameters a, b is obtained by iterating the expectation operator over n_1 :

 $\mathbb{E}[X_4; a, b] = \mathbb{E}[\mathbb{E}[X_4|n_1]] \longrightarrow \langle \mathcal{D} \rangle \langle \mathcal{D} \rangle$

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The Symmetric Stochastic Block Model SSBM(n, 2, a, b)Expectation of number of 4-cliques (2)

Since n_1 follows the binomial distribution $B(n, \frac{1}{2})$,

$$\mathbb{E}[n_1] = \frac{n}{2} , \ \mathbb{E}[n_1^2] = \frac{n^2 + n}{4}$$
$$\mathbb{E}[n_1^3] = \frac{n^2(n+3)}{8} , \ \mathbb{E}[n_1^4] = \frac{n(n+1)(n^2 + 5n - 2)}{16}$$

These expressions come from the moment generating function of the binomial distribution $M_X(t) = (1 - p + pe^t)^n$ which for $p = \frac{1}{2}$ becomes $M_{n_1}(t) = \frac{1}{2^n}(1 + e^t)^n$. Then the k^{th} moment is given by

$$\mathbb{E}[n_1^k] = \frac{d^k}{dt^k} M_{n_1}(t)|_{t=0}$$

See: http://mathworld.wolfram.com/BinomialDistribution.html for details. The expectation over n_1 is obtained by substituting $n_2 = n - n_1$, expanding the expression of $\mathbb{E}[X_4|n_1]$ and then using the moments of n_1, n_1^2, n_1^3, n_1^4 .

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The Symmetric Stochastic Block Model SSBM(n, 2, a, b)Expectation of number of 4-cliques (3)

Expanding, making the substitution $n_2 = n - n_1$ and combining the tems we get:

$$\begin{split} \mathbb{E}[X_4|n_1] &= \frac{a^6}{24} \left(2n_1^4 - 4nn_1^3 + (6n^2 - 18n + 22)n_1^2 + (-4n^3 + 18n^2 - 22n)n_1 + n^4 - 6n^3 + 11n^2 - 6n \right) + \\ &+ \frac{a^3b^3}{6} \left(-2n_1^4 + 4nn_1^3 + (-3n^2 + 3n - 4)n_1^2 + (n^3 - 3n^2 + 4n)n_1 \right) \\ &+ \frac{a^2b^4}{4} \left(n_1^4 - 2nn_1^3 + (n^2 + n - 1)n_1^2 + (-n^2 + n)n_1 \right) \end{split}$$

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The Symmetric Stochastic Block Model SSBM(n, 2, a, b)Expectation of number of 4-cliques (4)

$$\mathbb{E}[X_4] = \frac{a^6}{24} \left(2\mathbb{E}[n_1^4] - 4n\mathbb{E}[n_1^3] + (6n^2 - 18n + 22)\mathbb{E}[n_1^2] \right. \\ \left. + (-4n^3 + 18n^2 - 22n)\mathbb{E}[n_1] + n^4 - 6n^3 + 11n^2 - 6n \right) + \\ \left. + \frac{a^3b^3}{6} \left(-2\mathbb{E}[n_1^4] + 4n\mathbb{E}[n_1^3] + (-3n^2 + 3n - 4)\mathbb{E}[n_1^2] + (n^3 - 3n^2 + 4n)\mathbb{E}[n_1] \right) \right. \\ \left. + \frac{a^2b^4}{4} \left(\mathbb{E}[n_1^4] - 2n\mathbb{E}[n_1^3] + (n^2 + n - 1)\mathbb{E}[n_1^2] + (-n^2 + n)\mathbb{E}[n_1] \right) \right.$$

where the expectations $\mathbb{E}[n_1]$, $\mathbb{E}[n_1^2]$, $\mathbb{E}[n_1^3]$ and $\mathbb{E}[n_1^4]$ have been computed before.

Simulations •000

Numerical Computation of Number of Cliques

An Iterative Algorithm

We discuss two algorithms to compute X_q : iterative, and adjacency matrix based algorithm.

Framework: we are given a sequence $(G_t)_{t\geq 0}$ of graphs on n vertices, where G_{t+1} is obtained from G_t by adding one additional edge: $G_t = (\mathcal{V}, \mathcal{E}_t), \ \emptyset = \mathcal{E}_0 \subset \mathcal{E}_1 \subset \cdots$ and $|\mathcal{E}_t| = t$. **Iterative Algorithm**: Assume we know $X_q(G_t)$, the number of q-cliques of graph G_t . Then $X_q(G_{t+1}) = X_q(G_t) + D_q(e; G_t)$ where $D_q(e; G_t)$ denotes the number of q-cliques in G_{t+1} formed by the additional edge $e \in \mathcal{E}_{t+1} \setminus \mathcal{E}_t$.

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Computation of Number of Cliques

An Analytic Formula

Laplace Matrix $\Delta = D - A$ contains all connectivity information. *Idea*: Note the (i, j) element of A^2 is

$$(A^2)_{i,j} = \sum_{k=1}^n A_{i,k} A_{k,j} = |\{k : i \sim k \sim j\}|.$$

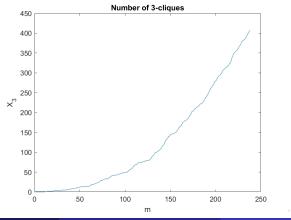
This means $(A^2)_{i,j}$ is the number of paths of length 2 that connect *i* to *j*. Hence $m = \frac{1}{2}trace(A^2)$. *Remark*: The diagonal elements of $A(A^2 - D)$ represent twice the number of 3-cycles (= 3-cliques) that contain that particular vertex. *Conclusion*:

$$X_3 = \frac{1}{6} trace \{A(A^2 - D)\} = \frac{1}{6} trace(A^3).$$

Simulations

Numerical results Graph of X_3 for the BKOFF dataset

Recall the dataset Bernard & Killworth Office. Weighted graph: Ordered m = 238 edges for n = 40 nodes. The plot of X_3 the number of 3-cliques:



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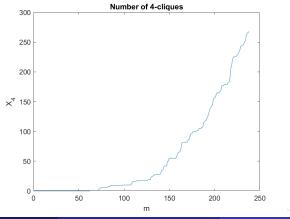
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Numerical results

Plot of X_4 for the BKOFF dataset

Weighted graph: Ordered m = 238 edges for n = 40 nodes. The plot of X_4 the number of 4-cliques:



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