Geometry of Exponential Random Graph Models

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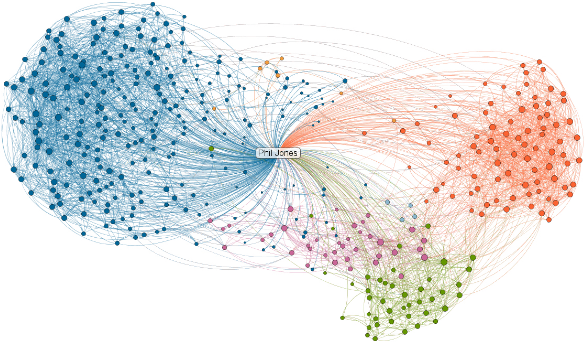
Big Statistical Challenge: *Researchers want to know how well a proposed model fits an observed network.*

- One of the most studied classes of network models are exponential random graph models, which are defined by network statistics (sufficient statistics).



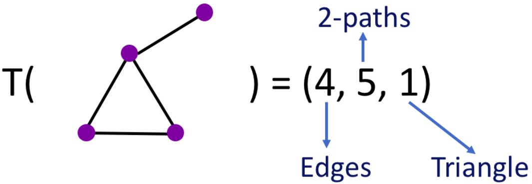
Exponential Random Graph Models

The model:

$$P_\theta(G) = Z(\theta)e^{\theta \cdot T(G)}, \ \theta \in \mathbb{R}^d$$

- $\theta \in \mathbb{R}^d$ is the **parameter vector**.
- $Z(\theta)$ is the **normalizing constant**.
- $T : \{\text{Graphs with } n \text{ vertices}\} \to \mathbb{Z}^d_{\geq 0}$ is the **sufficient statistic**.

Example to have in mind: Let $T(G)$ count the number of edges, 2-paths and triangles of the graph G.



Background and Notation

Adjacency Matrix: *Let $G = (V, E)$ be a graph with n vertices. Let A be the adjacency matrix of the graph, i.e.*

$$A_{ij} = \begin{cases} 1 & \text{if } (i,j) \in E, \\ 0 & \text{otherwise.} \end{cases} \tag{1}$$

Network Statistics: *The sufficient statistics of the edge-2path-triangle model are:*

- The number of edges of G: $t_1 = \sum_{i<j} A_{ij}$.
- The number of 2-paths in G: $t_2 = \sum_{i<j} (A^2)_{ij}$.
- The number of triangles in G: $t_3 = \frac{1}{6}\mathrm{tr}A^3$.

Adjacency Matrix: *Let $G = (V, E)$ be a graph with n vertices. Let A be the adjacency matrix of the graph, i.e.*

$$A_{ij} = \begin{cases} x_{ij} & \text{if } i < j, \\ 0 & \text{if } i = j, \\ x_{ji} & \text{if } i > j. \end{cases} \quad (2)$$

Network Statistics: *The sufficient statistics of the edge-2path-triangle model are:*

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Mantra of Algebraic Statistics

Statistical Models ⟷ Algebraic Varieties

Statistics | **Algebraic Geometry**

Algebraic Ideal

Definition

$k[x_1, \ldots, x_n]$ is the set of all polynomials in $x_1, \ldots, x_n$ with coefficients in k where k is a field.

Note: The field k can be $\mathbb{Q}$, $\mathbb{R}$, or $\mathbb{C}$.
Example: $x + y - z^2$ is a polynomial in $\mathbb{R}[x, y, z]$.

Definition

A subset $I \subset k[x_1, \ldots, x_n]$ is an **ideal** if it satisfies:

1. $0 \in I$.
2. If $f, g \in I$, then $f + g \in I$.
3. If $f \in I$ and $h \in k[x_1, \ldots, x_n]$, then $hf \in I$.

Algebraic Ideal

Definition

Let $f_1, \ldots, f_s$ be polynomials in $k[x_1, \ldots, x_n]$. Then we set

$$\langle f_1, \ldots, f_s \rangle = \left\{ \sum_{i=1}^{s} h_i f_i : h_1, \ldots, h_s \in k[x_1, \ldots, x_n] \right\}.$$

Lemma

If $f_1, \ldots, f_s \in k[x_1, \ldots, x_n]$, then $\langle f_1, \ldots, f_s \rangle$ is an ideal.
We will call $\langle f_1, \ldots, f_s \rangle$ the **ideal generated by** $f_1, \ldots, f_s$.

Example: $I = \langle x + y, x^2 - y + z^3 \rangle$ is an ideal of $\mathbb{R}[x, y, z]$ and it is generated by $x + y$ and $x^2 - y + z^3$.

Algebraic Variety

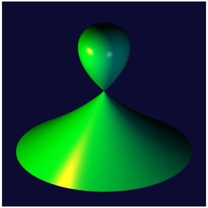
Definition

Let $f_1, \ldots, f_s$ be polynomials in $k[x_1, \ldots, x_n]$. Then we set

$$\mathbf{V}(f_1, \ldots, f_s) = \{(a_1, \ldots, a_n) \in k^n : f_i(a_1, \ldots, a_n) = 0 \ \forall 1 \le i \le s\}.$$

We call $\mathbf{V}(f_1, \ldots, f_s)$ the **affine variety** defined by $f_1, \ldots, f_s$.

Example:



$\mathbf{V}(x^2 + y^2 + z^3 - z^2)$

$\mathbf{V}((y^2 + z^2 - 1)^2 + (x^2 + y^2 - 1)^3)$

https://homepage.univie.ac.at/herwig.hauser/bildergalerie/gallery.html

Algebraic Variety

Interpretation: An affine variety $\mathbf{V}(f_1, \ldots, f_s) \subset k^n$ is the set of all solutions of the system of equations

$$f_1(x_1, \ldots, x_n) = \cdots = f_s(x_1, \ldots, x_n) = 0.$$

Similarly, given a polynomial ideal $\mathbf{I} = \langle g_1, \ldots, g_s \rangle \subset k[x_1, \ldots, x_n]$, $\mathbf{V}(\mathbf{I})$ is an affine variety in k^n. It is the set of all solutions of the system of equations where all the polynomials in $\mathbf{I}$ set equal to 0.

Research Goal

Goal: *Given the specific ERGM with edge, 2-paths, and triangle counts as sufficient statistics, we want to understand the geometry of the variety of the sufficient statistics by exploring*

1. *Dimension*
2. *Irreducibility*
3. *Singularities*

Review - Background and Notation

Adjacency Matrix: *Let $G = (V, E)$ be a graph with n vertices. Let A be the adjacency matrix of the graph, i.e.*

$$A_{ij} = \begin{cases} x_{ij} & \text{if } i < j, \\ 0 & \text{if } i = j, \\ x_{ji} & \text{if } i > j. \end{cases} \tag{3}$$

Network Statistics: *The sufficient statistics of the edge-2path-triangle model are:*

- The number of edges of G: $t_1 = \sum_{i<j} A_{ij}$.
- The number of 2-paths in G: $t_2 = \sum_{i<j} (A^2)_{ij}$.
- The number of triangles in G: $t_3 = \frac{1}{6}\text{tr}A^3$.

The Variety of Sufficient Statistics

Given a graph G and network statistic $t = T(G) = (t_1, t_2, t_3)$, the reference ideal of t is:

$$I_t = \langle \sum_{i<j} x_{ij} - t_1, \\ \sum_{i<j<k} (x_{ij}x_{jk} + x_{ij}x_{ik} + x_{ik}x_{jk}) - t_2, \\ \sum_{i<j<k} x_{ij}x_{jk}x_{ik} - t_3 \rangle \\ \subseteq k[x_{ij} \mid 1 \leq i < j \leq n].$$

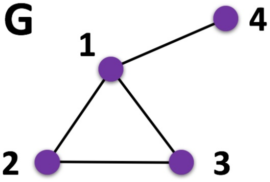
We will call the variety defined by I_t the reference variety:

$$V_t = V(I_t).$$

Example I

Consider the graph G in the figure below.

1. The number of edges of G: $t_1 = \sum_{i<j} A_{ij} = 4$.
2. The number of 2-paths in G: $t_2 = \sum_{i<j} (A^2)_{ij} = 5$.
3. The number of triangles in G: $t_3 = \frac{1}{6} tr(A^3) = 1$.



degree(I_t) = 6
dim(V_t) = 3

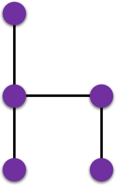
So, $t = T(G) = (4, 5, 1)$.

The reference ideal of G is:

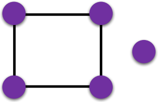
$$\begin{aligned} I_t = \langle & x_{12} + x_{13} + x_{23} + x_{14} + x_{24} + x_{34} - 4, \\ & x_{12}x_{13} + x_{12}x_{23} + x_{13}x_{23} + x_{12}x_{14} + x_{13}x_{14} + x_{14}^2 + x_{12}x_{24} + \\ & + x_{23}x_{24} + x_{24}^2 + x_{13}x_{34} + x_{23}x_{34} + x_{14}x_{34} + x_{24}x_{34} + x_{34}^2 - 5, \\ & x_{12}x_{13}x_{23} + x_{12}x_{14}x_{24} + x_{13}x_{14}x_{34} + x_{23}x_{24}x_{34} - 1 \rangle. \end{aligned}$$

Example II

$t_1 = (4, 4, 0)$, V_{t1} contains:

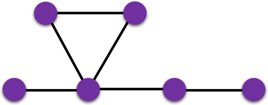


fork - chair



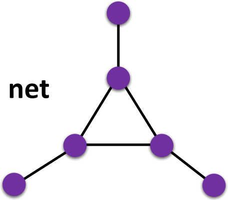
$C_4 \cup K_1$

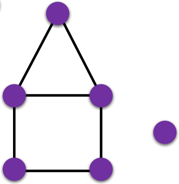
$t_2 = (6, 9, 1)$, V_{t2} contains:



X_{169}

net





co-4-fan

A Gröbner basis for I_t

Definition

Given an ideal $I \subset k[x_1, \dots, x_n]$. A finite subset G of I is a **Gröbner basis** with respect to the term order $\prec$ if the initial terms of the elements in G suffice to generate the initial ideal:

$$in_{\prec}(I) = \langle in_{\prec}(g) : g \in G \rangle.$$

Note: There is no minimality requirement for being a Gröbner basis. Hence, there is infinitely many Gröbner basis for an ideal I. But a **reduced Gröbner basis** is unique for every ideal I.

A Gröbner basis for I_t

Proposition

The polynomials

$$g_1 = f_1,$$
$$g_2 = \left(\sum_{i=2}^{n} x_{1i} + x_{2i}\right) f_1 - f_2,$$
$$g_3 = f_3 - \left(\sum_{i=3}^{n} x_{1i} x_{2i}\right) f_1 + x_{23} g_2$$

form a reduced Gröbner basis for I_t. In particular,

$$In(I_t) = \langle x_{12}, x_{13}^2, x_{23}^3 \rangle.$$

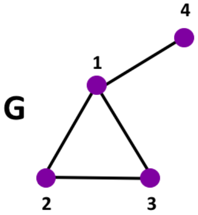
Dimension

Theorem

The ideal I_t has codimension 3.

That is, the dimension of the reference variety V_t is:

$$\dim(V_t) = \binom{n}{2} - 3.$$



$t = T(G) = (4, 5, 1)$

$$\dim(V_t) = \binom{4}{2} - 3$$
$$= 6 - 3 = 3$$

Irreducibility

Theorem

If $n \geq 4$, then I_t is prime.

In other words, if $n \geq 4$, then V_t is irreducible.

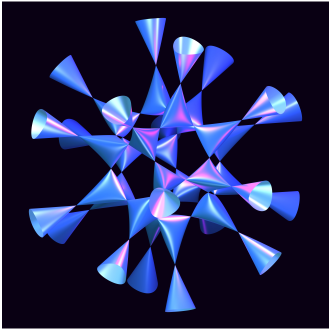
Proof.

- Fix $h_1, h_2 \notin I_t$ such that $h_1 h_2 \in I_t$. Based on the Gröbner basis, h_1 and h_2 have specific forms.
- $n = 4$: perform the polynomial long division on $h_1 h_2$ by g_2 and g_3 in Macaulay2. The result indicates that either $h_1 = 0$ or $h_2 = 0$.
- $n > 4$: by using division algorithm and induction, we show that the division of $h_1 h_2$ by g_2 and g_3 yields a remainder $r \neq 0$.

□

Definition

Intuitively, a **singular point** of $\mathbf{V}(f)$ is a point where the tangent line fails to exist.

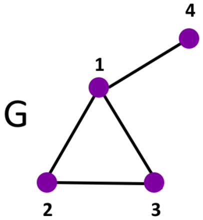


Bath Sextic - *https://imaginary.org/gallery/oliver-labs*

Edge-triangle Model:

Let G be a graph with n vertices. Let $t = T(G) = (t_1, t_3)$. The Jacobian of V_t at G, denoted $Jac(V_t)|_G$, is an $(n^2 - n) \times 2$ matrix whose rows are indexed by pairs (r, s) with $1 \leq r, s \leq n$ and $r \neq s$. The (r, s)th row of $Jac(V_t)|_G$ has the following form

$$[1 \quad \# \text{ of 2-paths between } r \text{ and } s].$$

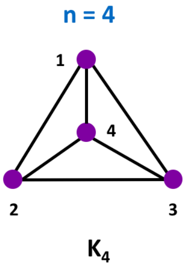


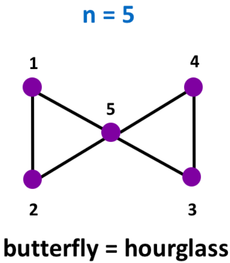
Rank 2 Jacobian

Edge-triangle Model:

Proposition

A graph G with n vertices is a singular point of a fiber of the edge-triangle model $\Leftrightarrow$ G is a windmill graph or a strongly regular graph of the form $(n, k, \frac{k^2-k}{n-1}, \frac{k^2-k}{n-1})$.





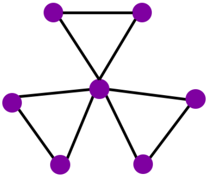
Singularitites

Remark

Just because a graph is singular in the edge-triangle model, it does not mean that it is singular in the edge-2path-triangle model.

n = 7

G



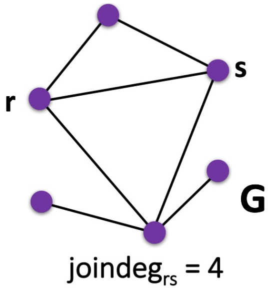
Edge-triangle Model:
Rank 1

Edge-2path-triangle Model:
Rank 3 (full rank)

Edge-2path-triangle Model:

Definition

Given a graph $G = (V, E)$ with adjacency matrix A and two vertices $r, s \in V$, let the joint degree of r and s in G be $jointdeg_{rs} := \deg r + \deg s - 2A_{rs}$.



The Jacobian of V_t at G, denoted $Jac(V_t)|_G$, is an $(n^2 - n) \times 3$ matrix whose rows are indexed by pairs (r, s) with $1 \leq r, s \leq n$ and $r \neq s$. The (r, s)th row of $Jac(V_t)|_G$ has the following form

$$[1 \quad \text{jointdeg}_{rs} \quad \# \text{ of 2-paths between } r \text{ and } s].$$

Singularities

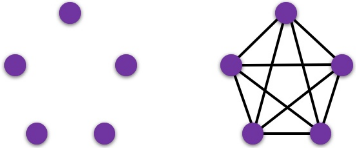
Edge-2path-triangle Model:

Proposition

Let G be a graph. If the automorphism group of G is the full symmetric group, then rank $Jac(V_t)_{|G} = 1$.

Proof.

Proof by contradiction: suppose rank $Jac(V_t)_{|G} \neq 1$.
Case 1: The number of 2-paths between r, s and u, v are different.
Case 2: The joint degrees between r, s and u, v are different.
In both cases, the permutation σ on G is not a graph automorphism (contradiction). Therefore, $Jac(V_t)_{|G} = 1$. □



Future Directions

1. Explore the relationship between singularity and degeneracy.
2. Can we use the geometry of the variety to develop a sampling algorithm for this statistical model?

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