The geometry of Markov random graphs Geometry and Combinatorics Seminar

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I. Random graphs

2. Encoding dependence

3. The stability of ERGMs

4. From stable to Lorentzian



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Random graphs

What are random graphs?

a set of graphs + some (measurable) uncertainty

a set of graphs + a probability distribution

Probability on a finite set

- Ω : a finite set
- $X: \Omega \to \{0,1\}$: discrete random variable
- $P:\Omega \rightarrow [0,1]$: a probability measure on Ω

 $\triangleright \ P(X=\Omega)=1$

Random subgraphs

- G = (V, E): a finite (undirected) graph
- $\mathcal{P}(E)$: power set of E
- A random subset $S \subseteq E$: a random variable $X : \mathcal{P}(E) \to \{0, 1\}$ that assigns a probability to each subset of edges

 \triangleright A random subset $S \subseteq E$ is a random element of $\mathcal{P}(E)$

Generating polynomials

• Well-developed ([BBL09], [ALGV19]) dictionary

 ${multivariate polynomials} \longleftrightarrow {probability distributions}$

• def. For X a random subgraph, its generating polynomial is

$$g_X := \sum_{S \subseteq E} P(X = S) \mathbf{x}^S$$

where $\mathbf{x}^S = \prod_{i \in S} x_i$ and $\mathbf{x} = (x_e)_{e \in E}$

Enhancing the dictionary

Operations

• Multiplication \longleftrightarrow disjoint union

 $\triangleright \ g_X \cdot g_Y = g_{X \sqcup Y}$

• Partial differentiation \longleftrightarrow conditioning

$$\triangleright \ \partial_i g_X = \sum_{S \ni i} P(X = S) \mathbf{x}^{S \setminus \{i\}}$$

 \triangleright i.e., $X \longmapsto (X \mid i \in S)$

• Specialization \longleftrightarrow conditioning

$$\triangleright \ g_X|_{x_i=0} = \sum_{S \not\supseteq i} P(X=S) \mathbf{x}^S$$

 $\triangleright \text{ i.e., } X \longmapsto (X \mid i \notin S)$

Enhancing the dictionary

Properties

- Positive coefficients \longleftrightarrow positive distribution
- Stability \longleftrightarrow negative dependence
 - Modelling repelling particles
 - ▷ Pairwise negative correlation: For $i \neq j$:

$$P(i,j\in S) \leq P(i\in S) \cdot P(j\in S)$$

Stable polynomials

- def. A nonzero polynomial g ∈ ℝ[x] is (real) stable if it does not have any roots in the open upper half of the complex plane H = {z ∈ ℂ^E : lm(z_e) > 0 for all e}.
- def. A probability distribution is strongly Rayleigh if g_X is stable.

Proposition [Brä07]

A multiaffine polynomial $g \in \mathbb{R}[\mathbf{x}]$ is stable if and only if for all $\mathbf{x} \in \mathbb{R}^E$ and $i, j \in E$ such that $i \neq j$,

$$\frac{\partial^2 g}{\partial x_i \partial x_j}(\mathbf{x}) g(\mathbf{x}) \le \frac{\partial g}{\partial x_i}(\mathbf{x}) \frac{\partial g}{\partial x_j}(\mathbf{x})$$

Lorentzian polynomials

 def. A subset J ⊆ N^E is M-convex when it satisfies the symmetric basis exchange property:

For any $\alpha, \beta \in J$ and an index i such that $\alpha_i > \beta_i$, there exists an index j such that $\alpha_j < \beta_j$ and $\alpha - e_i + e_j \in J$ and $\beta - e_j + e_i \in J$

Examples

- $\triangleright \quad G = (V, E)$: a finite connected graph
 - $J = \{\text{spanning trees of } G\} \subseteq \{0,1\}^E$
- $\triangleright M = matroid on a finite ground set E$
 - $\blacktriangleright J = \{ \text{bases of } M \}$
- $\triangleright \ J = \Delta^d_E \subseteq \mathbb{N}^E$
 - \blacktriangleright dth discrete simplex
 - Vectors with coordinate sum d

Lorentzian polynomials

- def. The support of a polynomial $g \in \mathbb{R}[\mathbf{x}]$ is

$$\operatorname{supp}(g) := \{ S \subseteq E : c_S \neq 0 \} \subseteq \mathbb{N}^E$$

where $g(\mathbf{x}) = \sum_{S \subseteq E} c_S \mathbf{x}^S$

• def. A polynomial $g \in \mathbb{R}[\mathbf{x}]$ is called positive if $\mathrm{supp}(g) = \{0, 1\}^E$

Lorentzian polynomials

Notation

- \triangleright H^d_E : homogeneous polynomials of degree d in variables $(x_e)_{e \in E}$
- $\triangleright M^d_E$: polynomials in H^d_E whose supports are M-convex
- $\,\triangleright\,\, L^2_E \subseteq H^2_E$: quadratic forms with non-negative coefficients that have at most one positive eigenvalue
- def. A homogeneous polynomial h ∈ H^d_E is Lorentzian if its support is M-convex and ∂_ih ∈ L^{d-1}_E for all i ∈ E. i.e., for d > 2:

$$L_E^d := \{ h \in M_E^d : \partial_i h \in L_E^{d-1} \text{ for all } i \in E \}$$

Lorentzian probability measures

• def. The homogenization of g_X is

$$h_X(z, \mathbf{x}) := \sum_{S \subseteq E} P(X = S) z^{|E| - |S|} \mathbf{x}^S$$

• def. A probability distribution is Lorentzian if h_X is Lorentzian.

Proposition [BH20]

If X is strongly Rayleigh, then X is Lorentzian.

A word on negative dependence

Proposition [BBL09]

Strongly Rayleigh probability measures are strongly conditionally negatively associated and pairwise negatively correlated.

Proposition [BH20]

Lorentzian probability measures are 2-Rayleigh: for all $\mathbf{x} \in \mathbb{R}^E_{\geq 0}$ and $i, j \in E$ such that $i \neq j$,

$$\frac{\partial^2 g}{\partial x_i \partial x_j}(\mathbf{x}) g(\mathbf{x}) \leq 2 \left(\frac{\partial g}{\partial x_i}(\mathbf{x}) \frac{\partial g}{\partial x_j}(\mathbf{x}) \right)$$

A word on negative dependence

- Negatively dependent probability measures have applications to determinantal point processes and machine learning ([AGV21, KT12])
- Identifying negatively dependent measures ([Pem00])



When is g_X stable or Lorentzian?

The first ideas and strides: Erdős-Rényi

- G = (V, E): finite
- Erdős-Rényi graphs G(p) for 0
 - I. Start with vertices V



- 2. Draw an edge between each pair of vertices with independent probability p
- Limitations: modelling complex systems

Erdős-Rényi graphs

- For
$$S \subseteq E$$
, $P(X = S) = p^{|S|}(1-p)^{|E|-|S|}$

Proposition

If X is Erdős-Rényi, then $g_X = \prod_{e \in E} (px_e + (1 - p))$ and this is a stable polynomial.



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Dependence

• Each edge in the Erdős-Rényi model is independent of the rest

How do we define a joint distribution where the random variables are not independent?

• Markov assumption: Adjacent edges are dependent



• def. A neighbourhood clique is a subset of pairwise dependent edges.

Markov random graphs

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- + G = (V, E): finite (undirected) graph with no self-loops
- def. The Markov random graph model on $\mathcal{P}(E)$ is:

$$P(X = G_S) \propto \exp\left(at_3(G_S) + \sum_{k \ge 1} b_k s_k(G_S)\right)$$

$$a, b_k \in \mathbb{R} : \text{parameters}$$

$$t_3(G_S) := \# \text{ triangles in } G_S$$

$$s_k(G_S) := \# k \text{-stars in } G_S$$

$$triangle$$

$$a, b_k \in \mathbb{R} : parameters$$

$$a, b_k$$

• def. The reduced Markov random graph is the above model reduced to only considering the edge and 2-star parameters.

The Markov-Gibbs correspondence

 $\{\text{positive Markov random fields}\} \longleftrightarrow \{\text{finite Gibbs distributions}\}$

Hammersley-Clifford theorem (1971)

A collection of positive random variables satisfy a Markov property if and only if it is a (finite) Gibbs distribution:

 $P(X = S) \propto \exp\left(-\mathcal{E}(S)\right)$

where ${\mathcal E}$ is an energy function that encodes the neighbourhood dependencies

• Every Gibbs distribution is positive

Cubic stable Markov random graphs

Proposition

If $G = C_3$, then the Markov random graph model is stable if and only if the triangle parameter a = 0.

Exponential random graphs (ERGMs)

- We can define a more general model with the following parameters:
 - \triangleright T > 0: temperature parameter
 - \triangleright F : a finite set of test graphs H
 - ▷ $\{a_H\}_{H \in F} \in \mathbb{R}^F$: a real parameter for each test graph
- def. $n_H(G_S) := \# \ln (H, G_S) = \# \{ H \hookrightarrow G_S \}$
- def. The exponential random graph model (ERGM) with the above parameters is

$$P(X = G_S) \propto \exp\left(\frac{1}{T} \sum_{H \in F} a_H n_H(G_S)\right)$$



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Behaviour with respect to temperature

• X : an ERGM

Variational question I

Fix $\{a_H\}_{H \in F}$. For which T is g_X stable?

Variational question 2

Fix T. For which parameters $\{a_H\}_{H\in F}$ is g_X stable?

Variational question I

Theorem I

Let X be an ERGM. If $a_H > 0$ for all $H \in F$, then $\lim_{T \to \infty} g_X$ is stable.

Variational question 2

Theorem 2

Let X be a reduced Markov ERGM and fix T > 0. Then, X is strongly Rayleigh for any choice of parameters b_1 and b_2 .

Proof sketch:

- Replace subgraph counts with homomorphism densities [Lov I 2]
- hom $(S_k, G) = \sum_{i \in V(G)} \deg(i)^{k-1}$
- $\hom(S_2, G) = 2|E(G)|$
- Specialize to a univariate polynomial [BBL09]
- Apply the Hermite-Sylvester theorem [Nat19]: a univariate polynomial is real-rooted iff its Hermite matrix is positive semidefinite

ERGMs on cycle graphs

Corollary

If n > 3, $G = C_n$, and X is the Markov random graph model on G, then X is strongly Rayleigh for any choice of parameters b_1 and b_2 .



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Lorentzian distributions and negative dependence

- Lorentzian is weaker than stability (but easier to test)
- Some negative dependence (i.e., the 2-Rayleigh property)

Proposition

If X is positive, then the support of h_X is M-convex.

Corollary

If X is an ERGM, then the support of h_X is M-convex.

Testing the Lorentzian condition for ERGMs

- Determining whether an ERGM is Lorentzian amounts to determining the signature of quadratic forms
 - \triangleright Quadratic forms \longleftrightarrow square symmetric matrices
- $Q: n \times n$ symmetric matrix
- $(n_+(Q), n_-(Q), n_0(Q))$: the number of positive, negative, and zero eigenvalues of Q

Testing the Lorentzian condition for ERGMs

- $Q: n \times n$ symmetric matrix
- $D_k(Q)$: leading $k \times k$ principal minor of Q

Proposition

If $D_k(Q) \neq 0$ for all k and $D_1(Q) > 0$, then

$$n_0(Q) = 0$$

$$n_+(Q) = \left| \left\{ 1 \le k \le n : \frac{D_k(Q)}{D_{k-1}(Q)} > 0 \right\} \right|$$

$$n_-(Q) = \left| \left\{ 1 \le k \le n : \frac{D_k(Q)}{D_{k-1}(Q)} < 0 \right\} \right|$$

where $D_0(Q) := 1$.

Testing the Lorentzian condition for ERGMs

- A quadratic form satisfies the Lorentzian condition iff $n_0(Q) = 0$ and $n_+(Q) \leq 1$

Corollary

If X is an ERGM and Q is a (relevant) quadratic form, then it satisfies the Lorentzian condition iff $D_k(Q) > 0$ for all odd k and $D_k(Q) < 0$ for all even k.

Lorentzian cubic Markov random graphs

Proposition

If $G = C_3$ then the Markov random graph model is Lorentzian if and only if the triangle parameter $a < \frac{9T}{2} \ln 2$.

Proof sketch:

• For ease of notation, let
$$B_1 := \exp\left(\frac{b_1}{3T}\right)$$
, $B_2 := \exp\left(\frac{b_2}{9T}\right)$, and
 $A := \exp\left(\frac{a}{27T}\right)$
 $h_X = z^3 + B_1^2 B_2^2 z^2 \left(\sum_{i=1}^3 x_i\right) + B_1^4 B_2^4 z \left(\sum_{\{i,j\}\in[3]} x_i x_j\right) + B_1^6 B_2^6 A^6 x_1 x_2 x_3$

Lorentzian cubic Markov random graphs: proof

• If
$$Q_0 = \frac{\partial}{\partial z} h_X$$
, then

$$\begin{split} D_1(Q_0) &= 3\\ D_2(Q_0) &= -4B_1^4B_2^4 < 0\\ D_3(Q_0) &= 5B_1^8B_2^8 > 0\\ D_4(Q_0) &= -6B_1^{12}B_2^{12} < 0 \end{split}$$

• The first relevant quadratic form satisfies the coniditon for any choice of edge and 2-star parameters b_1 and b_2

Lorentzian cubic Markov random graphs: proof

• For
$$i \in [3]$$
, let $Q_i = \frac{\partial}{\partial x_i} h_X$

$$D_1(Q_i) = B_1^2 B_2^2 > 0$$

$$D_2(Q_i) = -B_1^8 B_2^8 < 0$$

$$D_3(Q_i) = B_1^{14} B_2^{14} A^6 (2 - A^6)$$

• The remaining quadratic forms Q_i satisfy the Lorentzian condition iff

$$2 - A^{6} = 2 - \exp\left(\frac{2a}{9T}\right) > 0$$
$$a < \frac{9T}{2}\ln 2$$

Future directions

- Sequences of graphs as $V(G) \to \infty$
- Alternating-sign models
- ERGMs on finite graphs: acyclic condition
 - ▷ The random cluster model and the Tutte polynomial
- Connections to spin glass models and random matrix theory

Thank you!

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