Network Modeling

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Outline.

Introduction.

Random graph models.

 $\mathcal{G}(n, p)$. Definition of $\mathcal{G}(n, p)$. Sampling from $\mathcal{G}(n, p)$. Plausibility of $\mathcal{G}(n, p)$ as a model for social networks.

Towards more structured models.

Planted partition models. Preferential attachment.

Exponential random graph models.

Definition and examples. Sampling from an ERGM. Hammersley-Clifford Theorem. Near-degeneracy and multi-modality of ERGMs. Hypothesis testing.

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Statistical models for social network data.

Statistical models for social network data.

Social networks consist of actors and relations among them.

- actors: persons, organizations, companies, countries, ...
- relations: friendship, asking for advice, communication, collaboration, trade, war, ...



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Statistical models for social network data.

Data availability improved largely over the last decade.

- traditional data collection, e.g., by questionaires "please name your best friends"
- more and more automatically logged data from electronic communication and collaboration: telephone calls, email, online social networks, online markets, recommender systems, wikis, ...
- \Rightarrow opportunity and challenge for data-driven social science.

Statistical models for social network data.

Statistics can formulate precise statements about uncertainty.

What would happen, if we measured the data again?

- at a different point in time,
- on a different set of actors,
- with different environmental factors, ...

estimate expected outcome ± variability

 \Rightarrow to explain and predict social relations and behavior.

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Illustrative application: assessment of **social influence**.

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One American in ten tells the other nine how to vote, where to eat, and what to buy. They are The Influentials

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One American in ten tells the other nine how to vote, where to eat, and what to buy. They are The Influentials



Proposition is a bit too optimistic ... but approximate pattern might be empirically observable.

Social influence and network-based marketing. Empirical validation.

Hill, Provost, and Volinsky (2006): Network-Based Marketing. *Statistical Science* 21(2):256–276.

Data: Derived from a direct-mail marketing campaign of a telecommunications firm to promote a new product/service.

 "Traditional" variables: loyalty to firm, interest in high-tech products, early adopter, ...

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- Network variable: communicated with product adopter.
- Outcome: subsequently purchase or not.

Hypothesis: Customers connected to an adopter have a higher probability to purchase the product.

research question - graphically

One customer has already bought the product; some are connected to this early adopter.



Do customers connected to an early adopter have a higher probability to purchase the product?

Empirical validation (continued).

Research question: do customers connected to an early adopter have a higher probability to purchase the product?

Method: all potential customers are classified into *marketing segments* determined by traditional variables.

For each segment separately, compare

P(purchase | connected to adopter) P(purchase)

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Empirical validation (continued).

Method: all potential customers are classified into *marketing segments* determined by traditional variables.

For each segment separately, compare

P(purchase | connected to adopter) P(purchase)

Results: customers connected to product adopter have a purchase probability that is 3 to 5 times higher.

Network analysis can identify prospective customers ignored by traditional marketing strategies.

Social influence and network-based marketing. results – graphically

Customers connected to an early adopter do have a higher purchase probability!



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So, there is social influence - isn't it?

Other stories about social influence

Spread of obesity.

Christakis and Fowler (2007): The Spread of Obesity in a Large Social Network over 32 Years. *New England Journal of Medicine* 357:370–379.

Data (Framingham Heart Study): health data about 12,000 people from 1971–2003, including body mass index and various social relations.

Key result:

A person's chances of becoming obese increased by 57% [...] if he or she had a friend who became obese [...].

Is obesity contagious?

Spread of happiness and smoking behavior.

A person's chances of becoming obese increased by 57% [...] if he or she had a friend who became obese [...].

Other results on the same or similar datasets

- happy friends make an individual happier;
- individuals have a higher probability to start smoking if they are friends of smokers; ...

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Everything seems to spread through networks.

Criticism of popular network analysis methods.

Cohen-Cole and Fletcher (2008): Detecting Implausible Social Network Effects in Acne, Height, and Headaches. *British Medical Journal* 337:a2533.

Data: Add Health Study.

Results: using popular SNA methods it can be validated that

- people whose friends have skin diseases tend to develop skin diseases;
- individuals with tall friends become taller;
- the likelihood of headaches increases with the presence of a friend with headaches.

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Conclusion?

Revisiting social influence in purchase decisions.



One actor has bought the product.

His/her friends

- become aware of the product;
- receive recommendation;
- and/or desire to have it.



Some of them buy the product.

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Detailed mechanism (*middle*) has not been validated.

Alternative explanation of observed network data.

(2) Similar actors have a higher probability to become friends.



(3) Actors' characteristics influence purchase probabilities.

Alternative explanations for network effects.

Smokers' friends are often smokers.

individuals are influenced by their friends;

OR individuals chose those that are like them as friends.

Chances of becoming obese increase with obese friends.

individuals are influenced by their friends (e.g., eating behavior or acceptance of obesity);

- OR individuals chose those that are like them as friends;
- OR there are more fast-food restaurants in some regions; these cause obesity; and people living in the same region are more likely to become friends.

Social influence cannot be treated in isolation.

Actors who adopt a behavior might just have a higher probabiliy to be friends of early adopters. (not the other way round)

Need to model the relations as well-not just the behavior.

$$\begin{array}{c|c} \text{network}(t) & \rightarrow & \text{network}(t+1) \\ \hline & & & \\ \text{behavior}(t) & \rightarrow & \text{behavior}(t+1) \\ \end{array} \\ \begin{array}{c} \text{social influence} \\ \hline & & \\ \text{social influence} \\ \hline & & \\ \end{array} \\ \end{array}$$

Ignoring some of these dependencies may lead to spurious conclusions.

Statistical dependencies in network data.

Social influence.

- Network ties influence actors' behavior.
- E.g., friends of smokers start smoking.

Social selection.

- Actor characteristics influence network ties.
- E.g., smokers choose smokers as friends (homophily).

Network dependency.

- Ties influence other ties.
- E.g., friends of friends become friends (*transitivity*).

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Correlation of individual attributes.

E.g., eating behavior causes obesity.

Statistical models for social network data.

Specify realistic **probability distributions** for social networks (ties and behavior), where

- tie probabilities depend on other ties and behavior;
- behavior depends on social ties and behavior of others.

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Statistical network models serve several purposes.

Explaining social relations and/or behavior

 search for rules that govern the evolution of social networks.

Predicting social relations and/or behavior

learn from given data and predict the data yet to come.

Random generation of networks that look like real data

- algorithm engineering; empirical estimation of average runtime or performance;
- simulation of network processes (e.g., information spreading, spread of disease).

Structure of this lecture.

Varying amount of **time information** in the data requires different network models.

Networks observed at a single point in time

• model the probability of single networks P(G).

Networks observed at two or more points in time

model the conditional probability of later networks, given the previous ones P(G_t|G_{t-1}).

Continuously observed network changes or events

model the next network event, given the network of previous events P(e_t|G_{<t}).

Treated in three parts of this lecture.

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Definition and examples. Sampling from an ERGM. Hammersley-Clifford Theorem. Near-degeneracy and multi-modality of ERGMs. Hypothesis testing. Background: finite probability space.

Definition

A finite probability space is a pair (Ω, P) , where

- Ω is a finite set (*possible outcomes*)
- $P: \Omega \to [0, 1]$ a function satisfying $\sum_{\omega \in \Omega} P(\omega) = 1$.

Notation

- $P(\omega)$ is called the *probability* of $\omega \in \Omega$.
- The probability of a subset Ω' ⊆ Ω is defined by
 P(Ω') = ∑_{ω∈Ω'} P(ω).

Example (dice)

$$egin{aligned} \Omega &= \{1, 2, 3, 4, 5, 6\} \ P(\omega) &= 1/6 ext{ for all } \omega \in \Omega \ \Omega' &= \{1, 3, 5\} \end{aligned}$$

(possible outcomes when throwing a die) (uniform probability) (throwing an odd number) Background: finite probability space.

Definition

A finite probability space is a pair (Ω, P) , where

- Ω is a finite set (possible outcomes)
- $P: \Omega \to [0, 1]$ a function satisfying $\sum_{\omega \in \Omega} P(\omega) = 1$.

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Example (lottery)

$$\Omega = \{X \subset \{1, \dots, 49\}; |X| = 6\}$$
 (sets of 6 different numbers)
 $P(\omega) = {49 \choose 6}^{-1} = \frac{6!43!}{49!}$ for all $\omega \in \Omega$ (uniform probability)

Background: graphs.

Definition

A graph is a pair G = (V, E), where V is a finite set of vertices and E the set of edges.

- undirected graph: $E \subseteq {\binom{V}{2}} = \{\{u, v\}; u, v \in V\}$
- *directed* graph: $E \subseteq V \times V = \{(u, v); u, v \in V\}$
- loop: edge from a vertex to itself

Interpretation:

- vertices correspond to actors
- edges form the relation among them



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Random graph models.

Definition

A random graph model is a probability space (\mathcal{G}, P) , where \mathcal{G} is a (finite) set of graphs.

Example (uniform random graph model)

Let G be the set of all undirected, loopless graphs with vertex set $V = \{1, ..., n\}$ and let

$$P\colon \mathcal{G} \to \mathbb{R}; \ P(G) = rac{1}{2^{rac{n(n-1)}{2}}}$$

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Then (\mathcal{G}, P) is a random graph model.

Random graph models: notation.

- We consider only random graph models (G, P) in which all graphs in G have the same set of vertices; usually V = {1,...,n}.
- ► The set of *dyads D* consists of all elements that can be edges in a graph in *G*.
 - For undirected, loopless graphs:

 $D = \{ \{u, v\}; u, v \in V, u \neq v \}.$

- ► For directed, loopless graphs: $D = \{(u, v) : u, v \in V, u \neq v\}.$
- A dyad $e \in D$ is associated with a subset

$$\mathcal{G}_{\boldsymbol{e}} = \{ \boldsymbol{G} \in \mathcal{G} \; ; \; \boldsymbol{e} \in \boldsymbol{E}_{\boldsymbol{G}} \}$$

When we say *"probability of an edge e"*, we mean $P(\mathcal{G}_e)$, that is, the probability of \mathcal{G}_e .

Random graph models: edge probability.

A dyad $e \in D$ is associated with a subset of graphs

$${\mathcal G}_{m{e}} = \{ m{G} \in {\mathcal G} \ ; \ m{e} \in E_{m{G}} \}$$
 .

When we say "probability of an edge e", we mean $P(\mathcal{G}_e)$.

Thus, assigning a probability to each graph also determines the probability of individual edges.

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Does this also hold the other way round?

Independence and non-independence of edges.

In some cases the existence of an edge (or several edges) changes the probability of other edges.



For instance: does P(e) change when the nodes incident to e are indirectly connected via a third node? How? Why?

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Independence and non-independence of edges. small facebook network

769 nodes, 16656 edges \Rightarrow average edge probability is 0.056



186 722 dyads are indirectly connected via a third node; 16 556 of these are edges \Rightarrow average conditional edge probability for indirectly connected nodes is 0.089 Background: independence and conditional prob.

Definition

• Two subsets $A, B \subseteq \Omega$ are *independent* if

 $P(A \cap B) = P(A) \cdot P(B)$.

• If P(B) > 0, then the *conditional probability of A, given B* is

$$P(A|B) = \frac{P(A \cap B)}{P(B)}$$

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Example (probability space: dice) $A_{odd} = \{1, 3, 5\}$ and $A_{\leq 4} = \{1, 2, 3, 4\}$ are independent.

Background: independence and conditional prob.

Definition

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Example (probability space: dice) $A_{odd} = \{1, 3, 5\}$ and $A_{\leq 3} = \{1, 2, 3\}$ are **not** independent. Background: independence and conditional prob.

Definition

• Two subsets $A, B \subseteq \Omega$ are *independent* if

$$P(A \cap B) = P(A) \cdot P(B)$$
.

• If P(B) > 0, then the conditional probability of A, given B is

$$P(A|B) = rac{P(A \cap B)}{P(B)}$$

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Example (probability space: dice) $P(A_{odd}|A_{\leq 4}) = 1/2$, but $P(A_{odd}|A_{\leq 3}) = 2/3$ Independence of dyads in random graph models.

A dyad $e \in D$ is associated with a subset of graphs

$$\mathcal{G}_{\textit{e}} = \{\textit{G} \in \mathcal{G} \; ; \; \textit{e} \in \textit{E}_{\textit{G}} \}$$
 .

If G_{e1} and G_{e2} are independent, we say that "the dyads e₁ and e₂ are independent"

Definition

Let $D' \subset D$. A dyad $e \in D \setminus D'$ is said to be *independent* of D' if for all partitions $D' = D^+ \cup D^-$, the subset \mathcal{G}_e is independent of

$$\mathcal{G}_{D^+\cup D^-} = \{ G \in \mathcal{G} ; D^+ \subseteq E_G \text{ and } D^- \cap E_G = \emptyset \}$$

(all dyads in D^+ are edges in G and no dyad in D^- is an edge).

Structural balance theory (illustrating dependence).

Structural balance theory (Heider 1946) applies to triplets of 3 actors mutually connected by **positive** or **negative** ties:



not balanced

SBT claims that actors prefer balanced networks.

In an appropriate random graph model, it holds that

- all edges are pairwise independent;
- every edge depends on the two others.





For illustration, we treat in the following

- edge probability,
- independence of dyads,
- and expected number of edges

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of the uniform random graph model.

Uniform graph model: edge probability.

Lemma

The edge probability of a dyad $e \in D$ in the uniform random graph model is equal to 1/2.

Proof.

The two sets

$$\begin{array}{rcl} \mathcal{G}_{\boldsymbol{e}} &=& \{\boldsymbol{G} \in \mathcal{G} \; ; \; \boldsymbol{e} \in \boldsymbol{E}_{\boldsymbol{G}} \}, \\ \overline{\mathcal{G}_{\boldsymbol{e}}} &=& \{\boldsymbol{G} \in \mathcal{G} \; ; \; \boldsymbol{e} \notin \boldsymbol{E}_{\boldsymbol{G}} \} \end{array}$$

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- have the same cardinality $\Rightarrow P(\mathcal{G}_e) = P(\overline{\mathcal{G}_e})$,
- are disjoint $\Rightarrow P(\mathcal{G}_e) + P(\overline{\mathcal{G}_e}) = P(\mathcal{G}_e \cup \overline{\mathcal{G}_e}),$
- and their union equals $\mathcal{G} \Rightarrow \mathcal{P}(\mathcal{G}_e \cup \overline{\mathcal{G}_e}) = 1$.

$$\Rightarrow P(\mathcal{G}_e) = 1/2.$$

Uniform graph model: independence.

Lemma

The edge probability of a dyad $e \in D$ in the uniform random graph model is 1/2, **independent of all sets of dyads**.

Proof.

Let $D^+, D^- \subseteq D \setminus \{e\}$ be two disjoint subsets of dyads, not containing *e*. Consider

$$\mathcal{G}' = \{ G \in \mathcal{G} ; D^+ \subseteq E_G, \text{ and } D^- \cap E_G = \emptyset \}$$

(all dyads in D^+ are edges in G and no dyad in D^- is an edge).

Then, with $\mathcal{G}'_e = \{G \in \mathcal{G}' ; e \in E_G\}$ it follows $P(\mathcal{G}'_e | \mathcal{G}') = 1/2$ (as on the previous slide).

Background: random variable and expectation.

Let (Ω, P) be a probability space. Definition A random variable is a function $X \colon \Omega \to \mathbb{R}$.

Let $S = X(\Omega)$ be the set of values of X.

The *expectation* of the random variable X is defined by

$$\mathbb{E}(X) = \sum_{x \in S} x \cdot P(X = x) = \sum_{\omega \in \Omega} X(\omega) \cdot P(\omega)$$

Example

The prize assigned to lottery numbers is a random variable. Its expectation is the average gain that could be expected after "many" lottery draws (to be compared with the cost of a ticket). Background: linearity of expectation.

$$\mathbb{E}(X) = \sum_{\omega \in \Omega} P(\omega) \cdot X(\omega)$$
.

Lemma

If $X, Y : \Omega \to \mathbb{R}$ are two random variables and α a real number, then it is

$$\begin{split} \mathbb{E}(X+Y) &= \mathbb{E}(X) + \mathbb{E}(Y) \\ \mathbb{E}(\alpha \cdot X) &= \alpha \cdot \mathbb{E}(X) \ . \end{split}$$

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Background: density.

The *density* of a graph is the ratio

number of edges number of dyads

The density is between zero and one.

For undirected, loopless graphs with *n* vertices the denominator is equal to n(n-1)/2. For directed, loopless graphs with *n* vertices the denominator is equal to n(n-1).

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Uniform graph model: expected density.

Lemma

The expected density of graphs in $\mathcal{G}(n)$ equals 1/2.

Proof.

The number of edges of a graph G can be written as

$$\mathit{m}(\mathit{G}) = \sum_{\mathit{e} \in \mathit{D}} \chi_{\mathit{e}}(\mathit{G})$$

where $\chi_e \colon \mathcal{G} \to \{0,1\}$ is defined by

$$\chi_{e}(G) = \begin{cases} 1 & \text{if } e \in E_{G} \\ 0 & \text{else.} \end{cases}$$

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Uniform graph model: expected density.

Lemma

The expected density of graphs in $\mathcal{G}(n)$ equals 1/2.

Proof.

The number of edges of a graph G can be written as

$$\mathit{m}(\mathit{G}) = \sum_{\mathit{e} \in \mathit{D}} \chi_{\mathit{e}}(\mathit{G})$$

From the linearity of the expectation it follows that

$$\mathbb{E}[m] = \sum_{e \in D} \mathbb{E}[\chi_e] = \sum_{e \in D} P(e) \cdot 1 + (1 - P(e)) \cdot 0$$
$$= \sum_{e \in D} \frac{1}{2} \cdot 1 = \frac{1}{2} \frac{n(n-1)}{2}$$

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Uniform graph model: summary.

Characterizing properties:

- edges are mutually independent;
- all edges are equally likely;
- no preference for edges over non-edges or vice versa.

It has been found that empirical networks typically violate all of these properties:

- edges are not independent;
- have varying probabilities;
- networks are typically sparse (i. e., most dyads are non-edges).

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$\mathcal{G}(n, p)$ definition.

 $\mathcal{G}(n, p)$ is a model for undirected, loopless graphs.

Two parameters

 $n \in \mathbb{N}_{\geq 1}$ (number of vertices) $p \in [0, 1]$ (edge probability)

Definition of probability $P \colon \mathcal{G} \to [0, 1]$

Probability of graphs defined by specifying

- edge probability of each dyad is equal to p,
- each dyad is independent of all sets of dyads.

Probability of a graph in $\mathcal{G}(n, p)$.

Lemma

The probability of a graph G = (V, E) with m edges is

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

Proof.

For dyad $e \in D$ it is $P(e \in E) = p$, $P(e \notin E) = 1 - p$; multiply these probabilities over all dyads ... done. (multiplication is valid since edge probabilities are independent)

Remark

The uniform random graph model is identical with $\mathcal{G}(n, \frac{1}{2})$.

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 $\mathcal{G}(n, p)$ probability of a graph.

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

Proof.

(extended version)

$$P(G) = P({G})$$

$$= P\left(\left(\bigcap_{d \in E_G} \mathcal{G}_d \cap \bigcap_{d \in D \setminus E_G} \overline{\mathcal{G}}_d\right)\right)$$

$$= \prod_{d \in E_G} P(\mathcal{G}_d) \cdot \prod_{d \in D \setminus E_G} P(\overline{\mathcal{G}}_d)$$

$$= \prod_{d \in E_G} p \cdot \prod_{d \in D \setminus E_G} 1 - p$$

$$= p^m (1 - p)^{\frac{n(n-1)}{2} - m}.$$

Remark.

If every dyad is independent of all sets of dyads, then the probability of each graph is determined by the edge probabilities of all dyads.

In general (without independence), the edge probabilities do not uniquely determine the graph probability.

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Outline.

Introduction.

Random graph models.

$\mathcal{G}(n, p)$. Definition of $\mathcal{G}(n, p)$. Sampling from $\mathcal{G}(n, p)$.

Plausibility of $\mathcal{G}(n, p)$ as a model for social networks.

Towards more structured models.

Planted partition models. Preferential attachment.

Exponential random graph models.

Definition and examples. Sampling from an ERGM. Hammersley-Clifford Theorem. Near-degeneracy and multi-modality of ERGMs. Hypothesis testing. **Task:** design of a probabilistic algorithm returning a graph *G* with probability as in $\mathcal{G}(n, p)$.

Naive algorithm: iterate over all dyads $e \in D$

• draw a uniformly distributed random number $r \in [0, 1]$;

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• if $r \le p$ add e to the edge set.

Naive algorithm: iterate over all dyads $e \in D$

- draw a uniformly distributed random number $r \in [0, 1]$;
- if $r \le p$ add *e* to the edge set.

enumerate dyads

<i>d</i> ₁				
d ₂	d ₃			
d ₄	<i>d</i> 5	<i>d</i> ₆		
d ₇	d ₈	d ₉	<i>d</i> ₁₀	

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Naive algorithm: iterate over all dyads $e \in D$

- draw a uniformly distributed random number $r \in [0, 1]$;
- if $r \le p$ add e to the edge set.

*Is d*₁ *an edge?* (draw a random number...)

<i>d</i> ₁ ?				
d ₂	d ₃			
d ₄	<i>d</i> 5	<i>d</i> ₆		
d 7	d ₈	d ₉	<i>d</i> ₁₀	

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Naive algorithm: iterate over all dyads $e \in D$

- draw a uniformly distributed random number $r \in [0, 1]$;
- if $r \le p$ add e to the edge set.

 $\begin{array}{l} \textit{Is } \textit{d}_1 \textit{ an edge?} \\ \rightarrow \textit{NO (for instance)} \end{array}$

<i>d</i> ₁				
d ₂	d ₃			
d ₄	<i>d</i> 5	<i>d</i> ₆		
d 7	d ₈	d ₉	<i>d</i> ₁₀	

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Naive algorithm: iterate over all dyads $e \in D$

- draw a uniformly distributed random number $r \in [0, 1]$;
- if $r \le p$ add e to the edge set.

*Is d*₂ *an edge?* (draw a random number...)

<i>d</i> ₁				
<i>d</i> ₂ ?	d ₃			
<i>d</i> ₄	<i>d</i> 5	<i>d</i> ₆		
d ₇	<i>d</i> ₈	d ₉	<i>d</i> ₁₀	

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Naive algorithm: iterate over all dyads $e \in D$

- draw a uniformly distributed random number $r \in [0, 1]$;
- if $r \le p$ add e to the edge set.

Is d_2 *an edge*? → YES (for instance) ⇒ turn d_2 into the first edge



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Naive algorithm: iterate over all dyads $e \in D$

- draw a uniformly distributed random number $r \in [0, 1]$;
- if $r \le p$ add e to the edge set.

*Is d*₃ *an edge?* (draw a random number...)

<i>d</i> ₁				
<i>e</i> 1	<i>d</i> ₃ ?			
<i>d</i> ₄	d 5	<i>d</i> ₆		
d 7	<i>d</i> ₈	d ₉	<i>d</i> ₁₀	

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Naive algorithm: iterate over all dyads $e \in D$

- draw a uniformly distributed random number $r \in [0, 1]$;
- if $r \le p$ add e to the edge set.

 $\begin{array}{l} \textit{Is } \textit{d}_3 \textit{ an edge?} \\ \rightarrow \textit{NO (for instance)} \end{array}$

<i>d</i> ₁				
<i>e</i> 1	d ₃			
<i>d</i> ₄	<i>d</i> 5	<i>d</i> ₆		
d 7	d ₈	d ₉	<i>d</i> ₁₀	

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Naive algorithm: iterate over all dyads $e \in D$

- draw a uniformly distributed random number $r \in [0, 1]$;
- if $r \le p$ add e to the edge set.

go on . . .

<i>d</i> ₁				
<i>e</i> 1	d ₃			
d ₄	<i>d</i> 5	<i>d</i> ₆		
d 7	<i>d</i> ₈	d ₉	<i>d</i> ₁₀	

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Naive algorithm: iterate over all dyads $e \in D$

- draw a uniformly distributed random number $r \in [0, 1]$;
- if $r \le p$ add e to the edge set.

*Is d*₆ *an edge?* (draw a random number...)

<i>d</i> ₁				
<i>e</i> 1	d ₃			
d ₄	d 5	<i>d</i> ₆ ?		
d 7	d ₈	<i>d</i> 9	<i>d</i> ₁₀	

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Naive algorithm: iterate over all dyads $e \in D$

- draw a uniformly distributed random number $r \in [0, 1]$;
- if $r \le p$ add e to the edge set.

 $\begin{array}{l} \textit{Is } \textit{d}_6 \textit{ an edge?} \\ \rightarrow \texttt{YES} \textit{ (for instance)} \\ \Rightarrow \textit{turn } \textit{d}_6 \textit{ into the second edge} \end{array}$

<i>d</i> ₁				
<i>e</i> 1	d ₃			
d ₄	<i>d</i> 5	<i>e</i> ₂		
d 7	d ₈	d ₉	<i>d</i> ₁₀	

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Naive algorithm: iterate over all dyads $e \in D$

- draw a uniformly distributed random number $r \in [0, 1]$;
- if $r \le p$ add e to the edge set.

to be continued ...

<i>d</i> ₁				
<i>e</i> 1	d ₃			
d ₄	d 5	<i>e</i> ₂		
d 7	<i>d</i> ₈	<i>d</i> 9	<i>d</i> ₁₀	

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Background: sparse graphs and dense graphs.

Let *n* be the number of vertices and *m* the number of edges.

In undirected, loopless graphs it is $0 \le m \le n(n-1)/2 \in \Theta(n^2).$

A family of graphs with unbounded n = 1, 2, 3, ... is called

- dense if $m \in \Theta(n^2)$;
- sparse if $m \in \mathcal{O}(n)$;
- (in between: notation depends on context).

Density of sparse graphs tends to zero: $p \in O(1/n)$. Average degree of sparse graphs is bounded by constant: $\overline{d} \in O(1)$.

Empirical observation: social networks are typically sparse.

Generating graphs from $\mathcal{G}(n, p)$.

Naive algorithm: iterate over all dyads $e \in D$

• draw a uniformly distributed random number $r \in [0, 1]$;

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• if $r \le p$ add *e* to the edge set.

Runtime: is in $\Theta(n^2)$

 \Rightarrow asymptotically larger than the expected graph size, $\Theta(n + p \cdot n^2)$, if *p* is decreasing with *n* (sparse graphs).
Better ask the question:

How many dyads shall be left out before the next edge?

 \Rightarrow need only $\Theta(m)$ questions.

Randomly draw the number k of non-edges ...

draw $k = 1 \Rightarrow$ leave out one dyad; turn the second dyad into the first edge

draw $k = 3 \Rightarrow$ leave out the next three dyads (d_3 , d_4 , d_5); turn d_6 into the second edge



Better ask the question:

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 \Rightarrow need only $\Theta(m)$ questions.

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How many dyads shall be left out?

(Notation: q = 1 - p on the following slides.)

Observation: the next dyad that becomes an edge is preceeded by exactly k non-edges with probability $q^k p$.

⇒ randomly draw number k of non-edges (out of 0, 1,...) with probability $q^k p$ and add the k + 1th dyad to the edge set.

draw k = 1 (happens with probability qp)

draw k = 3 (happens with probability $q^3 p$)

<i>d</i> ₁				
d ₂	d ₃			
d ₄	d 5	<i>d</i> ₆		
d ₇	d ₈	d ₉	<i>d</i> ₁₀	

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d ₂	d ₃			
d ₄	d 5	<i>d</i> ₆		
d ₇	d ₈	d ₉	<i>d</i> ₁₀	

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<i>d</i> ₁				
<i>e</i> 1	d ₃			
d ₄	d 5	<i>d</i> ₆		
d ₇	d ₈	d ₉	<i>d</i> ₁₀	

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<i>d</i> ₁				
<i>e</i> 1	d ₃			
d ₄	<i>d</i> 5	<i>e</i> ₂		
d ₇	<i>d</i> 8	d ₉	<i>d</i> ₁₀	

How to draw numbers k = 0, 1, ... with probability $q^k p$?

Associate k = 0, 1, ... with interval $I_k \subset [0, 1]$ of length $q^k p$.



 $I_0 = [0, p], I_1 = [p, p + qp], I_2 = [p + qp, p + qp + q^2p], \dots$ Note that

$$\sum_{k=0}^{\infty} q^k p = p \cdot \sum_{k=0}^{\infty} q^k = p \cdot \frac{1}{1-q} = 1$$

For $r \leftarrow random([0, 1])$ choose k such that r is in I_k .

How to draw numbers k = 0, 1, ... with probability $q^k p$?



For $r \leftarrow random([0, 1])$ choose k such that r is in I_k .

The interval I_k ends at

$$\sum_{i=0}^{k} q^{i} p = p \cdot \sum_{i=0}^{k} q^{i} = p \cdot \frac{1-q^{k+1}}{1-q} = 1-q^{k+1}$$

For $r \leftarrow \text{random}([0, 1])$ compute the minimum k such that l_k ends after r, i. e., such that $1 - q^{k+1} > r$.

How to draw numbers k = 0, 1, ... with probability $q^k p$?

For $r \leftarrow \text{random}([0, 1])$ compute the minimum k such that $1 - q^{k+1} > r$.

The following inequalities are equivalent.

$$r < 1 - q^{k+1}$$

 $q^{k+1} < 1 - r$
 $(k+1)\log q < \log(1-r)$
 $k > \frac{\log(1-r)}{\log q} - 1$

Leave out $k := \left\lfloor \frac{\log(1-r)}{\log q} \right\rfloor$ dyads and insert the k + 1 dyad in the edge set.

 $\mathcal{G}(n, p)$ efficient generation (algorithm).

(Insert the
$$\left\lfloor \frac{\log(1-r)}{\log(1-p)} \right\rfloor + 1$$
 dyad in the edge set.)
 $E \leftarrow \emptyset$ 0 $n-1$
 $v \leftarrow 1 \ w \leftarrow -1$
while $v < n$ do
 $\left\lfloor \begin{array}{c} r \leftarrow random([0,1]) \\ w \leftarrow w + 1 + \left\lfloor \frac{\log(1-r)}{\log(1-p)} \right\rfloor \\ while \ w \ge v \text{ and } v < n \text{ do} \\ \ w \leftarrow w - v; \ v \leftarrow v + 1 \\ \text{if } v < n \text{ then} \\ \ \ E \leftarrow E \cup \{\{v, w\}\} \\ \text{return } G = (V, E)$

If $w \ge v$ then w is reduced by v and the row index v is incremented by one.

$\mathcal{G}(n, p)$ efficient generation (runtime).

$$E \leftarrow \emptyset$$

$$v \leftarrow 1 \ w \leftarrow -1$$
while $v < n$ do
$$\begin{bmatrix} r \leftarrow random([0, 1]) \\ w \leftarrow w + 1 + \left\lfloor \frac{\log(1 - r)}{\log(1 - p)} \right\rfloor \\$$
while $w \ge v$ and $v < n$ do
$$\begin{bmatrix} w \leftarrow w - v; \ v \leftarrow v + 1 \\ \text{if } v < n \text{ then} \\ \\ E \leftarrow E \cup \{\{v, w\}\} \end{bmatrix}$$
return $G = (V, E)$

 \Rightarrow runtime in $\mathcal{O}(m+n)$.

Outer while loop is executed m + 1 times (*m* is the number of edges of *G*).

Inner while loop is executed (in total) n - 1 times.

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Outline.

Introduction.

Random graph models.

$\mathcal{G}(n, p)$. Definition of $\mathcal{G}(n, p)$. Sampling from $\mathcal{G}(n, p)$. Plausibility of $\mathcal{G}(n, p)$ as a model for social networks.

Towards more structured models

Planted partition models. Preferential attachment.

Exponential random graph models.

Definition and examples. Sampling from an ERGM. Hammersley-Clifford Theorem. Near-degeneracy and multi-modality of ERGMs. Hypothesis testing. Can such a network be drawn from a $\mathcal{G}(n, p)$ model?

Graph has 769 vertices and about 16 600 edges.



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Which $\mathcal{G}(n, p)$? What is the most likely value for the parameter p?

Statistical inference of model parameters.

Problem: given a graph *G* generated from some parameterized random graph model (without knowing the parameter value).

What is the most likely parameter value?

Definition (maximum likelihood)

 $(\mathcal{G}, P_{\theta})$ random graph model parameterized by $\theta \in \Theta \subseteq \mathbb{R}^{k}$; $G_{\text{obs}} \in \mathcal{G}$ a graph (observation). *Likelihood* function associated with G_{obs}

$$L \colon \Theta \to \mathbb{R}; \ \theta \mapsto \mathcal{P}_{\theta}(\mathcal{G}_{\mathsf{obs}})$$

A parameter vector $\hat{\theta}$ maximizing *L*, i. e.,

$$\hat{\theta} = \arg \max_{\theta} L(\theta)$$

is called a *maximum likelihood estimate (MLE)* for θ .

Maximum likelihood estimate of p in $\mathcal{G}(n, p)$.

Assume that G_{obs} has exactly *m* edges; let $M = \frac{n(n-1)}{2}$.

$$L(p) = P_p(G_{obs}) = p^m (1-p)^{M-m} .$$

$$L'(p) = m \cdot p^{m-1} \cdot (1-p)^{M-m} - p^m \cdot (M-m) \cdot (1-p)^{M-m-1}$$

Setting L'(p) = 0 for 0 yields

$$m \cdot p^{m-1} \cdot (1-p)^{M-m} = p^m \cdot (M-m) \cdot (1-p)^{M-m-1}$$

$$m \cdot (1-p) = p \cdot (M-m)$$

$$m-pm = pM-pm$$

$$\frac{m}{M} = p$$

L(p) indeed assumes a maximum at $\hat{p} := \frac{m}{M}$ since [...].

Both graphs have 769 vertices and about 16 600 edges \Rightarrow both have the same probability in $\mathcal{G}(n, p)$. Maximum likelihood estimate for *p* is 0.056



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Which graph is drawn from a $\mathcal{G}(n, p)$ model?

Address this question by looking at two network properties:

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- 1. inhomogeneity of the graph density;
- 2. skewness of the degree distribution.

Inhomogeneity of the graph density



Colors encode the **dorm** variable (gray for missing value).

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Inhomogeneity of the graph density

Density of the whole network is 0.056



The subnetworks induced by the eight dorms have much higher densities, namely: 0.21, 0.37, 0.20, 0.35, 0.31, 0.24, 0.37, 0.25.

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Can this happen in a $\mathcal{G}(n, p)$ model?



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Comparing degree distributions.

Plotting vertex degree (y-axis) vs. rank of vertex degree.





max degree is 65 min degree is 21

max degree is 248 min degree is 1

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Plotting number of vertices (y-axis) with given degree (x-axis).



max degree is 65 min degree is 21

max degree is 248 min degree is 1

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$\mathcal{G}(n, p)$ probability of degree k.

Lemma

Let $v \in \{1, ..., n\}$ be any vertex. The probability that v has degree equal to $k \in \{0, ..., n-1\}$ in a graph drawn from $\mathcal{G}(n, p)$ is

$$P(d(v) = k) = \binom{n-1}{k} \cdot p^k q^{n-1-k}$$

Proof.

There are exactly $\binom{n-1}{k}$ different neighborhoods of *v* that have cardinality *k*. Each of them has probability $p^k q^{n-1-k}$.

$\mathcal{G}(n, p)$ probability of degree k.

details on the proof: let

$$\mathcal{N}_k(\mathbf{v}) = \{\{\mathbf{v}_1, \dots, \mathbf{v}_k\} \subseteq \mathbf{V} \setminus \{\mathbf{v}\}\}$$

be the set of *k*-element subsets of $V \setminus \{v\}$ (potential neighborhoods of size *k* of *v*). Define for $U \in \mathcal{N}_k(v)$ the subset

 $\mathcal{G}_U = \{ G \in \mathcal{G} ; \ \forall u \in U \colon \{u, v\} \in E_G \text{ and } \forall u \notin U \colon \{u, v\} \notin E_G \}$

(all graphs in which the neighborhood of *v* equals *U*). **Important fact:** \mathcal{G}_U and $\mathcal{G}_{U'}$ are disjoint for $U \neq U'$. Thus

$$P[d(v) = k] = \sum_{U \in \mathcal{N}_k(v)} P(\mathcal{G}_U) = \binom{n-1}{k} \cdot p^k q^{n-1-k}$$

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Histogram of degree2

Histogram of degree1





Degree distribution in $\mathcal{G}(n, p)$ (limit $n \to \infty$).

Theorem

Let $\lambda \in \mathbb{R}_{>0}$, $p_n := \lambda/(n-1)$ a sequence of edge probabilities, defined for $n \ge \lambda + 1$, $k \in \mathbb{N}_0$, $P_n[d(v) = k]$ probability that d(v) = k in $\mathcal{G}(n, p_n)$ for fixed v.

Then it is

$$\lim_{n\to\infty} P_n[d(v)=k] = e^{-\lambda} \cdot \frac{\lambda^k}{k!}$$

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(Is called Poisson distribution.)

Degree distribution in $\mathcal{G}(n, p)$ for large *n*.

Degree distribution of a graph drawn from $\mathcal{G}(n, p)$ with $n = 10^7$ and p = 10/(n-1); maximum observed degree is 30.

Histogram of degree.frequency



$$\lim_{n\to\infty} P_n[d(v)=k] = e^{-\lambda} \cdot \frac{\lambda^k}{k!}.$$



Histogram of degree2









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Towards more structured models.

Planted partition models. Preferential attachment.

Exponential random graph models.

Definition and examples. Sampling from an ERGM. Hammersley-Clifford Theorem. Near-degeneracy and multi-modality of ERGMs. Hypothesis testing. Two simple approaches to define more structured models.

- 1. **Planted partition models:** allow varying density between different classes of vertices (but keeping dyad independence as in the $\mathcal{G}(n, p)$ model).
- 2. **Incrementally defined models:** nodes and edges are incrementally added to the network; probability of later edges may depend on earlier ones (but not the other way round). Example: preferential attachment.

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Towards more structured models. Planted partition models.

Preferential attachment.

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Definition and examples. Sampling from an ERGM. Hammersley-Clifford Theorem. Near-degeneracy and multi-modality of ERGMs. Hypothesis testing. Recall: inhomogeneity of the graph density

Density of the whole network is 0.056



The subnetworks induced by the eight dorms have much higher densities, namely: 0.21, 0.37, 0.20, 0.35, 0.31, 0.24, 0.37, 0.25.

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Planted partition models.

Definition

A planted partition model is defined by

- ► A partition of the vertex set $V = V_1 \cup \cdots \cup V_k$ into *k* disjoint classes.
- ► Probabilities p_{ij} ∈ [0, 1] assigned to each pair (V_i, V_k) of classes.
- ► Two vertices u ∈ V_i and v ∈ V_j are connected by an edge with probability p_{ij}.

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Every dyad is independent of any set of dyads.

Planted partition models: example.

Matrix of edge probabilities for three vertex classes.

$p_1 \cdots p_1$	$p_2 \cdots p_2$	$p_3 \cdots p_3$
: :	: :	: :
$p_1 \cdots p_1$	$p_2 \cdots p_2$	$p_3 \cdots p_3$
$p_2 \cdots p_2$	$p_4 \cdots p_4$	$p_5 \cdots p_5$
: :	: :	: :
$p_2 \cdots p_2$	$p_4 \cdots p_4$	$p_5 \cdots p_5$
$p_3 \cdots p_3$	$p_5 \cdots p_5$	$p_6 \cdots p_6$
: :	: :	: :
$p_3 \cdots p_3$	$p_5 \cdots p_5$	$p_6 \cdots p_6$

For directed networks: matrix can be asymmetric. For loopless networks: diagonal elements are zero.

Planted partition models.

Definition

A planted partition model is defined by

- ► A partition of the vertex set $V = V_1 \cup \cdots \cup V_k$ into *k* disjoint classes.
- ► Probabilities p_{ij} ∈ [0, 1] assigned to each pair (V_i, V_k) of classes.
- ► Two vertices u ∈ V_i and v ∈ V_j are connected by an edge with probability p_{ij}.
- Every dyad is independent of any set of dyads.

Computation of probabilities and sampling in planted partition models is (almost) as simple as in $\mathcal{G}(n, p)$.
Outline.

Introduction.

Random graph models.

 $\mathcal{G}(n, p)$. Definition of $\mathcal{G}(n, p)$. Sampling from $\mathcal{G}(n, p)$. Plausibility of $\mathcal{G}(n, p)$ as a model for social networks.

Towards more structured models.

Planted partition models. Preferential attachment.

Exponential random graph models.

Definition and examples. Sampling from an ERGM. Hammersley-Clifford Theorem. Near-degeneracy and multi-modality of ERGMs. Hypothesis testing.

Recall: degree distributions.

sampled from $\mathcal{G}(n, p)$

empirical network.





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Other empirical dist. (Barabasi and Albert, 1999).

Note: logarithmic scaling of axes.



A Actor collaboration network n = 212,250 and $\overline{d} = 28.78$

- B WWW n = 325,729 and $\overline{d} = 5.46$
- C Power grid n = 4,941 and $\overline{d} = 2.67$

Preferential attachment: motivation and history.

Empirical observation: often a few nodes have very high degrees; degree-distribution resembles a *power-law*:

$$P(d(v)=k)pprox c\cdot rac{1}{k^\gamma}$$

Model idea (Barabási and Albert, 1999):

- 1. vertices are successively added to the network;
- new vertices create a fixed number of edges to already existing vertices;
- 3. probability of edge to vertex v is proportional to v's degree.

Interpretation high-degree vertices are more popular.

Experimental evidence for power-law distribution with $\gamma \approx$ 3.

Preferential attachment model.

Definition (Bollobás, Riordan, Spencer, and Tusnády)

Directed multi-graphs, including loops, with $n \ge 1$ vertices and constant outdegree equal to $b \ge 1$.

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Iterative definition:

start with empty graph $G = (V, E), V = E = \emptyset$

```
foreach v = 0, ..., n-1 do

put v into V

foreach j = 0, ..., b-1 do

attach an outgoing edge e = (v, \cdot) to v;

randomly select target w of e with probability

\frac{d_G(w)}{\sum_{w' \in V} d_G(w')};

put e = (v, w) into E;
```

Preferential attachment (algorithm).

uses: uniform random sampling of integer from $\{0, \ldots, k\}$

input : number of nodes $n \in \mathbb{N}_{>1}$, out-degree $b \in \mathbb{N}_{>1}$ data : array A[0...2nb-1] //collects endpoints of edges output multi-graph $G = (\{0, \ldots, n-1\}, E)$ $E \leftarrow \emptyset: m \leftarrow 0$ *//edge set and edge counter* foreach v = 0, ..., n - 1 do foreach i = 0, ..., b - 1 do $A[2m] \leftarrow v$ //v is source of next edge $w \leftarrow A[random(\{0, \dots, 2m\})]$ //randomly select target $\begin{bmatrix} A[2m+1] \leftarrow w; \\ E \leftarrow E \cup \{(v,w)\}; m \leftarrow m+1 \end{bmatrix}$ //put target in A //update edges

Note: number of occurences of *v* in *A* equals degree of $v \Rightarrow$ correct probability in selecting targets.

Preferential attachment leads to power law for low degree vertices.

Theorem (Bollobás, Riordan, Spencer, and Tusnády) For $a, b \in \mathbb{N}$ let δ be defined by

$$\delta(a,b) = \frac{2b(b+1)}{(a+b)(a+b+1)(a+b+2)}$$

For $n, a, b \in \mathbb{N}$ with $0 \le a \le n^{\frac{1}{15}}$ and $\varepsilon \in \mathbb{R}_{>0}$ it holds in the preferential attachment model that

$$P\left[(1-\varepsilon)\cdot\delta(a,b)\leq\frac{|\{v\in V_n: d_G^-(v)=a\}|}{n}\leq (1+\varepsilon)\cdot\delta(a,b)\right]$$

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Outline.

Introduction.

Random graph models.

 $\mathcal{G}(n, p)$. Definition of $\mathcal{G}(n, p)$. Sampling from $\mathcal{G}(n, p)$. Plausibility of $\mathcal{G}(n, p)$ as a model for social networks.

Towards more structured models.

Planted partition models. Preferential attachment.

Exponential random graph models.

Definition and examples. Sampling from an ERGM. Hammersley-Clifford Theorem. Near-degeneracy and multi-modality of ERGMs. Hypothesis testing.

Outline.

Introduction.

Random graph models.

 $\mathcal{G}(n, p)$. Definition of $\mathcal{G}(n, p)$. Sampling from $\mathcal{G}(n, p)$. Plausibility of $\mathcal{G}(n, p)$ as a model for social networks.

Towards more structured models. Planted partition models. Preferential attachment.

Exponential random graph models. Definition and examples.

Sampling from an ERGM. Hammersley-Clifford Theorem. Near-degeneracy and multi-modality of ERGMs. Hypothesis testing. Exponential random graph models (informal).

Exponential random graph models (ERGMs) are a **class** of random graph models.

Concrete ERG-model is specified by two components:

- 1. A set of network characteristics (*statistics*) that (may) have an influence on the probability of a graph.
- 2. A set of **parameters** (associated with statistics) that determine how network statistics increase or decrease the probabilities of graphs.

Choice of statistics often motivated by social science theory.

Parameters can be fitted to an observed network \Rightarrow hypothesis testing.

Exponential random graph models (ERGM).

Definition

The *ERGM class* consists of random graph models $(\mathcal{G}, P_{\theta})$ whose probability function P_{θ} can be written as

$$\mathcal{P}_{ heta}(G) = rac{1}{\kappa(heta)} \exp\left(\sum_{i=1}^k heta_i \cdot g_i(G)
ight)$$

with

- $g_i: \mathcal{G} \to \mathbb{R}$ for $i = 1, \dots, k$ (*statistics*);
- $\theta_i \in \mathbb{R}$ for i = 1, ..., k (parameters); $\theta = (\theta_1, ..., \theta_k)$;

normalizing constant κ defined by

$$\kappa(heta) = \sum_{m{G}'\in \mathcal{G}} \exp\left(\sum_{i=1}^k heta_i \cdot m{g}_i(m{G}')
ight)$$

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ERGM (example).

Consider undirected graphs with 3 vertices.

 $P(G) = \frac{1}{\kappa} \exp\left[-\log(2) \cdot m(G) + \log(16) \cdot \operatorname{triangles}(G)\right]$

	• •	•		
<i>m</i> (<i>G</i>)	0	1	2	3
triangles(G)	0	0	0	1
$P(G) \cdot \kappa$	1	$\frac{1}{2}$	$\frac{1}{2^2}$	$\frac{16}{2^3}$
# isomorphic graphs	1	3	3	1

 $\Rightarrow \kappa = 1 + 3 \cdot 1/2 + 3 \cdot 1/4 + 2 = 21/4$

Relation between statistics and probability.

Probability function

$$\mathcal{P}_{ heta}(G) = rac{1}{\kappa(heta)} \exp\left(\sum_{i=1}^k heta_i \cdot g_i(G)
ight),$$

Isolating the effect of one specific statistic g_{i_0} :

$$P_{ heta}(G) = \exp[heta_{i_0} \cdot g_{i_0}(G)] \cdot rac{1}{\kappa(heta)} \exp\left(\sum_{i
eq i_0} heta_i \cdot g_i(G)
ight)$$

 $\Rightarrow \text{ if } g_{i_0}(G') = g_{i_0}(G) + c \text{ and } g_i(G') = g_i(G) \text{ for all } i \neq i_0, \\ \text{then } P(G') = \exp(\theta_{i_0})^c \cdot P(G).$

It is $\exp(\theta_{i_0}) > 1 \Leftrightarrow \theta_{i_0} > 0$ and $\exp(\theta_{i_0}) < 1 \Leftrightarrow \theta_{i_0} < 0$.

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Relation between statistics and probability (example).

Let g_{i_0} count the number of triangles in *G*.

$$\mathcal{P}_{ heta}(G) = \exp[heta_{i_0} \cdot g_{i_0}(G)] \cdot rac{1}{\kappa(heta)} \exp\left(\sum_{i
eq i_0} heta_i \cdot g_i(G)
ight)$$



Positive $\theta_{i_0} \Rightarrow$ more likely;

Edge between 1 and 3 is $\exp(\theta_{i_0})$ -times as likely as between 1 and 4.

If other statistics change identically!

negative $\theta_{i_0} \Rightarrow$ less likely.

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Remark.

In this lecture we consider only ERGMs (\mathcal{G} , P) where \mathcal{G} is the set of all undirected, loopless graphs with vertex set $V = \{1, ..., n\}$.

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Example: $\mathcal{G}(n, p)$ belongs to the ERGM class.

Lemma

If $p \notin \{0,1\}$, then $\mathcal{G}(n,p)$ equals the ERGM defined by

$$P_1(G) = \exp\left[\theta \cdot m(G)\right] \cdot \kappa(\theta)^{-1}$$

where
$$\theta = \log\left(\frac{p}{1-p}\right)$$
.

Proof.

Let P_2 denote the probability function of the $\mathcal{G}(n, p)$ model.

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

= $\left(\frac{p}{1-p}\right)^{m(G)} \cdot (1-p)^{\binom{n}{2}}$
= $\exp \left[\theta \cdot m(G)\right] \cdot (1-p)^{\binom{n}{2}}$

Thus, $\frac{P_1(G)}{P_1(G')} = \frac{P_2(G)}{P_2(G')}$ for any two graphs G, G'.

Example: $\mathcal{G}(n, p)$ belongs to the ERGM class.

Proof. $P_1(G) = P_2(G) \frac{P_1(G')}{P_2(G')}$ for any two graphs *G*, *G*' implies that for arbitrary but fixed *G*' it is

$$\sum_{G \in \mathcal{G}} P_1(G) = \sum_{G \in \mathcal{G}} P_2(G) \cdot \frac{P_1(G')}{P_2(G')}$$
$$1 = 1 \cdot \frac{P_1(G')}{P_2(G')}$$

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Hence, $P_1(G') = P_2(G')$.

Interpretation of $\theta = \log \left(\frac{p}{1-p}\right)$.

Lemma If $p \neq 0, 1$, then $\mathcal{G}(n, p)$ equals the ERGM defined by

$$P_1(G) = \exp\left[\theta \cdot m(G)\right] \cdot \kappa(\theta)^{-1}$$

where $\theta = \log\left(\frac{p}{1-p}\right)$ and m(G) is the number of edges.

Relation between θ and p

- $\theta < 0 \iff$ expected density p < 1/2;
- $\theta = 0 \iff$ expected density p = 1/2;
- $\theta > 0 \iff$ expected density p > 1/2.

Does not hold in general (if the ERGM contains other statistics).

Commonly used network statistics (I).

Statistics g_i counting specific subgraphs (*configurations*).

$$\mathcal{P}_{ heta}(G) = rac{1}{\kappa(heta)} \exp\left(\sum_{i=1}^k heta_i \cdot g_i(G)
ight)$$

If a subgraph count is associated with a positive (negative) parameter, then those subgraphs are more (less) likely.

Example

► *m*(*G*) defined as the number of **edges**

models preference for edges over non-edges or vice versa.

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Commonly used network statistics (II).

$$\mathcal{P}_{ heta}(G) = rac{1}{\kappa(heta)} \exp\left(\sum_{i=1}^k heta_i \cdot g_i(G)
ight)$$

Example

assuming that actors have attribute values $a: V \rightarrow \{1, \ldots, c\}$, such as age, gender, ...

m_a(*G*) = |{{*u*, *v*} ∈ *E*; *a*(*u*) = *a*(*v*)}|, i. e., the number of edges connecting actors with the same attribute value

models tendency for (against) creating edges to similar actors **homophily (heterophily)**



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Commonly used network statistics (III).

Statistics g_i counting specific subgraphs (*configurations*).

$$\mathcal{P}_{ heta}(G) = rac{1}{\kappa(heta)} \exp\left(\sum_{i=1}^k heta_i \cdot g_i(G)
ight)$$

Example

► *t*(*G*) defined as the number of **triangles**

models preference (reluctance) to close triangles (transitivity).



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Commonly used network statistics (IV).

$$\mathcal{P}_{ heta}(G) = rac{1}{\kappa(heta)} \exp\left(\sum_{i=1}^k heta_i \cdot g_i(G)
ight)$$

Example

► $s_{\ell}(G)$ defined as the number of ℓ -stars, $\ell = 2, ..., n-1$ models tendency for (against) connecting to high-degree vertices.



Note: a vertex of degree *d* contributes $\binom{d}{\ell}$ to the ℓ -star count.

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Implication on dyad dependency.



Using some of these statistics make edge probabilities **dependent**.

Implication on dyad dependency.



Edge dependency (example).

Consider undirected graphs with 3 vertices; 2-star count s_2 .

Let e, e' be two different dyads.

$$\begin{array}{rcl} P(\mathcal{G}_{e}|\mathcal{G}_{e'}) &=& (2+8)/(1+2\cdot 2+8) = 10/13 \\ P(\mathcal{G}_{e}) &=& (1+2\cdot 2+8)/(1+3\cdot 1+3\cdot 2+8) = 13/18 \end{array}$$

Thus, dyads e and e' are statistically dependent.

Outline.

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Towards more structured models.

Planted partition models. Preferential attachment.

Exponential random graph models.

Definition and examples.

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Hammersley-Clifford Theorem. Near-degeneracy and multi-modality of ERGMs. Hypothesis testing.

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Sampling from an ERGM: why is this difficult?

We want to design a probabilistic algorithm that

- returns at each call a graph G from \mathcal{G} ;
- with probability equal to P(G).

So far, algorithms for sampling from $\mathcal{G}(n, p)$ or the preferential attachment model decided about the inclusion/exclusion of edges one after the other.

(In general) this is not feasible for ERGMs

we cannot compute edge probabilities

$$P(e \in E) = P(\mathcal{G}_e) = P(\{G \in \mathcal{G}; e \in E_G\})$$

in an efficient way;

► we cannot even compute P(G) for a single graph G since the normalizing constant has 2ⁿ(ⁿ) terms.

Markov chain simulation (informal).

A Markov chain consists of a set of states and transition probabilities to jump from one state to another.

Here, given an ERGM (\mathcal{G}, P)

- the set of states is G (all graphs);
- transition probabilities π are a function of *P*
- in such a way that
 - ► the probability to be on a graph G converges to P(G), when the number of simulation steps tends to ∞.
- \Rightarrow Simulate many steps and return the current graph.



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Finite stationary Markov chain (simplified definition).

Note: Markov chains are usually defined as *random processes* that satisfy certain properties. The following is a more intuitive definition for stationary Markov chains.

Definition

A (finite stationary) Markov chain is a pair (\mathcal{G}, π) , where

- \mathcal{G} is a finite set $\mathcal{G} = \{G_1, \ldots, G_N\}$ (*state space*);
- π is a matrix $\pi \in \mathbb{R}^{N \times N}$ (*transition matrix*) satisfying
 - ▶ for all *i*, *j* it is π_{ij} ∈ [0, 1];
 - for all *i* it is $\sum_{j=1}^{N} \pi_{ij} = 1$.

 π_{ij} interpreted as the probability to jump from state G_i to G_j .



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How to define the transition probabilities.

Goal: given an ERGM (\mathcal{G}, P)

▶ define transition probabilities π on the set of graphs G in such a way that the probability to **be on a graph** G converges to P(G), when the number of simulation steps tends to ∞.

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Background: eigenvectors and eigenvalues.

Let $A \in \mathbb{R}^{n \times n}$ be a matrix and $x \in \mathbb{C}^n$ be a vector. If there is a $\lambda \in \mathbb{C}$ such that

 $\boldsymbol{A}\cdot\boldsymbol{x}=\boldsymbol{\lambda}\cdot\boldsymbol{x} \ ,$

then x is called an *eigenvector* of A and (if $x \neq 0$) λ is called an *eigenvalue* of A.

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Stationary state space distributions.

A *Markov chain* is a pair (\mathcal{G}, π) , where π_{ij} is the probability to jump from state G_i to state G_i .

$$\begin{array}{c} P(G_1) \xrightarrow{\pi_{12}} P(G_2) \xleftarrow{\pi_{32}} P(G_3) \\ & & \uparrow \\ P(G_4) & P(G_5) & \cdots \end{array}$$

A probability distribution *P* on *G* is called *stationary* if for all *j* it is $P(G_j) = \sum_{i=1}^{N} P(G_i) \pi_{ij}$.

Satisfied if and only if (with $P = [P(G_1) \dots P(G_N)] \in \mathbb{R}^N$ written as a row vector) it is

$$\mathsf{P}=\mathsf{P}\pi$$
 ,

i.e., *P* is an eigenvector of π with eigenvalue one.

Irreducible and aperiodic Markov chains.

 π_{ij} interpreted as the probability to jump from state G_i to G_j .



A sequence of states $G_{i_1}, G_{i_2}, \ldots, G_{i_k}$ is called a *(directed) path* if for all $j = 1, \ldots, k - 1$ it is $\pi_{i_j i_{j+1}} > 0$.

Definition

The Markov chain (\mathcal{G}, π) is called

- *irreducible* if for any two states G_i, G_j ∈ G there is a path from G_i to G_j;
- aperiodic if the greatest common divisor of the length of all cycles (i. e., paths from a state to itself) equals one.

Stationary distribution of reversible Markov chains.

Theorem

If a probability distribution P on G satisfies for all graphs G_i , G_j

$$P(G_i)\pi_{ij}=P(G_j)\pi_{ji}$$

(Markov chain is then called reversible) and the Markov chain is irreducible and aperiodic then P is the unique stationary distribution of the Markov chain and for any initial distribution P' it is

$$\lim_{K\to\infty} P'\pi^K = P \;\;.$$

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Conditions will be used to find an appropriate π if *P* is given.

Background: Perron-Frobenius Theorem.

spectral radius $\rho(A) = \max\{|\lambda|; \lambda \text{ is eigenvalue of } A\}$

Theorem (Perron-Frobenius)

The spectral-radius $\rho(A)$ of a non-negative, irreducible, aperiodic matrix A is an eigenvalue of multiplicity one, all entries of an associated eigenvector are non-zero and have the same sign, and the absolute values of all smaller eigenvalues are strictly smaller than ρ .

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Background: power iteration.

Theorem (power iteration)

Let A be a non-negative, irreducible, aperiodic matrix and x a normalized eigenvector with associated eigenvalue $\rho(A)$. For a vector $y^{(0)}$ whose projection onto x is not zero define a sequence of vectors by

$$y^{(i+1)} = \frac{\boldsymbol{A} \cdot \boldsymbol{y}^{(i)}}{\|\boldsymbol{A} \cdot \boldsymbol{y}^{(i)}\|}$$

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Then $\lim_{i\to\infty} y^{(i)} = x$.
Stationary distribution of reversible Markov chains. Theorem

If a probability distribution P on G satisfies for all graphs G_i , G_j

$$\mathsf{P}(G_i)\pi_{ij}=\mathsf{P}(G_j)\pi_{ji}$$

and the Markov chain (\mathcal{G}, π) is irreducible and aperiodic then P is the unique stationary distribution of (\mathcal{G}, π) and for any initial distribution P' it is

$$\lim_{K
ightarrow\infty}oldsymbol{P}'\pi^K=oldsymbol{P}$$
 .

Proof.

Matrix π satisfies the conditions of the theorems on the previous slides. We show that

- *P* is an eigenvector of π with eigenvalue one;
- the spectral radius ρ of π is one.

P is an eigenvector of π with eigenvalue one.

From

$$\mathsf{P}(\mathsf{G}_{i})\pi_{ij}=\mathsf{P}(\mathsf{G}_{j})\pi_{ji}$$

it follows that for all $G_i \in \mathcal{G}$ it is

$$\sum_{G_j \in \mathcal{G}} P(G_j) \pi_{ji} = \sum_{G_j \in \mathcal{G}} P(G_i) \pi_{ij} = P(G_i)$$

(since the rows of π sum up to one).

Thus, *P* and π satisfy the matrix equation $P\pi = P$, i.e., *P* is an eigenvector of π with eigenvalue one.

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The spectral radius ρ of π is one.

We have that for all *i* it is $\sum_{j=1}^{N} \pi_{ij} = 1$.

Let *x* be an eigenvector of π with eigenvalue ρ .

For all *j* it is $\rho x_j = \sum_{i=1}^N x_i \pi_{ij}$. Thus

$$\rho \sum_{j=1}^{N} x_j = \sum_{j=1}^{N} \rho x_j = \sum_{j=1}^{N} \sum_{i=1}^{N} x_i \pi_{ij}$$
$$= \sum_{i=1}^{N} \sum_{j=1}^{N} x_i \pi_{ij} = \sum_{i=1}^{N} x_i \sum_{j=1}^{N} \pi_{ij} = \sum_{i=1}^{N} x_i$$

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Since $\sum_{i=1}^{N} x_i \neq 0$, it must be $\rho = 1$.

Stationary distribution of reversible Markov chains.

Theorem

If a probability distribution P on G satisfies for all graphs G_i , G_j

$$P(G_i)\pi_{ij}=P(G_j)\pi_{ji}$$

(Markov chain is called reversible) and the Markov chain is irreducible and aperiodic then P is the unique stationary distribution of the Markov chain and for any initial distribution P' it is

$$\lim_{K o\infty} {m P}' \pi^K = {m P}$$
 .

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Gibbs sampling.

Given *P*, define π such that

$$\mathsf{P}(\mathsf{G}_{i})\pi_{ij}=\mathsf{P}(\mathsf{G}_{j})\pi_{ji}$$
 .

Gibbs sampling: define π as follows

- $\pi_{ij} = 0$ if G_i and G_j differ in more than one dyad;
- ▶ if G_i and G_i differ in exactly one dyad, then

$$\pi_{ij} = \frac{P(G_j)}{\binom{n}{2}(P(G_i) + P(G_j))}$$

• $\pi_{ii} = \sum \frac{P(G_i)}{\binom{n}{2}(P(G_i) + P(G))}$

(sum over all G that differ from G_i in exactly one dyad)

Show: π is normalized, irreducible, aperiodic, reversible.

Gibbs sampling.

Transition probabilities defined by

$$\pi_{ij} = rac{P(G_j)}{\binom{n}{2}(P(G_i) + P(G_j))}$$
.

Didn't we claim that it is intractable to compute P(G)?

$$egin{array}{rcl} P_{ heta}(G) &=& rac{1}{\kappa(heta)}\exp\left(\sum_{i=1}^k heta_i\cdot g_i(G)
ight) \ \kappa(heta) &=& \sum_{G'\in\mathcal{G}}\exp\left(\sum_{i=1}^k heta_i\cdot g_i(G')
ight) \end{array}$$

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Gibbs sampling (algorithm).

initialize G by any graph from G; repeat *many* times

- select a dyad {*i*, *j*} uniformly at random;
- with probability $\frac{P(G^{+ij})}{P(G^{+ij})+P(G^{-ij})}$
 - ▶ replace G = (V, E) by $G^{+ij} = (V, E \cup \{i, j\})$
 - otherwise replace G = (V, E) by $G^{-ij} = (V, E \setminus \{i, j\})$;

return G;

Note: (in practice) the statistics $g_{\ell}(G^{+ij})$ and $g_{\ell}(G^{-ij})$ can be efficiently derived by computing changes to the statistics $g_{\ell}(G)$.

The ability to sample from an ERGM enables us to efficiently estimate quantities that are computationally intractable. For instance,

▶ the expected number of edges, triangles, ℓ-stars,...;

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- the normalizing constant κ ;
- the probability P(G) of a specific graph G.

Estimation of the expected number of edges.

Let (\mathcal{G}, P) be an ERGM. By definition it is

$$\mathbb{E}(m) = \sum_{G \in \mathcal{G}} P(G) \cdot m(G) \; .$$

To approximate $\mathbb{E}(m)$ draw *K* random samples G_1, \ldots, G_K from (\mathcal{G}, P) and compute

$$\widehat{\mathbb{E}(m)} = \sum_{i=1}^{K} \frac{1}{K} \cdot m(G_i) \; .$$

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 $\widetilde{\mathbb{E}}(m)$ converges to $\mathbb{E}(m)$ in probability when $K \to \infty$.

Outline.

Introduction.

Random graph models.

 $\mathcal{G}(n, p)$. Definition of $\mathcal{G}(n, p)$. Sampling from $\mathcal{G}(n, p)$. Plausibility of $\mathcal{G}(n, p)$ as a model for social networks.

Towards more structured models.

Planted partition models. Preferential attachment.

Exponential random graph models.

Definition and examples. Sampling from an ERGM.

Hammersley-Clifford Theorem.

Near-degeneracy and multi-modality of ERGMs. Hypothesis testing.

Recall: some statistics make edge probabilities dependent – others not.

$$P_{ heta}(G) = rac{1}{\kappa(heta)} \exp\left(\sum_{i=1}^{k} heta_i \cdot g_i(G)
ight)$$



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Conditional independence of edges (informally).

Two dyads d_1 and d_2 are said to be *conditionally independent* (given the rest of the graph) if—under the condition that all other dyads are fixed—the state of the dyad d_2 does not provide any additional information about the probability $P(d_1 \in E)$.



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Conditional independence of edges.

Let (\mathcal{G}, P) be a random graph model where *D* is the set of dyads of graphs in \mathcal{G} and assume that P(G) > 0 for all $G \in \mathcal{G}$. Let $d_1, d_2 \in D$ be two different dyads.

For a partition $D^+ \uplus D^- = D \setminus \{d_1, d_2\}$ of the set of dyads different from d_1 and d_2 let the subset $\mathcal{G}_{D^+ \uplus D^-}$ be defined by

$$\mathcal{G}_{D^+ \uplus D^-} = \{ G \in \mathcal{G} \ ; \ D^+ \subseteq E_G \ \text{and} \ D^- \cap E_G = \emptyset \}$$

We say that d_1 and d_2 are *conditionally independent* (given the rest of the graph) if for all partitions $D^+ \uplus D^- = D \setminus \{d_1, d_2\}$ it is

$$P(\mathcal{G}_{d_1}|\mathcal{G}_{D^+\uplus D^-}) = P(\mathcal{G}_{d_1}|\mathcal{G}_{D^+\uplus D^-}\cap \mathcal{G}_{d_2})$$
.

Informally: if we know the state of all dyads in $D \setminus \{d_1, d_2\}$, the state of the dyad d_2 does not provide any additional information about the probability $P(d_1 \in E)$.

Markov random graphs.

Definition

Markov random graphs are a class of random graph models satisfying (1) the probability of every graph is positive and (2) for every set of four pairwise different vertices $\{i, j, u, v\}$ the dyads $\{i, j\}$ and $\{u, v\}$ are conditionally independent, given the rest of the graph.

Example

 $\{i, j\}$ and $\{u, v\}$ conditionally independent;

 $\{i, j\}$ and $\{j, u\}$ might be conditionally dependent;



We'll see later that Markov graphs are a subclass of the ERGM class.

Dependence graph (of a random graph model).

Definition

Let (\mathcal{G}, P) be a random graph model and let *D* be the set of dyads of graphs in \mathcal{G} .

The dependence graph $\mathcal{D} = (D, E)$ of (\mathcal{G}, P) has vertex set D,

 $\{d_i, d_j\} \in E$ if d_i and d_j are conditionally dependent, given the rest of the graph.

Example

the dependence graph of a Markov graph on vertices $V = \{1, 2, 3, 4\}$ is



Hammersley-Clifford Theorem; special case.

Theorem (first part)

Let (\mathcal{G}, P) be a random graph satisfying P(G) > 0 for all $G \in \mathcal{G}$, let D be the set of dyads and \mathcal{D} the dependence graph.

There are constants { $\alpha_A \in \mathbb{R}$; $A \subseteq D$ }, satisfying $\alpha_A = 0$ if A is not a clique in \mathcal{D} , such that

$$P(G) = \frac{1}{\kappa} \exp\left(\sum_{A \subseteq E(G)} \alpha_A\right), \quad \text{where} \quad (1)$$

$$\kappa = \sum_{G' \in \mathcal{G}} \exp\left(\sum_{A \subseteq E(G')} \alpha_A\right). \quad (2)$$

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Note: A is a clique in \mathcal{D} if dyads in A are pairwise dependent. $A \subseteq E(G)$ means that all dyads in A are edges in G. Hammersley-Clifford Theorem; special case.

Theorem (second part)

Conversely, if the probability P on G is defined by

$$\begin{split} \mathcal{P}(G) &= \frac{1}{\kappa} \exp\left(\sum_{A \subseteq E(G)} \alpha_A\right) \ , \qquad \textit{where} \\ \kappa &= \sum_{G' \in \mathcal{G}} \exp\left(\sum_{A \subseteq E(G')} \alpha_A\right) \ , \end{split}$$

then two dyads d_1 and d_2 are conditionally independent in (\mathcal{G}, P) , unless there is a subset $A \subseteq D$ with $d_1, d_2 \in A$ and $\alpha_A \neq 0$.

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Conclusion from the Hammersley-Clifford Theorem.

There are constants { $\alpha_A \in \mathbb{R}$; $A \subseteq D$ }, such that

$$P(G) = \frac{1}{\kappa} \exp\left(\sum_{A \subseteq E(G)} \alpha_A\right)$$

Every random graph model (\mathcal{G}, P) with P > 0 is an ERGM

- ► statistics: for $A \subseteq D$ define $g_A(G) = \begin{cases} 1 & A \subseteq E(G) \\ 0 & \text{else} \end{cases}$
- parameters: α_A

$$P(G) = \frac{1}{\kappa} \exp\left(\sum_{A \subseteq D} \alpha_A \cdot g_A(G)\right)$$

Cliques in the dependence graph of a Markov graph.

Markov random graphs: edges $\{i, j\}$ and $\{u, v\}$ are conditionally independent, unless they have a vertex in common.

Cliques in the dependence graph of a Markov graph are



No other subgraphs are cliques in the dependence graph.

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ERGM of general Markov graphs.

Corollary Let (\mathcal{G}, P) be a Markov random graph on vertices $V = \{1, ..., n\}$. Then there are real constants

$$\begin{array}{ll} \eta_{uv} & \text{for all} & \text{dyads} \{u, v\} \\ \tau_{uvw} & \text{for all} & \text{triangles} \{u, v, w\} \\ \sigma_{uv_1 \dots v_\ell} & \text{for all} & 2 \leq \ell \leq n-1, \text{ and all} \\ \ell \text{-stars} (u, \{v_1, \dots, v_\ell\}) \end{array}$$

such that the probability of a graph $G \in \mathcal{G}$ can be written as

$$P(G) = \frac{1}{\kappa} \exp\left(\sum_{uv \in E(G)} \eta_{uv} + \sum_{uvw \in T(G)} \tau_{uvw} + \sum_{\ell=2}^{n-1} \sum_{uv_1 \dots v_\ell \in S_\ell(G)} \sigma_{uv_1 \dots v_\ell}\right)$$

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ERGM of general Markov graphs (remarks).

$$P(G) = \frac{1}{\kappa} \exp\left(\sum_{uv \in E(G)} \eta_{uv} + \sum_{uvw \in T(G)} \tau_{uvw} + \sum_{\ell=2}^{n-1} \sum_{uv_1 \dots v_\ell \in S_\ell(G)} \sigma_{uv_1 \dots v_\ell}\right)$$

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Each dyad, triangle, ℓ -star can contribute differently to the probability of a graph.

 \Rightarrow unreasonably high number of parameters.

Homogeneous random graph model.

Two graphs G = (V, E) and H = (W, F) are called *isomorphic* if there is a bijection $\varphi \colon V \to W$ such that

$$\forall u, v \in V \colon \{u, v\} \in E \Leftrightarrow \{\varphi(u), \varphi(v)\} \in F .$$

Definition

A random graph model (\mathcal{G}, P) is called *homogeneous* if for any pair of isomorphic graphs *G* and *H* it is P(G) = P(H).

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ERGM of homogeneous Markov graphs.

Corollary

Let (\mathcal{G}, P) be a homogeneous Markov random graph. Then there are real constants η , τ , and σ_{ℓ} for $\ell = 2, ..., n-1$ such that the probability of a graph $G \in \mathcal{G}$ can be written as

$$P(G) = \frac{1}{\kappa} \exp\left(\eta \cdot m(G) + \tau \cdot t(G) + \sum_{\ell=2}^{n-1} \sigma_{\ell} \cdot s_{\ell}(G)\right)$$

Proof.

Start from the ERGM of a general Markov graph.

Show that any two edge parameters are equal...

For $\ell = 2, \ldots, n-1$, show that any two ℓ -star parameters are equal...

Show that any two triangle parameters are equal...

Example: dependence graph of $\mathcal{G}(n, p)$.

 $\mathcal{G}(n, p)$ is a homogeneous random graph model whose dependence graph has no edges. Thus,

$$P(G) = rac{1}{\kappa} \exp\left(\eta \cdot m(G)
ight)$$
 .

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Hammersley-Clifford Theorem; special case.

Theorem (first part)

Let (\mathcal{G}, P) be a random graph satisfying P(G) > 0 for all $G \in \mathcal{G}$, let D be the set of dyads and \mathcal{D} the dependence graph.

There are constants { $\alpha_A \in \mathbb{R}$; $A \subseteq D$ }, satisfying $\alpha_A = 0$ if A is not a clique in \mathcal{D} , such that

$$egin{array}{rcl} \mathcal{P}(G) &=& rac{1}{\kappa} \exp\left(\sum_{A\subseteq E(G)} lpha_A
ight) \ , & ext{ where } \ & \kappa &=& \sum_{G'\in\mathcal{G}} \exp\left(\sum_{A\subseteq E(G')} lpha_A
ight) \ . \end{array}$$

Möbius Inversion Theorem.

Needed for the proof of the Hammersley-Clifford Theorem.

Let S be a finite set and

$$f: \mathcal{P}(S) \to \mathbb{R}; \qquad g: \mathcal{P}(S) \to \mathbb{R};$$

two functions defined on the set of subsets of *S*.

Then, for all subsets $A \subseteq S$ it is

$$f(A) = \sum_{B \subseteq A} g(B)$$

if and only if for all subsets $A \subseteq S$ it is

$$g(A) = \sum_{B\subseteq A} (-1)^{|A\setminus B|} f(B)$$
.

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Want to show
$$P(G) = \frac{1}{\kappa} \exp \left(\sum_{A \subseteq E(G)} \alpha_A \right)$$

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For a set $B \subseteq D$ define $G_B = (V, B) \in \mathcal{G}$ to be the graph whose edge set is equal to B.

For $A \subseteq D$ define

$$lpha_{\mathcal{A}} := \sum_{B \subseteq \mathcal{A}} (-1)^{|\mathcal{A} \setminus B|} \log \mathcal{P}(\mathcal{G}_B) \; \; .$$

Motivation (Möbius Inversion Theorem)

$$f(A) = \sum_{B \subseteq A} g(B) \Longleftrightarrow g(A) = \sum_{B \subseteq A} (-1)^{|A \setminus B|} f(B)$$
.

By definition we have

$$lpha_{\mathcal{A}} = \sum_{B \subseteq \mathcal{A}} (-1)^{|\mathcal{A} \setminus \mathcal{B}|} \log \mathcal{P}(\mathcal{G}_{\mathcal{B}}) \; \; .$$

Möbius Inversion Theorem:

$$f(A) = \sum_{B \subseteq A} g(B) \Longleftrightarrow g(A) = \sum_{B \subseteq A} (-1)^{|A \setminus B|} f(B)$$
.

Thus, for $A \subseteq D$ it is

$$\log P(G_A) = \sum_{B \subseteq A} \alpha_B$$

In particular, for A = E(G) we get

$$P(G) = \exp\left(\sum_{B \subseteq E(G)} \alpha_B\right)$$

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We have

$$P(G) = \exp\left(\sum_{A \subseteq E(G)} lpha_A\right)$$

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It remains to show that $\alpha_A = 0$ if A is not a clique in \mathcal{D} ; and we are done with the first part of the theorem.

Want to show that $\alpha_A = 0$ if *A* is not a clique in \mathcal{D} .

Let $d, d' \in D$ be two conditionally independent dyads and $B \subseteq D$ with $d, d' \notin B$. It is

$$\frac{P(G_{B \cup \{d,d'\}})}{P(G_{B \cup d'}) + P(G_{B \cup \{d,d'\}})} = \frac{P(G_{B \cup \{d\}})}{P(G_B) + P(G_{B \cup \{d\}})}$$

and, hence

$$\frac{P(G_{B\cup\{d,d'\}})}{P(G_{B\cup\{d'\}})} = \frac{P(G_{B\cup\{d\}})}{P(G_B)} \quad . \tag{3}$$

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$$lpha_{\mathcal{A}} = \sum_{B\subseteq \mathcal{A}} (-1)^{|\mathcal{A}\setminus B|} \log \mathcal{P}(\mathcal{G}_B)$$
 .

Let $A \subseteq D$, contain two conditionally independent dyads d, d'.

$$\begin{aligned} \alpha_{A} &= \sum_{\substack{B \subseteq A \\ d,d' \in B}} (-1)^{|A \setminus B|} \log P(G_{B}) + \sum_{\substack{B \subseteq A \\ d \in B, d' \notin B}} (-1)^{|A \setminus B|} \log P(G_{B}) + \sum_{\substack{B \subseteq A \\ d \notin B, d' \notin B}} (-1)^{|A \setminus B|} \log P(G_{B}) + \sum_{\substack{B \subseteq A \\ d, d' \notin B}} (-1)^{|A \setminus B|} \log P(G_{B}) \\ &= \sum_{\substack{B \subseteq A \setminus \{d, d'\}}} (-1)^{|A \setminus B|} \log \left(\frac{P(G_{B \cup \{d, d'\}})}{P(G_{B \cup \{d'\}})} \middle/ \frac{P(G_{B \cup \{d\}})}{P(G_{B})} \right) \\ &= 0 \quad , \text{ follows from (3)} \end{aligned}$$

Thus, $\alpha_A = 0$ if *A* is not a clique in \mathcal{D} .

Hammersley-Clifford Theorem.

Theorem (second part)

Conversely, if the probability P on G is defined by

$$\begin{split} \mathsf{P}(G) &= \frac{1}{\kappa} \exp\left(\sum_{A \subseteq E(G)} \alpha_A\right) \ , \qquad \textit{where} \\ \kappa &= \sum_{G' \in \mathcal{G}} \exp\left(\sum_{A \subseteq E(G')} \alpha_A\right) \ , \end{split}$$

then two dyads d and d' are conditionally independent in (\mathcal{G}, P) , unless there is a subset $A \subseteq D$ with d, d' $\in A$ and $\alpha_A \neq 0$.

Suppose that *d*, *d'* are two dyads such that there is no subset $A \subseteq D$ with $\alpha_A \neq 0$ and $d, d' \in A$.

We show that d and d' are conditionally independent.

Equivalently, for any $B \subseteq D$ with $d, d' \notin B$ it is



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(*d*, *d'* are two dyads for which there is no subset $A \subseteq D$ with $\alpha_A \neq 0$ and $d, d' \in A$; $d, d' \notin B$)

$$\log\left(\frac{P(G_{B\cup\{d,d'\}})}{P(G_{B\cup\{d'\}})}\right) = \sum_{A\subseteq B\cup\{d,d'\}} \alpha_A - \sum_{A\subseteq B\cup\{d'\}} \alpha_A$$
$$= \sum_{\substack{A\subseteq B\cup\{d,d'\}\\d\in A}} \alpha_A$$
$$= \sum_{\substack{A\subseteq B\cup\{d\}\\d\in A}} \alpha_A$$
$$= \sum_{\substack{A\subseteq B\cup\{d\}\\d\in A}} \alpha_A - \sum_{\substack{A\subseteq B\\d\in B}} \alpha_A$$
$$= \log\left(\frac{P(G_{B\cup\{d\}})}{P(G_B)}\right).$$

Hammersley-Clifford Theorem; special case.

Theorem

Let (\mathcal{G}, P) be a random graph satisfying P(G) > 0 for all $G \in \mathcal{G}$.

There are constants { $\alpha_A \in \mathbb{R}$; $A \subseteq D$ }, satisfying $\alpha_A = 0$ if A is not a clique in \mathcal{D} , such that

$$P(G) = \frac{1}{\kappa} \exp\left(\sum_{A \subseteq E(G)} \alpha_A\right)$$
 (4)

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Conversely, if P is defined by (4), then two dyads $d, d' \in D$ are conditionally independent, unless there is a subset $A \subseteq D$ with $d, d' \in A$ and $\alpha_A \neq 0$.

Outline.

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Towards more structured models.

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Definition and examples. Sampling from an ERGM. Hammersley-Clifford Theorem.

Near-degeneracy and multi-modality of ERGMs.

Hypothesis testing
Many Markov random graphs give rise to multi-modal probability distributions:

- probability mass centered on a small set of graphs
- other graphs are very unlikely.

For instance, only near-empty or near-complete graphs have a non-vanishing probability.

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Near-degeneracy and multi-modality of ERGMs.

Consider the following ERGM

$$P(G) = \frac{1}{\kappa} \exp\left(\eta \cdot m(G) + \tau \cdot t(G)\right)$$
 with $\eta < 0, \tau > 0$.

Then, in very **sparse** networks

- there are few possibilities to close triangles;
- creation of edges is unlikely;
- \Rightarrow very unlikely to leave the set of near-empty graphs.

In contrast, in very dense networks

- an edge can close many triangles (up to n-2);
- deletion of edges is unlikely;
- \Rightarrow very unlikely to leave the set of near-complete graphs.

Near-degeneracy and multi-modality of ERGMs.

Degeneracy is undesirable for two reasons.

- 1. Convergence of the Markov chain towards the stationary distribution is very slow.
- 2. Degenerate models seem to be unreasonable models for empirical networks.

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Avoiding near-degeneracy of ERGMs.

Assumed linear marginal effect of closed triangles:

- closing one triangle contributes τ to the log-probability;
- closing two triangles contributes $2\tau \dots$



Geometrically-weighted edgewise shared partner (GWESP) statistic:

- ▶ a *k*-triangle counts more than a single triangle,
- but less than k-times as much.

Typically leads to less degenerate models.

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Testing hypotheses with ERGMs.

Given a hypothesis (e. g., *transitivity*) and an observed network G_{obs} .

• Decide on a reasonable set of statistics g_i , i = 1, ..., k

$$P(G) = \frac{1}{\kappa} \exp\left(\sum_{i=1}^{k} \theta_i g_i(G)\right)$$

- ▶ including a statistic related to the hypothesis,
 e. g., g_k = number of triangles.
- Compute maximum likelihood estimates $\hat{\theta} = (\hat{\theta}_1, \dots, \hat{\theta}_k)$.
- Compute probability of observing a network in the null model defined by (θ̂₁,..., θ̂_{k-1}, 0) that gives rise to θ_k as large as θ̂_k.

Estimation of ERGM Parameters.

Definition (maximum likelihood)

 $(\mathcal{G}, P_{\theta})$ random graph model parameterized by $\theta \in \Theta \subseteq \mathbb{R}^{k}$; $G_{\text{obs}} \in \mathcal{G}$ a graph (observation). *Likelihood* function associated with G_{obs}

 $L: \Theta \to \mathbb{R}; \ \theta \mapsto P_{\theta}(G_{obs})$

A parameter vector $\hat{\theta}$ maximizing *L*, i. e.,

 $\hat{\theta} = \arg \max_{\theta} L(\theta)$

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is called a *maximum likelihood estimate (MLE)* for θ .