Introduction to statistical network analysis

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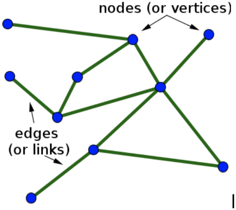
Basic concepts

Basic concepts

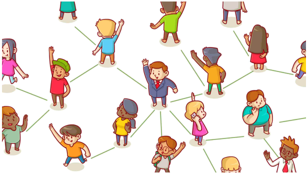


- Nodes (Vertices): participants in the network
  Network size: number of nodes n
- Edges (Links): connections or relationships between nodes
- **Examples [nodes (edges)]:**
  - people (friendship)
  - webpages (hyperlinks)
  - paper (citation)
  - genes (regulatory actions)
  - brain regions (oxygen level correlation)
- Adjacency matrix: $A_{i,j}$ is the edge between nodes (i, j)

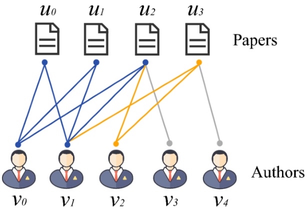
Basic concepts

Classification of network data: (1) partite

- Unipartite network: any node may connect to anyone else



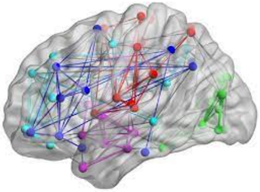
- Bipartite network: nodes partitioned into two groups, only between-group edges are possible



Basic concepts

Classification of network data: (2) edge direction

- Undirected (Symmetric) network: $A_{i,j} = A_{j,i}$
- Directed (Asymmetric) network: $A_{i,j}$ and $A_{j,i}$ might not equal



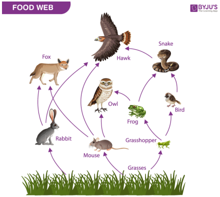


Figure: Left: undirected network; right: directed network

Basic concepts

Classification of network data: (3) edge weight

- Binary: $A_{i,j} \in \{0,1\}$
  Example: friend (1) or non-friend (0)
- Signed: $A_{i,j} \in \{0,1,-1\}$
  Example: friend (1) or foe (-1) or no interaction (0)
- Weighted: $A_{i,j} \in \mathbb{R}$
  Example: trade surplus/deficit between countries

Research topics

Statistical research aims:

- modeling network formation
- finding roles of individual nodes
  Examples: community detection, node embedding
- stochastic behavior of network features
  Examples: network moments
- link prediction

Research topics

Network data vs conventional data:

- Networks: **no individual observation**, only relational data
- Deriving "**network analogues** of classical techniques"
  Examples:
  - one-/two-sample test
  - cross-validation
  - method-of-moments
  - goodness-of-fit test
  - re/subsampling

Popular network models

Overview

Now we survey Network models: Erdos-Renyi model

- Simple $\rightarrow$ complex
- For simplicity, focus on undirected, binary networks
- Model probability matrix:

$$P_{i,j} := \mathbb{P}(A_{i,j} = 1)$$

Network models: Erdos-Renyi

Erdos-Renyi (ER) model (Newman 2018)

- Model formula:

$$P_{i,j} := \mathbb{P}(A_{i,j} = 1) \equiv p$$

- **Definition:** network density/sparsity is the (asymptotic order of) average edge probability:

$$\rho_n \asymp \bar{P} := \binom{n}{2}^{-1} \sum_{1 \le i < j \le n} P_{i,j}$$

  In ER model, $\rho_n \asymp p$

- Density is usually a crucial measure for assessing the **problem difficulty** of estimation/testing

Erdos-Renyi model

$$P_{i,j} := \mathbb{P}(A_{i,j} = 1) \equiv p \asymp \rho_n$$

Model estimation:

- **Moment estimator:**

$$\widehat{p} := \binom{n}{2}^{-1} \sum_{1 \le i < j \le n} A_{i,j}$$

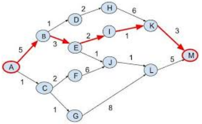
- **Consistency** (Chen et al. 2021): When $\binom{n}{2} p \to \infty$, $\widehat{p}/p \xrightarrow{p} 1$
  Roughly speaking

$$\frac{|\widehat{p} - p|}{p} \overset{\text{approx.}}{\asymp} \frac{1}{\sqrt{n^2 p}}$$

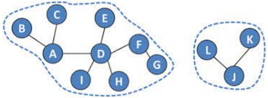
Erdos-Renyi model

ER model:

- Too simple to fit real-world data well
- But a good null model (“no structure/pattern”) for testing (Gao & Lafferty 2017*a*)
- Neat for studying some network properties
  - **Example:** average shortest path (Katzav et al. 2018)



  - **Example:** is the network connected? (Erdos & Rényi 1960)



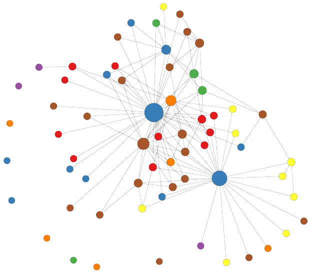
Answers to these questions are the same for: (i) ER model; and (ii) general model with all $P_{i,j} \asymp \rho_n$

β-model

- **Definition:** degree is the total number of edges of a node

$$d_i := \sum_{j:j \neq i} A_{i,j}$$

- Average degree: $\bar{d} := \frac{1}{n} \sum_{i=1}^{n} d_i \asymp \rho_n n$
- Degree describes the node's **popularity** (hub, leaf)



β-model

Degree-driven network model:

- Network structure entirely determined by degrees
- Network $\rightarrow$ degrees: easy to compute
- Degree sequence $\stackrel{?}{\rightarrow}$ network model

Configuration model (Chung & Lu 2002):

- Not a probabilistic model for "network population"
- Given a degree sequence $d_1, \ldots, d_n$, generate network
  1. Set $S := \{1, \ldots, 1, 2, \ldots, 2, \ldots, n, \ldots, n\}$, each i repeats d_i times
  2. Randomly select two entries from S, make an edge, delete them from S
  3. Repeat step 2 until S is exhausted

β-model

β**-model** (Chatterjee et al. 2011):

- **Formula:**

$$P_{i,j} = \frac{e^{\beta_i+\beta_j}}{1+e^{\beta_i+\beta_j}}$$

  Parameters $\beta_i \in \mathbb{R}$

- **Estimation: MLE**, negative log-likelihood:

$$L(\beta) := \sum_{1\le i<j\le n} \log\left(1+e^{\beta_i+\beta_j}\right) - \sum_{i=1}^{n} \beta_i d_i$$

  Then

$$\widehat{\beta} := \arg\min_{\beta} L(\beta)$$

- **Consistency:** if true β_i's are $O(1)$ (i.e., $\rho_n \asymp 1$, can be relaxed to $\rho_n \gg n^{-1/2}$), then $\|\widehat{\beta} - \beta\|_\infty \xrightarrow{p} 0$

β-model

β-model:

$$P_{i,j} = \frac{e^{\beta_i+\beta_j}}{1+e^{\beta_i+\beta_j}}$$

$$L(\beta) := \sum_{1\le i<j\le n} \log\left(1+e^{\beta_i+\beta_j}\right) - \sum_{i=1}^{n} \beta_i d_i$$

Pros and cons:

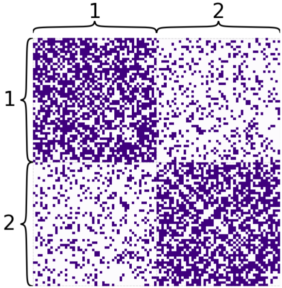
- (+) Scalable to very large and sparse networks (Shao et al. 2023)
- (+) Privacy protection (only publicize degrees) (Karwa & Slavković 2016)
- ($-$) Limited expressivity

Stochastic block model (SBM)

- Nodes are partitioned into K communities (blocks, groups)
- **Formula** (Holland et al. 1983)

$$P_{i,j} := \rho_n B_{c_i,c_j}$$

c_i: which community node i belongs to
ρ_n: network sparsity rescaler



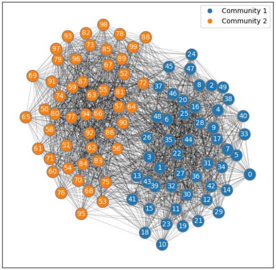


Figure: Left: heatmap of adjacency A; right: network plot (nodes have been sorted)

Stochastic block model (SBM)

SBM:

$$P_{i,j} := \rho_n B_{c_i,c_j}$$

where B: community-level edge probability matrix

- **Estimation:** MLE:

$$L(c,B) := \sum_{1\le i<j\le n} \left\{ A_{i,j} \log B_{c_i,c_j} + (1-A_{i,j}) \log(1-B_{c_i,c_j}) \right\}$$

$$(\widehat{c},\widehat{B}) := \mathop{\arg\max}_{c_i\in[1:K],B\in[0,1]^{K\times K}} L(c,B)$$

- Estimating c_{true} is community detection (Abbe 2018)
- If $\rho_n \gg n^{-1}\log n$, then MLE is consistent: as $n\to\infty$,
  - $\widehat{c} = c_{\text{true}}$ a.s. (Bickel & Chen 2009)
  - $\widehat{B} \xrightarrow{p} B_{\text{true}}$

Question: How to understand this requirement on ρ_n?

Stochastic block model (SBM)

$$L(c,B) := \sum_{1\leq i<j\leq n} \left\{ A_{i,j} \log B_{c_i,c_j} + (1-A_{i,j}) \log(1-B_{c_i,c_j}) \right\}$$

- Exact MLE infeasible (combinatorial optimization for c)
- In practice: Tabu search (Zhao et al. 2012)
  1. Initialize c and B
  2. Iterate until convergence:
     - For $i \in [1:n]$: update c_i
     - Update B

Stochastic block model (SBM)

SBM:

$$P_{i,j} := \rho_n B_{c_i,c_j}$$

MLE is too slow, can we do better?

- **Alternative formula:**

  $$P = \rho_n Z B Z^T$$

  where membership matrix Z may look like:

  $$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

  corresponding to $c = (1, 1, 4, \ldots, 2)$, i.e., each row of Z is a one-hot vector indicating membership
- Verify: $P_{i,j} = \rho_n Z_{i,\cdot} B Z_{j,\cdot}^T = \rho_n B_{c_i,c_j}$

Stochastic block model (SBM)

SBM (matrix form):

$$P = \rho_n Z B Z^T$$

Therefore:

- P is rank-K
- **Spectral decomposition** of P:

$$P = USU^T$$

  where $S : K \times K$ diagonal; $U : n \times K$ orthonormal: $U^T U = I$
- U only has K **different rows**, one for each community (Qin & Rohe 2013)
- cluster rows of $U \Rightarrow$ true community labels

Stochastic block model (SBM)

SBM (matrix form):

$$P = \rho_n Z B Z^T$$

In practice, we only observe A ...

- Suppose we know K
- Leading-K SVD of A:

$$A \approx \widehat{U}\widehat{S}\widehat{U}^T$$

  (network sparsity absorbed into $\widehat{S}$)
- Cluster the rows of $\widehat{U} \Rightarrow$ community detection
- The above method is called spectral clustering (Lei & Rinaldo 2015)
- **Consistency:** $\rho_n \gg n^{-1} \log n \Rightarrow$ misclassification rate $\xrightarrow{p} 0$

Stochastic block model (SBM)

SBM:

$$P_{i,j} := \rho_n B_{c_i,c_j}$$

- We only explained "block model"
- What about "stochastic"?
- **Two-stage** generation (Bickel & Chen 2009):
  1. "Stochastic": each node chooses its community:

     $$c_1, \ldots, c_n \overset{\text{i.i.d.}}{\sim} \text{Multinomial}(q_1, \ldots, q_K)$$

  2. "Block model":

     $$P_{i,j} := \rho_n B_{c_i,c_j}$$

- Stochastic or not doesn't matter so much in practice

Stochastic block model (SBM)

Arguably the "most famous" network model

- Simple, yet expressive
- Communities are very interpretable
  Examples:
  - social circles (friendship network) (Yang et al. 2013)
  - functional regions (brain image network) (Wu et al. 2022)
  - research areas (citation network) (Ji et al. 2022)
- Towards general models: SBM with growing K

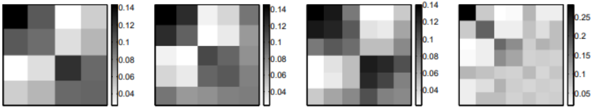
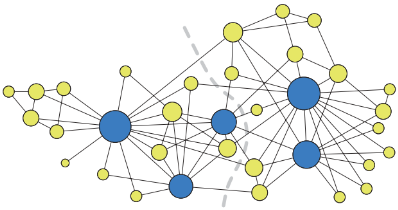


Figure: Choi et al. (2012): as K increases, SBM captures more structural details

Degree-corrected SBM



- What may go wrong with SBM?
- Why? (Recall spectral clustering ...)
- In community detection, we want to **adjust for degree heterogeneity**

Degree-corrected SBM

- **Formula:**

$$P_{i,j} = \rho_n \theta_i \theta_j B_{c_i,c_j}$$

where θ_i: degree correction

- **Matrix form:**

$$P = \rho_n \Theta Z B Z^T \Theta$$

where $\Theta = \mathrm{diag}(\theta_1, \ldots, \theta_n)$

- **Identifiability:** require $\sum_{i:c_i=k} \theta_i = 1$ for each community k

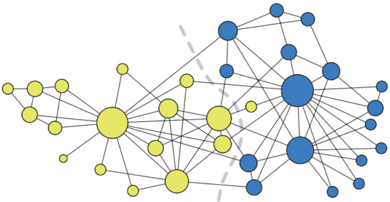


Figure: Karrer & Newman (2011): DCSBM adjusts for degrees

Degree-corrected SBM

- **Spectral clustering** (Von Luxburg 2007):
  1. Compute Laplacian:
  $$L := D^{-1/2}AD^{-1/2}$$
  where $D = \mathrm{diag}(d_1, \ldots, d_n)$
  Interpretation: reweighted edges
  $$L_{i,j} = \frac{A_{i,j}}{\sqrt{d_i d_j}}$$
  (how much attention do we pay to our relationship?)
  2. Leading-K SVD of L:
  $$L \approx \widehat{U}\widehat{S}\widehat{U}^T$$
  3. Cluster rows of $\widehat{U}$

Degree-corrected SBM

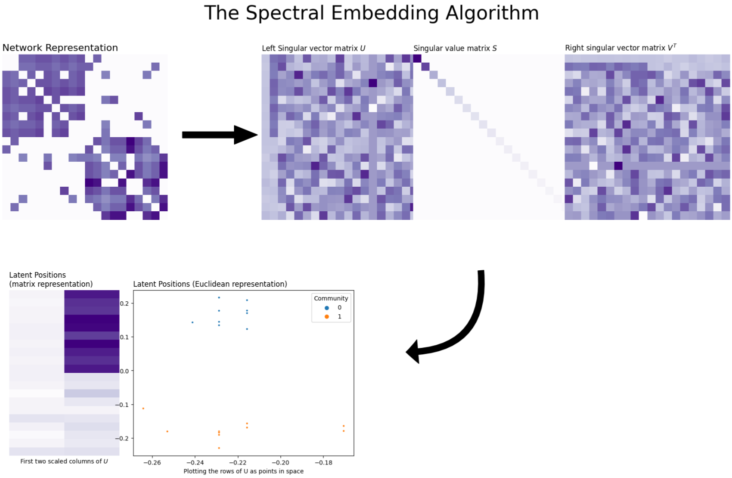


Figure: Illustration of spectral community detection for SBM (Bridgeford et al. 2022)

Quick recap

Which methods have we seen so far?

- Moment estimator for ER model
- MLE for β-model and SBM
- Spectral method for SBM

More about SBM/DCSBM

Overlapping communities:

- Airoldi et al. (2008) **Mixed-Membership Stochastic Blockmodel (MMSB):**
  1. Prior step:
  $$\vec{\pi}_i \overset{\text{i.i.d.}}{\sim} \text{Dirichlet}$$
  2. For each (i,j), draw $c_i \sim \text{Multinom.}(\vec{\pi}_i)$, do the same for j. Then generate $P_{i,j}$:
  $$P_{i,j} = B_{c_i,c_j}$$

  * **Parameter estimation:** EM algorithm
- Zhang et al. (2020) **Overlapping Continuous Community Assignment Model (OCCAM):**
  - **Matrix form:**
  $$P = \rho_n \Theta Z B Z^T \Theta$$
  but now Z may have continuous rows, satisfying $\|Z_{i,\cdot}\|_2 = 1$
  Similarly, (Jin et al. 2024): $\|Z_{i,\cdot}\|_1 = 1$
  - **Parameter estimation:** spectral clustering

More about SBM/DCSBM

Other estimation methods:

- Modularity (Girvan & Newman 2002, Newman 2006)

$$\frac{1}{2m}\sum_{i<j}\left(A_{i,j}-\frac{d_i d_j}{2m}\right)\mathbb{1}_{[c_i=c_j]}$$

  m: total number of edges

- Analytical approximate EM algorithm (Ball et al. 2011)
- Semi-definite programming (SDP)

$$\arg\max_X \langle A, X\rangle, \quad \text{s.t., } X_{ii}\equiv 1, X\succeq 0$$

  Then spectral cluster X (Cai & Li 2015, Amini & Levina 2018)

- “SCORE” (Jin 2015)
- Spectral clustering + majority vote refinement (Gao et al. 2018)

More about SBM/DCSBM

Extension: popularity-adjusted SBM (Sengupta & Chen 2018):

- **Motivation:** overall sparse but locally dense networks
  DCSBM cannot describe this scenario:
  - $i, j \in$ same community k
  - i is globally more popular than j
  - ... but not among members of some community ℓ
- **Formulation:** for $i \in$ community k, $j \in$ community ℓ:

$$P_{i,j} = \Lambda_i^{(\ell)} \Lambda_j^{(k)}$$

  where Λ encodes:
  - community-level edge probabilities
  - node's popularity in each community

  You can think: $\Lambda_i^{(\ell)} = \theta_i^{(\ell)} \sqrt{\rho_n B_{k,\ell}}$ (recall $c_i = k$)
- **Reduce to DCSBM:**

$$\Lambda_i^{(\ell)} = \theta_i \sqrt{\rho_n B_{k,\ell}} \quad \Rightarrow \quad P_{i,j} = \rho_n \theta_i \theta_j B_{k,\ell}$$

- MLE for Λ's $\Rightarrow$ community detection

More about SBM/DCSBM

popularity-adjusted SBM (Cont'd)

$$P_{i,j} = \Lambda_i^{(\ell)} \Lambda_j^{(k)}$$

This is subtle: MLE for Λ's $\Rightarrow$ community detection

- MLE gives you all $\Lambda_i^{(\ell)}$'s ..
- ... but that's insufficient for determining $P_{i,j}$
- For each (i, j):

$$P_{i,j} = \Lambda_i^{(?)} \Lambda_j^{(?)}$$

Random dot-product model (RDPG)

- Generalization of SBM/DCSBM (Young & Scheinerman 2007)
- **Formula:** recall DCSBM (no ρ_n):

$$P = \Theta Z B Z^T \Theta$$

  Suppose $B \succ 0$ (diagonal all positive), then

$$P = (\Theta Z B^{1/2}) \cdot (\Theta Z B^{1/2}) =: X X^T$$

  where $X \in \mathbb{R}^{n \times K}$: latent space matrix
- In other words:
  - Each node has an embedding $X_{i,\cdot}$
  - Edge probability: $P_{i,j} = \langle X_{i,\cdot}, X_{j,\cdot} \rangle$
- **Estimation:** can estimate X up to a rotation/reflection O: Under mild conditions, $\widehat{X}$ by SVD: $\|\widehat{X} - XO\|_{2\to\infty} \xrightarrow{p} 0$ (Cape et al. 2019); CLT (Athreya et al. 2022)

Random dot-product model (RDPG)

Approximately low-rank structure is ubiquitous

- Udell & Townsend (2019): for any A

$$\inf_{\mathrm{rank}(\widehat{A}) \leq C \log n/\varepsilon^2} \|A - \widehat{A}\|_{\max} \leq \varepsilon \|A\|$$

- Xu (2018): Holder smoothness in graphon (will explain later) $\Rightarrow$ polynomial eigenvalue decay

$$\sum_{i>r} \lambda_i^2 = O(r^{-\beta} + n^{-1})$$

Random dot-product model (RDPG)

$$P = XX^T, \quad A \approx \widehat{X}\widehat{X}^T, \quad \widehat{X} \approx XO$$

Assortativity constraint?

- Generalized RDPG (Rubin-Delanchy et al. 2022)

$$P = X \begin{pmatrix} I_p & 0 \\ 0 & -I_q \end{pmatrix} X^T$$

Estimation: still SVD A:

$$A = \widehat{U}\widehat{S}\widehat{V}^T$$

compare the signs of columns: $\widehat{U}_{\cdot,i}$ vs $\widehat{V}_{\cdot,i}$ to know which of I_p or $-I_q$ this eigenvalue/vector belong to

Random dot-product model (RDPG)

$$P = XX^T, \quad A \approx \widehat{X}\widehat{X}^T, \quad \widehat{X} \approx XO$$

Interpretability

- Rows i of $\widehat{X}$: embedding of node i

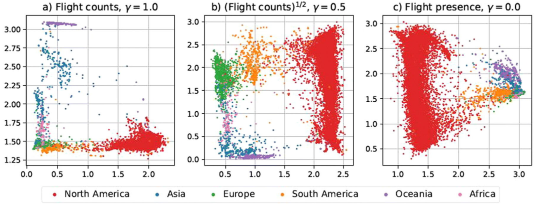


Figure: Gallagher et al. (2024): embedding of airports in flight network

- However, this embedding is limited to that particular network, due to the unknown O
  Cannot be directly used for comparing nodes' roles across networks

Latent space models

Distance model (Hoff et al. 2002)

- **Formulation:**

$$\mathrm{Logit}(P_{i,j}) := \alpha + \beta x_{i,j} + \|z_i - z_j\|$$

  where
  - $x_{i,j}$: observable edge covariate
    (two node covariates $\rightarrow$ edge covariate)
  - z_i: latent space position
- **Identifiability:** $\sum_{i=1}^n z_i = \vec{0}$
- **Estimation:** Variational EM

Multiplicative Z term (Ma et al. 2020)

- **Formulation:**

$$\mathrm{Logit}(P_{i,j}) := \alpha + \beta x_{i,j} + \langle z_i, z_j \rangle$$

  Identifiability condition omitted here
- **Estimation:** (regularized) MLE by (projected) gradient

ERGM

Exponential random graph models (ERGM) (Hunter et al. 2008)

- Directly model the distributions of subgraphs (motifs)
- Dependent edge generation
- Not a convenient generative model (model $\stackrel{?}{\rightarrow}$ data)

ERGM

Formula:

- Set of motifs (subgraphs) $\mathscr{R}_1, \ldots, \mathscr{R}_m$
  Examples: `edge`, `triangle`, `three-star`
- Given an adjacency matrix a, let $R(a)$ count the frequency of $\mathscr{R}$ in a
- Network likelihood (Hunter & Handcock 2006):

$$\mathbb{P}(A = a) \propto \exp\Big\{\sum_{i=1}^{m} \theta_i R_i(a)\Big\}$$

To fit an ERGM to data:

- Choose the set of motifs, compute $R_i(a)$'s
- Estimate θ_i's

ERGM

$$\mathbb{P}(A = a) \propto \exp\Big\{\sum_{i=1}^{m} \theta_i R_i(a)\Big\}$$

Given θ, how to generate data?

- Start with an initial adjacency
- Each time, decide whether to flip an edge (i, j), resulting A (before flip) $\to A'$ (after flip)
- **Metropolis-Hastings** (Liu & Liu 2001):
  accept the flip w.p.

$$\min\Big(1, \exp\Big[\sum_i \theta_i \{R_i(A') - R_i(A)\}\Big]\Big)$$

- Iterate many rounds (with burn-in and thinning)
  - Burn-in: discard the first few rounds (e.g., first 1000 rounds)
  - Thinning: take data from every few rounds, as if they were i.i.d.

$$\mathbb{P}(A=a) \propto \exp\Big\{\sum_{i=1}^{m} \theta_i R_i(a)\Big\}$$

Given $A=a$, how to estimate θ?

- MLE is hard, don't know normalizing constant
- Score equation:

  $$\nabla \ell(\theta) = 0,$$

  that is, for each i,

  $$R_i(a) = \mathbb{E}[R_i(A)]$$

- Robbins–Monro update (Snijders 2002):

  $$\theta_i^{(n+1)} = \theta_i^{(n)} + \alpha_n \Big\{R_i(a) - \widehat{\mathbb{E}}^{\theta^{(n)}}[R_i(A)]\Big\},$$

  where: $\widehat{\mathbb{E}}[R_i(A)]$ evaluated by MH-MC
  step size α_i: $\sum_i \alpha_i = \infty$, $\sum_i \alpha_i^2 < \infty$

Graphon model

Overview:

- A very general framework
- Contains the aforementioned models as special cases

Two-stage network generation:

1. Latent node positions: $X_1, \ldots, X_n \stackrel{\text{i.i.d.}}{\sim}$ Uniform$[0,1]$
2. Latent graphon function:

$$P_{i,j} = f(X_i, X_j) \tag{1}$$

Understandings:

- X_i describes "what kind of node"
- f captures all structural information in the network

Graphon model

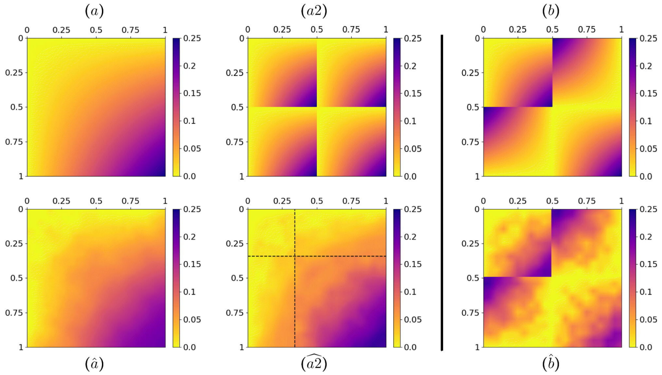


Figure: Illustration of some graphons (Sischka & Kauermann 2025)

Graphon model

Examples:

- ER model: $f(x,y) \equiv p$
- β-model:

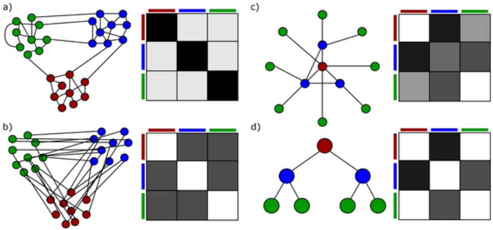
$$\beta_i = g(X_i)$$
$$f(x,y) = \text{Logit}^{-1}(g(X_i) + g(X_j))$$

for proper $g(\cdot)$

Graphon model

Examples: SBM

- K communities $\Leftrightarrow$ partition $[0,1]$ into K sub-intervals
- $X_i \in k$th interval $\Leftrightarrow i \in$ community k
- Graphon f: piece-wise constant



Graphon model

Aldous-Hoover theorem (Zhao 2023)

- Exchangeable network: for any permutation $\pi : \mathbb{N} \to \mathbb{N}$,

$$(A_{i,j}) \stackrel{d}{=} (A_{\pi(i),\pi(j)})$$

- Aldous-Hoover: Exchangeable network has the representation

$$A_{i,j} \sim \text{ Bernoulli}(f(X_i, X_j)),$$

  for $X_i \stackrel{\text{i.i.d.}}{\sim}$ Uniform$[0,1]$
- Exchangeability $\Rightarrow$ graphon model
- All nodes i.i.d. choose their roles $\Rightarrow$ exchangeabililty

Graphon model

Examples:

- RDPG with i.i.d. latent positions $\Rightarrow$ graphon model
- Latent space model with i.i.d. latent positions $\Rightarrow$ graphon model
- Recall ERGM:

$$\mathbb{P}(A = a) \propto \exp\left\{ \sum_{i=1}^{m} \theta_i R_i(a) \right\}$$

where each $R_i(a)$: some motif count
Chatterjee & Diaconis (2013): ERGM $\approx$ graphon model (as $n \to \infty$)

Graphon model

$$X_1, \ldots, X_n \overset{\text{i.i.d.}}{\sim} \text{Uniform}[0,1]$$
$$P_{i,j} = f(X_i, X_j)$$

Graphon estimation:

- Cannot estimate f or X_i's (not identifiable)
- May estimate $P_{i,j}$'s
- Smoothness assumption on f [in equiv. class]
- How to estimate $P_{i,j}$'s?

Graphon model

$$X_1, \ldots, X_n \overset{\text{i.i.d.}}{\sim} \text{Uniform}[0,1]$$
$$P_{i,j} = f(X_i, X_j)$$

Graphon estimation:

- **Method 1:** universal singular value thresholding (USVT) (Chatterjee 2015)
  1. SVD A:
  $$A = \widehat{U}\widehat{S}\widehat{V}^T, \quad (S \text{ diag. sorted})$$
  2. Keep singular values above $C\sqrt{n}$ for $C > 2$
  Say, keep the first $K \Rightarrow (\widetilde{U}, \widetilde{S}, \widetilde{V}) = (\widehat{U}_{\cdot,1:K}, \widehat{S}_{1:K,1:K}, \widehat{V}_{\cdot,1:K})$
  3. Estimator:
  $$\widehat{P} := \widetilde{U}\widetilde{S}\widetilde{V}^T$$

Achieves SOTA MSE (Xu 2018, Luo & Gao 2024)

Graphon model

$$X_1, \ldots, X_n \overset{\text{i.i.d.}}{\sim} \text{Uniform}[0,1]$$
$$P_{i,j} = f(X_i, X_j)$$

Graphon estimation:

- **Method 2:** Neighborhood smoothing (NS) (Zhang et al. 2017)
  1. Dissimilarity measure of graphon slices $f(\cdot, X_i)$ and $f(\cdot, X_j)$:
     $$d(i,j) := \max_{i' \neq i,j} |\langle A_{i,\cdot} - A_{j,\cdot}, A_{i',\cdot} \rangle| / n$$
  2. For each node i, set neighborhood
     $\mathcal{N}_i := \{j : \text{smallest } h = \log n / n \text{ proportion of } d(i,j)\text{'s}\}$
  3. Estimator:
     $$\widehat{P}_{i,j} := \frac{1}{|\mathcal{N}_i|} \sum_{i' \in \mathcal{N}_i} A_{i',j}$$

Achieves state-of-the-art "$2 \to \infty$ error"; explicit formula

Selected research topics

Overview

We will cover these selected topics

- Method-of-moments
- Goodness-of-fit tests
- Cross-validation
- Graph matching
- Extensions to weighted, directed, bipartite graphs
- Other topics (briefly mention)

Method-of-moments

Network moments

- **Definition:** a network moment indexed by a motif R is

$$\widehat{U}_n := \binom{n}{r}^{-1} \sum_{i_1 < \cdots < i_r} \mathbb{1}_{[A_{i_1,\ldots,i_r} \cong R]}$$

- **Examples:** triangle count

$$\widehat{U}_n = \binom{n}{3}^{-1} \sum_{i<j<k} A_{i,j} A_{j,k} A_{k,i}$$

- **CLT:**

$$\frac{\widehat{U}_n - \mathbb{E}[U_n]}{\widehat{S}_n} \xrightarrow{p} N(0,1),$$

  where S_n is some variance estimator (Bickel et al. 2011, Zhang & Xia 2022)

- Moments can be used to identify network models
  Application: network two-sample test

Goodness-of-fit tests

Is the network “structureless”? (Gao & Lafferty 2017*b*)

- $H_0 : P_{i,j} \equiv p$ (ER as null model)
- H_a : non-constant graphon model
- **Method-of-moment test:** null distribution:

$$n^{3/2} g(p) \cdot (T_2, T_3)^T \xrightarrow{d} N(0, I_2), \tag{2}$$

where $T_2 = E^3 - T$ and $T_2 = 3E^2(1-E) - V$, here:

- E counts edges
- T counts triangles
- V counts V-shapes

$g(\cdot)$ is known function; easy to estimate p

Goodness-of-fit tests

GoF test for SBM (Lei 2016)

- $H_0 : K = K_0$ vs $H_a : K > K_0$
- Based on observed A, fit SBM with $K = K_0$, get $\widehat{P}$
- **Idea:** is the residual network "pure noise"?
- Test statistic:

$$\widetilde{A}_{i,j} := \frac{A_{i,j} - \widehat{P}_{i,j}}{\sqrt{(n-1)\widehat{P}_{i,j}(1-\widehat{P}_{i,j})}}, \quad i \neq j$$

  Then under H_0,

$$n^{2/3} \cdot \left\{ \pm \lambda_1(\widetilde{A}) - 2 \right\} \xrightarrow{d} \text{Tracy-Widom}(1),$$

  where $\lambda_1 \geq \cdots \geq \lambda_n$ are sorted eigenvalues
- **Application: decide** K

Goodness-of-fit tests

Key to build valid GoF method:

- Number of continuous parameters is small under H_0
- **Example:** ER model has 1 parameter
- **Example:** SBM has $O(n+K^2)$, but the n memberships can be perfectly recovered for not-very-sparse networks, so we just deal with $O(K^2)$ parameters
- **Example:** DCSBM (Zhang & Amini 2023, Jin et al. 2025)
  H_0 : model is an SBM (no degree corrections)

No known method to test GoF for:

- β-model
- Latent space models, including RDPG
- General graphon model

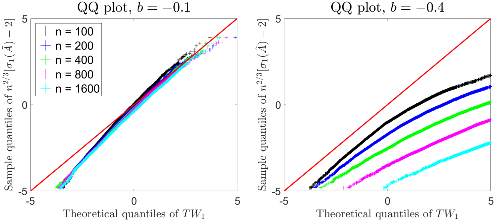


Figure: Shao et al. (2023): exactly mimicking Lei (2016) for β-model won't work (each curve)

Cross-validation

CV for network data?

- **Motivation:** select tuning parameter(s)
  Example: number of communities K in SBM
  Example: bandwidth h in neighborhood smoothing
- **Challenge:** we may observe only one A, how to split data?

Method 1 (node-split CV) (Chen & Lei 2018)

1. Write
$$A = \begin{pmatrix} A^{(11)} & A^{(12)} \\ A^{(21)} & A^{(22)} \end{pmatrix}$$
2. Use $[A^{(11)}, A^{(12)}]$ to train model (say, SBM)
3. Validation: look at how well fitted model predicts $A^{(22)}$
   (beware $A^{(21)} = \{A^{(12)}\}^T$ already used for training)

Cross-validation

Method 2 (edge-splitting CV): (Li et al. 2020)

1. Randomly sample $M_{i,j} \overset{\text{i.i.d.}}{\sim}$ Bernoulli(q); set $M_{j,i} = M_{i,j}$
   Training data: $\{(i,j) : M_{i,j} = 1\}$
   Validation data: $\{(i,j) : M_{i,j} = 0\}$
2. Fit a model to training data using, say, low-rank method
   May fill in zeros to validation data spots
   This outputs $\widetilde{A}$, then $\widehat{A} = \widetilde{A}/q$ is link predictor
3. See how well $\widehat{A}$ predicts A entries on validation data

Graph matching

- **Data:** two adjacency matrices $A^{(1)}, A^{(2)} \in \{0,1\}^{n \times n}$
- **Problem:** estimate a permutation matrix Π minimizing

$$\|A^{(1)} - \Pi A^{(2)} \Pi^T\|_F^2 \tag{3}$$

- **Applications** (Conte et al. 2004, Lyzinski et al. 2015):
  - Account matching in different social networks
  - Connectome alignment in brain imaging
  - Structurally similar chemical particles
  - Network two-sample test
- **Complexity:** (3) is NP (not known to be P)
- Statistical question: if A's are structured, would the problem be more solvable?

Graph matching

Approach 1: low-rank approximation

- Assume model is low-rank: $A \sim P = XX^T$
- Leading-k SVD:
$$A \approx \widehat{X}\widehat{X}^T$$
- **Davis-Kahan theorem:**
$$\widehat{X} \approx XO$$
for (inestimable) orthonormal $O : O^T O = I$
- Minimize:
$$\|\widehat{X}^{(1)} - \Pi\widehat{X}^{(2)}O\|_F$$
over Π and O

Graph matching

$$\|\widehat{X}^{(1)} - \Pi\widehat{X}^{(2)}O\|_F \tag{4}$$

Approach 1: low-rank approximation (cont'd)

- joint optimization of (4) is still difficult
- Zhang (2018): first estimate O, then Π (no iteration!)
- **Key idea:** match row distributions, get $\widehat{O}$; then easy to estimate Π
- Alternatively, Tang et al. (2014) uses a rotation-invariant kernel to run MMD (Gretton et al. 2012) on X-rows

Graph matching

Approach 2: local network moments

- **Correlated ER model:**

$$\mathrm{Cor}\left(A_{i,j}^{(1)}, A_{\pi^*(i),\pi^*(j)}^{(2)}\right) = \rho$$

  for some true permutation π^*

- **Method 1: degree profile** (Ding et al. 2021):
  1. For each node i, compute degree distribution of its neighbors: F_i
  2. Similarity matrix:

$$S_{i,j} := \mathrm{distance}(F_i, F_j)$$

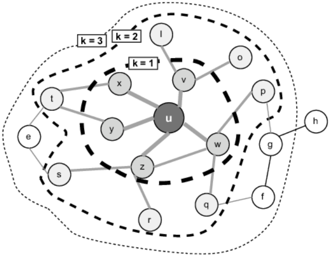
  3. Estimate π by Hungarian algorithm

Approach 2: local network moments (cont'd)

- **Method 2: large neighborhood statistics** (Mossel & Xu 2020):
  1. Seed I_0: a small set of correctly matched nodes
  2. For each k and each $j_1 \in$ net 1, $j_2 \in$ net 2, compute

     $$w_{k;j_1,j_2} := \{i : i \in I_0, i \in \{k\text{-hop neighborhoods of both } i \text{ and } j\}\}$$

     k : tuning parameter; if $|w_{k;j_1,j_2}|$ is large, match (j_1, j_2)
- Many recent (strong) results (Ding & Du 2023, Mao et al. 2024) and more ...



Extensions to weighted, directed, bipartite graphs

Weighted networks:

- $A_{i,j} \sim$ Bernoulli $\Rightarrow A_{i,j} \sim \mathscr{F}_\theta$
- **Example: Poisson β-model** (Yan et al. 2016)

$$\mathbb{P}(A_{i,j} = x) = \frac{e^{(\beta_i + \beta_j)x}}{x!} e^{-e^{\beta_i + \beta_j}}$$

- **Example: weighted SBM** (Xu et al. 2020)

$$A_{i,j} \sim \mathscr{F}_{c_i, c_j}$$

  There are $\binom{K}{2}$ different $\mathscr{F}$'s
- Typically the same methods (MLE, spectral, ...) work for the weighted version

Extensions to weighted, directed, bipartite graphs

Directed networks:

- Each node may have two roles: sender and receiver
- **Example: directed SBM** (Wang & Wong 1987)

$$\mathbb{P}(A_{i,j} = 1) = P_{c_i, d_j},$$

  where

  - c_i: community label as sender
  - d_j: community label as receiver

- Spectral clustering:

$$A \approx \widehat{U} S \widehat{V}^T,$$

  then:

  - Cluster rows of $\widehat{U}$ to estimate $\vec{c}$
  - Cluster rows of $\widehat{V}$ to estimate $\vec{d}$

Extensions to weighted, directed, bipartite graphs

Bipartite networks:

- Two node sets of distinct meanings
  Example: recommender system: buyers $\leftrightarrow$ goods
  Example: drug-target network
- A is $m \times n$
- Method and theory: mostly similar to directed networks
  Some differences:
  - Unlike directed networks, no self-loops
  - Asymptotics: m, n may grow at different rates

Other topics

Resampling networks

Problem description:

- **Observe:** one A
- **Goal:** sampling distribution of some model functional (e.g., triangle count)

Recall i.i.d. case: observe $X_1, \ldots, X_n$, goal: sample mean

- **Parametric bootstrap:** use X to fit a model $F_{\widehat{\theta}}$, resample from F, repeatedly get $X_1^*, \ldots, X_n^*$ and bootstrapped $\bar{X}^*$
- **Non-parametric bootstrap:** resample from X, repeatedly get $X_1^*, \ldots, X_n^*$ and bootstrapped $\bar{X}^*$
- These two methods produce similar $\bar{X}^*$ distributions

Resampling networks

Network? ... observe A, goal: triangle count

- **Method 1:** use A to fit $\widehat{P}$, then repeatedly generate A^* from $\widehat{P}$ and compute triangle count
- **Method 2** (Green & Shalizi 2017): repeatedly resample nodes, each time induce A^*, count triangles
  Specifically, $k_1^*, \ldots, k_n^*$ resampled from $[n]$, then

$$A^*_{i,j} := A_{k_i,k_j}$$

- Methods 1 and 2 may give you very different triangle count sampling distributions!

What happened?

- **Method 1.5:** use A to fit $\widehat{P}$, then still resample nodes, each time induce $\widehat{P}^*$, then sample A^* from $\widehat{P}^*$, count triangles
- Method 1.5 $\approx$ Method 2 $\neq$ Method 1
- Reading: Zhang & Xia (2022)

Dynamic networks

What do data look like?

- **Scenario 1: network snapshots:** $\{A^{(t)}\}_{t=1}^{T}$ (Sewell & Chen 2015, Pensky 2019)
  Examples: friendship, international trade
- **Scenario 2: stream of edges:** (i, j, t), where t : time stamp (Less studied) (Perry & Wolfe 2013, Fang et al. 2024)
  Examples: emails, contact (epidemiology)

Network snapshots:

- Build model for each layer
- Parameters evolve over time / across layers
- Different layers may have similar/shared parameters
- Tensor analysis (Dr. Xia's tutorial tomorrow)
- Some works: convert edge stream to snapshots

Nodal covariates

Sometimes you observe more than a network ...

- **Data:** $A \in \mathbb{R}^{n\times n}$ and $X \in \mathbb{R}^{n\times p}$
- **Examples:** individual covariates (gender, age, job, ...)
- Structure of X may relate to structure of A

Use X to help modeling A
Example: covariate-assisted community detection (Binkiewicz et al. 2017)

- **Method:**

$$\text{Apply spectral clustering to:} \quad A + \lambda X X^T$$

  λ : tuning parameter
- Edge covariates can be utilized similarly

Nodal covariates

Use A to model/predict X

Example: network regression (Le & Li 2022)

- **Data:** on each node, observe (X_i, Y_i)
- **Goal:** use X and A to predict Y
- **Model:** $C_X := \text{ColumnSpace}(X)$, $C_P := \text{ColumnSpace}(P)$,

$$\mathbb{E}[Y|X] = \underbrace{X\beta}_{\in C_X} + \underbrace{X\theta}_{\in C_X \cap C_P} + \underbrace{\alpha}_{\in C_P}$$

  and $(X\beta) \perp (X\theta)$ and $(X\theta) \perp \alpha$

- **Estimation strategy:** first estimate θ

Nodal covariates

Some understandings

- Beware of differences in X and A structures (considering X might or might not help A's model fitting) (Zhang et al. 2016, Deshpande et al. 2018)
- Be careful when building joint models
  Example: shall we worry about this model for joint community detection?

$$P_{i,j} \propto \exp\left\{B_{c_i,c_j} + C_{X_i,X_j}\right\}$$

where suppose each $X_i \in [K]$, here

- c_i: network community label
- X_i: covariate community label

Sampling network

What if we have to explore the network?

- We might not be able to sample nodes i.i.d. from $\{$all kinds of nodes$\}$
- **Example (snowball):** start from an initial set of people, ask them to refer friends to our study, and friends ask their further friends, ...
- Study strategy:
  1. Model the true (complete) network
  2. Specify a sampling scheme
  3. Analyze what the sampling scheme will produce

Sampling network

Example: random walk (Athreya & Röllin 2016)

- Mechanism. Start from i_0; randomly pick a neighbor, walk to i_1; randomly pick a neighbor of i_1, walk to i_2, ... Obtain the induced network observation
- **Theorem.** Network $\sim$ graphon $f(u,v)$, then the network surveyed by random walk is approximately generated by

  $$\text{degree-weighted graphon:} \quad f(X_i, X_j),$$

  but now X_i is **not** Uniform$[0,1]$, instead, has pdf:

  $$p_X(u) := \frac{\int_0^1 f(u,v)\mathrm{d}v}{\int_0^1\int_0^1 f(u',v)\mathrm{d}u'\mathrm{d}v} \propto \mathbb{E}[\text{degree}] \text{ at } u$$

- Many more other sampling schemes (non-backtracking, snowball, ...) (Rohe 2019)

Core periphery structure

- Aforementioned models attempt to model **all** nodes
- But often there are seclusive nodes with few connections (Rombach et al. 2014)
- **Core:** dense and structured subnetwork
- **Periphery:** the rest of network

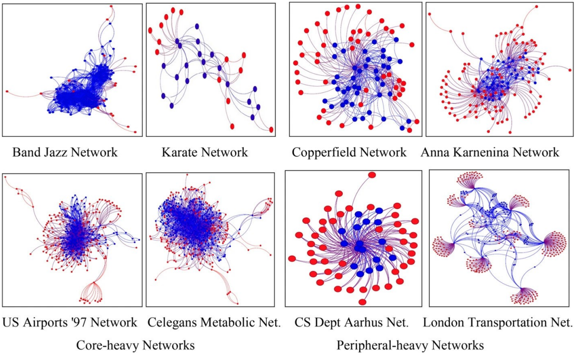


Figure: Blue: core; red: periphery (Meghanathan 2024)

Core periphery structure

Miao & Li (2023)

- Informative model for core part
- Non/Less-informative model for periphery part

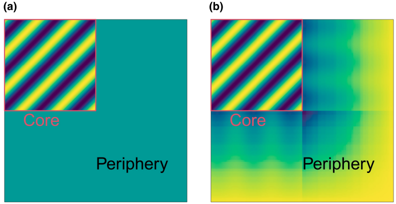


Figure: Two periphery models: left: ER; right: configuration (Miao & Li 2023)

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