Graph Limits & Subgraph Counts

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Introduction

- In 1970 Paul Holland and Samuel Leinhardt (1970, AJS) introduced the triad census.
  - counts of all 4 (16) unique triad isomorphisms in an undirected (directed) graph
  - can construct transitivity index (TI) from triad census...
  - ...as well as the mean and variance of the degree sequence
- Holland and Leinhardt (1976, SM) provide variance expressions for these counts

Introduction (continued)

- In early work normality of these counts was assumed (w/o proof)

- Nowicki (1989, 1991) showed asymptotic normality of counts for homogenous random graphs

- Bickel, Chen & Levina (2011, AS) demonstrated asymptotic normality in the "general" case

Introduction (continued)

- Large literature in sociology which uses triad counts to "test" various hypotheses
  - see Holland and Leinhardt (1976, SM) and Wasserman and Faust (1994)
  - cf., computational biology (e.g., Milo et al., 2002)
- Asymptotic distribution theory puts these tests on firmer ground

Introduction (continued)

- Subgraph frequencies might be used to (partially) identify structural models of network formation (e.g., de Paula et al., 2015)

- indirect inference approach:

  - use structural model to simulate networks...and count subgraphs

  - compare simulated counts with actual counts

Setup

Let $G(\mathcal{V}, \mathcal{E})$ be a finite undirected random graph with

- agents/vertices $\mathcal{V} = \{1, \ldots, N\}$,

- links/edges $\mathcal{E} = \{\{i, j\}, \{k, l\}, \ldots\}$, and

- adjacency matrix $\mathbf{D} = \left[D_{ij}\right]$ with

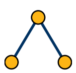
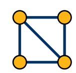
$$D_{ij} = \begin{cases} 1 & \text{if } \{i, j\} \in \mathcal{E} \\ 0 & \text{otherwise} \end{cases}$$

Subgraphs

- (Partial Subgraph) Let $\mathcal{V}(S) \subseteq \mathcal{V}(G)$ be any subset of the vertices of G and $\mathcal{E}(S) \subseteq \mathcal{E}(G) \cap \mathcal{V}(S) \times \mathcal{V}(S)$, then $S = (\mathcal{V}(S), \mathcal{E}(S))$ is an *partial subgraph* of G.

- (Induced Subgraph) Let $\mathcal{V}(S) \subseteq \mathcal{V}(G)$ be any subset of the vertices of G and $\mathcal{E}(S) = \mathcal{E}(G) \cap \mathcal{V}(S) \times \mathcal{V}(S)$, then $S = (\mathcal{V}(S), \mathcal{E}(S))$ is an *induced subgraph* of G.

Subgraphs (continued)

- The induced subgraph S includes *all* edges in G connecting any two agents in $\mathcal{V}(S)$
  - a (partial) subgraph may include only a subset of such edges
  - $S =$  is a partial subgraph of $G =$ , but not an induced subgraph

Graph Isomorphism

- Consider two graphs, R and S, of the same order.

- Let $\varphi : \mathcal{V}(R) \to \mathcal{V}(S)$ be a bijection from the nodes of R to those of S.

- The bijection $\varphi : \mathcal{V}(R) \to \mathcal{V}(S)$

  – *maintains adjacency* if for every dyad $i, j \in \mathcal{V}(R)$ if $\{i, j\} \in \mathcal{E}(R)$, then $\{\varphi(i), \varphi(j)\} \in \mathcal{E}(S)$;

  – *maintains non-adjacency* if for every dyad $i, j \in \mathcal{V}(R)$ if $\{i, j\} \notin \mathcal{E}(R)$, then $\{\varphi(i), \varphi(j)\} \notin \mathcal{E}(S)$.

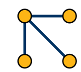
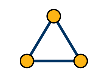
Graph Isomorphism (continued)

- If the bijection maintains both adjacency and non-adjacency we say it *maintains structure*.

- (Graph Isomorphism) The graphs R and S are *isomorphic* if there exists a structure-maintaining bijection $\varphi : \mathcal{V}(R) \to \mathcal{V}(S)$.

- Notation: $R \cong S$ means "R is isomorphic to S."

Induced Subgraph Density

- S is a p^{th}-order graphlet of interest (e.g., $S =$  or $S =$ )

- G_N is the network/graph under study

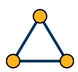
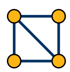
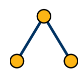
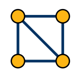
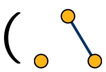
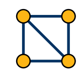
- $\mathbf{i}_p \subseteq \{1, 2, \ldots, N\}$ is a set of p integers with $i_1 < i_2 < \cdots < i_p$
  - $\mathcal{C}_{p,N}$ is set of all $\binom{N}{p}$ such integer sets
  - $G[\mathbf{i}_p]$ is the induced subgraph of G associated with vertex set $\mathbf{i}_p$

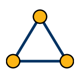
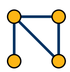
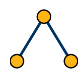
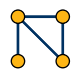
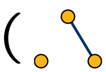
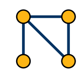
Induced Subgraph Density (continued)

- The induced subgraph density of S in G_N, denoted by $t_{\text{ind}}(S, G_N)$ or $P_N(S)$ equals the probability that $G_N[\mathbf{i}_p]$, for $\mathbf{i}_p$ chosen uniformly at random from $C_{p,N}$, is isomorphic to S:

$$\begin{aligned} t_{\text{ind}}(S, G_N) &= \binom{N}{p}^{-1} \sum_{\mathbf{i}_p \in C_{p,N}} \mathbf{1}(S \cong G_N[\mathbf{i}_p]) \\ &= \Pr(S \cong G_N[\mathbf{i}_p]) \\ &= P_N(S) \end{aligned}$$

Induced Subgraph Density (Examples)

- $t_{\text{ind}}($  $,$  $) = \frac{2}{4}$, $t_{\text{ind}}($  $,$  $) = \frac{2}{4}$ and $t_{\text{ind}}($  $,$  $) = \frac{0}{4}$

- $t_{\text{ind}}($  $,$  $) = \frac{1}{4}$, $t_{\text{ind}}($  $,$  $) = \frac{2}{4}$ and $t_{\text{ind}}($  $,$  $) = \frac{1}{4}$

Induced Subgraph Density: Graphon Case

- Let $h\left(U_i, U_j\right)$ be a valid graphon.

- $\text{iso}(S)$ is the group of isomorphisms of S, and $|\text{iso}(S)|$ its cardinality

- Under the "Aldous-Hoover DGP" the *ex ante* probability that an induced p-subgraph is isomorphic to S is given by

$$\begin{aligned} t_{\text{ind}}(S,h) &= |\text{iso}(S)| \\ &\times \mathbb{E}\left[\prod_{\{i,j\}\in\mathcal{E}(S)} h\left(U_i, U_j\right) \prod_{\{i,j\}\in\mathcal{E}(\bar{S})} \left[1 - h\left(U_i, U_j\right)\right]\right] \\ &= P(S). \end{aligned}$$

Graph Limits

Let $\{G_N\}_{N=1}^{\infty}$ be a sequence of networks. If

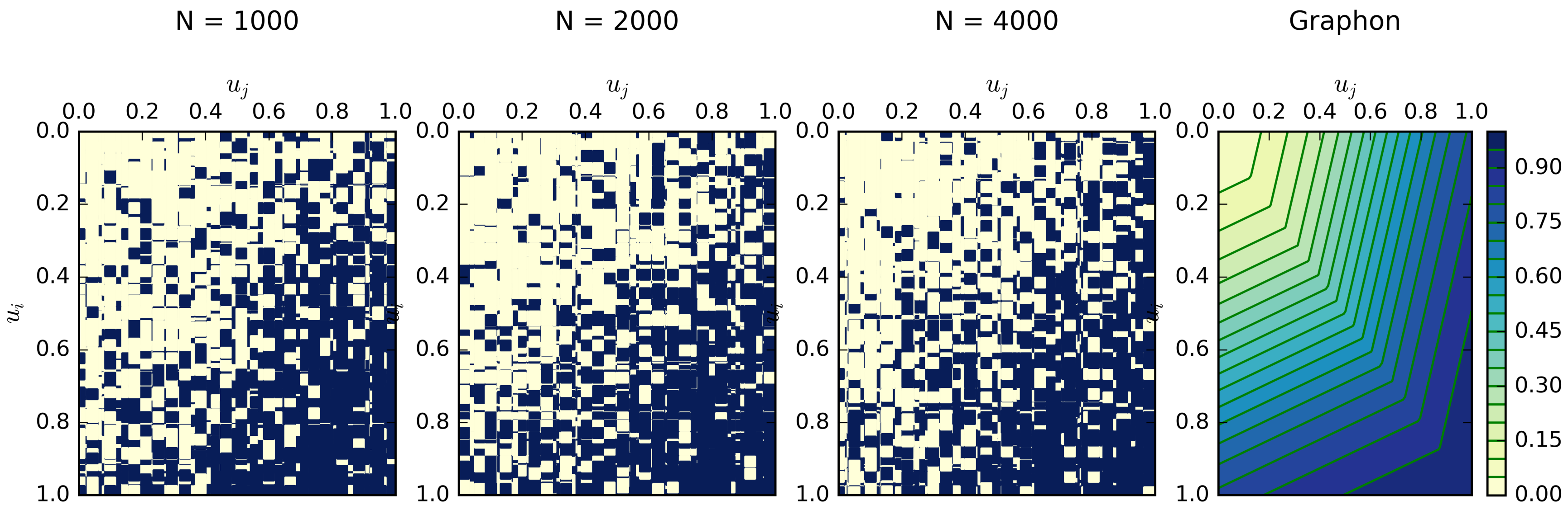
$$\lim_{N\to\infty} t_{\text{ind}}(S, G_N) = t_{\text{ind}}(S, h)$$

for some graphon $h(\cdot,\cdot)$ and all fixed subgraphs S, then we say that G_N converges to $h(\cdot,\cdot)$.

- Lovász (2012) for complete development

- Diaconis and Janson (2008) for connections with Aldous-Hoover Theorem

Graph Limits: Example



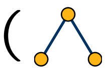
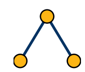
(Injective) Homomorphism Density

- The homomorphism density gives the probability that S is (isomorphic to) a subgraph of a randomly selected induced subgraph of G_N of order $p = |\mathcal{V}(S)|$

- Alternatively the homomorphism density equals fraction of injective mappings $\varphi : \mathcal{V}(S) \to \mathcal{V}(G_N)$ that preserve edge adjacency

$$\begin{aligned} t_{\text{hom}}(S, G_N) &= \frac{1}{\binom{N}{p} |\text{iso}(S)|} \sum_{R \subseteq K_N, R \cong S} \mathbf{1}(R \subseteq G_N) \\ &= \frac{1}{\binom{N}{p} |\text{iso}(S)|} \sum_{R \subseteq K_N, |V(R)|=p} \mathbf{1}(R \cong S) \prod_{\{i,j\} \in \mathcal{E}(R)} D_{ij} \\ &= Q_N(S) \end{aligned}$$

Homomorphism Density (continued)

- Summation in $t_{\text{hom}}(S, G_N) = Q_N(S)$ is over the $\binom{N}{3}$ |iso()| $= \frac{3}{6}N(N-1)(N-2)$ (partial) subgraphs of K_N (the complete graph) which are isomorphic to $S =$ ) .

- We count the number of these subgraphs which are also *partial* subgraphs of G_N

Homomorphism Density (continued)

- The expected value of $Q_N(S)$ is:

$$\begin{aligned}
\mathbb{E}\left[Q_N(S)\right] &= \frac{1}{\binom{N}{p}\left|\text{iso}(S)\right|} \sum_{R \subseteq K_N, |V(R)|=p} \left\{ \mathbf{1}\left(R \cong S\right) \right. \\
&\quad \left. \times \mathbb{E}\left[\mathbb{E}\left[\prod_{\{i,j\} \in \mathcal{E}(R)} D_{ij} \middle| U_1, \ldots, U_N\right]\right]\right\} \\
&= \mathbb{E}\left[\prod_{\{i,j\} \in \mathcal{E}(S)} h\left(U_i, U_j\right)\right] \\
&= Q(S) = t_{\text{hom}}(S, h)
\end{aligned}$$

- Can use $t_{\text{hom}}(S, G_N)$ to define graph convergence

Recap

- *Induced subgraph density*, $P_N(S)$: probability that $G_N[\mathbf{i}_p]$, for $\mathbf{i}_p$ chosen uniformly at random from $C_{p,N}$, is isomorphic to S

- *Homomorphism density*, $Q_N(S)$: probability that *a subgraph of* $G_N[\mathbf{i}_p]$, for $\mathbf{i}_p$ chosen uniformly at random from $C_{p,N}$, is isomorphic to S

- If $\lim_{N\to\infty} P_N(S) = t_{\text{ind}}(S,h)$ for some graphon $h(\cdot,\cdot)$ and all fixed subgraphs S, then we say that G_N converges to $h(\cdot,\cdot)$.

One more tool! Graphlet Stitchings

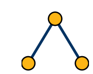
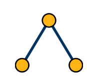
- Graph union: $T \cup U = G\left(\mathcal{V}\left(T\right) \cup \mathcal{V}\left(U\right), \mathcal{E}\left(T\right) \cup \mathcal{E}\left(U\right)\right)$

- Let $W_{q,R,S}$ be a union of two isomorphisms, respectively T and U, of the graphlets R and R with

  1. $|\mathcal{V}\left(R\right)| = |\mathcal{V}\left(S\right)| = p$
  2. $|\mathcal{V}\left(R\right) \cap \mathcal{V}\left(S\right)| = q$ vertices in common
  3. identical structures across all vertices in common

- The multiset of all such graphlet stitchings (including isomorphisms) is denoted by $\mathcal{W}_{q,R,S}$ (with $\mathcal{W}_{q,S,S} = W_{q,S}$)

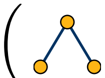
Graphlet Stitching: Example #1

- Let the graphlets $R =$  and $S =$  share one vertex in common.
  - There is just one possible way to join them: $R \cup S \cong$ 
- We therefore have that $\mathcal{W}_{1,}$ $= \{$  $\}$

Graphlet Stitching: Example #1 (continued)

- Define the probability of observing an element of $\mathcal{W}_{1,}$  as a subgraph of a randomly sampled triad as

$$Q\left(\mathcal{W}_{1,}\right.$$  $$\left.\right) = \sum_{W \in \mathcal{W}_{1,}} Q(W)$$ 

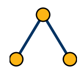
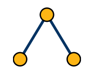
$$= Q\left(\right.$$  $$\left.\right)$$

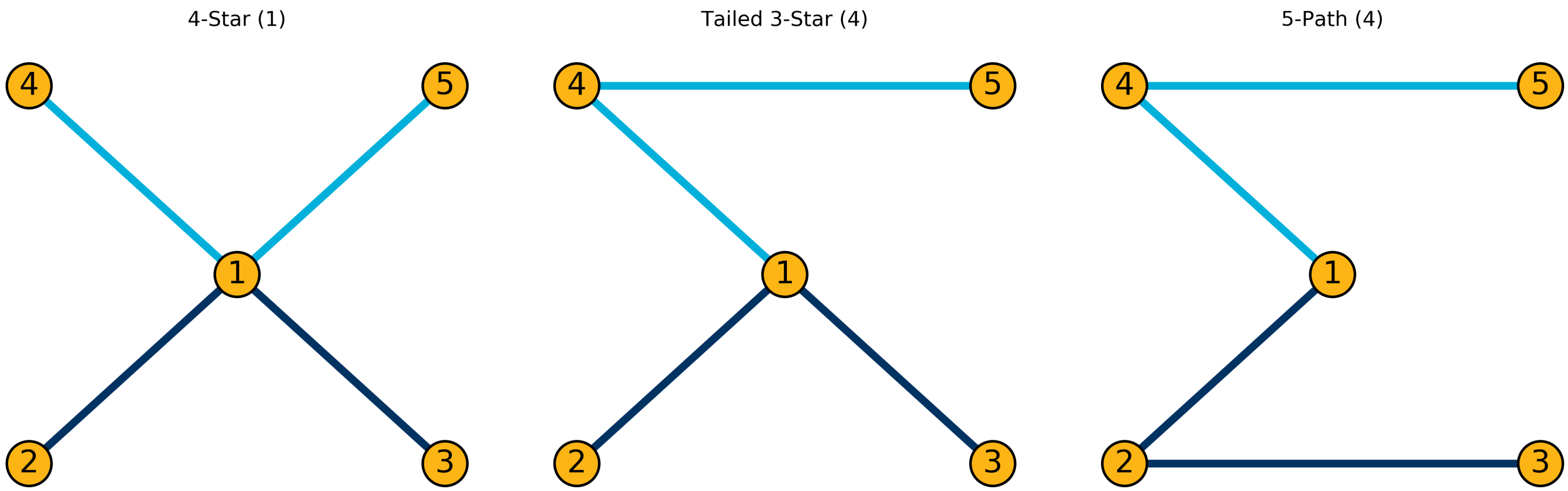
$$= \mathbb{E}\left[D_{12} D_{13}\right]$$

with $Q(W)$ the homomorphism density introduced above

- For $q = 2$ (two nodes in common) we have, of course, $\mathcal{W}_{2,}$  $= \{$  $\}$

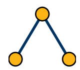
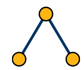
Graphlet Stitching: Example #2

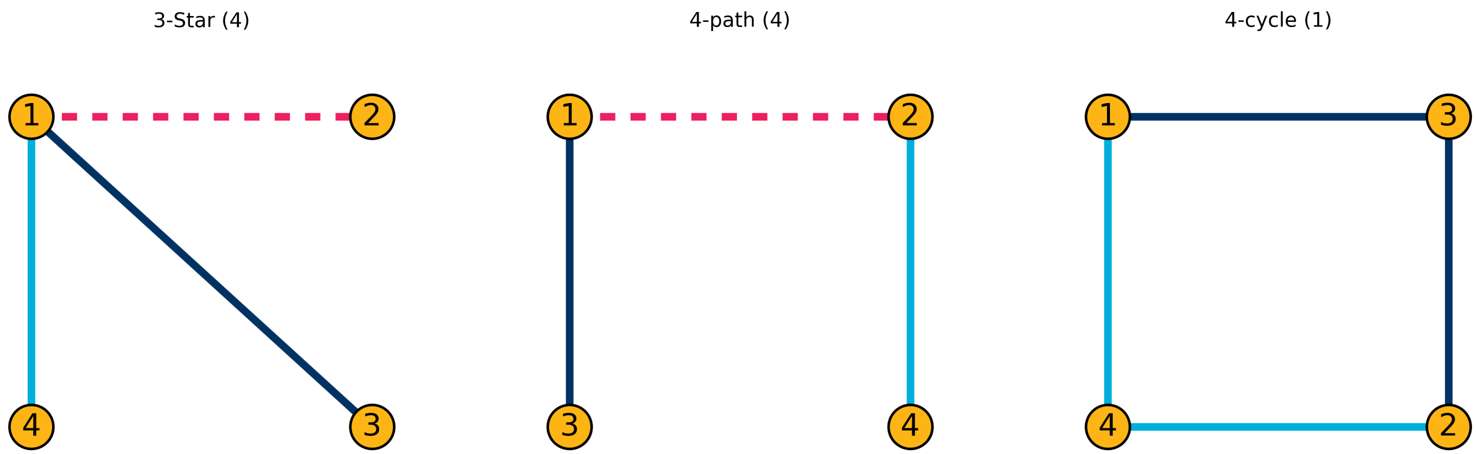
There are nine ways (three up to isomorphisms) to join the graphlets $R =$  and $S =$ , sharing one vertex in common.



Notes: Number of isomorphisms of each graphlet in $\mathcal{W}_{1,q}$ given in parentheses.

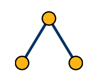
Graphlet Stitching: Example #2 (continued)

There are nine ways (three up to isomorphisms) to join the graphlets $R =$  and $S =$ , sharing two vertices in common.



Notes: Number of isomorphisms of each graphlet in $\mathcal{W}_{2,q}$ given in parentheses.

Estimation of Subgraph Frequencies

- We will develop explicit results for two subgraph frequencies
  - the frequency of connected dyads: $S =$ 
  - the frequency of two star triads: $S =$ 

- General case involves no new ideas...
  - ...but can be *very* tedious in practice

Density

- We estimate $\rho_N = \text{Pr}\left(D_{ij} = 1\right)$ by

$$\widehat{\rho}_N = \frac{2}{N\left(N-1\right)} \sum_{i<j} D_{ij}$$

- Projecting onto $U_1, ..., U_N$ yields the decomposition:

$$\begin{aligned} \widehat{\rho}_N &= \underbrace{\frac{2}{N\left(N-1\right)} \sum_{i<j} h_N\left(U_i, U_j\right)}_{\text{U-Statistic}} + \underbrace{\frac{2}{N\left(N-1\right)} \sum_{i<j} \left(D_{ij} - h_N\left(U_i, U_j\right)\right)}_{\text{"Poisson Binomial R.V''}} \\ &= U_N + T_N \end{aligned}$$

- Observe that T_N is mean independent of U_N

Density: Variance Calculation

We have

$$\begin{aligned}\mathbb{V}\left(\hat{\rho}_N\right) &= \mathbb{V}\left(U_N\right) + \mathbb{V}\left(T_N\right) + 2\mathbb{C}\left(U_N, T_N\right) \\ &= \mathbb{V}\left(U_N\right) + \mathbb{V}\left(T_N\right).\end{aligned}$$

A Hoeffding (1948) variance decomposition gives

$$\mathbb{V}\left(U_N\right) = \binom{N}{2}^{-2} \sum_{q=1}^{2} \binom{N}{2}\binom{2}{q}\binom{N-2}{2-q}\Omega_q$$

for

$$\Omega_q = \mathbb{C}\left(h_N\left(U_{i_1}, U_{i_2}\right), h_N\left(U_{j_1}, U_{j_2}\right)\right)$$

with $\{i_1, i_2\}$ and $\{j_1, j_2\}$ sharing $q = 1, 2$ indices in common

Density: Variance Calculation (continued)

Evaluating Ω_1 yields

$$\begin{aligned}\Omega_1 &= \mathbb{E}\left[h_N\left(U_1, U_2\right) h_N\left(U_1, U_3\right)\right] - \mathbb{E}\left[h_N\left(U_1, U_2\right)\right] \mathbb{E}\left[h_N\left(U_1, U_3\right)\right] \\ &= Q\left(\mathcal{W}_{1, \circ\!-\!\circ}\right) - P\left(\circ\!-\!\circ\right) P\left(\circ\!-\!\circ\right) \\ &= Q\left(\overset{\circ}{\wedge}\right) - P\left(\circ\!-\!\circ\right) P\left(\circ\!-\!\circ\right)\end{aligned}$$

Evaluating Ω_2 yields

$$\begin{aligned}\Omega_2 &= \mathbb{E}\left[h_N\left(U_1, U_2\right)^2\right] - \mathbb{E}\left[h_N\left(U_1, U_2\right)\right] \mathbb{E}\left[h_N\left(U_1, U_2\right)\right] \\ &= \mathbb{V}\left(\mathbb{E}\left[D_{12} \middle| \mathbf{U}\right]\right)\end{aligned}$$

Density: Variance Calculation (continued)

Evaluating the variance of $\mathbb{V}(T_N)$ we get

$$\begin{aligned}
\mathbb{V}(T_N) &= \mathbb{V}\left(\mathbb{E}\left[T_N \mid \mathbf{U}\right]\right) + \mathbb{E}\left[\mathbb{V}\left(T_N \mid \mathbf{U}\right)\right] \\
&= 0 + \left(\frac{2}{N(N-1)}\right)^2 \mathbb{V}\left(\left.\sum_{i<j}\left(D_{ij} - h_N\left(U_i, U_j\right)\right)\right| \mathbf{U}\right) \\
&= \left(\frac{2}{N(N-1)}\right)^2 \sum_{i<j} \mathbb{V}\left(D_{ij} - h_N\left(U_i, U_j\right)\Big| \mathbf{U}\right) \\
&= \frac{2}{N(N-1)} \mathbb{E}\left[\mathbb{V}\left(D_{12} \mid \mathbf{U}\right)\right]
\end{aligned}$$

Density: Variance Calculation (continued)

Collecting terms we have:

$$
\begin{aligned}
\mathbb{V}\left(\widehat{\rho}_N\right) &= \frac{4\left(N-2\right)}{N\left(N-1\right)}\left[Q\left(\wedge\right) - P\left(\circ\!\!-\!\!\circ\right)P\left(\circ\!\!-\!\!\circ\right)\right] \\
&+ \frac{2}{N\left(N-1\right)}\mathbb{V}\left(\mathbb{E}\left[\left.D_{12}\right|\mathbf{U}\right]\right) + \frac{2}{N\left(N-1\right)}\mathbb{E}\left[\mathbb{V}\left(\left.D_{12}\right|\mathbf{U}\right)\right] \\
&= \frac{4\left(N-2\right)}{N\left(N-1\right)}\left[Q\left(\wedge\right) - P\left(\circ\!\!-\!\!\circ\right)P\left(\circ\!\!-\!\!\circ\right)\right] \\
&+ \frac{2}{N\left(N-1\right)}P\left(\circ\!\!-\!\!\circ\right)\left(1 - P\left(\circ\!\!-\!\!\circ\right)\right)
\end{aligned}
$$

Density: Variance Calculation (continued)

- To allow for graph sequences where $\rho_N \to 0$ as $N \to \infty$ we normalize
  - Let $\tilde{Q}\left(\;\right) = \frac{Q\left(\;\right)}{\rho^2}$ and $\tilde{P}\left(\;\right) = \frac{P\left(\;\right)}{\rho_N}$
  - Recall that $\lambda_N = (N-1)\,\rho_N$

Density: Variance Calculation (continued)

- After normalization:

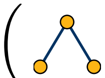
$$\begin{aligned}\mathbb{V}\left(\frac{\widehat{\rho}_N}{\rho_N}\right) &= \frac{4\,(N-2)}{N\,(N-1)}\left[\tilde{Q}\left(\wedge\right) - \tilde{P}\left(\circ\!-\!\circ\right)\tilde{P}\left(\circ\!-\!\circ\right)\right] \\ &\quad + \frac{2}{N\lambda_N}\tilde{P}\left(\circ\!-\!\circ\right) - \frac{2}{N\,(N-1)}\tilde{P}\left(\circ\!-\!\circ\right)^2 \\ &= O\left(\frac{1}{N}\right) + O\left(\frac{1}{N\lambda_N}\right) + O\left(\frac{1}{N^2}\right)\end{aligned}$$

- If $\lambda_N \to \infty$ first term dominates

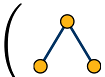
- If $\lambda_N \to \lambda_0 > 0$, first two terms dominate

Asymptotic Inference

- Asymptotic theory for U-Statistics gives, for $\lambda_N \to \infty$ as $N \to \infty$

$\sqrt{N}\left(\frac{\widehat{\rho}_N}{\rho_N} - 1\right) \xrightarrow{D} \mathcal{N}\left(0, 4\left[\tilde{Q}\left(\right.\right.\right.$  $\left.\right) - \tilde{P}\left(\right.$  $\left.\right)\tilde{P}\left(\right.$  $\left.\left.\left.\right)\right]\right)$

- Result due to Bickel, Chen and Levina (2011, *Annals of Statistics*)

- <u>Comment:</u> Under Erdos-Renyi $\tilde{Q}\left(\right.$  $\left.\right) = \tilde{P}\left(\right.$  $\left.\right)\tilde{P}\left(\right.$  $\left.\right)$

Variance Estimation

We can estimate the asymptotic variance using the analog estimators:

$$\hat{Q}\left(\quad\right) = \binom{N}{3}^{-1} \sum_{i<j<k} \frac{1}{3}\left\{D_{ij}D_{ik} + D_{ij}D_{jk} + D_{ik}D_{jk}\right\}$$
$$= \binom{N}{3}^{-1} \frac{1}{3}\left[T_{\mathsf{TS}} + 3T_{\mathsf{T}}\right]$$

and

$$\hat{P}\left(\quad\right) = \binom{N}{2}^{-1} \sum_{i<j} D_{ij}$$

Variance Estimation for $\widehat{P}\left(\circ\!\!-\!\!\circ\right)$: Nyakatoke

For Nyakatoke we have

$$\widehat{Q}\left(\wedge\right) \cong 0.006105$$

and

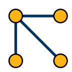
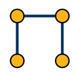
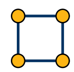
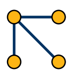
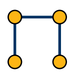
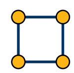
$$\widehat{P}\left(\circ\!\!-\!\!\circ\right) \simeq 0.0698$$

which gives

$$\begin{array}{c} \widehat{\rho}_N \\ \text{(a.s.e)} \end{array} = \begin{array}{c} 0.0698 \\ (0.0064) \end{array}$$

<u>Note</u>: Estimate of excluded higher order variance term is 4.6×10^{-6}

Limit Distribution of $\widehat{P}(\wedge)$

- Define the multiset of graphlet stitchings:
  - $\mathcal{W}_{1,\wedge} = (\{$  ,  ,  $\}, m)$
  - Here $m = \{($  $, 4), ($  $, 4), ($  $, 1)\}$ gives the multiplicity of each unique graphlet in $\mathcal{W}_{1,\wedge}$
- Normalize graphlet according to number of edges in it.
  - $\tilde{P}(\wedge) = \dfrac{P(\wedge)}{\rho_N^2}$ and $\tilde{Q}\left(\mathcal{W}_{1,\wedge}\right) = \dfrac{Q\left(\mathcal{W}_{1,\wedge}\right)}{\rho_N^4}$

Limit Distribution of $\widehat{P}(\wedge)$

If $\lambda_N \to \infty$ as $N \to \infty$, then

$$\sqrt{N}\left(\frac{\widehat{P}(\wedge)}{\rho_N^2} - \tilde{P}(\wedge)\right) \xrightarrow{D} \mathcal{N}\left(0, 9\left[\tilde{Q}\left(\mathcal{W}_{1,\wedge}\right) - \tilde{P}\left(\wedge\right)\tilde{P}\left(\wedge\right)\right]\right).$$

- Analysis involves a variance calculation along the lines outlined above

- And the characterization of the limiting variance of a 3rd order U-Statistics

Wrapping Up

- In large graphs subgraph counting is computationally challenging
  - implications for feasibility of both estimation and inference
  - see Bhattacharya and Bickel (2015) for a subsampling approach
- Very little (i.e., almost none) empirical work using these results
- Tremendous scope for using these methods in empirical analysis; but not easy!