# CS-E5745 <br> Mathematical Methods for Network Science 

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## This lecture

1. Basic concepts and notation (remind CS-E5740)
2. Basic network models (remind CS-E5740)
3. Common approximations:

- Tree-like approximations
- "Thermodynamic limit"


## Basic definitions and notation (1/8)

- Graph $G=(V, E)$, where $V$ is the set of nodes and $E \subseteq V \times V$ is the set of edges
- Usually no self-edges: $(v, v) \notin E$ for any $v \in V$.
- In this course: undirected networks, no multiedges or weighted edges (unless otherwise mentioned)
- We will use both vertices/edges and nodes/links.
- $N=|V|$ and $L=|E|$


## Basic definitions and notation (2/8)

- Two nodes $v, u$ are adjacent or neighbors if there is a link $(v, u) \in E$, and $(v, u)$ is incident to $v$ and $u$.
- Neighborhood of node $v$ is the set of nodes adjacent it: $\Gamma(v)=\{u \mid(v, u) \in E\}$
- Degree of node $v$ is the number of adjacent nodes: $k_{v}=|\Gamma(v)|$


## Basic definitions and notation (3/8)

- Walk is a sequence of nodes and connected by links $\left(v_{0}, e_{1}, v_{1}, e_{2}, \ldots, e_{l}, v_{l}\right)$, where $e_{i}=\left(v_{i-1}, v_{i}\right) \in E$
- Length of the walk is the number of edges in it
- Path is a walk where all nodes are distinct, with the exception that the first and the last node can be the same.
- Cycle is a path where the first and the last node are the same
- Distance between two nodes is the length of the shortest path between those nodes
- Note! Some sources might have different definitions for walk and path! Always define these concept (outside of this course) for clarity.


## Basic definitions and notation (4/8)

- Two nodes are connected if there is a path between them
- Component is a maximal set of nodes that are connected
- Connectivity partitions an undirected graph into components (i.e., each node is in exactly one component)
- The size of the component is the number of nodes in it
- The largest component is the one with largest size
- Connected graph is a graph with a single component
- Giant component is the component that spans non-zero fraction of an infinitely large network


## Basic definitions and notation (5/8)

- Percolation theory in networks describes the properties of connected components
- Site percolation: paths are allowed only through occupied nodes
- Bond percolation: paths are allowed only through occupied edges
- Identical to removing nodes/edges
- Physics: regular lattices, nodes or edges set independently and uniformly occupied with occupation probability


## Basic definitions and notation (6/8)

- We assume that the nodes are (or are implicitly mapped to) numbers from 0 to $N-1$
- Adjacency matrix:

$$
A_{u v}= \begin{cases}1, & \text { if }(u, v) \in E \\ 0, & \text { if }(u, v) \notin E\end{cases}
$$

- Useful when working with networks, e.g.,
- Degree: $k_{v}=\sum_{u} A_{u v}$
- Number of walks of length $n$ starting at $v$ and ending at $u$ : $\left(A^{n}\right)_{u v}$
- $\ldots$


## Basic definitions and notation (7/8)

- Global clustering coefficient or transitivity is

$$
C=\frac{\# \text { of triangles }}{\# \text { connected triplets }}=\frac{\sum_{u v h} A_{u v} A_{v h} A_{h u}}{\sum_{u v h} A_{u v} A_{h u}}=\frac{\operatorname{Tr}\left(A^{3}\right)}{\operatorname{Tr}(A F A)}
$$

- Tr is the trace operator and $F$ is the adjacency matrix of a full graph
- Local clustering coefficient for node $u$ is

$$
c_{u}=\frac{\sum_{v h} A_{u v} A_{v h} A_{h u}}{\sum_{v h} A_{u v} A_{h u}}=\frac{\left(A^{3}\right)_{u u}}{(A F A)_{u u}}=\frac{\left(A^{3}\right)_{u u}}{k_{u}\left(k_{u}-1\right) / 2}
$$

## Basic definitions and notation (8/8)

- Tree is a connected graph with no loops
- Equivalently, a connected graph with $N-1$ edges
- Forest is a graph that consists of trees


## Random graph models

- Create an artificial random network with desired properties
- = probability distributions over all graphs $P(G)$
- (Physicist jargon: probability distribution is an "ensemble")
- Can be roughly divided to two categories:

1. Null models that have some set of structural properties but otherwise maximally random: Usually closed form formula for $P(G)$
2. Stylised models to analyse particular microscopic generation rules: No closed form formula for $P(G)$, only algorithm for sampling

## Erdős-Rényi random graphs

- "soft" and "hard" versions:
- $G(N, p)$ : $N$ nodes, each link exists with probability $p$
- $G(N, L): N$ nodes and $L$ links distributed uniformly randomly between the nodes
- (Physicist jargon: These are some times called "canonical ensemble" and "microcanonical ensemble")
- $G\left(N, p=\frac{L}{N(N-1) / 2}\right) \approx G(N, L)$, because $\langle L\rangle=p N(N-1) / 2$
- Often used interchangeably for large networks
- Differences in these two discussed later in the course
- $G(N, p)$ AKA Bernoulli random graphs


## Configuration model (1/6)

- Configuration model: a completely random graph with given degree sequence $\left\{k_{u}\right\}_{u}$
- Again "soft" and "hard" variants can be constructed:
- Each graph with the exactly the given degree sequence is sampled uniformly randomly
- The expected value of degrees is given by the degree sequence, but there can be slight deviations
- More on these on the 5th lecture
- In practise also other variants and complications, see a recent review article: https://arxiv.org/abs/1608.00607
- Note: Often only the "hard" variant is said to be a configuration model, and "soft" variants have different names (e.g., Chung-Lu model)


## Configuration model (2/6)

- The "hard" variant of the configuration:

$$
P\left(G \mid\left\{k_{u}\right\}\right)= \begin{cases}\frac{1}{\Omega\left(\left\{k_{u}\right\}\right)}, & \text { if } k(G)=\left\{k_{u}\right\} \\ 0, & \text { otherwise }\end{cases}
$$

- The sequence $\left\{k_{u}\right\}$ is a graphic sequence iff
- $\sum_{u} k_{u}$ is even, and
- $\sum_{u=0}^{r} k_{u} \leq r(r-1)+\sum_{i=r+1}^{N-1} \min \left(r, k_{u}\right)$, for all $r \leq N-2$ (where in the sums $\left\{k_{u}\right\}$ ordered such that $k_{u} \geq k_{u+1}$ )


## Configuration model (3/6)

- The configuration model can be relaxed by allowing multi-links and self-loops
- Only requirement is that $\sum_{u} k_{u}$ is even
- Large sparse networks will have small number of multi-links and loops
- Easy generation algorithm based on stubs
- Node $u$ has $k_{u}$ stubs
- Select two stubs uniformly randomly and connect


## Configuration model (4/6)

- Example: $\left\{k_{u}\right\}=\{2,2,1,1\}$. Stubs:



## Configuration model (5/6)

- Example: $\left\{k_{u}\right\}=\{2,2,1,1\}$. Two of the possible solutions:



## Configuration model (6/6)

- A "soft configuration model": each edge ( $u, v$ ) (including $u=v)$ is present independently with probability

$$
P\left((u, v) \in G \mid\left\{k_{u}\right\}\right)= \begin{cases}\frac{k_{u} k_{v}}{\sum_{u} k_{u}}, & \text { if } u \neq v \\ \frac{k_{u} k_{v}}{2 \sum_{u} k_{u}}, & \text { if } u=v .\end{cases}
$$

- This leads to the expected value of the degree of each node to follow the given sequence $\langle k(G)\rangle=\left\{k_{u}\right\}$
- Very similar formula can be derived for the expected number of edges between two nodes in the "hard" configuration model variant with multiedges
- ... but the edges do not appear independently of each other
- Few variants exist (see Hofstad: inhomogeneous random graphs, Chung-Lu model, Norros-Reittu model)


## Assumption and approximations

- Analytical calculations are often impossible if you want to do them precisely for finite networks
- We want the big picture, and don't care about minor details or extreme accuracy of our calculations
- We do simplifying assumptions and approximations, such as
- Concentrate on what happens at the infinite network size
- Assume that we can disregard some aspects of the network structure
- Leave out higher order terms in series expansions
- ...


## Infinitely large networks

- Assumption: Network is big enough that it behaves like an infinitely large system
- It is often convenient to study some class of networks when $N \rightarrow \infty$
- (Physicist jargon: Taking infinite limit on a size of the system keeping some other variables constant is called the "thermodynamic limit")
- Calculations and results often become simpler: only the largest effects matters, details and higher order effects can be omitted
- Example: $G(N, p)$ and $G(N, L)$ become in effect the same ensemble at the thermodynamic limit
- Warning: it is often assumed that all "soft" and "hard" distributions become the same, but this is not necessarily true, see Squartini et al. "Breaking of Ensemble Equivalence in Networks" PRL (2015)


## Tree-like approximations

- Assumption: Network doesn't have any loops, or the loops only have a minor effect to the phenomena that is studied
- Many calculations for trees are often easier than for general graphs
- Example: Calculate the number of nodes that can be reached from a node
- Sparse random networks are locally tree-like [Exercise 1.4]
- Many results can be shown to be precise for infinitely large networks using this idea (see Hofstad)
- The tree-like assumption is very common in networks literature and often implicit
- Real networks have high clustering coefficient but the theory still seems to work, see melnik et al. "The unreasonable effectiveness of
tree-based theory for networks with clustering" PRE (2011)


## Mean-field-type approximations

- Assumption: Parts of the network can be grouped together in a way that we can concentrate on the average behavior of each group
- Example: All nodes of the same degree have the same probability of being infected in epidemics
- Calculations relying on this assumption are called "mean field theory"
- Very common approach in network science


## Does my theory work for real networks?

- Often in the literature no formal tools are given to determine if the theory works for particular network
- Example: How much fluctuations from the theory I should expect to have when my network has $N$ nodes?
- Typical approach: compare analytical results to example data or detailed simulations


## Does my theory work for real networks?



Figure from: Melnik et al. "The unreasonable effectiveness of tree-based theory for networks with clustering" PRE (2011)

## Following a link leads to high degree nodes

- A node with degree $k$ has probability proportional to $k$ of being reached when a link is followed
- Selecting a random link, and one of its endpoints (in general)
- Selecting a random node and one of its neighbors (when no degree-degree correlations)

$$
p^{\prime}(k) \propto k p(k)
$$

- Recurring theme in calculations
- Spreading process is more likely to reach high degree nodes, high degree nodes are more effective spreaders ...
- Neighboring nodes have higher degree than uniformly random nodes, high degree nodes are more likely to belong to the giant component ...
- Your friends have more friends than you do


## Following a link leads to high degree nodes

- Selecting a random link and following one of its neighbors, the degree of the node is always distributed according to:

$$
p^{\prime}(k) \propto k p(k)
$$

- Selecting a random node and one of its neighbors differs from above in the real world since the degrees of adjacent nodes are often correlated.


## Following a link leads to high-degree nodes

- Example: $\left\{k_{u}\right\}=\{2,2,1,1\}$. Probabilities to reach node when following a link $\left\{\frac{2}{6}, \frac{2}{6}, \frac{1}{6}, \frac{1}{6}\right\}$.



## Excess degrees

- Follow a link, how many new links does the node have (i.e., not counting the link used to come to the node)

$$
q(k) \propto(k+1) p(k+1)
$$

- Network is a forest, start breadth first search from any node...
- Excess degree is the branching factor
- Tree can be infinitely large iff avg. excess degree larger than one


## Excess degrees

- Example: $\left\{k_{u}\right\}=\{2,2,1,1\}$. Excess degree sequence (one element for each stub) $\{1,1,1,1,0,0\}$.


