Lecture 12: Introduction to Network Modeling Approaches

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Lecture 12 overview

- Models, metrics and architecture
 - Understanding
 - Practice
- Overview of model types
- "Poisson Random graphs
- "Small Worlds"
- Random graphs "generalized" for degree sequences
- System formation models
 - Cumulative advantage (aka preferential attachment)
 - Node copying and others
- Structure-Property models
 - Cascades, epidemics and other initial "applications"

The Materials Science Metaphor

- PROCESSING> STRUCTURE> PROPERTIES
- Structure determines/affects properties
 - **Structure** is a multi-dimensional term that includes many scales and concepts simultaneously (and thus is not a "simple invisible")
 - **Properties** include attributes that encompass dynamics, behavior and "ilities".
 - Relationships between Structure and Properties are plentiful and became strongest as material classes under detailed study increased
 - Solid Mechanics, dislocation theory, atomic theory are some of the key enablers for deriving mechanisms to propose structure/property relationships in materials.
- In materials, properties of interest (almost always) **simultaneously** depend on **several** structural parameters. There is every reason to believe that engineering systems will similarly require numerous structural parameters to make real progress.

The Materials Science Metaphor II

• **Processing** determines **Structure**

- Different Processing Modes (e-beam deposition, casting, forging, crystal growth, etc.) have different *control parameters* (Temperature gradient, stresses, pressure, magnetic and electrical fields, composition, etc.) that affect/determine properties.
- **Design** is thus modifying the processing modes and control parameters to obtain the desired combination of properties. **Understanding structure is the chief enabler of effective design**
- Thermodynamics, phase transformations, thermal and fluid sciences, solid mechanics are useful fundamentals underlying Process/structure relationship
- Linking the framework to Engineering Systems requires discussing the structure and properties analogues in such systems.

The Materials Science Metaphor III

- Structure Characterization
 - Materials-Multiple Dimensional and very broadly construed
- Engineering Systems Possibilities for Architecture Characterization as Networks.. are also very broad

Network metrics; structural characteristics

- size, sparseness, degree, average degree, degree sequence
- degree distribution, power laws, exponents, truncation
- geodesic, path length, graph diameter
- transitivity (clustering)
- connectivity, reciprocity
- centrality (degree, closeness, betweenness, information, eigenvector)
- prestige, acquaintance

- hierarchy
- community structure, cliques
- homophily, assortative mixing, degree correlation coefficient
- motifs, coarse- graining
- self-similarity, scale-free, scale-rich
- dendograms, cladograms and relationship strength
- modularity vs. integrality

The Materials Science Metaphor IV

- Structure Characterization
 - Materials-Multiple Dimensional and very broadly construed
- Engineering Systems Possibilities for Architecture Characterization.. are also very broad (but nonetheless almost surely needs to grow)
- Engineering System Properties are also numerous (but some of the most important are not yet adequately quantified)
 - Robustness (congestion, failure of nodes and links etc.)
 - Flexibility
 - Rates of propagation (disease, ideas etc.)
 - Performance efficiency
- The **Processing > Structure > Properties** "Mantra" from materials becomes for engineering systems
 - Formation mechanisms + constraints > architecture (structure) > Properties (ilities +)

Schematic of Engineering System Model Purposes







The math models of properties allow trade-off of Architectural variables and patterns of interaction on properties to drive choice of desirable structure. The math models of formation mechanisms allow choice of lowest cost or feasible sets of desirable structural metrics to be selected and evolved.

Model types

- Models of Systems (networks)
- Models for predicting/explaining Structure
 - Models for formation/growth processes of systems
 - Most network models such as random, small-world etc. implicitly fall in this category
 - Cumulative advantage, preferential attachment, bipartite community formation, heuristic optimization relative to constraints, hierarchy (or heuristics) + random
- Models for predicting/explaining properties of systems
 - Predicting properties from structure architecture
 - Flexibility, robustness, performance of functions
 - Operational processes or functions
 - Communication, problem solving, decision-making, learning
 - Search and navigation
 - Failures and cascades, epidemics
- Models/algorithms used to "observe" systems (why care?)
 - Calculation of structural metrics
 - Communities, motifs, coarse-graining, hierarchy

The Iterative Learning Process

Objectively obtained quantitative data (facts, phenomena)





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Poisson Random Graph

- Rapaport and later Erdos and Renyi and others such as Bollobas have studied a very simple model *in some depth*. This is the one where each node in a network is connected with probability p to other nodes. Ensembles with variable numbers of links <k> are studied and the degree distribution is $p_k \cong \frac{\langle k \rangle^k e^{-\langle k \rangle}}{k!}$
- The path length can be formally shown to be and is thus consistent with a "Small World" $l \cong \frac{\ln n}{\ln \langle k \rangle}$
- Clustering is simply equal to the random probability of a link between 2 nodes and is

$$C = < k > / n$$

Poisson Random Graph II

- It is generally stated that this model is nice for intuition but describes no real networks. It also provides a **benchmark**.
- Let us look again at the Metrics Table from Newman with addition of some estimated quantities from the random network model.

Poisson Random Graph II

- It is generally stated that this model is nice for intuition but describes no real networks. It also provides a **benchmark**.
- Let us look again at the Metrics Table from Newman with addition of some estimated quantities from the random network model.
- What do we see? (more in assignment # 3)
- Path Length, *l*, is generally small (small worlds) and often approximately equal to that given by Poisson random network
- Clustering is usually orders of magnitude higher than predicted by random networks for the large networks and is ~constant with n

Small World Problem as seen by Watts

Lattice Random graph $L(N) = N^{1/d}$ $L(N) = \log N$ $C(N) \approx N^{-1}$ $C(N) \approx const$



Professor C. Magee, 2006 Figures by MIT OCW. Page 16

Small World Network Model (1D)

K is the number of nearest neighbors originally with links (=3 below)



Figure by MIT OCW.



Small-world networks



Small World Clustering Estimation

- Watts and Strogatz got results from simulation
- Later Work by Barrett and Weigt

 on their model derived
 a clustering coefficient of
- An improved model by Newman and Watts and independently by Monasson *C* gives for the clustering coefficient
- These estimates are sufficiently high for real networks



$$C = \frac{3(K-1)}{2(2K-1)}(1-p)^3$$

 $=\frac{3(K-1)}{2(2K-1)+4Kp(p+2)}$

Small World Model Path Lengths

- Simulation based by Watts and Strogatz showed that path lengths were small and scaled with ln n
- No exact solution (yet) but Barthelemy and Amaral proposed a scaling relation that was later derived by Newman and Watts. It shows that the transition to "Small World Path Length Dependence" occurs at smaller p as n increases. Indeed, *the number of shortcuts needed to give small world behavior is constant* (for given K) *as n increases*

Ubiquity of small-world networks





Small World Models

- Small world models thus
 - Show that it is relatively easy to have higher clustering and yet short paths. In large networks a few long paths is all that is needed- brain now understood this way as are some other large scale complex systems
- However, the specific models have only marginal connection to any real systems as they are stylistic and notional
- Small World Models have been relatively widely used as a "substrate" for studies of such as iterated games, epidemics. The rewiring approach has also proven useful even if the specific models are not real (more on model utility in later lectures)

Generalized Random Graphs I

- Since the 1970's, many papers have been published that generalize the random graph model for various purposes. Recent work has emphasized degree distribution and clustering
- The "configuration model" allows the "degree sequence" to be preset and then random connections made.
- Clustering comparison to real networks is "better" than for random networks
- For Generalized Random Graphs with Power laws, clustering depends on α

$$C = \frac{\langle k \rangle}{n} \left[\frac{\langle k^2 \rangle - \langle k \rangle}{\langle k \rangle^2} \right]^2$$
$$C \cong n^{-\left[\frac{3\alpha - 7}{\alpha - 1}\right]}$$

• Low α (less than 7/3)"power law but random" networks can thus have significant clustering.

Generalized Random Graphs II

- Generalized Random Graphs have also been developed for
 - Directed graphs
 - Bipartite graphs are of particular interest as the clustering coefficient does not vanish as n becomes large
 - Most interesting, recent work has shown that the number of types of nodes can be expanded beyond two (Multipartite) and mixing of arbitrary types ("non-pure homophily") can be allowed and still allow calculation of many metrics.
- Work on other generalized random network models (exponential and Markov for example) continue but for now the most useful is the bipartite/multipartite models as they are the only ones showing transitivity. They are limited to bipartite/multipartite networks but there are more examples of these than *generally realized*
- Putting enough structure (and constraints) in to a model so it reflects reality and making random additions is attractive

System Formation (Network Growth) Models

- (Most) real Networks grow (adding nodes and links)
- As (attempts at realistic) rules for attachment were devised, the first simple "reality-related" models for system formation were developed
- Barabasi and Albert model
- Citation networks and D. J. de S. Price (following a Simon skew distribution concept)

- Price/Barasi and Albert model generalizations
- Other growth models

Schematic of Engineering System Model Purposes



Barabasi and Albert Model

- Insights
 - Real Networks are growing (adding nodes and links). *Attachment* will not occur randomly but will tend to be *preferential* (the rich get richer)
- Assumptions
 - Undirected network (and first applied to citations and the Internet which are directed)
 - Each node is added with a *fixed* number of links ϖ_{new} which must be positive and an integer.
 - Probability of attaching to node i is (equal to degree centrality)

$$p_i = \frac{k_i}{\sum_j k_j}$$

Results: Simulation using the model yielded power laws with $\alpha = 3$ independent of ϖ_{new}

and led to idea that scale-free structures with hubs exist when power laws are found (but we now realize that power laws are ubiquitous)

D. J. de S. Price's work I

- 1965- described first example of a scale free network
 - He showed that the Scientific Citations Network shows a power law.
 - Initially he estimated that α was 2.5 3 and later (1976) gave a more accurate value of 3.04
- 1976- presented the first "growth" model for a network to explain the power law he had found in 1965.
 - He based it on work by (again) Herb Simon (1955) who had shown that *power laws arise* when "the rich get richer" –the amount you get goes up with the amount you already have ("The Matthew effect"). The power laws Simon was "explaining" were wealth effects (Pareto) and some of the power laws shown by George Zipf.
- "For to everyone who hath shall be given"...

Patterns 2



D. J. de S. Price's work II

- 1965- described first example of a "scale free" network
 - He showed that the Scientific Citations Network follows a power law for degree distribution.
 - Initially he estimated that α was 2.5 3 and later (1976) gave a more accurate value of 3.04
- 1976- presented the first "growth" model for a network to explain the power law he had found in 1965.
 - He based it on work by (again) herb Simon (1955) who had shown that *power laws arise* when "the rich get richer" –the amount you get goes up with the amount you already have ("The Matthew effect"). The power laws Simon was "explaining were some of those shown by George Zipf.
 - → Price was the *first to use this concept* (he called it *cumulative advantage*) to discuss network growth and to explain degree distributions on networks (although others used Simon's approach to develop similar models before Price was rediscovered in 2003 or so).

Price's Model

- Assumptions
 - Directed graph-appropriate for citation network
 - Nodes are added with variable (and permanent) outdegree ϖ^{O} but average out degree $< k^{O} >$ is stable
 - Assumes starting point for in-degree of a new paper at

$$\varpi_{new}^{I} = 1$$
 but discusses general case

• Result

$$p_k \cong k^{-(2+1/\varpi^0)}$$

• Price in 1976 makes a decent case for agreement with his 1965 results

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Generalizations of Price/Barabasi-Albert Models I

- The Albert and Barabasi review (2002) identifies about 15 variants involving non- linear preference, time-dependent growth, mean degree increase with time, **multiple node fitnesses**, and many others
 - Many allow $\alpha < 3$ and thus can "improve" agreement with actual networks
 - Costs for links (and aging of nodes) has been modeled and this also "improves agreement" with real networks

Classes of small-world networks: Truncation due to Costs and Constraints



Courtesy of National Academy of Sciences, U.S.A. Used with permission. Source: Amaral, L. A. N., A. Scala, M. Barthelemy, and H. E. Stanley. "Classes of small-world networks." *Proc Natl Acad Sci* 97 (2000): 11149-11152. (c) National Academy of Sciences, U.S.A.

Proc Nat Acad Sci USA 97, 11149 (2000)

Generalizations of Barabasi-Albert Models II

• Albert-Barabasi (2002) review identifies about 15 variants involving non- linear preference, time-dependent growth, mean degree increase with time, multiple node fitness, and many others

Some remaining limitations of all Barabasi-Albert models

- Model is undirected but the real Web is directed
- If it is regarded as directed then it only generates acyclic graphs (the web is not acyclic)
- The out-degree of the web is a power law whereas the model gives constant out-degree
- Note that Price's model is also acyclic but it is directed and his network of interest is acyclic so his model is reasonable in its limited sphere. (Citation out-degree is constant)

Generalized Growth Models

- Callaway model as generalized by Krapivsky and Redner
 - Nodes and links are added separately to the network so many new nodes have no links. This model yields a full directed network with separate preferential attachment of ingoing and outgoing links
 - Extensions of K-R models that incorporate realistic system constraints heuristically- have been developed as well.
- Node Copying Models –see next slide

Node Copying Models

- Kleinberg et. al. have suggested network growth involves a mixture of *copying* existing nodes and links along with stochastic additions
- Assumptions: copy an existing node, assume a number of links, *M*, to add to it. The nodes for the other end of the links are found by choosing a random node and *copying its linked nodes* and do this sequentially until *M* links in total have been copied.
- This copying gives power laws similarly to cumulative advantage where $2 < \alpha < 3$ depending upon the ratio of

copying to stochastic addition for the network.

• Although the model was first suggested for the web, it is more descriptive for biochemical (protein) interaction networks. Much later work extending this model has focused on this domain.

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- Structure-Property models
 - Robustness, cascades, epidemics and other initial "applications" with robustness as the "property"

Structure-Property Models for Networked Systems

- Newman, 2003 review article (P 2 closure for Introduction)
 - "As we will see, the scientific community has, by drawing on ideas from a broad variety of disciplines, made an excellent start on the first two of these aims, the characterization and modeling of network structure. Studies of the effect of structure on system behavior on the other hand are still in their infancy. It remains to be seen what the crucial theoretical developments will be in this area."
 - CM (2006) All areas require coordinated development??..
- For the rest of this lecture, we will briefly look at some of the early work (prior to the quote above). A number of later lectures will explore developments after Newman's review.
- Modeling developments in this area must concern themselves with defining the property being modeled and the operational process in the system being studied.

Network Resilience and Robustness

- The term resilience in the network literature is very similar to robustness as we use it and as defined in the T & D
 - *Robustness: ability to deliver desired function in spite of* changes to the environment, internal variations or emergent properties
 - Thus we will look at resilience studies to determine how structure might affect (certain kinds of) robustness
- An important aspect of this discussion is that robustness will not be found to depend upon structure in a simple way. For example, one structure may be more robust to one type and level of disturbance or change while another will be more robust to another type or level of disturbance/change
- Psuedometric: $\Gamma = 1/(\frac{\Delta P}{C^D})$ Robustness equals the •

inverse delta (decrease) in performance divided by the change/disturbance level C^{D} leading to that decrease.

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Function in a network where connection is essential: *function is connectivity and/or path length*



Performance deterioration can be estimated by connectivity or path length increase and disturbance by # of nodes removed.

Connectivity and path length upon node failure: random network



Figure by MIT OCW.

Source: Statistical Mechanics of Complex Networks, Reka Albert and Albert-Laszlo Barabasi, Fig. 32, 2001



Connectivity and path length upon node failure: scale free network



Figure by MIT OCW.

Source: Statistical Mechanics of Complex Networks, Reka Albert and Albert-Laszlo Barabasi, Fig. 32, 2001





Application to these actual networks (particularly the Internet) has been shown to be mistakenly based upon assumptions about the structure of the Internet being known because of a power law degree distribution

Source: Statistical Mechanics of Complex Networks, Reka Albert and Albert-Laszlo Barabasi, 2001

Robustness summary #1

- Targeted attack on *selected* nodes is a more severe test of robustness in networks where communication distance and/or connectivity is an indicator of functional performance
- Scale free structure (vs. random) is positive for random failure but is a negative feature for targeted attack.
- Prior level of connectivity is positive for robustness for either type of vulnerability
- At the model-definition level of approximation, most other structural features are not important for robustness
- As far as structure-property relationships, this work results in a sort of **"Duh".**

Cascades

- Cascades can be thought of as "multipliers" of the functional performance change for a given initial disturbance
- Why do some relatively small initial disturbances cause a very large system response?
 - *Cascades* (blackouts, fads, innovation diffusion, organizational breakdown)
 - In this case, robustness ~ inverse probability of cascade
- What is the influence of network structure on such phenomena?
 - Connectivity, degree distribution
 - Node heterogeneity
- Watts (2002) developed a simple model to address these questions based on *percolation in generalized random networks*

The Watts Model for Global Cascades I

- Model
 - Binary Decisions with Externalities
 - nodes decide based on *fraction of linked nodes* making the same decision

Local Dependency



Figure by MIT OCW. After Watts.

Source: Six Degrees: The Science of a Connected Age, Duncan J. Watts, Fig. 8.2, 2003



The Watts Model for Global Cascades II

- Model
 - Binary Decisions with Externalities
 - nodes decide based on *fraction of linked nodes* making the same decision
 - There is *heterogeneity* in the number of links, k, (degree distribution) *and in the vulnerability of each node*

Hetereogeneity of Resistance



Figure by MIT OCW. After Watts.

Source: Six Degrees: The Science of a Connected Age, Duncan J. Watts, Fig. 8.3, 2003





Figure by MIT OCW. After Watts. Source: *Six Degrees: The Science of a Connected Age*, Duncan J. Watts, Fig. 8.4, 2003



The Watts Model for Global Cascades III

- Model
 - Binary Decisions with Externalities
 - nodes decide based on *fraction of linked nodes* making the same decision
 - There is *heterogeneity* in the number of links, k, (degree distribution) and in the susceptibility of each node

- This model differs from many others that seem the same in having *local dependencies, fractional thresholds and heterogeneity*. All of these factors turn out to be important in cascades.
 - Changeover (or failure) is triggered by a small seed (as small as one node)
 - Sparse networks

The Watts Model for Global Cascades IV

- Outputs of model
 - Phase transformations at critical values of <k> and threshold (two different boundaries)

"Phase Diagram" for Cascades



Courtesy of National Academy of Sciences, U.S.A. Used with permission. Source: Watts, D. J. "A Simple model of global cascades on random networks." *Proc Natl Acad Sci* 99 (2002): 5766-5771. (c) National Academy of Sciences, U.S.A.

Source: A simple model of global cascades on random networks, Duncan J. Watts, Fig. 1, 2001

The Watts Model for Global Cascades V

- Outputs of model
 - Phase transformations at critical values of <k> and threshold

 - Probability of global cascade
 Vulnerable nodes and clusters
 The size of the global cascade



Courtesy of National Academy of Sciences, U.S.A. Used with permission.

Source: Watts, D. J. "A Simple model of global cascades on random networks." *Proc Natl Acad Sci* 99 (2002): 5766-5771. (c) National Academy of Sciences, U.S.A.

Source: A simple model of global cascades on random networks, Duncan J. Watts, Fig. 2, 2001

The Watts Model for Global Cascades VI

- Outputs of model
 - Phase transformations at critical values of <k> and threshold –at the high <k> end, they are improbable but
 - total- a particularly nasty kind of vulnerability
 - Probability of global cascade
 - Vulnerable nodes and clusters
 - The size of the global cascade
 - Influence of structure on global cascade

Structural Effects on Cascade Phase Diagrams



Courtesy of National Academy of Sciences, U.S.A. Used with permission. Source: Watts, D. J. "A Simple model of global cascades on random networks." *Proc Natl Acad Sci* 99 (2002): 5766-5771. (c) National Academy of Sciences, U.S.A.

Source: A simple model of global cascades on random networks, Duncan J. Watts, Figs. 4a, 4b, 2001



The Watts Model for Global Cascades VII

- Outputs of model
 - Phase transformations at critical values of <k> and threshold
 - Probability of global cascade
 - Vulnerable nodes and clusters
 - The size of the global cascade
 - Influence of structure on global cascade
 - Heterogeneity effects differ between susceptibility and nodal degree
 - Targeted attack at high k nodes is still a vulnerability but not when <k> is high
- Further progress needs *observations and specific functions described*

Epidemics and viruses

- Robustness also relates to the ability of a system to reject an infectious disease
 - This is clearly similar to the Cascade problem and many models have been developed but all involve 1on- 1 disease spreading
- SIR model

SIR Model for Epidemics



Figure by MIT OCW. After Watts.

Source: Six Degrees: The Science of a Connected Age, Duncan J. Watts, Fig. 6.1, 2003



Epidemics and viruses

- Robustness also relates to the ability of a system to reject an infectious disease
 - This is clearly similar to the Cascade problem and many models have been developed but all involve 1on- 1 disease spreading
- SIR model
 - Susceptible individuals ,S, who can get the disease
 - Infected individuals, i, who can pass it on and
 - Recovered individuals, R, who are immune (or dead)

This is an old model but solving it for realistic networks is new.

$$\frac{dS}{dt} = -\beta iS,$$
$$\frac{di}{dt} = \beta iS - \gamma i,$$
$$\frac{dR}{dt} = \gamma i$$

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Applying network theory to epidemics: Healthcare Institution Network



Courtesy of U.S. Centers for Disease Control.

Source: L. A. Meyers, M. E. J. Newman, M. Martin and S. Schrag.

"Applying network theory to epidemics: Control measures for outbreaks of Mycoplasma pneumoniae."

Emerg Infect Dis (February 2003).

Source: Applying network theory to epidemics: Control measures for outbreaks of Mycoplasma pneumoniae, Ancel, Newman, Fig. 1

Simulated (1000runs) Outbreak Sizes



Courtesy of U.S. Centers for Disease Control.

Source: L. A. Meyers, M. E. J. Newman, M. Martin, and S. Schrag.

"Applying network theory to epidemics: Control measures for outbreaks of Mycoplasma pneumoniae." *Emerg Infect Dis* (February 2003).

Source: Applying network theory to epidemics: Control measures for outbreaks of Mycoplasma pneumoniae, Ancel, Newman, Fig. 6

Comparison of simulation and analytical prediction



Courtesy of U.S. Centers for Disease Control.

Source: L. A. Meyers, M. E. J. Newman, M. Martin, and S. Schrag.

"Applying network theory to epidemics: Control measures for outbreaks of Mycoplasma pneumoniae." *Emerg Infect Dis* (February 2003).

Source: Applying network theory to epidemics: Control measures for outbreaks of Mycoplasma pneumoniae, Ancel, Newman, Fig. 7



Comparison to actual outbreak at Evansville Indiana Hospital



Courtesy of U.S. Centers for Disease Control.

Source: L. A. Meyers, M. E. J. Newman, M. Martin, and S. Schrag.

"Applying network theory to epidemics: Control measures for outbreaks of Mycoplasma pneumoniae." *Emerg Infect Dis* (February 2003).

Source: Applying network theory to epidemics: Control measures for outbreaks of Mycoplasma pneumoniae, Ancel, Newman, Fig. 7

Evansville Case Study

- Use of Case study leads to a well-grounded simulation
- Simulation allows many details to be studied and policy options explored
- The work demonstrated the criticality of the number of wards served by a caregiver despite the fact that low numbers of caregivers are infected.

SIS Model

• No immunity just re-infection

$$\frac{dS}{dt} = -\beta iS, \quad \frac{di}{dt} = \beta iS - \gamma i$$

- Phase transitions between regions where disease persists and where it does not
- Power law degree distributions results in no non-zero epidemic threshold and no non-zero value for disease persistence (computer viruses may live forever on the web)

SIS Network Structural Effects



Figure by MIT OCW. After Watts.

Source: Six Degrees: The Science of a Connected Age, Duncan J. Watts, Fig. 6.10, 2003



Robustness Observations

- Almost all models and observations thus far show a difficult mixture of robustness and fragility
- Robustness is very dependent on the specific regime of change/disruption that is of importance. The quantitative results thus far (are limited in their own robustness but) indicate that the influence of structure changes is very different in these different regimes. We will return to a richer robustness study in a lecture on "organizational modeling". Nonetheless, practical architecting for robustness is *challenging*.
- Generalization seems inappropriate but specific grounded cases appear to lead to better understanding (and thus indicate a path to better engineering practice)

References for lecture 12

- Watts, *Six Degrees;* Newman, "Structure and Function of Complex Networks"; Albert, R. and Barabasi, A-L., "Statistical Mechanics of Complex Networks"
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