Lecture 6: Mid-Semester Review - Prediction in Random Graphs

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Models and Data Sets

The overarching problem is the following:

Main Problem

Given a dynamical graph-based data set, discover if data can be explained as a structured data graph, or just as a random graph.

To do so, we need to understand: (1) how to generate dynamical graphs; (2) how to analyze these graphs.
Random graphs: two main classes, $\mathcal{G}_{n,p}$ and $\Gamma^{n,m}$.
Structured graphs: weighted graphs or percolation graphs $\rightarrow$ sequence of nested graphs.
What to look for:

1. complete subgraphs (cliques)
2. connectivity (number and size of connected components)
3. spectral gap and optimal partitions (Cheeger constant)

Sequence of Nested Graphs

We fix the number of vertices n. Sequence: $(G_m)_{0\leq m\leq M}$ of graphs $G_m=(\mathcal{V},\mathcal{E}_m)$, where each G_m has exactly n vertices, $|\mathcal{V}|=n$, and m edges, $|\mathcal{E}_m|=m$. Additionally we require $\mathcal{E}_m\subset\mathcal{E}_{m+1}$ (nestedness).

Examples: see movies

- Quasi-Regular percolation graph : PercGraph_n100N10d2_sig0.100000_lp2.000000.mp4
- Vertices are permuted randomly : PercGraph_scrambled_n100N10d2_sig0.100000_lp2.000000.mp4
- Edges are permuted randomly : PercGraph_random_n100N10d2_sig0.100000_lp2.000000.mp4

Random Graphs

The *Erdös-Rényi class* $\mathcal{G}_{n,p}$ of random graphs: the number of vertices is fixed to n, and each edge is selected independently with probability p. The probability mass function, $P(G)$ for a graph G with n vertices and m edges is

$$P(G) = p^m(1-p)^{n(n-1)/2-m} \quad , \quad \frac{n(n-1)}{2} = \binom{n}{2}.$$

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The class $\Gamma^{n,m}$ is the set of all graphs with n vertices and exactly m edges. In this class, the graph probability distribution is uniform:

$$P(G) = 1 / \binom{n(n-1)/2}{m}.$$

Distribution of Cliques

Expected Values

Let X_q denote the number of q-cliques in a random graph G. Then the expectation of X_q in $\mathcal{G}_{n,p}$ class is

$$\mathbb{E}[X_q] = \binom{n}{q} p^{q(q-1)/2}$$

The expectation of X_q in the class $\Gamma^{n,m}$ is approximated by the above formula for $p = \frac{2m}{n(n-1)}$:

$$\mathbb{E}[X_q] \approx \binom{n}{q} \left(\frac{2m}{n(n-1)}\right)^{q(q-1)/2} \sim \theta_q \frac{m^{q(q-1)/2}}{n^{q(q-2)}}$$

$$\mathbb{E}[X_3] \sim \theta \frac{m^3}{n^3} \quad , \quad \mathbb{E}[X_4] \sim \theta \frac{m^6}{n^8}$$

3-Cliques and 4-cliques

Thresholds

Theorem

Let $m = m(n)$ be the number of edges in $\Gamma^{n,m}$.

1. *If $m \gg n$ (i.e. $\lim_{n\to\infty} \frac{m}{n} = \infty$) then* $\lim_{n\to\infty} Prob[G \in \Gamma^{n,m}\ has\ a\ 3-clique] \to 1$.
2. *If $m \ll n$ (i.e. $\lim_{n\to\infty} \frac{m}{n} = 0$) then* $\lim_{n\to\infty} Prob[G \in \Gamma^{n,m}\ has\ a\ 3-clique] \to 0$.

Theorem

Let $m = m(n)$ be the number of edges in $\Gamma^{n,m}$.

1. *If $m \gg n^{4/3}$ (i.e. $\lim_{n\to\infty} \frac{m}{n^{4/3}} = \infty$) then* $\lim_{n\to\infty} Prob[G \in \Gamma^{n,m}\ has\ a\ 4-clique] \to 1$.
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q-Cliques
Thresholds

Theorem

Let $p = p(n)$ be the edge probability in $\mathcal{G}_{n,p}$. Let $q \geq 3$ be and integer.

1. *If $p \gg \frac{1}{n^{2/(q-1)}}$ (i.e. $\lim_{n\to\infty} n^{2/(q-1)} p = \infty$) then $\lim_{n\to\infty} Prob[G \in \mathcal{G}_{n,p}\ has\ a\ q - clique] \to 1$.*
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Theorem

Let $m = m(n)$ be the number of edges in $\Gamma^{n,m}$. Let $q \geq 3$ be and integer.

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3-Cliques and 4-Cliques

Behavior at the threshold

In general we obtain a "coarse threshold". Recall a Poisson process X with parameter λ has p.m.f. $Prob[X=k] = e^{-\lambda}\frac{\lambda^k}{k!}$.

Theorem

In $\mathcal{G}_{n,p}$,

1. *For $p = \frac{c}{n}$, X_3 is asymptotically Poisson with parameter $\lambda = c^3/6$.*
2. *For $p = \frac{c}{n^{2/3}}$, X_4 is asymptotically Poisson with parameter $\lambda = c^6/24$.*

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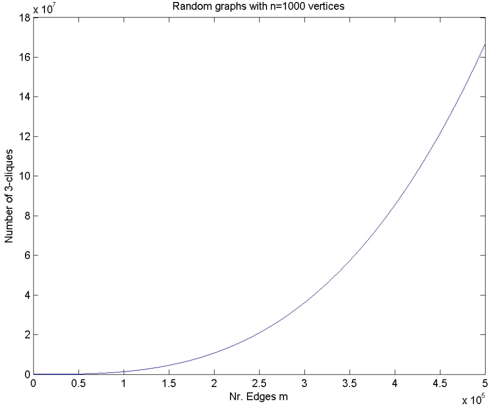
Theorem

In $\Gamma^{n,m}$,

1. *For $m=cn$, X_3 is asymptotically Poisson with parameter $\lambda=4c^3/3$.*
2. *For $m=cn^{4/3}$, X_4 is asymptotically Poisson with parameter $\lambda=8c^6/3$.*

Numerical Results

3-cliques for random graph with $n = 1000$ vertices



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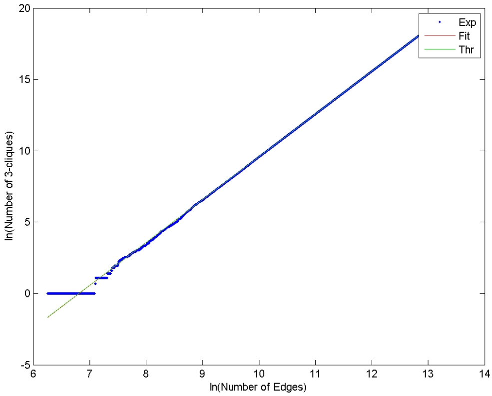

Connectivity
Strong threshold

Theorem

1. *Let* $m = m(n)$ *satisfies* $m \ll \frac{1}{2}n\log(n)$. *Then*
$$\lim_{n\to\infty} Prob[G \in \Gamma^{n,m} \text{ is connected}] = 0$$
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3. *Assume* $m = \frac{1}{2} n \log(n) + tn + o(n)$, *where* $o(n) \ll n$. *Then*
$$\lim_{n \to \infty} Prob[G \in \Gamma^{n,m} \text{ is connected}] = e^{-e^{-2t}}$$

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In this case $\frac{1}{2} n \log(n)$ is known as a *strong threshold*.

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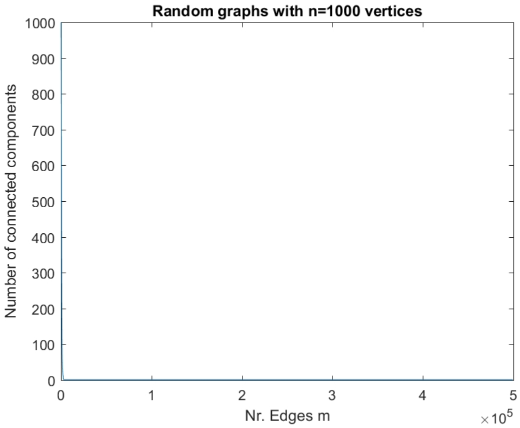

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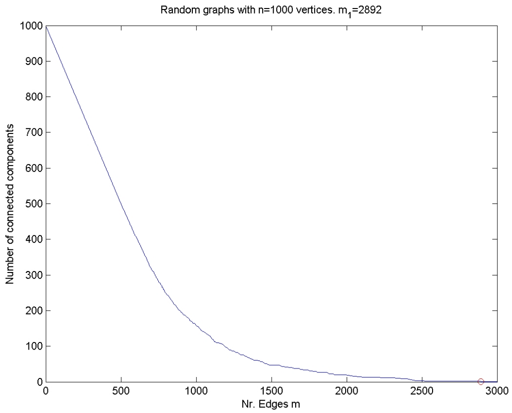

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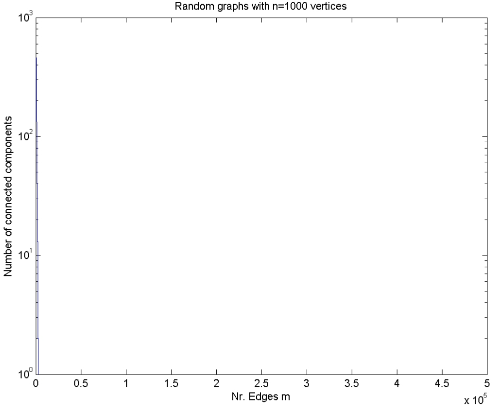

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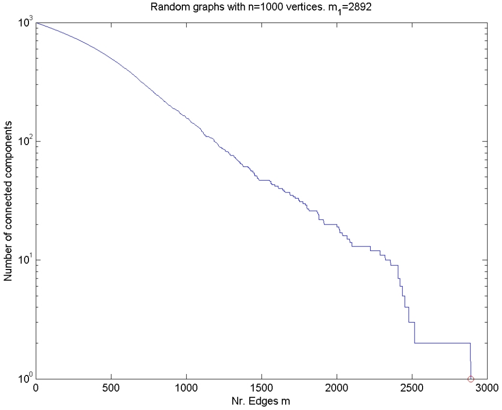

Graph Laplacians
$\Delta, L, \tilde{\Delta}$

Recall the Laplacian matrices:

$$\Delta = D - A \quad , \quad \Delta_{ij} = \begin{cases} d_i & \textit{if} \quad i = j \\ -1 & \textit{if} \quad (i,j) \in \mathcal{E} \\ 0 & \quad \textit{otherwise} \end{cases}$$

$$L = D^{-1}\Delta \quad , \quad L_{i,j} = \begin{cases} 1 & \textit{if} \quad i = j \text{ and } d_i > 0 \\ -\frac{1}{d(i)} & \textit{if} \quad (i,j) \in \mathcal{E} \\ 0 & \quad \textit{otherwise} \end{cases}$$

$$\tilde{\Delta} = D^{-1/2}\Delta D^{-1/2} \quad , \quad \tilde{\Delta}_{i,j} = \begin{cases} 1 & \textit{if} \quad i = j \text{ and } d_i > 0 \\ -\frac{1}{\sqrt{d(i)d(j)}} & \textit{if} \quad (i,j) \in \mathcal{E} \\ 0 & \quad \textit{otherwise} \end{cases}$$

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Remark: $D^{-1}, D^{-1/2}$ are the pseudoinverses.

Eigenvalues of Laplacians
$\Delta, L, \tilde{\Delta}$

What do we know about the set of eigenvalues of these matrices for a graph G with n vertices?

1. $\Delta = \Delta^T \geq 0$ and hence its eigenvalues are non-negative real numbers.
2. $eigs(\tilde{\Delta}) = eigs(L) \subset [0, 2]$.
3. 0 is always an eigenvalue and its multiplicity equals the number of connected components of G,

$$dim\, ker(\Delta) = dim\, ker(L) = dim\, ker(\tilde{\Delta}) = \#connected\ \ components.$$

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Let $0 = \lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_{n-1}$ be the eigenvalues of $\tilde{\Delta}$. Denote

$$\lambda(G) = \max_{1 \leq i \leq n-1} |1 - \lambda_i|.$$

Note $\sum_{i=1}^{n-1} \lambda_i = trace(\tilde{\Delta}) = n$. Hence the average eigenvalue is about 1. $\lambda(G)$ is called *the absolute gap* and measures the spread of eigenvalues away from 1.

The spectral absolute gap
$\lambda(G)$

The main result in [8]) says that for connected graphs w/h.p.:

$$\lambda_1 \geq 1 - \frac{C}{\sqrt{\text{Average Degree}}} = 1 - \frac{C}{\sqrt{p(n-1)}} = 1 - C\sqrt{\frac{n}{2m}}.$$

Theorem (For class $\mathcal{G}_{n,p}$)

Fix $\delta > 0$ and let $p > (\frac{1}{2} + \delta)log(n)/n$. Let $d = p(n-1)$ denote the expected degree of a vertex. Let $\tilde{G}$ be the giant component of the Erdös-Rényi graph. For every fixed $\varepsilon > 0$, there is a constant $C = C(\delta, \varepsilon)$, so that

$$\lambda(\tilde{G}) \leq \frac{C}{\sqrt{d}}$$

with probability at least $1 - Cn\exp(-(2-\varepsilon)d) - C\exp(-d^{1/4}log(n))$.

Connectivity threshold: $p \sim \frac{log(n)}{n}$.

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Theorem (For class $\Gamma^{n,m}$)

Fix $\delta > 0$ and let $m > \frac{1}{2}(\frac{1}{2} + \delta)n\log(n)$. Let $d = \frac{2m}{n}$ denote the expected degree of a vertex. Let $\tilde{G}$ be the giant component of the Erdös-Rényi graph. For every fixed $\varepsilon > 0$, there is a constant $C = C(\delta, \varepsilon)$, so that

$$\lambda(\tilde{G}) \leq \frac{C}{\sqrt{d}}$$

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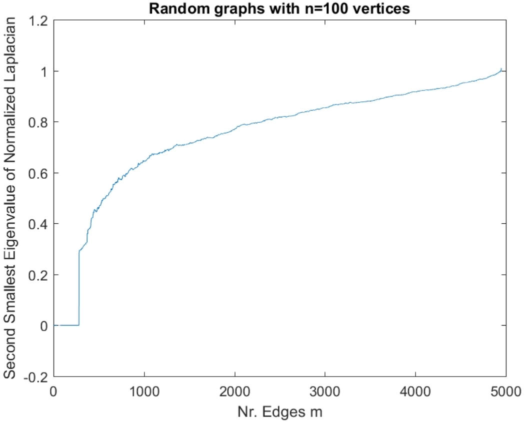
Connectivity threshold: $m \sim \frac{1}{2}n\log(n)$.

Numerical Results

λ_1 for random graphs

Results for $n = 100$ vertices: $\lambda_1(\tilde{G}) \approx 1 - \frac{C}{\sqrt{m}}$.



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$1 - \lambda_1$ for random graphs

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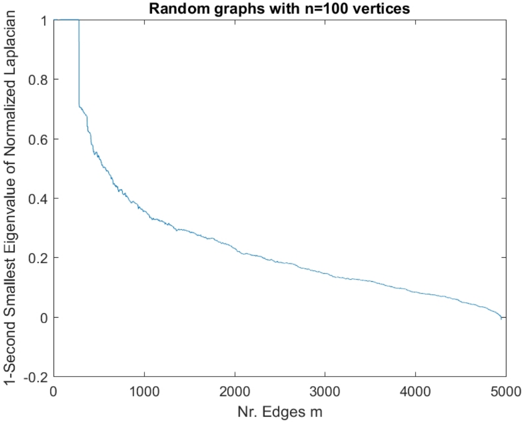

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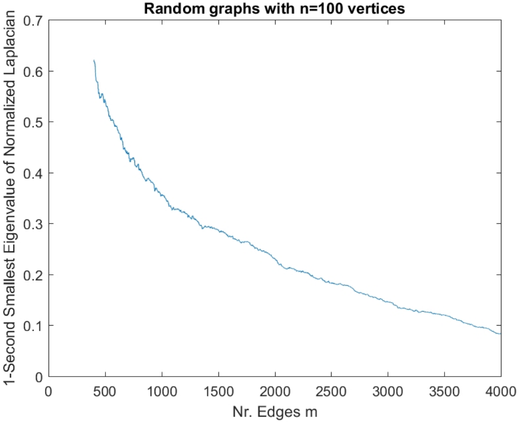

Numerical Results

$log(1-\lambda_1)$ vs. $log(m)$ for random graphs

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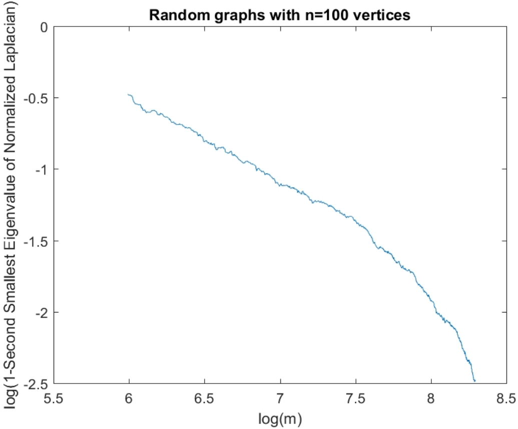

The Cheeger constant
h_G and Optimal Partitions

Fix a graph $G = (\mathcal{V}, \mathcal{E})$ with n vertices and m edges. The *Cheeger constant* h_G is the optimum value of

$$h_G = \min_{S \subset \mathcal{V}} \frac{|E(S, \bar{S})|}{min(vol(S), vol(\bar{S}))}$$

where

1. For two disjoint sets of vertices A abd B, $E(A,B)$ denotes the set of edges that connect vertices in A with vertices in B:
$$E(A,B) = \{(x,y) \in \mathcal{E} \ \ , \ \ x \in A \ , \ \ y \in B\}.$$
2. The *volume* of a set of vertices is the sum of its degrees:
$$vol(A) = \sum_{x \in A} d_x.$$
3. For a set of vertices A, denote $\bar{A} = \mathcal{V} \setminus A$ its complement.

The Cheeger inequalities

h_G and λ_1

Theorem

For a connected graph

$$2h_G \geq \lambda_1 > 1 - \sqrt{1 - h_G^2} > \frac{h_G^2}{2}.$$

Equivalently:

$$\sqrt{2\lambda_1} > \sqrt{1 - (1 - \lambda_1)^2} > h_G \geq \frac{\lambda_1}{2}.$$

Proof of upper bound reveals a "good" initial guess of the optimal partition:

1. Compute eigenpair (λ_1, g^1) for the second smallest eigenvalue;
2. Form the partition:

$$S = \{k \in \mathcal{V} \ , \ g_k^1 \geq 0\} \ , \ \bar{S} = \{k \in \mathcal{V} \ , \ g_k^1 < 0\}$$

Min-cut Problems

Weighted Graphs

The Cheeger inequality holds true for weighted graphs, $G = (\mathcal{V}, \mathcal{E}, W)$.

- $\Delta = D - W$, $D = diag(w_i)_{1 \leq i \leq n}$, $w_i = \sum_{j \neq i} w_{i,j}$
- $\tilde{\Delta} = D^{-1/2} \Delta D^{-1/2} = I - D^{-1/2} W D^{-1/2}$
- $eigs(\tilde{\Delta}) \subset [0, 2]$
- $h_G = \min_S \frac{\sum_{x \in S, y \in \bar{S}} W_{x,y}}{min(\sum_{x \in S} W_{x,x}, \sum_{y \in \bar{S}} W_{y,y})}$
- $2h_G \geq \lambda_1 \geq 1 - \sqrt{1 - h_G^2}$
- Good initial guess for optimal partition: Compute the eigenpair (λ_1, g^1) associated to the second smallest eigenvalue of $\tilde{\Delta}$; set:

$$S = \{k \in \mathcal{V} \;\; , \;\; g_k^1 \geq 0\} \;\; , \;\; \bar{S} = \{k \in \mathcal{V} \;\; , \;\; g_k^1 < 0\}$$

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