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

Radu Balan

Department of Mathematics, AMSC, CSCAMM and NWC University of Maryland, College Park, MD

March 9, 2017

(日) (四) (문) (문) (문)

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:

- complete subgraphs (cliques)
- ② connectivity (number and size of connected components)
- Spectral gap and optimal partitions (Cheeger constant)

Sequence of Nested Graphs

We fix the number of vertices *n*. Sequence: $(G_m)_{0 \le m \le M}$ 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 *Erdöd-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

$$P(G) = p^{m}(1-p)^{n(n-1)/2-m}$$
, $\frac{n(n-1)}{2} = \begin{pmatrix} n \\ 2 \end{pmatrix}$

Random Graphs

The *Erdöd-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

$$P(G) = p^m (1-p)^{n(n-1)/2-m}$$
, $\frac{n(n-1)}{2} = \begin{pmatrix} n \\ 2 \end{pmatrix}$

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:

$$P(G) = 1/\left(egin{array}{c} n(n-1)/2 \\ m \end{array}
ight).$$

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

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

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 $\Gamma^{n,m}$.

• 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

q-Cliques

Theorem

Let p = p(n) be the edge probability in G_{n,p}. Let q ≥ 3 be and integer.
If p ≫ 1/(q-1) (i.e. lim_{n→∞} n^{2/(q-1)}p = ∞) then lim_{n→∞} Prob[G ∈ G_{n,p} has a q - clique] → 1.
If p ≪ 1/(q-1) (i.e. lim_{n→∞} n^{2/(q-1)}p = 0) then lim_{n→∞} Prob[G ∈ G_{n,p} has a q - clique] → 0.

q-Cliques

Theorem

Theorem

Let m = m(n) be the number of edges in Γ^{n,m}. Let q ≥ 3 be and integer.
If m ≫ n^{2(q-2)/(q-1)} (i.e. lim_{n→∞} m/(n^{2(q-2)/(q-1)}) = ∞) then lim_{n→∞} Prob[G ∈ Γ^{n,m} has a q - clique] → 1.
If m ≪ n^{2(q-2)/(q-1)} (i.e. lim_{n→∞} m/(n^{2(q-1)/(q-1)}) = 0) then lim_{n→∞} Prob[G ∈ Γ^{n,m} has a q - clique] → 0.

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

• 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 $\lambda = c^6/24$.

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

• 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 $\lambda = c^6/24$.

Theorem

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

For m = cn, X₃ is asymptotically Poisson with parameter λ = 4c³/3.
 For m = cn^{4/3}, X₄ is asymptotically Poisson with parameter λ = 8c⁶/3.

Numerical Results 3-cliques for random graph with n = 1000 vertices



Models and Graphs

Numerical Results 3-cliques for random graph with n = 1000 vertices



March 8, 2017

Connectivity Strong threshold

Theorem

Image: A matrix and a matrix

Connectivity Strong threshold

Theorem

Let m = m(n) satisfies m ≪ ¹/₂n log(n). Then

$$\lim_{n \to \infty} Prob[G \in \Gamma^{n,m} \text{ is connected}] = 0$$

Let m = m(n) satisfies m ≫ ¹/₂n log(n). Then

$$\lim_{n \to \infty} Prob[G \in \Gamma^{n,m} \text{ is connected}] = 1$$

Assume m = ¹/₂n log(n) + tn + o(n), where o(n) ≪ n. Then

$$\lim_{n \to \infty} Prob[G \in \Gamma^{n,m} \text{ is connected}] = e^{-e^{-2t}}$$

Connectivity Strong threshold

Theorem

• Let
$$m = m(n)$$
 satisfies $m \ll \frac{1}{2}n\log(n)$. Then

$$\lim_{n \to \infty} Prob[G \in \Gamma^{n,m} \text{ is connected}] = 0$$
• Let $m = m(n)$ satisfies $m \gg \frac{1}{2}n\log(n)$. Then

$$\lim_{n \to \infty} Prob[G \in \Gamma^{n,m} \text{ is connected}] = 1$$
• Assume $m = \frac{1}{2}n\log(n) + tn + o(n)$, where $o(n) \ll n$. Then

$$\lim_{n \to \infty} Prob[G \in \Gamma^{n,m} \text{ is connected}] = e^{-e^{-2t}}$$
In this case $\frac{1}{2}n\log(n)$ is known as a strong threshold.



Radu Balan (UMD)

March 8, 2017



Random graphs with n=1000 vertices. m₁=2892





Radu Balan (UMD)

March 8, 2017

$\overline{Graph Laplacians}$

Recall the Laplacian matrices:

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

Ã

$\begin{array}{l} \text{Graph Laplacians} \\ {}_{\Delta,\,\textit{L},\,\tilde{\Delta}} \end{array}$

Recall the Laplacian matrices:

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

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

Ãι

< □ > < 同 >

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?

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

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

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?

- $\Delta = \Delta^T \ge 0$ and hence its eigenvalues are non-negative real numbers.
- eigs($\tilde{\Delta}$) = eigs(L) \subset [0, 2].
- 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.

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

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

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. Redu Balan (UMD) Graphs 5 March 8, 2017

The spectral absolute gap $\lambda(G)$

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

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

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

The spectral absolute gap $\lambda(G)$

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

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

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

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

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

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

Numerical Results λ_1 for random graphs

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



March 8, 2017

Numerical Results $1 - \lambda_1$ for random graphs

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



Numerical Results $1 - \lambda_1$ for random graphs

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



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

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



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

• 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:

$$vol(A) = \sum_{x \in A} d_x.$$

• For a set of vertices A, denote $\overline{A} = \mathcal{V} \setminus A$ its complement.

The Cheeger inequalities h_G and λ_1

Theorem

For a connected graph

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

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:

- Compute eigenpair (λ_1, g^1) for the second smallest eigenvalue;
- Porm the partition:

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

Min-cut Problems Weighted Graphs

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

- $\Delta = D W$, $D = diag(w_i)_{1 \le i \le n}$, $w_i = \sum_{j \ne i} w_{i,j}$
- $\tilde{\Delta} = D^{-1/2} \Delta D^{-1/2} = I D^{-1/2} W D^{-1/2}$
- $\mathit{eigs}(ilde{\Delta}) \subset [0,2]$

•
$$h_G = \min_S \frac{\sum_{x \in S, y \in \overline{S}} W_{x,y}}{\min(\sum_{x \in S} W_{x,x}, \sum_{y \in \overline{S}} W_{y,y})}$$

- $2h_G \ge \lambda_1 \ge 1 \sqrt{1 h_G^2}$
- Good initial guess for optimal partition: Compute the eigenpair (λ₁, g¹) associated to the second smallest eigenvalue of Δ̃; set:

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

References

- B. Bollobás, **Graph Theory. An Introductory Course**, Springer-Verlag 1979. **99**(25), 15879–15882 (2002).
- F. Chung, Spectral Graph Theory, AMS 1997.
- F. Chung, L. Lu, The average distances in random graphs with given expected degrees, Proc. Nat.Acad.Sci. 2002.
- F. Chung, L. Lu, V. Vu, The spectra of random graphs with Given Expected Degrees, Internet Math. 1(3), 257–275 (2004).
- R. Diestel, **Graph Theory**, 3rd Edition, Springer-Verlag 2005.
- P. Erdös, A. Rényi, On The Evolution of Random Graphs
- G. Grimmett, **Probability on Graphs. Random Processes on Graphs and Lattices**, Cambridge Press 2010.

> < = > < = >

- C. Hoffman, M. Kahle, E. Paquette, Spectral Gap of Random Graphs and Applications to Random Topology, arXiv: 1201.0425 [math.CO] 17 Sept. 2014.
- J. Leskovec, J. Kleinberg, C. Faloutsos, Graph Evolution: Densification and Shrinking Diameters, ACM Trans. on Knowl.Disc.Data, $\mathbf{1}(1)$ 2007.