Topics in concentration of measure: Lecture III

Sourav Chatterjee

Courant Institute, NYU

St. Petersburg Summer School, June 2012

Lecture III: Large deviations for dense random graphs

Main objective: how to count graphs with a given property

- Only consider finite undirected graphs without self-loops in this talk.
- $2^{n(n-1)/2}$ such graphs on n vertices.
- Question: Given a property P and an integer n, roughly how many of these graphs have property P?
- For example, P may be: $\#\text{triangles} \geq tn^3$, where t is a given constant.
- To make any progress, need to assume some regularity on P. For example, we may demand that P be continuous with respect to some metric.
- What metric? What space?

Another motivation

- Let $G(n,p)$ be the Erdős-Rényi random graph on n vertices where each edge is added independently with probability p.
- Number of triangles in $G(n,p)$ roughly $\binom{n}{3}p^3 \sim n^3p^3/6$.
- What if, just by chance, #triangles turns out to be $\approx tn^3$ where $t > p^3/6$? What would the graph look like, conditional on this rare event?

An abstract topological space of graphs

- Beautiful unifying theory developed by Lovász and coauthors V. T. Sós, B. Szegedy, C. Borgs, J. Chayes, K. Vesztergombi, A. Schrijver and M. Freedman. Related to earlier works of Aldous, Hoover, Kallenberg.
- Let G_n be a sequence of simple graphs whose number of nodes tends to infinity.
- For every fixed simple graph H, let $\hom(H, G)$ denote the number of homomorphisms of H into G (i.e. edge-preserving maps $V(H) \to V(G)$, where $V(H)$ and $V(G)$ are the vertex sets).
- This number is normalized to get the homomorphism density

$$t(H, G) := \frac{\hom(H, G)}{|V(G)|^{|V(H)|}}.$$

This gives the probability that a random mapping $V(H) \to V(G)$ is a homomorphism.

Abstract space of graphs contd.

- Suppose that $t(H, G_n)$ tends to a limit $t(H)$ for every H.
- Then Lovász & Szegedy proved that there is a natural "limit object" in the form of a function $f \in \mathcal{W}$, where $\mathcal{W}$ is the space of all measurable functions from $[0,1]^2$ into $[0,1]$ that satisfy $f(x,y) = f(y,x)$ for all x, y.
- Conversely, every such function arises as the limit of an appropriate graph sequence.
- This limit object determines all the limits of subgraph densities: if H is a simple graph with k vertices, then

$$t(H, f) = \int_{[0,1]^k} \prod_{(i,j) \in E(H)} f(x_i, x_j)\, dx_1 \cdots dx_k.$$

- A sequence of graphs $\{G_n\}_{n \geq 1}$ is said to converge to f if for every finite simple graph H,

$$\lim_{n \to \infty} t(H, G_n) = t(H, f).$$

Example

- For any fixed graph H,

$$t(H, G(n,p)) \to p^{|E(H)|} \quad \text{almost surely as } n \to \infty.$$

- On the other hand, if f is the function that is identically equal to p, then $t(H, f) = p^{|E(H)|}$.
- Thus, the sequence of random graphs $G(n,p)$ converges almost surely to the non-random limit function $f(x,y) \equiv p$ as $n \to \infty$.

Abstract space of graphs contd.

- The elements of $\mathcal{W}$ are sometimes called 'graphons'.
- A finite simple graph G on n vertices can also be represented as a graphon f^G is a natural way:

$$f^G(x,y) = \begin{cases} 1 & \text{if } (\lceil nx \rceil, \lceil ny \rceil) \text{ is an edge in } G, \\ 0 & \text{otherwise.} \end{cases}$$

- Note that this allows *all* simple graphs, irrespective of the number of vertices, to be represented as elements of the single abstract space $\mathcal{W}$.
- So, what is the topology on this space?

The cut metric

- For any $f, g \in \mathcal{W}$, Frieze and Kannan defined the cut distance:

$$d_\square(f,g) := \sup_{S,T \subseteq [0,1]} \left| \int_{S \times T} [f(x,y) - g(x,y)] dx dy \right|.$$

- Introduce an equivalence relation on $\mathcal{W}$: say that $f \sim g$ if $f(x,y) = g_\sigma(x,y) := g(\sigma x, \sigma y)$ for some measure preserving bijection σ of $[0,1]$.
- Denote by $\widetilde{g}$ the closure in $(\mathcal{W}, d_\square)$ of the orbit $\{g_\sigma\}$.
- The quotient space is denoted by $\widetilde{\mathcal{W}}$ and τ denotes the natural map $g \to \widetilde{g}$.
- Since $d_\square$ is invariant under σ one can define on $\widetilde{\mathcal{W}}$ the natural distance $\delta_\square$ by

$$\delta_\square(\widetilde{f}, \widetilde{g}) := \inf_\sigma d_\square(f, g_\sigma) = \inf_\sigma d_\square(f_\sigma, g) = \inf_{\sigma_1, \sigma_2} d_\square(f_{\sigma_1}, g_{\sigma_2})$$

making $(\widetilde{\mathcal{W}}, \delta_\square)$ into a metric space.

Cut metric and graph limits

To any finite graph G, we associate the natural graphon f^G and its orbit $\widetilde{G} = \tau f^G = \widetilde{f}^G \in \widetilde{\mathcal{W}}$. One of the key results of the is the following:

Theorem (Borgs, Chayes, Lovász, Sós & Vesztergombi)

A sequence of graphs $\{G_n\}_{n\geq 1}$ converges to a limit $f \in \mathcal{W}$ if and only if $\delta_\square(\widetilde{G}_n, \widetilde{f}) \to 0$ as $n \to \infty$.

Our result

- For any Borel set $\widetilde{A} \subseteq \widetilde{\mathcal{W}}$, let
$$\widetilde{A}_n := \{\widetilde{h} \in \widetilde{A} : \widetilde{h} = \widetilde{G} \text{ for some } G \text{ on } n \text{ vertices}\}.$$
- Let $I(u) := \frac{1}{2}u \log u + \frac{1}{2}(1-u)\log(1-u)$.
- For any $\widetilde{h} \in \widetilde{\mathcal{W}}$, let $I(\widetilde{h}) := \int\int I(h(x,y))dxdy$, where h is any element of $\widetilde{h}$.

Theorem (Chatterjee & Varadhan, 2010)

The function I is well-defined and lower-semicontinuous on $\widetilde{\mathcal{W}}$. If $\widetilde{F}$ is a closed subset of $\widetilde{\mathcal{W}}$ then

$$\limsup_{n\to\infty} n^{-2} \log |\widetilde{F}_n| \le -\inf_{\widetilde{h}\in\widetilde{F}} I(\widetilde{h})$$

and if $\widetilde{U}$ is an open subset of $\widetilde{\mathcal{W}}$, then

$$\liminf_{n\to\infty} n^{-2} \log |\widetilde{U}_n| \ge -\inf_{\widetilde{h}\in\widetilde{U}} I(\widetilde{h}).$$

Erdős-Rényi graphs

- Counting graphs can be related to finding large deviation probabilities for Erdős-Rényi random graphs.
- For example,

$$\begin{aligned}&\#\text{graphs on } n \text{ vertices satisfying } P\\ &= 2^{n(n-1)/2}\mathbb{P}(G(n,1/2) \text{ satisfies } P).\end{aligned}$$

- Indeed, the main result in our paper is stated as a large deviation principle for the Erdős-Rényi graph, which can be easily proved to be equivalent to the graph counting principle stated before.

Large deviation principle for ER graphs

- The random graph $G(n,p)$ induces probability distribution $\widetilde{\mathbb{P}}_{n,p}$ on the space $\widetilde{\mathcal{W}}$ through the map $G \to \widetilde{G}$.
- Let $I_p(u) := \frac{1}{2}u\log\frac{u}{p} + \frac{1}{2}(1-u)\log\frac{1-u}{1-p}$.
- For $\widetilde{h} \in \widetilde{\mathcal{W}}$, let $I_p(\widetilde{h}) := \int\int I_p(h(x,y))dxdy$, where h is any element of $\widetilde{h}$.

Theorem (Chatterjee & Varadhan, 2010)

For any closed set $\widetilde{F} \subseteq \widetilde{\mathcal{W}}$,

$$\limsup_{n\to\infty} \frac{1}{n^2}\log \widetilde{\mathbb{P}}_{n,p}(\widetilde{F}) \le -\inf_{\widetilde{h}\in\widetilde{F}} I_p(\widetilde{h}).$$

and for any open set $\widetilde{U} \subseteq \widetilde{\mathcal{W}}$,

$$\liminf_{n\to\infty} \frac{1}{n^2}\log \widetilde{\mathbb{P}}_{n,p}(\widetilde{U}) \ge -\inf_{\widetilde{h}\in\widetilde{U}} I_p(\widetilde{h}).$$

Method of proof

- The LDP can be proved by standard techniques for the weak topology on $\widetilde{\mathcal{W}}$. (Fenchel-Legendre transforms, Gärtner-Ellis theorem, etc.)
- However, the weak topology is not very interesting. For example, subgraph counts are not continuous with respect to the weak topology.
- The LDP for the topology of the cut metric does not follow via standard methods.

Szemerédi's lemma

- Let $G = (V, E)$ be a simple graph of order n.
- For any $X, Y \subseteq V$, let $e_G(X, Y)$ be the number of X-Y edges of G and let
$$\rho_G(X, Y) := \frac{e_G(X, Y)}{|X||Y|}$$
- Call a pair (A, B) of disjoint sets $A, B \subseteq V$ ϵ-regular if all $X \subseteq A$ and $Y \subseteq B$ with $|X| \geq \epsilon|A|$ and $|Y| \geq \epsilon|B|$ satisfy $|\rho_G(X, Y) - \rho_G(A, B)| \leq \epsilon$.
- A partition $\{V_0, \ldots, V_K\}$ of V is called an ϵ-regular partition of G if it satisfies the following conditions: (i) $|V_0| \leq \epsilon n$; (ii) $|V_1| = |V_2| = \cdots = |V_K|$; (iii) all but at most ϵK^2 of the pairs (V_i, V_j) with $1 \leq i < j \leq K$ are ϵ-regular.

Theorem (Szemerédi's lemma)

Given $\epsilon > 0$, $m \geq 1$ there exists $M = M(\epsilon, m)$ such that every graph of order $\geq M$ admits an ϵ-regular partition $\{V_0, \ldots, V_K\}$ for some $K \in [m, M]$.

Finishing the proof using Szemerédi's lemma

- Suppose G is a graph of order n with ϵ-regular partition $\{V_0, \ldots, V_K\}$.
- Let G' be the random graph with independent edges where a vertex $u \in V_i$ is connected to a vertex $v \in V_j$ with probability $\rho_G(V_i, V_j)$.
- Using Szemerédi's regularity lemma, one can prove that $\delta_\square(G, G') \simeq 0$ with high probability if K and n are appropriately large and ϵ is small.
- Let f be the probability density of the law of $G(n,p)$ with respect to the law of G'. (This is easily computed; gives rise to the entropy function.) Then

$$\mathbb{P}(G(n,p) \approx G) \approx f(G)\mathbb{P}(G' \approx G) \approx f(G).$$

- Since the space $\widetilde{\mathcal{W}}$ is compact, this allows us to approximate $\mathbb{P}(G(n,p) \in A)$ for any nice set A by approximating A as a finite union of small balls.

Conditional distributions

Theorem

Take any $p \in (0,1)$. Let $\widetilde{F}$ be a closed subset of $\widetilde{\mathcal{W}}$ satisfying

$$\inf_{\widetilde{h} \in \widetilde{F}^o} I_p(\widetilde{h}) = \inf_{\widetilde{h} \in \widetilde{F}} I_p(\widetilde{h}) > 0.$$

Let $\widetilde{F}^*$ be the subset of $\widetilde{F}$ where I_p is minimized. Then $\widetilde{F}^*$ is non-empty and compact, and for each n, and each $\epsilon > 0$,

$$\mathbb{P}(\delta_\square(G(n,p), \widetilde{F}^*) \geq \epsilon \mid G(n,p) \in \widetilde{F}) \leq e^{-C(\epsilon, \widetilde{F})n^2}$$

where $C(\epsilon, \widetilde{F})$ is a positive constant depending only on ϵ and $\widetilde{F}$.

Proof: Follows from the compactness of $\widetilde{\mathcal{W}}$ (a deep result of Lovász and Szegedy, involving recursive applications of Szemerédi's lemma and martingales).

Large deviations for triangle counts

- Let $T_{n,p}$ be the number of triangles in $G(n,p)$.
- Objective: to evaluate the limit

$$\lim_{n\to\infty} \frac{1}{n^2} \log \mathbb{P}(T_{n,p} \geq (1+\epsilon)\mathbb{E}(T_{n,p}))$$

  as a function of p and ϵ.
- Exact evaluation of limit due to Chatterjee & Dey (2009): for a certain explicit set of (p,t),

$$\lim_{n\to\infty} \frac{1}{n^2} \log \mathbb{P}(T_{n,p} \geq tn^3) = -I_p((6t)^{1/3}),$$

  when $I_p(u) := \frac{1}{2}u \log \frac{u}{p} + \frac{1}{2}(1-u)\log\frac{1-u}{1-p}$.
- Unfortunately, the result does not cover all values of (p,t).

Large deviations for triangle counts contd.

- Recall: $\mathcal{W}$ is the space of symmetric measurable functions from $[0,1]^2$ into $[0,1]$.
- For each $f \in \mathcal{W}$, let

$$T(f) := \frac{1}{6}\int_0^1 \int_0^1 \int_0^1 f(x,y)f(y,z)f(z,x)\, dx\, dy\, dz$$

and let $I_p(f) = \iint I_p(f(x,y))dxdy$.

- For each $p \in (0,1)$ and $t \geq 0$, let

$$\phi(p,t) := \inf\{I_p(f) : f \in \mathcal{W},\ T(f) \geq t\}. \tag{1}$$

Theorem (Chatterjee & Varadhan, 2010)

For each $p \in (0,1)$ and each $t \geq 0$,

$$\lim_{n\to\infty} \frac{1}{n^2} \log \mathbb{P}(T_{n,p} \geq tn^3) = -\phi(p,t).$$

Moreover, the infimum is attained in the variational problem (1).

The 'replica symmetric' phase

Theorem (Chatterjee & Varadhan, 2010)

Let $h_p(t) := I_p((6t)^{1/3})$. Let $\hat{h}_p$ be the convex minorant of h_p. If t is a point where $h_p(t) = \hat{h}_p(t)$, then $\phi(p,t) = h_p(t)$. Moreover, for such (p,t), the conditional distribution of $G(n,p)$ given $T_{n,p} \geq tn^3$ is indistinguishable from the law of $G(n,(6t)^{1/3})$ in the large n limit.

Remarks: This result recovers the result of Chatterjee & Dey and gives more. However, the theorem of Chatterjee & Dey gives an error bound of order $n^{-1/2}$, which is impossible to obtain via Szemerédi's lemma.

'Replica symmetry breaking'

The following theorem shows that given any t, for all p small enough, the conditional distribution of $G(n,p)$ given $T_{n,p} \geq tn^3$ does not resemble that of an Erdős-Rényi graph.

Theorem (Chatterjee & Varadhan, 2010)

Let $\widetilde{C}$ denote the set of constant functions in $\widetilde{\mathcal{W}}$ (representing all Erdős-Rényi graphs). For each t, there exists $p' > 0$ and $\epsilon > 0$ such that for all $p < p'$,

$$\lim_{n\to\infty} \mathbb{P}(\delta_\square(G(n,p), \widetilde{C}) > \epsilon \mid T_{n,p} \geq tn^3) = 1.$$

The double phase transition

Theorem (Chatterjee & Varadhan, 2010)

There exists $p_0 > 0$ such that if $p \leq p_0$, then there exists $p^3/6 < t' < t'' < 1/6$ such that the replica symmetric picture holds when $t \in (p^3/6, t') \cup (t'', 1/6)$, but there is a non-empty subset of (t', t'') where replica symmetry breaks down.

The small p limit

The following theorem says that when t is fixed and p is very small, then conditionally on the event $\{T_{n,p} \geq tn^3\}$ the graph $G(n,p)$ must look like a clique.

Theorem (Chatterjee & Varadhan, 2010)

For each t,

$$\lim_{p \to 0} \frac{\phi(p,t)}{\log(1/p)} = \frac{(6t)^{2/3}}{2}.$$

Moreover, if

$$\chi_t(x,y) := 1_{\{\max\{x,y\} \leq (6t)^{1/3}\}}$$

is the graphon representing a clique with triangle density t, then for each $\epsilon > 0$,

$$\lim_{p \to 0} \lim_{n \to \infty} \mathbb{P}(\delta_\square(\widetilde{G(n,p)}, \widetilde{\chi}_t) \geq \epsilon \mid T_{n,p} \geq tn^3) = 0.$$

Lower tails

- Given a fixed simple graph H,

$$\lim_{u \to 0} \lim_{n \to \infty} \frac{\log \mathbb{P}(t(H, G(n,p)) \le u)}{n^2} = -\frac{1}{2(\chi(H)-1)} \log \frac{1}{1-p},$$

  where $\chi(H)$ is the chromatic number of H.
- Closely related to the Erdős-Stone theorem from extremal graph theory.
- In fact, the precise result implies the following: given that $t(H, G(n,p))$ is very small (or zero), the graph $G(n,p)$ looks like a complete $(\chi(H)-1)$-equipartite graph with $(1-p)$-fraction of edges randomly deleted.
- However, if $t(H, G(n,p))$ is just a little bit below its expected value, the graph continues to look like an Erdős-Rényi graph as in the upper tail case.

An application

- Exponential random graph models (ERGMs) popular in social network literature
- Previously, could not be tackled mathematically.
- Using the LDP for Erdős-Rényi graphs, several such models can be fully analyzed (joint work with Persi Diaconis).
- Gives interesting phase transitions, confirming predictions from the non-rigorous literature.

Open questions

- There are many questions that remain unresolved, even in the simple example of upper tails for triangle counts. For example:
- What is the set of optimal solutions of the variational problem defining the rate function in the broken replica symmetry phase (i.e. where the optimizer is not a constant)?
- Is the solution unique in the quotient space $\widetilde{\mathcal{W}}$, or can there exist multiple solutions?
- Is it possible to explicitly compute a nontrivial solution for at least some values of (p, t) in the broken replica symmetry region?
- Is it possible to even numerically evaluate or approximate a solution using a computer?
- What is the full characterization of the replica symmetric phase? What is the phase boundary?
- What happens in the sparse case where p and t are both allowed to tend to zero?

Acknowledgment

Special thanks to: Amir Dembo, who suggested the problem to me in 2005. An old manuscript due to Bolthausen, Comets and Dembo (2003) provided a partial solution to the question but was never published.