A Survey of Modern Analysis on Graphs: Open Problems

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A Model Problem

A large class of graph algorithms based on heuristic analogies to physical systems (e.g. heat or electrical flow) are motivated by physical diffusion processes involving a discrete Poisson equation:

$$\Delta \mathbf{f}(x) = \mathbf{g}(x)$$

For supervised and semi-supervised learning problems, $\mathbf{g}(x)$ is typically related to a problem-specific seed set S

For example, take $\mathbf{g} = \chi_S$ or some scaling thereof

A Meta-Algorithm

A by no means exhaustive list:

- PageRank [2]
- Centered Commute Times [8]
- Consistency-based Learning [4]
- Harmonic Functions [3]
- Green's Function Recommender [1]

Modulo minor variations, these are motivated by the (generalized) inversion of a discrete Laplace operator Δ

Discrete Green's Functions on Graphs

Typically one solves the Poisson problem by convolving the source term with the discrete Green's function $\mathcal{G}$ for Δ:

$$\mathbf{f} = \mathcal{G}\mathbf{g}$$

For a graph without boundary the Green's function $\mathcal{G}$ is just the Moore-Penrose pseudoinverse $\mathcal{L}^\dagger$ of the graph Laplacian [6]:

$$\mathcal{G} = \mathcal{L}^\dagger = \sum_{\lambda_j > 0} \frac{1}{\lambda_j} \mathbf{u}_j \mathbf{u}_j^T.$$

Hence we "solve" the linear system:

$$\mathcal{L}\mathbf{f} = \mathbf{g}$$

Three "Query" Regimes

This is a data science analogue of approximating the solution of a PDE by convolving a source with a Green's function

Three (general) techniques...

- Implicit convolution of $\mathcal{G}$ with the given source term $\mathbf{g}$
- Approximate ad-hoc reconstruction of $\mathcal{G}$ via a low-rank eigendecomposition of $\mathcal{L}$
- Explicit computation of $\mathcal{G}$ by direct methods

The latter is notionally an $O(n^3)$ proposition, so most work focuses on the first two methods

Laplacians of Graphs & Notation

Let A be the $n \times n$ adjacency matrix of a graph G on n nodes:

$$A_{ij} = \begin{cases} w_{ij}, & \text{if } i \sim j \\ 0, & \text{otherwise} \end{cases}$$

Likewise, denote by D the diagonal matrix of row sums:

$$D_{ij} = \begin{cases} d_i, & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases}$$

The **combinatorial graph Laplacian** is defined as $\mathcal{L} = D - A$

Brief Facts about Graph Matrices

Let $E : C^1 \to C^0$ be the $n \times m$ edge-incidence matrix

Denoting by e_k^+ and e_k^- the respective head and tail vertices of the k'th edge, E has columns of the form $\mathbf{e}_k = \delta_{e_k^+} - \delta_{e_k^-}$

$$E = \begin{array}{c} \\ e_k^+ \\ \\ e_k^- \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \end{array} \begin{pmatrix} | & | & & \mathbf{e}_k & & | & | \\ | & | & & \vdots & & | & | \\ | & | & & 1 & & | & | \\ \mathbf{e}_1 & \mathbf{e}_2 & \cdots & \vdots & \cdots & \mathbf{e}_{m-1} & \mathbf{e}_m \\ | & | & & -1 & & | & | \\ | & | & & \vdots & & | & | \end{pmatrix}$$

Brief Facts about Graph Matrices

The Laplacian $\mathcal{L}$ has the well-known following properties:

- $\mathcal{L}$ factors as $\mathcal{L} = D - A = EWE^T$
- $\mathcal{L}$ is positive semidefinite with eigenvalues $0 = \lambda_n \leq \lambda_{n-1} \leq ... \leq \lambda_1 \leq \text{vol}(G)$
- The multiplicity of the eigenvalue $\lambda_n = 0$ is equal to the number of connected components of G
- The indicator vectors of the connected components of G span the corresponding eigenspace

If G is connected, then the vector $\mathbf{u}_n = \mathbf{1}_n$ is harmonic.

Effective Resistances & Commute Times

The **commute time** between nodes s and t is the symmetrized hitting time, $H(s,t)$, for a random walk between s and t:

$$C(s,t) = H(s,t) + H(s,t) = C(s,t).$$

$C(s,t)$ is then just the expected number of hops for a random walk starting at s to reach t and then return to s.

$C(s,t)$ is proportional to the **effective resistance** $R(s,t)$ [5]:

$$R(s,t) = \min\left\{ \sum_{e \in E} r_e i_e^2 \;\middle|\; i = (i_e)_{e \in E} \text{ unit } s-t \text{ flow} \right\}$$

$C(s,t)$ may be obtained from a quadratic form with kernel matrix $\mathcal{L}^\dagger$ for any s and t...

Effective Resistances & Commute Times

Theorem (Fouss et al. [7])

The commute time $C(s,t)$ between nodes s and t may be written as:

$$\begin{aligned}
\frac{1}{N} C(s,t) &= (\mathbf{e}_s - \mathbf{e}_t)^T \mathcal{L}^\dagger (\mathbf{e}_s - \mathbf{e}_t) \\
&= \sum_{k=1}^{n-1} \frac{1}{\lambda_k} (\mathbf{u}_k(s) - \mathbf{u}_k(t))^2 \\
&= \mathcal{L}^\dagger(s,s) - 2\mathcal{L}^\dagger(s,t) + \mathcal{L}^\dagger(t,t). \\
&= R(s,t)
\end{aligned}$$

A Geometric View

It doesn't always work...

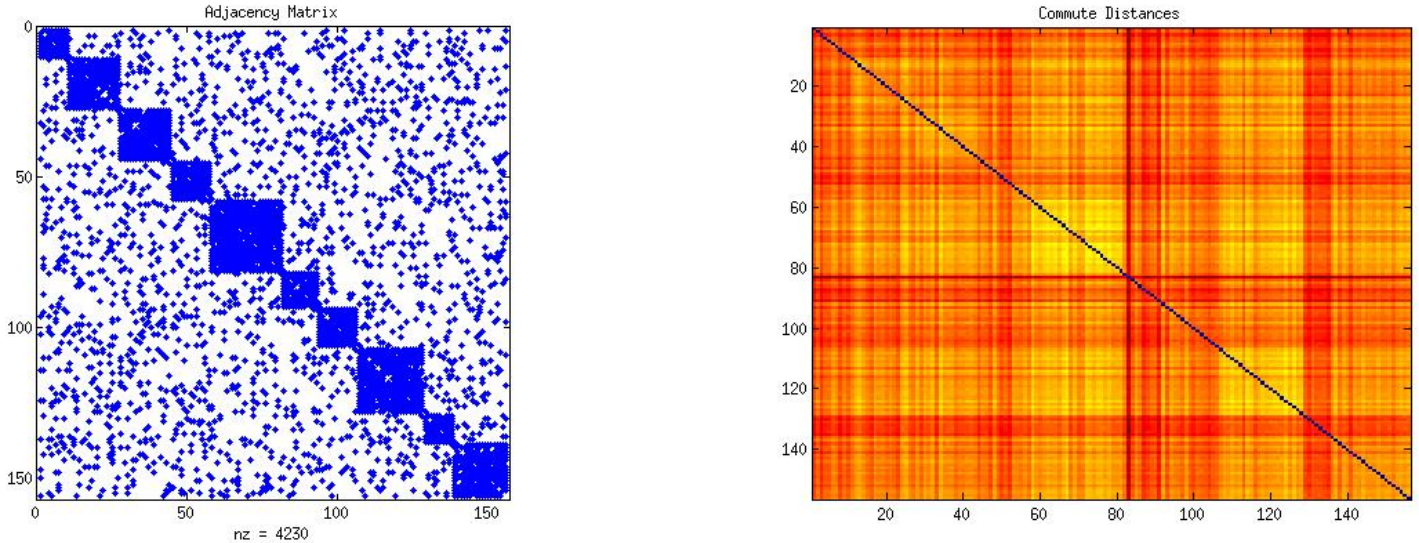

Figure: Exact Commute Times

What Went Wrong(?)

Empirically, the raw commute distance can be strongly affected by the node degree.

(von Luxburg et al.) For certain classes of random graphs, known concentration results yield [9]

$$C(s,t) \to \frac{1}{d_s} + \frac{1}{d_t}.$$

This is worthless as a distance measure on a graph, as all nodes then have the same nearest-neighbor, second nearest-neighbor, etc.

Moreover, it was empirically observed that $\mathcal{L}^\dagger(s,s) \approx \frac{1}{d_s}$, implying that $\mathcal{L}^\dagger(s,t) \to 0$.

Commute Times & the Combinatorial Laplacian

Fortunately, exact commute times are **not** what one obtains by solving the model Poisson problem presented earlier:

$$\mathbf{f} = \mathcal{G}\mathbf{g} = \mathcal{L}^{\dagger}\mathbf{g}$$

Specifically, a doubly-centered version of $C(s,t)$ is obtained [8]

Hence, only the weighted off-diagonals of the pseudoinverse are used:

$$f(s) = \sum_{k \in V} \mathcal{L}^{\dagger}(s,k) g(k)$$

A Model Distance?

It seems to work...

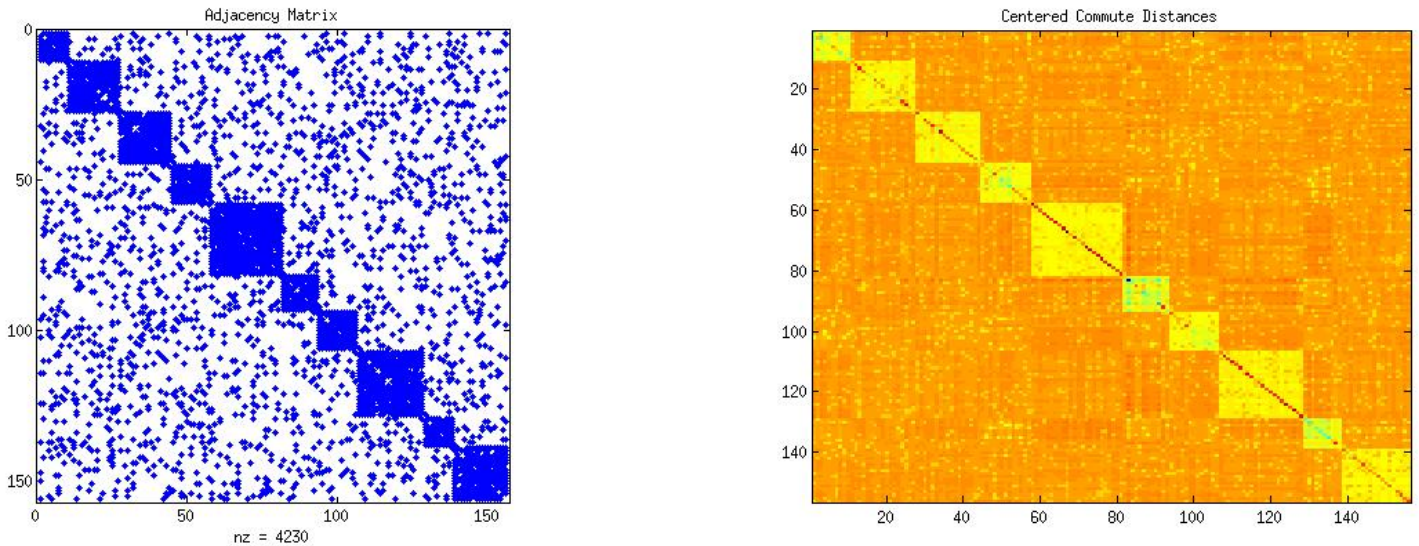

Figure: Centered Commute Times

Or a Band-Aid?

Centering seems to resolve the interference by the self-correlations $\mathcal{L}^\dagger(s,s)$, but perhaps **not** the underlying problem if $\mathcal{L}^\dagger(s,t) \longrightarrow 0$!

However, there is a generalization of the effective resistance that mitigates this pathological behavior...

for certain classes of *random geometric graphs* arising in machine-learning applications

Random Geometric Graphs

A useful taxonomy for graphs (AI Hero - GraphEx 2016):

- **Relational graphs**: links are observed (e.g. social networks, computer or biological networks, etc)
- **Attributional graphs**: links are imputed from node characteristics (e.g. Markov random fields)

Random geometric graphs are attributional graphs: node $s \in V(G)$ is associated to an $X_s \in \mathbb{R}^d$

Edges are then imputed by similarity of node vectors in the ambient Euclidean space

Random Geometric Graphs

Relevant random geometric graph models include: [10]:

- ϵ-**ball graphs**: assume $X_1, \ldots, X_n$ are drawn i.i.d. from an underlying density f on $\mathbb{R}^d$ with $M \doteq \text{supp}(f)$ and connect each X_i to any X_j with Euclidean distance smaller than ϵ

- k-**NN graphs**: assume $X_1, \ldots, X_n$ are drawn i.i.d. from an underlying density f on $\mathbb{R}^d$ with $M \doteq \text{supp}(f)$ connect each X_i to its k nearest neighbors by an undirected, unweighted edge

- **Lattice graphs**: uniform lattices such as the square lattice or triangular lattice in $\mathbb{R}^d$. Note that these have constant marginals

p-Resistances of Graphs

Recall the classical formulation of the effective resistance:

$$R(s,t) = \min\Big\{ \sum_{e\in E} r_e i_e^2 \;\Big|\; i = (i_e)_{e\in E} \text{ unit } s-t \text{ flow} \Big\}$$

for $r_e \doteq \frac{1}{w_e}$. This suggests the natural generalization:

$$R_p(s,t) = \min\Big\{ \sum_{e\in E} r_e |i_e|^p \;\Big|\; i = (i_e)_{e\in E} \text{ unit } s-t \text{ flow} \Big\} \qquad (*)$$

As noted, $R(s,t)$ is proportional to the commute time $C(s,t)$

Phase Transitions of p-Resistances

The p-resistance interpolates several well-known graph distances:

Theorem (Alamgir & von Luxburg [10])

For any weighted graph G the following hold:

- *For $p = 1$, the p-resistance coincides with the shortest path distance on the graph*
- *For $p = 2$, the p-resistance reduces to the standard resistance distance defined above*
- *For $p \to \infty$, $R_p(s,t)^{p-1} \to \frac{1}{m}$ where m is the unweighted $s-t$-mincut*

Something even more intriguing happens for $1 < p < 2$...

Phase Transitions of p-Resistances

Let $\left(G_n\right)_{n\in\mathbb{N}}$ be a family of graphs with $|V| \longrightarrow \infty$ with n

Let r, R be constants depending on n, $C \geq R/r$ a constant, and $\mathcal{N}(s)$ the ball or radius $C \cdot r$ around s

For i^* the optimal flow from the previous slide, define:

$$\begin{aligned} R_p^{local}(s) &\doteq \sum_{e\in\mathcal{N}(s)} r_e |i_e^*|^p \\ R_p^{local}(s,t) &\doteq R_p^{local}(s) + R_p^{local}(t) \\ R_p^{global}(s,t) &\doteq R_p(s,t) - R_p^{local}(s,t) \end{aligned}$$

Phase Transitions of p-Resistances

The notation $e \in \mathcal{N}_s$ is meant to signify that the edge e has both endpoints (not necessarily s) within $\mathcal{N}_s$

$R_p^{local}(s,t)$ is then just the contribution to $R_p(s,t)$ exclusively from nodes in $\mathcal{N}(s) \cup \mathcal{N}(t)$

Conversely, $R_p^{global}(s,t)$ is the contribution to the effective resistance from edges with endpoints outside of $\mathcal{N}_s$ and $\mathcal{N}_t$

Regard τ_n as an "average degree" of the graph G_n (for now)...

Phase Transitions of p-Resistances

Theorem (Alamgir & von Luxburg [10])

Consider a family of unweighted geometric graphs on $\mathbb{R}^d$ satisfying some general assumptions (listed below). Fix two vertices s and t and define two critical thresholds $p^* \doteq 1 + \frac{1}{d-1}$ and $p^{**} \doteq 1 + \frac{1}{d-2}$. Then as $n \to \infty$:

- *If $p < p^*$ and τ_n is sub-polynomial in n, then $\frac{R_p^{global}(s,t)}{R_p^{local}(s,t)} \to \infty$*
- *If $p > p^{**}$ and $\tau_n \to \infty$, then $\frac{R_p^{global}(s,t)}{R_p^{local}(s,t)} \to \frac{1}{d_s^{p-1}} + \frac{1}{d_t^{p-1}}$*

Phase Transitions of p-Resistances

In words: "...there exists a non-trivial point of phase transition in the behavior of p-resistances: if $p < p^*$, then p-resistances are informative about the global topology of the graph, whereas if $p > p^{**}$ the p-resistances converge to trivial distance functions that do not depend on any global properties of the graph."

- Morteza Alamgir & Ulrike von Luxburg [10]

Geometric Assumptions

Let $(G_n)_{n\in\mathbb{N}}$ be a family of unweighted geometric graphs constructed from $X_1, \ldots, X_n \in M \subset \mathbb{R}^d, d > 2$. Assume that there exist r, R satisfying $0 < r \leq R$ such that the following hold for all $x \in \{X_1, \ldots, X_n\}$:

- **Distribution of Points**: For $\rho \in \{r, R\}$ the number of sample points in $B(x, \rho)$ is of the order $\Theta(n \cdot \rho^d)$
- **Graph connectivity**: x is connected to all sample points within $B(x, r)$ and to no sample points outside of $B(x, R)$
- **Regularity of the boundary**: M is compact, connected with $M \setminus \partial M$ connected. There exist constants $\alpha > 0$, $\epsilon_0 > 0$ such that if $\epsilon < \epsilon_0$ then for all $x \in \partial M$ we have:

$$\text{vol}(B_\epsilon(x) \cap M) \geq \alpha \text{vol}(B_\epsilon(x))$$

Geometric Assumptions

The phase transition for p-resistances holds for: [10]:

- ϵ-**ball graphs**: if $M \doteq \text{supp}(f)$ satisfies condition 3 above
- k-**NN graphs**: if $M \doteq \text{supp}(f)$ satisfies condition 3 above
- **Lattice graphs**: only the lower bound of the theorem holds, as the upper bound requires that $\tau_n \to \infty$ while $\tau_n = \Theta(1)$ for a uniform lattice as these have constant degrees

Geometric Assumptions

Open Question: are the geometric conditions on the preceding slide sufficient/necessary to ensure L^p upper-regularity of a graphon corresponding to each class of random graphs?

Non-Open Question(s): what is L^p upper-regularity? What is a graphon? And why should we care if this is in fact the case?

Graphons: an Inadequate Introduction

Definition (Graphon)

A **graphon** $W : [0,1]^2 \longrightarrow [0,1]$ is a symmetric, measurable function on two variables

- Morally, think of $W(i,j) \in [0,1]$ as the probability of an edge connecting i, j in an ensemble of random graphs
- A graphon is then just a generative model for a family of random graphs
- Convergence of sequence of graphs G_n to a graphon W will preserve a desirable property: graph homomorphisms

Graphons: an Inadequate Introduction

Definition (Graph Homomorphism)

Let H, G be finite, simple graphs. A function $\varphi : V(H) \to V(G)$ is called an **graph homomorphism** if:

$$(u, v) \in E(H) \Longrightarrow (\varphi(u), \varphi(v)) \in E(G)$$

Now define the homomorphism density of a graph H in G:

$$t(H, G) \doteq \frac{\#\text{hom}(H, G)}{|V(G)|^{|V(H)|}}$$

Intuitively, $t(H, G)$ is the fraction of a maps from $V(H)$ to $V(G)$ which are graph homomorphisms

Graphons: an Inadequate Introduction

Define the homomorphism density of a graph H in a graphon W as:

$$t(H, W) \doteq \int_{[0,1]^{|V(H)|}} \prod_{\substack{(i,j)\in E(H) \\ i<j}} W(x_i, x_j) dx dy$$

A sequence of graphs $(G_n)_{n\in\mathbb{N}}$ is said to converge to a graphon W if the following holds for all finite, simple graphs H:

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

The space of graphons may be endowed with a metric wherein compactness is implied by an analytic version of the Weak Regularity Lemma from combinatorics

The Cut Norm & Cut Distance on Graphons

The *cut norm* on integral kernels over $[0,1]^2$ is defined as:

$$\begin{aligned} \|W\|_{\square} &\doteq \sup_{S,T\subseteq[0,1]} \left| \int_{S\times T} W(x,y)dxdy \right| \\ &= \sup_{f,g:[0,1]\to[0,1]} |\langle f, Wg\rangle| \end{aligned}$$

The *cut distance* between graphons W, V is then defined as:

$$d_{\square}(W,V) = \|W - V\|_{\square}$$

Intuitively: find the subset of the unit square on which W, V maximally disagree - this maximum **is** obtained

The Weak Regularity Lemma for Graphons

A graphon U is termed a *stepfunction with at most k steps* if there is a partition $\mathcal{P} = \{V_1, \ldots, V_k\}$ of $[0,1]$ such that U is piecewise constant on the $V_i \times V_j$

Theorem (Lovász & Szegedy [20])

For every graphon W and $\epsilon > 0$, there is a stepfunction W' with at most $\lceil 2^{2/\epsilon^2} \rceil$ steps such that $\|W - W'\|_\square \leq \epsilon$

Compactness of Graphons in the Cut Metric

Let $\sigma : [0,1] \to [0,1]$ be a measure-preserving bijection and define:

$$W^{\sigma}(x,y) \doteq W(\sigma(x),\sigma(y))$$

The cut metric is then defined to be:

$$\delta_{\square}(W,V) \doteq \inf_{\sigma} \|W^{\sigma} - V\|_{\square}$$

The Weak Regularity Lemma for graphons is equivalent to compactness of the space of graphons under $\delta_{\square}$

Extensions to Sparse Graphs and General L^p Norms

Almost all of the foundational theory of graph limits and graph regularity surveyed so far applies to *dense* graphs

Extensions to sparse graphs are possible [15] [19]

Extensions to general L^p norms are also possible [16] [17]

We will discuss in detail the existence criteria for L^p graphons, as I believe that this illustrates a possible connection to the phase transition of p-resistances phenomenon discussed last time

L^p Graphons

An L^p graphon is a graphon for which the following norm is finite [16]:

$$\|W\|_p \doteq (\mathbb{E}[|W|^p])^{\frac{1}{p}} = \left(\int_{[0,1]^2} |W(x,y)|^p dxdy \right)^{\frac{1}{p}}$$

Note the similarity to the matrix norm proposed by von Luxburg & Alamgir for Laplacian regularization in [10]:

$$\|A\|_{m,n} \doteq \left(\sum_i ((\sum_j a_{ij}^m)^{\frac{1}{m}})^n \right)^{\frac{1}{n}}$$

A sequence of graphs G_n will converge to an L^p graphon when the sequence is *L^p Upper Regular*...

L^p Upper Regularity

Let $\alpha_i > 0$ and β_{ij} ($\beta_{ij} = 0$ if $ij \notin E(G)$) be vertex and edge weights, respectively, and $\alpha_U \doteq \sum_{i \in U} \alpha_i$ for $U \subset V(G)$

For simple, unweighted graphs $\beta_{ij} = 1$ if $i \sim j$, $\alpha_i = 1$ for all $i \in V(G)$. Following [16] define:

$$\begin{aligned} \|G\|_p &\doteq \left(\sum_{i,j \in V(G)} \frac{\alpha_i \alpha_j}{\alpha_G^2} |\beta_{ij}|^p \right)^{\frac{1}{p}} \\ \|G\|_\infty &\doteq \max_{i,j \in V(G)} |\beta_{ij}| \end{aligned}$$

If G is simple $\|G\|_1$ may be viewed as an edge density

L^p Upper Regularity

For any $S, T \subseteq V(G)$ define the edge density between S, T as:

$$\rho_G(S,T) \doteq \sum_{s\in S, t\in T} \frac{\alpha_s \alpha_t}{\alpha_S \alpha_T} \beta_{st}$$

G is said to be *(C,η)-upper L^p regular* if $\alpha_i \leq \eta \alpha_G$ for all $i \in V(G)$ and the condition:

$$\sum_{i,j=1}^{m} \frac{\alpha_{V_i}\alpha_{V_j}}{\alpha_G^2} \left| \frac{\rho_G(V_i,V_j)}{\|G\|_1} \right|^p \leq C^p$$

holds for every partition $V_1 \cup \ldots \cup V_m$ of $V(G)$ for which $\alpha_{V_k} \geq \eta \alpha_G$ for all K

L^p Upper Regularity

In words: "Informally, a graph G is (C, η)-upper L^p regular if $G/\|G\|_1$ has L^p norm at most C after we average over any partition of the vertices into blocks of at least $\eta|V(G)|$ in size (and no vertex has weight greater than $\eta\alpha_G$)."

- Christian Borgs, Jennifer T. Chayes, Henry Cohn, Yufei Zhao [16]

L^p Upper Regular Sequences

A sequence of graphs $(G_n)_{n>0}$ is said to be a *C-upper L^p regular sequence* if for any $\eta > 0$, (G_n) is $(C+\eta, \eta)$-upper L^p regular in the tails [16]

Theorem (Borgs, Chayes, Cohn, Zhao [16])

Let $p > 1$ and $(G_n)_{n\geq 0}$ be a C-upper L^p regular sequence of weighted graphs. There exists an L^p graphon W with $\|W\|_p \leq C$ so that

$$\liminf_{n\to\infty} \delta_\square \left(\frac{G_n}{\|G_n\|_1}, W \right) = 0$$

i.e. an L^p upper regular sequence has a subsequence that converges to an L^p graphon in the cut metric

Open(?) Questions

- Are the upper regularity criteria for the existence of an L^p graphon compatible with the phase transition phenomenon?
- Can non-local operators for the $p < 2$ case be obtained for L^p graphons analogous to the construction in [22]
- Can the phase transition of p-resistances be related to compactness/non-compactness (in cut-norm) of such a non-local operator?
- Are there any computational implications for recent techniques in deep-learning/signal-processing on graphs/manifolds?

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