SOME PROBLEMS AND RESULTS IN THE GEOMETRY OF GRAPHS

NATI LINIAL

- Hebrew University
- Jerusalem, Israel
- http://www.cs.huji.ac.il/∼nati/

Some of the main issues

1. The different faces of expansion.

2. Local vs. global views of graphs.

3. Lifts of graphs.

4. Eigenvectors of graphs (Differential geometry of graphs?)

5. Analogous questions for hypergraphs (On to the realm of topology?)

A quick review on expansion in graphs

There are three main perspectives of expansion:

- Combinatorial - isoperimetric
- Linear Algebraic
- Probabilistic - Rapid convergence of the random walk

For more on this: Our survey article with Hoory and Wigderson

The combinatorial definition

A graph $G = (V, E)$ is said to be ϵ-edge-expanding if for every partition of the vertex set V into X and $X^c = V \setminus X$, where X contains at most a half of the vertices, the number of cross edges

$$e(X, X^c) \geq \epsilon |X|.$$

In words: in every cut in G, the number of cut edges is at least proportionate to the size of the smaller side.

The combinatorial definition (contd.)

The edge expansion ratio of a graph $G = (V, E)$, is

$$h(G) = \min_{S \subseteq V,\, |S| \leq |V|/2} \frac{|E(S, \overline{S})|}{|S|}.$$

This is the combinatorial analogue of Cheeger's constant.

The linear-algebraic perspective

The **Adjacency Matrix** of an n-vertex graph G, denoted $A = A(G)$, is an $n \times n$ matrix whose (u, v) entry is the number of edges in G between vertex u and vertex v. Being real and symmetric, the matrix A has n real eigenvalues which we denote by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$.

A combinatorial analogue of the Laplacian.

Some simple things the spectrum of $A(G)$ tells about G

- If G is d-regular, then $\lambda_1 = d$. The corresponding eigenvector is $v_1 = \mathbf{1}/\sqrt{n}$
- The graph is connected iff $\lambda_1 > \lambda_2$. We call $\lambda_1 - \lambda_2$ the spectral gap.
- The graph is bipartite iff $\lambda_1 = -\lambda_n$
- $\chi(G) \geq -\frac{\lambda_1}{\lambda_n} + 1$
- A substantial spectral gap implies logarithmic diameter.

Spectrum vs. expansion

Theorem 1. *Let G be a d-regular graph with spectrum $\lambda_1 \geq \cdots \geq \lambda_n$. Then*

$$\frac{d-\lambda_2}{2} \leq h(G) \leq \sqrt{(d+\lambda_2)(d-\lambda_2)}.$$

The bounds are tight.

- Left inequality is easy and powerful.
- Right inequality is deeper. It is even surprising but, unfortunately, it is weak.

High expansion can coexist with a poor spectral gap

- The line graph of $G = (V, E)$ is a graph L whose vertex set is $E(G)$.
- Two vertices in L are adjacent if the corresponding edges in G share a vertex.
- If G is d-regular, then L is $(2d - 2)$-regular.
- If G is an excellent expander, then so is L.
- The first eigenvalue of L is $2d - 2$ and the second one is $> d$. This spectral gap is poor (compared e.g., with Ramanujan Graphs).

Random walks on expanders converge rapidly

Consider $\hat{A} = \frac{1}{d}A(G)$, the normalized adjacency matrix (i.e. the transition matrix of the random walk on G).

Theorem 2. *Let G be an (n,d)-graph with $|\lambda_2|, |\lambda_n| \leq \alpha d$. Then for any distribution vector $\mathbf{p}$ and any positive integer t:*

$$\|\hat{A}^t\mathbf{p} - \mathbf{u}\|_2 \leq \|\mathbf{p} - \mathbf{u}\|_2 \alpha^t \leq \alpha^t$$

where $\mathbf{u}$ is the uniform (=limit) distribution on $V(G)$.

How do you measure speed of convergence?

Even this can be done in many different ways:

- L_2 distance of the random walk's distribution to the limit distribution. This is essentially equivalent to spectral gap.
- Same with L_1 ("total variation") - the traditional measure in probability.
- Other norm?
- K-L divergence (a common way of measuring distance among distributions) to the limit distribution. In the regular case this means - how fast does the entropy converge. This leads to the study of log-Sobolev inequalities.

What would make us happy and why do we complain?

We need to capture "expansion" in a way that

- Is efficiently computable (eigenvalues are good for this).
- Works well at different scales of size (the combinatorial definition works fine at every scale).
- Extends naturally to contexts more general than graphs.

Is there a combinatorial equivalent to spectral gap?

Granted, it is fairly surprising that expansion (a combinatorial condition) and spectral gap (a linear-algebraic condition) are qualitatively equivalent. However, for a long time I was wondering if the spectral gap can also be quantitatively captured in combinatorial terms.
This was solved in joint work with Yonatan Bilu. It is based on the notion of discrepancy.

A main reason why expanders are so important for computer science is their pseudo-random nature. In many ways, expanders behave as if they were random graphs. One major example of this principle is:

Theorem 3 (The expander mixing lemma). *Let $G = (V, E)$ be a d-regular graph on n vertices, and let $\lambda = \lambda_2(G)$ be the second largest eigenvalue of (the adjacency matrix of) G.*
Then for any two disjoint sets of vertices $X, Y \subseteq V$, the number of edges connecting X and Y satisfies

$$|e(X,Y) - \frac{d}{n}|X||Y|| \le \lambda\sqrt{|X||Y|}$$

Discrepancy and spectral gap are essentially equivalent

Theorem 4 (Yonatan Bilu, L.). *Let $G = (V, E)$ be a d-regular graph on n vertices and suppose that for any two disjoint sets of vertices $X, Y \subseteq V$, the number of edges connecting X and Y satisfies*

$$|e(X,Y) - \frac{d}{n}|X||Y|| \leq \alpha\sqrt{|X||Y|}$$

for some $\alpha > 0$. Then the second eigenvalue of G is at most $O(\alpha \log(\frac{d}{\alpha}))$. The bound is tight

Expansion at different scales

- The combinatorial definition(s) of expansion are very coarse.
- Smaller sets can expand beyond $h(G)$.
- Generally, we define an expansion profile: For every $1 \leq k \leq n$ we define:

$$\Phi_E(G,k) = \min\{|E(S,\bar{S})| : |S| = k\}.$$

- Likewise, the vertex expansion profile:

$$\Phi_V(G,k) = \min\{|\Gamma(S) \setminus S| : |S| = k\}.$$

Understanding expansion profiles

There are many classes of graphs G for which it is desirable to determine/estimate the quantities $\Phi_E(G,k)$ and $\Phi_V(G,k)$. An important example is the d-dimensional cube, where

- The optimal edge isoperimetric sets are sub-cubes.
- The optimal vertex isoperimetric sets are hamming balls.

These facts are applicable in many situations.

The shortcoming of the spectral approach

Theorem 5 (Kahale). *For every (n, d, α)-graph G, every $\rho > 0$ and every set S of $\leq \rho n$ vertices*

$$\Gamma(S) \geq |S|(d/2) \cdot (1 - \sqrt{1 - 4(d-1)/(d^2\alpha^2)}) \cdot (1 - c \log d / \log(1/\rho))$$

Combined with the Alon Boppana bound and with $\rho \to 0$ this yields vertex expansion of $d/2$ for small linear sized sets.

This is nearly tight. A slightly modified Ramanujan graph can have two vertices with the same neighbor set, i.e. expansion $\leq d/2$, but $\lambda(G) \leq 2\sqrt{d-1} + o(1)$.

What's worse...

- Even the (nearly) strongest possible information on the spectral gap yields very little on the expansion of small, linear-sized sets of vertices...
- .... and says essentially nothing about the expansion of sets of $O(\sqrt{n})$ vertices.

The computational difficulty

Theorem 6. *The following computational problem is co-NP hard*

Input: *A graph G, and $\epsilon > 0$.*

Output: *Is G an ϵ-edge-expander?*

The challenge - Methods for estimating expansion

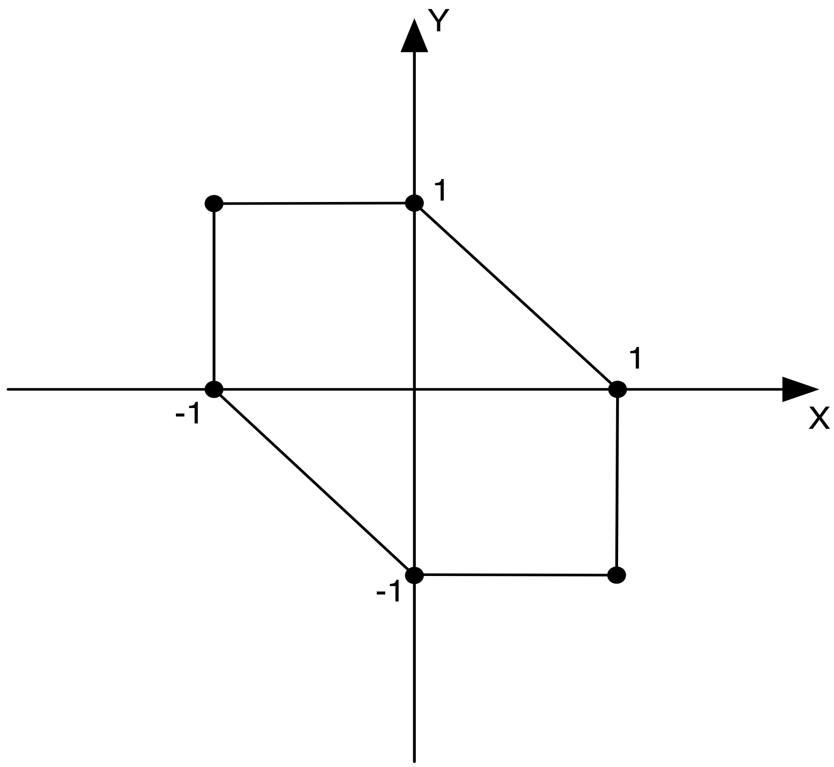
The computational hardness and the limitations of the spectral method make it interesting to develop methods to estimate expansion even for special classes of graphs. E.g. the (old) Margulis Expanders:

Theorem 7 (L. + London). *For any planar set A of finite positive measure,*

$$\frac{|S(A) \cup T(A) \cup A|}{|A|} \geq \frac{4}{3},$$

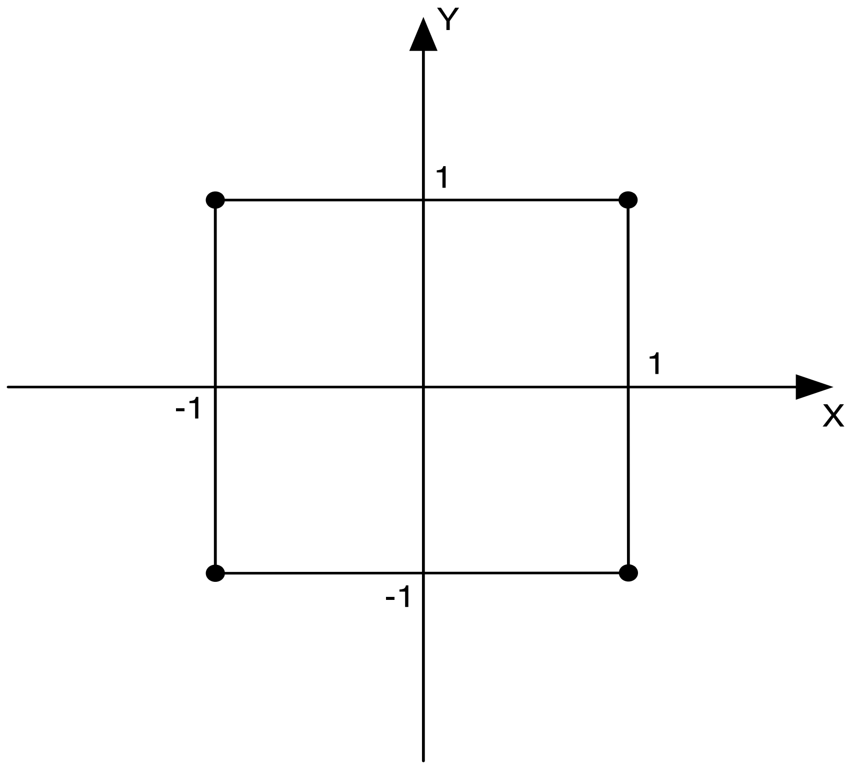
where $S(x, y) = (x, x + y)$, $T(x, y) = (x + y, y)$. The bound $\frac{4}{3}$ is tight.

The extremal example



The hexagon $A = \{(x, y); |x|, |y|, |x + y| \leq 1\}$ has area 3

... and its image



$S(A) \cup T(A) \cup A$ is the square $\{(x,y); |x|, |y| \leq 1\}$ of area 4.

So, what's missing?

Conjecture 1. *The same statement holds when everything is done* $\bmod 1$.

If true that would give the first nontrivial family of expanders with an exactly determined expansion.

Expansion in metric spaces?

The (combinatorial) definition of expansion can be naturally extended to general metric spaces (For every set S of size $\leq n/2$ at least $(1+\epsilon)|S|$ elements of the space are at distance $\leq \delta$ from S.)

To make this definition useful it may be necessary to impose additional conditions that hold in (say regular) graphs but not necessarily in general metric spaces. E.g.

$$|B(2r, x)| \leq O(|B(r, x)|^2).$$

Much remains to be studied here.

...and while we are at it...

Random walks (and diffusion, heat kernels etc.) on general metric spaces have been considered in the more geometric realm as well in more practically inclined studies (machine learning, computer vision - Clustering, segmentation etc.).
Can this be made rigorous and concrete?

Is there a good connection with metric expansion?.

Expansion at different scales

- We usually start with the extremal problem: What is the largest possible expansion at a given scale. Random graphs are often optimal (or at least close to optimal).

- However, as we'll see, at the small scale, random graphs are often far from being optimal, so even the extremal problems at the small scale are challenging.

- Expansion at small scale is useful for a variety of problems in graph theory (e.g. work by Sudakov, Krivelevich and others).

- ... and for a whole range of problems in theoretical computer science and coding theory.

The expansion of small sets in random graphs

Theorem 8. *Let $d \geq 3$ be a fixed integer. Then for every $\delta > 0$ there exists $\epsilon > 0$ such that:*

1. For almost every (n, d)-graph G and every set S of $\leq \epsilon n$ vertices

$$|E(S, \bar{S})| \geq (d - 2 - \delta)|S|$$
$$|\Gamma(S)| \geq (d - 1 - \delta)|S|.$$

2. For a bipartite G and a one-sided S,

$$|\Gamma(S)| \geq (d - 1 - \delta)|S|.$$

In simple words...

Small (but linear-sized) sets in a random graphs are nearly forests.

As we shall see later, it is very difficult to understand what happens when the nearly is removed and we speak about graphs of high girth.

The constructive challenge

To find explicit constructions of graphs with such excellent expansion parameters at the small scale. Two comments are in order:

- As mentioned, (the best possible) spectral methods allow you to conclude an expansion rate of up to $d/2$. There are several important problems for which this is exactly the threshold for usefulness. Any better bound would be useful...

- Using the technique of zigzag products (which we won't review here), it is possible to make some progress in this direction.

But this is just a tip of something much larger, or, should I say something much smaller?

Local theory of graphs

There is a whole world of wonderful questions that arise from the following perspective: Suppose that you have to investigate a graph that is much too big to be stored and processed by your computer. What can you do? You do not seem to have much choice but to sample sets of vertices

of reasonably small cardinality k and examine the induced subgraph. The questions are:

- What are the possible views at this level? (local problems.)
- What does this view tell you about the graph as a whole? (local-global problems.)

Two local problems

The graph-copy problem: (the very special case $k = 3$). Let G be a large graph and let $p = p(G)$ be the four-dimensional vector where p_i is probability that a random triple of vertices have i induced edges ($i = 0, 1, 2, 3$). Obviously,

$$\sum p_i = 1 \quad p_i \geq 0.$$

So let us consider the following three-dimensional subset of $\mathbb{R}^4$,

$$\{p(G)|G \text{ a graph}\}.$$

Can you describe this set? Its closure? Its convex hull?

Some comments on the graph-copy problem

- $p_0 + p_3 \geq \frac{1}{4} - o(1)$ (Goodman '64).
- Razborov has recently solved the following closely related question: How small can p_3 be in a large graph with given edge density.
- These problems are not as innocent as you might think. They are related to arithmetic progressions in dense sets of integers - a deep and beautiful subject. For a glimpse in this direction, see Trevisan's problem on triangles and diamonds (on Terry Tao's home page).
- The theory of graph limits (Lovász, Szegedy et. al.) provides interesting insights on these problems.

Graphs of high girth

The girth of a graph G is defined as the shortest length of a cycle in G. Define $g(d,n)$ to be the largest possible girth of a d-regular graph on n vertices. The following bounds are known:

$$(2+o(1))\frac{\log n}{\log(d-1)} \geq g(d,n) \geq (\frac{4}{3}-o(1))\frac{\log n}{\log(d-1)}.$$

- The lower bound is from [LPS].

- The upper bound is very simple ("Moore's bound").

A clarification

...and why is this a local issue?

Because a graph has girth$\geq g$ iff the $\lfloor \frac{g}{2} \rfloor$ ball around each vertex induces a tree.

A heretical conjecture on graphs of high girth

Conjecture 2. *There is an* $\epsilon_0 > 0$ *for which*

$$(2 - \epsilon_0 + o(1))\frac{\log n}{\log(d-1)} \geq g(d,n).$$

This should be contrasted with the trivial

$$(2 + o(1))\frac{\log n}{\log(d-1)} \geq g(d,n).$$

Some evidence for this heresy

- The Moore bound is the graph-theoretic analogue of the sphere-packing bound in coding theory which is known to always be exponentially far from being tight.

- The cases where the Moore bound (in its precise form) is tight are "under control". In particular (Feit, Higman, Biggs) Moore graphs do not exist for any $d \geq 3$ and $g \geq 13$. This is analogous to the characterization of all perfect codes.

- Shlomo Hoory's thesis.

The metrical implications of high girth

Theorem 9 (L., Magen, Naor). *For every $k \geq 3$, the l_2 distortion of every k-regular graph of girth g is at least $\Omega(\sqrt{g})$.*

Two outstanding questions:

Problem 1. *Is it true with $\Omega(g)$ as well?*

The situation in l_1 is even more mysterious:

Problem 2. *Can you prove anything about embedding into l_1?*

... a challenge for combinatorialists

Can you find a proof for

$$g(d,n) \geq (1+\epsilon_0)\frac{\log n}{\log(d-1)}$$

with any $\epsilon_0 > 0$?

There are numerous proof for this inequality with $\epsilon_0 = 0$ (the oldest of which is due to Erdős and Sachs '63), but proving this with a positive ϵ_0 (let alone $\epsilon_0 > \frac{1}{3}$ to improve on [LPS]) seems challenging and interesting.

The shape of things to come - Local-global phenomena in graph theory?

It's a bit scary (premature?) to contemplate, but here is a fantastic example.

Recall the quantitative version of Ramsey's Theorem: Every n-vertex graph contains a clique or an anticlique of cardinality $\Omega(\log n)$. The bound is asymptotically tight.

Conjecture 3 (Erdős-Hajnal). *For every graph H there is an $\epsilon = \epsilon(H) > 0$ such that every n-vertex graph which does not contain an induced copy of H has a clique or an anticlique of cardinality $\geq \Omega(n^{\epsilon})$.*

Why induced?

By the quantitative version of Ramsey's Theorem, if G is an n-vertex graph that contains no k-clique, then G has a clique of size

$$\geq \Omega\big(n^{1/(k-1)}\big)$$

What's a "large" spectral gap?

An instinct that most combinatorialists have is to ask about any new parameter they encounter "how large/small can it be?"
In this spirit we ask:
Problem 3. *How small can λ_2 be in a d-regular graph? (i.e., how large can the spectral gap get)?*

This was answered as follows:
Theorem 10 (Alon, Boppana).

$$\lambda_2 \geq 2\sqrt{d-1} - o(1)$$

The largest possible spectral gap and the number $2\sqrt{d-1}$

A good approach to extremal combinatorics and questions of the form "How large/small can this parameter get" is to guess a/the extremal case (the ideal example), and show that there are no better instances.
What, then, is the ideal expander?
Funny answer: It's the infinite d-regular tree. Do you see why?
In fact, something like eigenvalues (spectrum) can also be defined for infinite graphs. It turns out that the supremum of the spectrum for the d-regular infinite tree is....

$$2\sqrt{d-1}$$

Can we emulate phenomena from infinite graphs in the finite realm?

Part of the business of asking extremal problems is to ask for any bound you find whether it is tight.

Problem 4. *Are there d-regular graphs with second eigenvalue*

$$\lambda_2 \leq 2\sqrt{d-1} \quad ?$$

When such graphs exist, they are called Ramanujan Graphs.

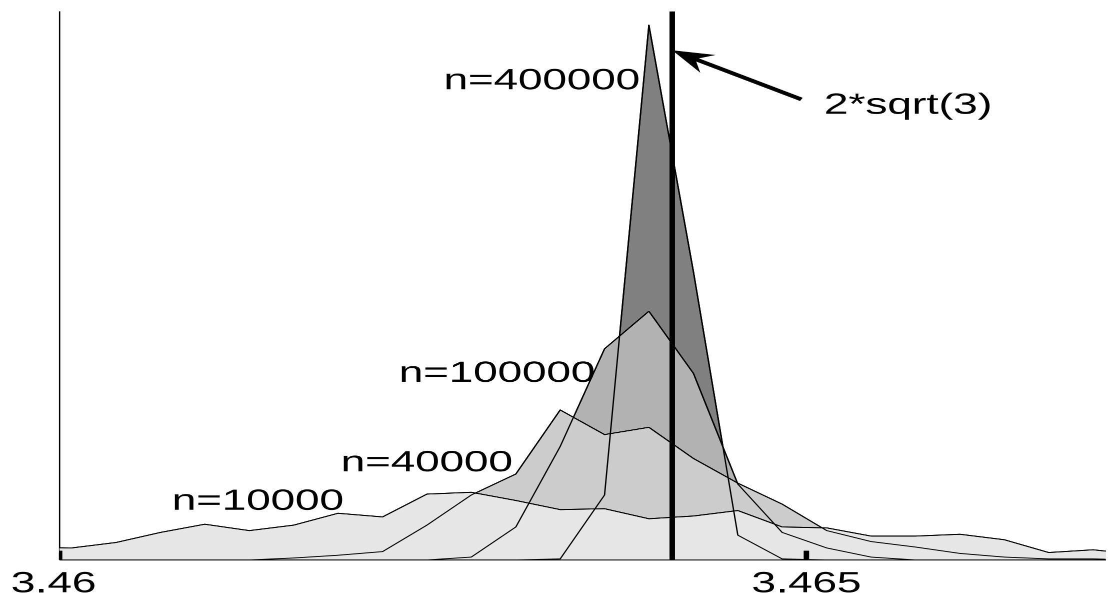
We also want to understand the typical behavior.

Problem 5. *How likely is a (large) random d-regular graph to be Ramanujan?*

A few words about Ramanujan Graphs

Margulis; Lubotzky-Phillips-Sarnak; Morgenstern: d-regular Ramanujan Graphs exist when $d-1$ is a prime power. The construction is easy, but the proof uses a lot of heavy mathematical machinery.

Friedman: If you are willing to settle for $\lambda_2 \leq 2\sqrt{d-1}+\epsilon$, they exist. Moreover, almost every d-regular graph satisfies this condition.


n=400000
2*sqrt(3)
n=100000
n=40000
n=10000
3.46
3.465

Some open problems on Ramanujan Graphs

- Can we construct arbitrarily large d-regular Ramanujan Graphs for every d? Currently no one seems to know. $d = 7$ is the first unknown case.

- Can we find elementary methods of proof for graphs with large spectral gap (or even Ramanujan)? Some recent progress: constructions based on random lifts of graphs (Bilu-L.) can get $\lambda_2 \leq O(\sqrt{d}\log^{3/2} d)$.

The signing conjecture

The following, if true, would prove the existence of arbitrarily large d-regular Ramanujan graphs for every $d \geq 3$.

Conjecture 4. *Every d regular graph G has a signing with spectral radius $\leq 2\sqrt{d-1}$.*

A signing is a symmetric matrix in which some of the entries in the adjacency matrix of G are changed from $+1$ to -1. The spectral radius of a matrix is the largest absolute value of an eigenvalue.

This conjecture, if true, is tight.

Expansion at various size scales

- We have defined expansion in terms of worst-case. In particular a d-regular graph can have edge expansion at most $(1 - o(1))\frac{d}{2}$. On the other hand, in almost every d-regular graph, sets S of size $|S| \leq \epsilon n$ have at least $(d - 2 - \delta)|S|$ neighbors.
  (For every $d \geq 3$ and for every $\delta \geq 0$ there is an $\epsilon > 0$ such that in a random d-regular graph the following holds with probability $\geq 1 - \delta$: Every set S of $\leq \epsilon n$ vertices has $(d - 2 - \delta)|S|$ outside neighbors.)

- By a result of Kahale such conclusions cannot be derived from spectral information. Can we explicitly construct such graphs? The zig-zag method by Reingold-Vadhan-Wigderson goes a long way in this direction, but the problem is still far from being resolved.

- This is also closely related to the girth problem: What is the largest $g = g(n, d)$ such that there exist d-regular graphs on n vertices with no cycles of length $< g$?

- Even more generally this leads to local-global problems on graphs. How can a large graph look at the micro level? How does this affect the graph's global properties?

More computationally-motivated challenges

There are many nice properties that expanders may have which we are still unable to accomplish.

Problem 6. *Can we construct expanders on which can efficiently solve:*

- *Shortest path problems.*
- *Routing problems.*

Problem 7. *Which NP-hard computational problem on graph remain hard when restricted to expander graphs? Is the situation similar to what you see with random graphs?*

Enough with eigenvalues. What about the eigenvectors?

There is a rich and classical theory concerning the eigenvectors of Laplacians of Riemannian Manifolds. Is there an interesting analogous theory for graphs?

If A is the adjacency matrix of a graph $G = (V, E)$ and f is an eigenfunction of A. Let $C = C_f \subseteq E$ be the set of edges on which f changes sign i.e., those edges $xy \in E$ for which $f(x)f(y) \leq 0$.

The connected components of the graph $G \setminus C$ are called the nodal domains of f.

If $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ are the eigenvalues of A with the corresponding eigenfunctions $f_1, f_2, \ldots, f_n$, then a classical theorem of Courant says (I am a bit sloppy here, but this is precise e.g. when G has no repeated eigenvalues).

Theorem 11 (Courant's Nodal Domain Theorem). *The eigenfunction f_k has at most k nodal domains.*

Eigenvectors of graphs (contd.)

We started with some numerical experiments that show very clearly:
Numerical Observation 1. *For almost every graph every eigenfunction has exactly two nodal domains.*

In addition, it seems (from experiments) that:

Numerical Observation 2. *For every* $1 > p > 0$ *and every* n *large enough, almost every graph every eigenfunction of a graph in* $G(n, p)$ *has exactly two nodal domains.*

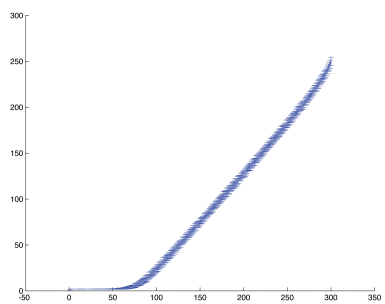
Eigenvectors of graphs - What we already know

Theorem 12 (Yael Dekel, James Lee, L.). *For every $1 > p > 0$ there is a constant C, such that for almost every graph from $G(n, p)$, every eigenfunction has one positive domain and one negative domain which together contain all but at most C of the n vertices.*

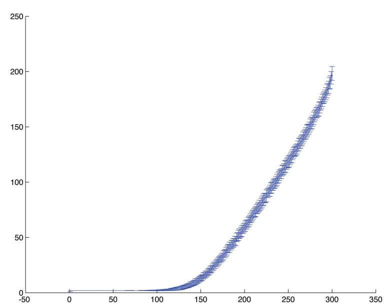
Eigenvectors of graphs - What we'd like to know

Experiments with random regular graphs reveal the "great blue yonder"

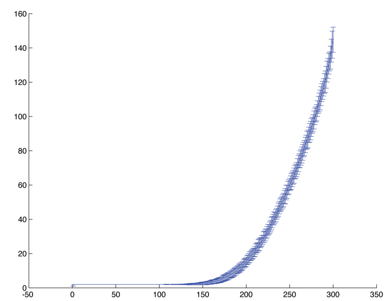
$d = 3$



$d = 4$



$d = 5$



Moving up in dimension

Problem 8. *Is there a theory of expander hypergraphs?*

More concretely:

Problem 9. *How do you generate random 3-uniform hypergraphs that cover each edge d times? (Random Steiner Triple Systems.)*

What about a theory of random hypergraphs?

Here there is already a beginning of theory (work of Meshulam $+$ L.). In particular, for higher-dimensional simplicial complexes there are several natural notions of connectedness and there is some progress in understanding the threshold functions in the 2-dimensional and higher situation.