Shannon Entropy and Bipartite Graphs

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- IT inspires work in combinatorics and graph theory.
- Entropy-based proofs in extremal combinatorics (focus of this talk).
- This interplay between IT $\leftrightarrow$ Discrete Math has been proved fruitful.

Results of mutual interest to IT & CS researchers.

Proposition (Shearer's Lemma)

Let

- $X_1, \ldots, X_n$ *be discrete random variables,*
- $\mathcal{S}_1, \ldots, \mathcal{S}_m \subseteq [1:n]$ *include every element* $i \in [1:n]$ *in* at least $k \geq 1$ *of these subsets.*

Then,

$$k \, \mathrm{H}(X^n) \leq \sum_{j=1}^{m} \mathrm{H}(X_{\mathcal{S}_j}),$$

with $X^n \triangleq (X_1, \ldots, X_n)$.

A Nice Geometric Application of Shearer's Lemma

Problem

Let $\mathcal{P} \subseteq \mathbb{R}^3$ be a set of points that has at most r projections on each of the XY, XZ and YZ planes. How large can this set be ?

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Solution

$$|\mathcal{P}| \leq r^{\frac{3}{2}}.$$

The bound on the cardinality of $\mathcal{P}$ is achieved by a grid of $\sqrt{r} \times \sqrt{r} \times \sqrt{r}$ points, provided that r is a square of an integer.

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- Pick uniformly at random a point $(X, Y, Z) \in \mathcal{P}$.
- $\Rightarrow\ \mathrm{H}(X, Y, Z) = \log|\mathcal{P}|$.

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- $\Rightarrow \ \mathrm{H}(X, Y, Z) = \log |\mathcal{P}|$.
- By Shearer's lemma,

$$2\,\mathrm{H}(X, Y, Z) \leq \mathrm{H}(X, Y) + \mathrm{H}(X, Z) + \mathrm{H}(Y, Z).$$

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- At most r projections of $\mathcal{P}$ on each of the XY, XZ and YZ planes

$$\Rightarrow \ \mathrm{H}(X, Y) \leq \log r, \quad \mathrm{H}(X, Z) \leq \log r, \quad \mathrm{H}(Y, Z) \leq \log r.$$

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$$\Rightarrow \; \mathrm{H}(X, Y) \leq \log r, \quad \mathrm{H}(X, Z) \leq \log r, \quad \mathrm{H}(Y, Z) \leq \log r.$$

- This gives

$$2 \log |\mathcal{P}| \leq 3 \log r \quad \Rightarrow \quad |\mathcal{P}| \leq r^{\frac{3}{2}}.$$

Bipartite Graphs

- A graph G is called bipartite if it has two types of vertices, and an edge $e \in \mathsf{E}(G)$ cannot connect two vertices of the same type.
- The two types of vertices are referred to as left and right vertices.

Applications of Bipartite Graphs

Properties of bipartite graphs are of great interest in, e.g., modern coding theory, and communication networks:

- Tanner graphs.
- LDPC codes.
- Message-passing decoding algorithms operating on bipartite graphs.
- Modelling complex networks by bipartite graphs.

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Notation:

- $\mathcal{I}(G)$ denotes the set of all the independent sets in G.

Theorem (Jeff Kahn, 2001)

If G is a bipartite d-regular graph with n vertices, then

$$\big|\mathcal{I}(G)\big| \leq \big(2^{d+1} - 1\big)^{\frac{n}{2d}}.$$

If $(2d)|n$, then the bound is achieved by a disjoint union of $\frac{n}{2d}$ complete d-regular bipartite graphs $(K_{d,d})$.

He also conjectured the tight bound for general (irregular) bipartite graphs.

J. Kahn, "An entropy approach to the hard-core model on bipartite graphs," *Combinatorics, Probability and Computing*, vol. 10, no. 3, pp. 219–237, May 2001.

J. Kahn, "Entropy, independent sets and antichains: a new approach to Dedekind's problem," *Proceedings of the American Mathematical Society*, vol. 130, no. 2, pp. 371–378, June 2001.

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  - D. Galvin and Y. Zhao, "The number of independent sets in a graph with small maximum degree", March 2011.
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- In 2019, Y. Zhao passed on the challenge to his fearless students at MIT, sophomore Ashwin Sah & junior Mehtaab Sawhney.
- Together with their friend, David Stoner (an undergraduate student from Harvard), they solved this problem in a month !

Their approach, not relying on IT, led to the generalized result:

Theorem (A. Sah, M. Sawhney, D. Stoner and Y. Zhao, 2019)

Let G be an undirected graph without isolated vertices or multiple edges connecting any pair of vertices. Let d_r be the degree of $r \in \mathsf{V}(G)$. Then,

$$\left|\mathcal{I}(G)\right| \leq \prod_{(u,v) \in \mathsf{E}(G)} \left(2^{d_u} + 2^{d_v} - 1\right)^{\frac{1}{d_u \, d_v}},$$

with equality if G is a disjoint union of complete bipartite graphs.

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Publication

https://news.mit.edu/2019/mit-undergraduates-solve-combinatorics-problem-0225

Ashwin Sah, Mehtaab Sawhney, David Stoner and Yufei Zhao, "The number of independent sets in an irregular graph," *Journal of Combinatorial Theory, Series B*, Volume 138, Sept. 2019, pp. 172-195.

Follow-Up Work

The techniques that they found to solve that conjecture quickly led to solve several other related open problems, including "A Reverse Sidorenko Inequality," related to graph colorings and graph homomorphisms.

Kahn's IT Proof (2001) and Left Challenge

- Kahn's proof for regular bipartite graphs made a clever use of Shearer's entropy inequality.
- It remained unclear how to apply Shearer's inequality in a lossless way in the irregular case, despite previous attempts during the last decade (including Sah *et al.*, who proved it in a clever non-IT approach).

Kahn's IT Proof for Regular Bipartite Graphs (2001)

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- Regularity of $G \;\Rightarrow\; |\mathcal{A}| = |\mathcal{B}| = \frac{n}{2}$.

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- Let $\mathcal{S} \subseteq [1:n]$ be an independent set of G, selected uniformly at random from $\mathcal{I}(G)$.
- Let $X_i = \mathbb{1}\{i \in \mathcal{S}\} \in \{0,1\}$, for $i \in [1:n]$, indicating which vertices in G belong to the independent set $\mathcal{S}$.

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- Let $X_i = \mathbb{1}\{i \in \mathcal{S}\} \in \{0,1\}$, for $i \in [1:n]$, indicating which vertices in G belong to the independent set $\mathcal{S}$.
- Uniform selection of $\mathcal{S} \in \mathcal{I}(G) \quad \Rightarrow \quad \mathrm{H}(X_1,\ldots,X_n) = \log\big|\mathcal{I}(G)\big|$.
- Denote $X_{\mathcal{A}} = (X_i)_{i\in\mathcal{A}}$, $X_{\mathcal{B}} = (X_i)_{i\in\mathcal{B}}$.
- $$\mathrm{H}(X_1,\ldots,X_n) = \mathrm{H}(X_{\mathcal{A}}, X_{\mathcal{B}}) = \mathrm{H}(X_{\mathcal{A}}) + \mathrm{H}(X_{\mathcal{B}}|\,X_{\mathcal{A}}).$$

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- G is bipartite $\Rightarrow \mathcal{N}(b) \subseteq \mathcal{A}$ for all $b \in \mathcal{B}$.

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- G is bipartite $\Rightarrow$ $\mathcal{N}(b) \subseteq \mathcal{A}$ for all $b \in \mathcal{B}$.
- $$\mathrm{H}(X_{\mathcal{B}} | X_{\mathcal{A}}) \leq \sum_{b \in \mathcal{B}} \mathrm{H}(X_b | X_{\mathcal{A}}) \leq \sum_{b \in \mathcal{B}} \mathrm{H}(X_b | X_{\mathcal{N}(b)}).$$

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- For $b \in \mathcal{B}$, let
$$Q_b \triangleq \mathbb{1}\{\mathcal{S} \cap \mathcal{N}(b) = \emptyset\}$$
be the indicator function of the event that non of the neighbors of b is included in the independent set $\mathcal{S}$.

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- $Q_b = 0 \Rightarrow b \notin \mathcal{S}$ ($\exists$ neighbor of b in $\mathcal{S}$) $\Rightarrow \mathrm{H}(X_b|Q_b = 0) = 0$.
- $Q_b = 1 \Rightarrow X_b \in \{0, 1\}$ and equiprobable $\Rightarrow \mathrm{H}(X_b|Q_b = 1) = 1$ [bits]. (it is equiprobable since $\mathcal{S} \in \mathcal{I}(G)$ is random with equiprobable dist.).

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- By DPI,

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$$\omega_b \triangleq \Pr[Q_b = 1], \quad b \in \mathcal{B},$$

then

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- Combining all this gives

$$\mathrm{H}(X_{\mathcal{B}} | X_{\mathcal{A}}) \leq \sum_{b \in \mathcal{B}} \omega_b.$$

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$$\mathrm{H}(X_{\mathcal{A}}) \leq \frac{1}{d} \sum_{b \in \mathcal{B}} \mathrm{H}\big(X_{\mathcal{N}(b)}\big).$$

- Since the binary RV Q_b is uniquely determined by the vector $X_{\mathcal{N}(b)} \in \{0,1\}^d$, for all $b \in \mathcal{B}$,

$$\begin{aligned} \mathrm{H}\big(X_{\mathcal{N}(b)}\big) &= \mathrm{H}\big(X_{\mathcal{N}(b)}, Q_b\big) \\ &= \mathrm{H}(Q_b) + \mathrm{H}\big(X_{\mathcal{N}(b)} | Q_b\big) \\ &= \mathsf{H_b}(\omega_b) + \mathrm{H}\big(X_{\mathcal{N}(b)} | Q_b\big). \end{aligned}$$

Kahn's IT Proof (Cont.)

- Recall that $\omega_b \triangleq \Pr[Q_b = 1]$, so

$$\mathrm{H}\big(X_{\mathcal{N}(b)} | Q_b\big) = \omega_b \, \mathrm{H}\big(X_{\mathcal{N}(b)} | Q_b = 1\big) + (1 - \omega_b) \, \mathrm{H}\big(X_{\mathcal{N}(b)} | Q_b = 0\big).$$

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- If $Q_b = 1$, then $i \notin \mathcal{S}$ for all $i \in \mathcal{N}(b)$, so $X_{\mathcal{N}(b)}$ is a zero vector.

$$\Rightarrow \mathrm{H}\big(X_{\mathcal{N}(b)} | Q_b = 1\big) = 0, \quad b \in \mathcal{B}.$$

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- If $Q_b = 0$, then $X_{\mathcal{N}(b)} \in \{0,1\}^d$ cannot be a zero vector (there exists at least one element $i \in \mathcal{N}(b)$ in $\mathcal{S}$).

$$\Rightarrow \mathrm{H}\big(X_{\mathcal{N}(b)} | Q_b = 0\big) \leq \log(2^d - 1), \quad b \in \mathcal{B}.$$

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- Combining all this, gives

$$\mathrm{H}(X_{\mathcal{A}}) \leq \frac{1}{d} \sum_{b \in \mathcal{B}} \Big\{ \mathsf{H_b}(\omega_b) + (1-\omega_b) \, \log(2^d - 1) \Big\}.$$

Kahn's IT Proof (Cont.)

Overall (with $\log$ on base 2),

$$\begin{aligned}
\log\bigl|\mathcal{I}(G)\bigr| &= \mathrm{H}(X_1, \dots, X_n) \\
&= \mathrm{H}(X_{\mathcal{B}} | X_{\mathcal{A}}) + \mathrm{H}(X_{\mathcal{A}}) \\
&\leq \sum_{b \in \mathcal{B}} \omega_b + \frac{1}{d} \sum_{b \in \mathcal{B}} \Bigl\{ \mathsf{H_b}(\omega_b) + (1-\omega_b)\, \log(2^d - 1) \Bigr\} \\
&= \frac{1}{d} \sum_{b \in \mathcal{B}} \left\{ \mathsf{H_b}(\omega_b) + \omega_b\, \log\left(\frac{2^d}{2^d - 1} \right) \right\} + \frac{n}{2d}\, \log(2^d - 1).
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Let $f \colon [0,1] \to \mathbb{R}$ be given by

$$f(x) \triangleq \mathsf{H_b}(x) + x \log\biggl(\frac{2^d}{2^d - 1} \biggr), \quad x \in [0,1].$$

$$\Rightarrow \qquad \max_{x \in [0,1]} f(x) = f\biggl(\frac{2^d}{2^{d+1} - 1} \biggr).$$

Kahn's IT Proof (Cont.)

$$\begin{aligned}\log\bigl|\mathcal{I}(G)\bigr| &\leq \frac{1}{d}\sum_{b\in\mathcal{B}}\left\{\mathsf{H_b}(\omega_b)+\omega_b\,\log\left(\frac{2^d}{2^d-1}\right)\right\}+\frac{n}{2d}\,\log(2^d-1)\\ &\leq \frac{|\mathcal{B}|}{d}\,f\left(\frac{2^d}{2^{d+1}-1}\right)+\frac{n}{2d}\,\log(2^d-1)\\ &= \frac{n}{2d}\left[f\left(\frac{2^d}{2^{d+1}-1}\right)+\log(2^d-1)\right]\\ &= \frac{n}{2d}\,\log(2^{d+1}-1),\end{aligned}$$

which gives, after exponentiation of both sides,

$$\bigl|\mathcal{I}(G)\bigr| \leq \left(2^{d+1}-1\right)^{\frac{n}{2d}}.$$

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- $|\,\mathsf{V}(K_{d,d})| = 2d.$
- If $(2d)|n$, and G is a bipartite graph of $\frac{n}{2d}$ separate $K_{d,d}$ subgraphs, then
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The entropy-based upper bound is tight for regular bipartite graphs.

Tensor Product

The tensor product $G \times H$ of two graphs G and H is a graph such that

- The vertex set of $G \times H$ is the Cartesian product $\mathsf{V}(G) \times \mathsf{V}(H)$,
- Two vertices $(g, h), (g', h') \in \mathsf{V}(G \times H)$ are adjacent

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Graph K_2

The graph $K_2 \triangleq K_{1,1}$ is specialized to two vertices that are connected by an edge. We label the two vertices in K_2 by 0 and 1.

Bipartite Double Cover

For a graph G, the tensor product $G \times K_2$ is a bipartite graph, called the bipartite double cover of G.

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An edge $(u, v) \in \mathsf{E}(G)$ is mapped into edges

- $\big((u, 0), (v, 1)\big) \in \mathsf{E}(G \times K_2)$
- $\big((v, 0), (u, 1)\big) \in \mathsf{E}(G \times K_2)$

(G is undirected).

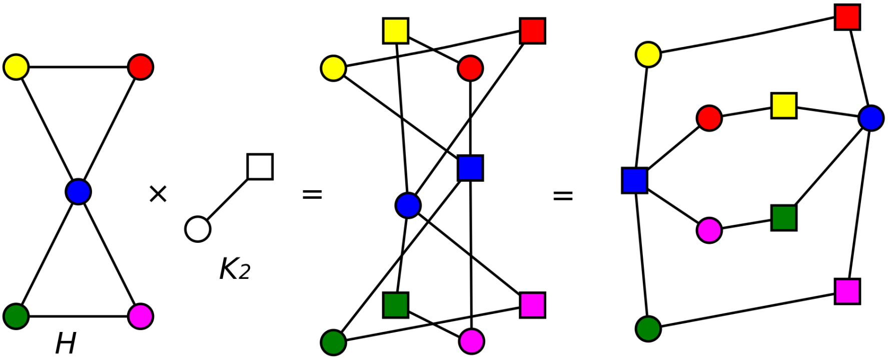

Figure: A graph G (left) and the bipartite double cover $G \times K_2$ (right). (The figure is reproduced from wikipedia.)

Zhao's Inequality

Theorem (Zhao 2010)

For every finite graph G: $\big|\mathcal{I}(G)\big|^2 \leq \big|\mathcal{I}(G \times K_2)\big|.$

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- $$\Rightarrow \quad \left|\mathcal{I}(G)\right|^2 \leq \left|\mathcal{I}(G \times K_2)\right| \leq (2^{d+1} - 1)^{\frac{2n}{2d}},$$

  and taking square roots implies that Khan's inequality continues to hold even when the regular graph G is not necessarily bipartite.

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  and taking square roots implies that Khan's inequality continues to hold even when the regular graph G is not necessarily bipartite.
- The same kind of a simple extension can be done from bipartite (irregular) graphs to general graphs (Galvin & Zhao, 2011).

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A Recent Publication

I. Sason, "A generalized information-theoretic approach for bounding the number of independent sets in bipartite graphs," *Entropy*, vol. 23, no. 3, paper 270, pp. 1–14, March 2021.

Outline of our Analysis

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- some complications that arise from the non-regularity of the bipartite graphs,
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It deviates from Khan's proof already at its starting point, by a proper adaptation to the general setting of irregular bipartite graphs.

Outline of our Analysis

- Consider a general bipartite graph G with a number of vertices $|\mathsf{V}(G)| = n$, and where none of its vertices is isolated.
- Label the vertices by the elements of $[1 : n]$.
- Let $\mathcal{L}$ and $\mathcal{R}$ be the vertices of the two types in $\mathsf{V}(G)$ (called, respectively, the left and right vertices in G).
- $\mathsf{V}(G) = \mathcal{L} \cup \mathcal{R}$ is a disjoint union.
- Let $\mathcal{D}_{\mathrm{L}}$ and $\mathcal{D}_{\mathrm{R}}$ be, respectively, the sets of all possible degrees of vertices in $\mathcal{L}$ and $\mathcal{R}$.
- Let $X_{\mathcal{L}} = (X_i)_{i \in \mathcal{L}}$ and $X_{\mathcal{R}} = (X_i)_{i \in \mathcal{R}}$.
- For all $d \in \mathcal{D}_{\mathrm{L}}$, let
  - $\mathcal{L}_d$ be the set of vertices in $\mathcal{L}$ with degree d,
  - $\mathcal{R}_d$ be the set of vertices in $\mathcal{R}$ that are adjacent to vertices in $\mathcal{L}_d$.

Outline of our Analysis (Cont.)

$$\begin{aligned}
\mathrm{H}(X^n) &= \mathrm{H}(X_{\mathcal{L}}, X_{\mathcal{R}}) \\
&= \mathrm{H}(X_{\mathcal{L}}) + \mathrm{H}(X_{\mathcal{R}} | X_{\mathcal{L}}) \\
&\leq \sum_{d \in \mathcal{D}_{\mathrm{L}}} \mathrm{H}(X_{\mathcal{L}_d}) + \mathrm{H}(X_{\mathcal{R}} | X_{\mathcal{L}}) \\
&\leq \sum_{d \in \mathcal{D}_{\mathrm{L}}} \mathrm{H}(X_{\mathcal{L}_d}) + \sum_{d \in \mathcal{D}_{\mathrm{L}}} \mathrm{H}(X_{\mathcal{R}_d} | X_{\mathcal{L}}) \\
&= \sum_{d \in \mathcal{D}_{\mathrm{L}}} \big\{ \mathrm{H}(X_{\mathcal{L}_d}) + \mathrm{H}(X_{\mathcal{R}_d} | X_{\mathcal{L}}) \big\},
\end{aligned}$$

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Although the first summand on the RHS of last equality is an entropy of $X_{\mathcal{L}_d}$, the conditioning on $X_{\mathcal{L}}$ (rather than just on $X_{\mathcal{L}_d}$) in the second term is essential for the analysis, while it also leads to a stronger upper bound on $\mathrm{H}(X^n)$ (since $\mathcal{L}_d \subseteq \mathcal{L}$).

Outline of our Analysis (Cont.)

Due to the irregularity of the bipartite graph, for $r \in \mathcal{R}_d$, the set $\mathcal{N}(r)$ is not necessarily a subset of $\mathcal{L}_d$. The following variant of Shearer's lemma is therefore crucial in our analysis.

Outline of our Analysis (Cont.)

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A Variant of Shearer's Lemma

The inequality in Shearer's lemma holds even if the sets $\mathcal{S}_1, \ldots, \mathcal{S}_m$ are not necessarily included in $[1 : n]$.

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The inequality in Shearer's lemma holds even if the sets $\mathcal{S}_1, \ldots, \mathcal{S}_m$ are not necessarily included in $[1:n]$.

Proof

- Define the subsets $\mathcal{S}'_j \triangleq \mathcal{S}_j \cap [1:n]$ for all $j \in [1:m]$.
- The subsets $\mathcal{S}'_1, \ldots, \mathcal{S}'_m$ are all included in $[1:n]$, and every element $i \in [1:n]$ continues to be included in at least $k \geq 1$ of these subsets.
- $\Rightarrow$ Shearer's Lemma can be applied to the subsets $\mathcal{S}'_1, \ldots, \mathcal{S}'_m$.
- $\mathcal{S}'_j \subseteq \mathcal{S}_j \Rightarrow \mathrm{H}(X_{\mathcal{S}'_j}) \leq \mathrm{H}(X_{\mathcal{S}_j})$ for $j \in [1:m]$, proving our claim.

Outline of our Analysis (Cont.)

This gives, after some analysis (following the recipe of Kahn's proof),

$$\log\left|\mathcal{I}(G)\right| = \mathrm{H}(X^n)$$
$$\leq \sum_{d \in \mathcal{D}_{\mathrm{L}}} \left\{ \frac{1}{d} \sum_{r \in \mathcal{R}_d} \left\{ \mathsf{H}_{\mathsf{b}}(\omega_r) + \omega_r \log\left(\frac{2^d}{2^{\mathsf{d}_r} - 1} \right) + \log(2^{\mathsf{d}_r} - 1) \right\} \right\}$$

with

$$Q_r \triangleq \mathbb{1}\{\mathcal{S} \cap \mathcal{N}(r) = \emptyset\},$$
$$\omega_r \triangleq \Pr[Q_r = 1].$$

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with

$$Q_r \triangleq \mathbb{1}\{\mathcal{S}\cap\mathcal{N}(r) = \emptyset\}, \\ \omega_r \triangleq \Pr[Q_r = 1].$$

Maximization over $\omega_r \in [0,1]$ term-by-term (for each $d \in \mathcal{D}_{\mathrm{L}}$) gives

$$\big|\mathcal{I}(G)\big| \leq \prod_{d\in\mathcal{D}_{\mathrm{L}}} \prod_{r\in\mathcal{R}_d} \left(2^d + 2^{\mathsf{d}_r} - 1\right)^{\frac{1}{d}}.$$

Outline of our Analysis (Cont.)

The bound is tight if G is a bipartite graph that is d-regular on one side (w.o.l.o.g., it can be assumed to be regular on the left side), and it may be irregular on the other side:

$$\prod_{r \in \mathcal{R}} \left(2^d + 2^{\mathsf{d}_r} - 1\right)^{\frac{1}{d}} = \prod_{r \in \mathcal{R}} \left(\left(2^d + 2^{\mathsf{d}_r} - 1\right)^{\frac{1}{d\,\mathsf{d}_r}}\right)^{\mathsf{d}_r}$$
$$= \prod_{(u,v) \in \mathsf{E}(G)} \left(2^{\mathsf{d}_u} + 2^{\mathsf{d}_v} - 1\right)^{\frac{1}{\mathsf{d}_u\,\mathsf{d}_v}}.$$

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We prove, however, that this approach leads to a loose bound if the bipartite graph is irregular on both sides of the graph

Number of Walks of a Given Length in Bipartite Graphs

- Lower bounds on the number of walks of a given length in bipartite graphs rely on the work by Alon, Hoory and Linial on the Moore bound and its extension (2002).
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Contribution

New bounds, expressed in terms of entropies of probability mass functions that are induced by the degree distributions of the bipartite graph.

Lower Bounds on the Number of Walks of a Given Length

Proposition

Let

- G *be a bipartite graph,*
- $\mathcal{U}$ *and* $\mathcal{V}$ *be the left and right vertices of* G*.*
- $|\mathcal{U}| = m$ *and* $|\mathcal{V}| = n$*.*

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- $\mathcal{P}_k$ *be the set of walks of length* $k \in \mathbb{N}$ *in* G *(edges may be repeated).*
- d_r *denote the degree of a vertex* $r \in \mathsf{V}(G)$.
- P *and* Q *be PMFs defined, respectively, on* $\mathcal{U}$ *and* $\mathcal{V}$ *as follows:*

$$\mathsf{P}(u) \triangleq \frac{d_u}{|\,\mathsf{E}(G)|}, \quad u \in \mathcal{U},$$

$$\mathsf{Q}(v) \triangleq \frac{d_v}{|\,\mathsf{E}(G)|}, \quad v \in \mathcal{V}.$$

Lower Bounds on the Number of Walks of a Given Length (cont.)

1. If k is odd, then

$$\begin{aligned} \left|\mathcal{P}_k\right| &\geq \left|\,\mathsf{E}(G)\right|^k \exp\left(-\tfrac{1}{2}(k-1)[\mathrm{H}(P)+\mathrm{H}(Q)]\right) \\ &\geq \frac{\left|\,\mathsf{E}(G)\right|^k}{(mn)^{\frac{k-1}{2}}}. \end{aligned}$$

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The last inequality on each of the two cases holds with equality if the bipartite graph G is regular.

Lower Bounds on the Number of Walks of a Given Length (cont.)

Derivation of these lower bounds:

I. Sason, "Entropy-based proofs of combinatorial results on bipartite graphs," *Proceedings of ISIT 2021*, pp. 3225-3230, July 2021.

Counting Independent Sets

It is left for future work to study if our analysis (I.S., Entropy, March '21)

- can be adapted to yield a tight bound on the number of independent sets of a bipartite graph when both sides of the graph are irregular;
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Number of Trails and Paths of a Given Length (cont.)

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Thanks a lot, Amos and Prakash, for the organization & invitation !