Independent Sets and Graph Energy

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Preliminaries

Let:

- G be a connected, simple, undirected graph on n nodes
- the independence number $\alpha(G) = \alpha$ be the size of the largest set of nodes in G with no edges between them
- $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$ be eigenvalues of the adjacency matrix $A(G) = A$ corresponding to graph G
- n^+ and n^- be the number of positive and negative eigenvalues of A respectively
- the energy of G, $\mathcal{E}(G)$, be defined as

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|$$

Basics

- Since G is simple, A has trace zero
- So, $\operatorname{tr}(A) = \sum_{i=1}^{n} \lambda_i = 0$ which implies

$$\sum_{\lambda_i > 0} \lambda_i + \sum_{\lambda_i < 0} \lambda_i = 0 \iff \sum_{\lambda_i > 0} \lambda_i = -\sum_{\lambda_i < 0} \lambda_i$$

- So,

$$\begin{aligned} \mathcal{E}(G) &= \sum_{i=1}^{n} |\lambda_i| \\ &= \sum_{\lambda_i > 0} \lambda_i - \sum_{\lambda_i < 0} \lambda_i \\ &= 2 \sum_{\lambda_i > 0} \lambda_i \end{aligned}$$

The Problem

Conjecture

Let G be a connected, simple, undirected graph on n nodes. Then

$$\mathcal{E}(G) \geq 2(n - \alpha)$$

Equivalently,

$$\sum_{\lambda_i > 0} \lambda_i \geq n - \alpha$$

Graffiti

- Developed in the mid 1980s, Graffiti is a mainly graph theoretic conjecture-making software
- The program consists of a set of heuristics to eliminate trivially true statements and a library of graphs for proposed, nontrivial conjectures [?]
- Originally proposed by Graffiti, the problem was verified by Liu et al in 2023 for *all* graphs on at most 10 nodes [?].

ChatGPT

ChatGPT 3.5:

Since r is the number of positive eigenvalues, we can say that $r \geq \alpha(G)$ because an independent set of size $\alpha(G)$ would have $\alpha(G)$ non-zero eigenvalues, making r at least as large as $\alpha(G)$.

So, we have:

$\sum_{i=1}^{r} \lambda_i \geq \alpha(G) \times n^{\frac{1}{\alpha(G)}}$

This inequality implies that the sum of positive eigenvalues of the adjacency matrix of a graph is greater than or equal to the number of nodes minus the independence number of the graph.

ChatGPT 4:

Bounding the Sum of Non-positive Eigenvalues:

Since there are at least $n - \alpha(G)$ non-positive eigenvalues, we can bound their sum:

$$\sum_{i=k+1}^{n} \lambda_i \leq -(n - \alpha(G)).$$

This follows because the sum of these non-positive eigenvalues is negative and there are at least $n - \alpha(G)$ such terms.

$n - \alpha << \alpha$

One useful bound for the positive sum involving the matching number of the graph:

$$\mu \leq \sum_{\lambda_i > 0} \lambda_i$$

Utilizing Structure

Various graph properties have well-defined connections to graph energy. For example,

- $\sum_{\lambda_i > 0} \lambda_i \geq r$ where r is the radius
- $\sqrt{m} \leq \sum_{\lambda_i > 0} \lambda_i \leq m$ where m is the number of edges

However, this algorithmic thinking is what Graffiti and like-minded programs have tried for 30 years!

Utilizing Algebra

Reframing the problem in matrix theoretic terms may provide some insight. There is an α by α principal submatrix of A containing all zeroes such that $\lambda_k(A) \leq 0 \leq \lambda_{n-\alpha+k}$ for all $i = 1, 2, ..., \alpha$ via the Interlacing Theorem. So,

$$\begin{aligned} n - \alpha \leq \sum_{\lambda_i > 0} \lambda_i &\iff n \leq \sum_{i=n-\alpha+1}^{n} \lambda_i + \alpha \\ &\iff n \leq \sum_{i=n-\alpha+1}^{n} \lambda_i(A) + \sum_{i=n-\alpha+1}^{n} \lambda_i(\mathbb{I}_n) \\ &\iff \operatorname{tr}(A + \mathbb{I}_n) \leq \sum_{i=n-\alpha+1}^{n} \lambda_i(A + \mathbb{I}_n) \end{aligned}$$

Fundamental Facts About Graphs

- From Cvetković, we know $\alpha(G) \leq \min\{n - n^-, n - n^+\}$ [?].
- Thus, if proven true or proven true for a specific subset of graphs, the conjecture immediately implies $\sum_{\lambda_i > 0} \lambda_i \geq \max\{n^-, n^+\}$.
- Moreover, since $\sum_{\lambda_i > 0} \lambda_i = -\sum_{\lambda_i < 0} \lambda_i$, we can also say

$$1 \leq \frac{1}{n^+} \sum_{\lambda_i > 0} \lambda_i \quad \text{and} \quad 1 \leq \frac{1}{n^-} \sum_{\lambda_i < 0} |\lambda_i|$$

In other words, for a connected, simple, undirected graph, the average positive and average negative eigenvalue must be larger than 1.

Applications

- Graph energy has intimate ties with π-electron energy in molecules
- The most computationally efficient algorithm to find an independent set is $\mathcal{O}(1.1996^n)$ derived by Xiao in 2017 [?]
- Meanwhile, the most efficient algorithms for finding eigenvalues of a symmetric matrix are about $\mathcal{O}(n^2)$
- For a field with a wide variety of applications, computational savings in spectral graph theory is ideal!

Conclusion

Thanks!

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References