Inequalities Related to Spectral Graph Theory

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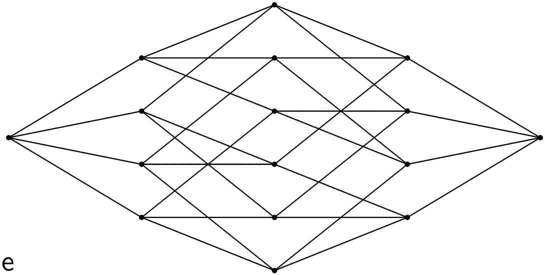
Distance Matrices

1. Throughout let $G = (VG, EG)$ be a connected graph of order n and diameter D.
2. Let A_i be the i-th distance matrix, i.e., an $n \times n$ matrix with rows and columns indexed by the vertex set VG such that

$$(A_i)_{uv} = \begin{cases} 1, & \text{if } \partial(u,v) = i; \\ 0, & \text{else.} \end{cases}$$

3. In particular, $A_0 = I$ is the identity matrix and $A_1 = A$ is the adjacency matrix.

The 4-cube



The 4-cube

$A_0 + A_1 + A_2 + A_3 + A_4 = J$ of 4-cube

$$\begin{pmatrix}
1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1\\
1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1\\
1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1\\
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1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1\\
1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1
\end{pmatrix}$$

The inner product

Definition

For two $n \times n$ symmetric matrices M, N over $\mathbb{R}$, define

1. the inner product $\langle M, N \rangle := \frac{1}{n} \sum_{i,j} M_{ij} N_{ij}$,
2. the norm $\|M\| := \sqrt{\langle M, M \rangle}$, and
3. the projection of M into N

$$\text{Proj}_N(M) := \frac{\langle N, M \rangle}{\|N\|^2} N.$$

Remark

1. Note that $A_0, A_1, \ldots, A_D$ form an orthogonal basis of the space they span.
2. The study of how a given matrix projects into some space spanned by $A_0, A_1, \ldots, A_D$ has long been concerned.
3. For example, the study of error-correcting codes concerns with finding a large subset $C \subseteq VG$ and a larger integer i such that

$$\mathrm{Proj}_{A_{\geq i}}(J_C) = J_C,$$

where

$$(J_C)_{xy} := \begin{cases} 1, & \text{if } x, y \in C \text{ and } x \neq y; \\ 0, & \text{else,} \end{cases}$$

and

$$A_{\geq i} := A_i + A_{i+1} + \cdots + A_D.$$

Perron-Frobenius vector

1. Let λ_0 be the largest eigenvalue of A with corresponding eigenvector α, normalized to have $< \alpha, \alpha >= n$.
2. Note that $\alpha = (1, 1, \ldots, 1)^T$ iff G is regular.
3. In general a nonnegative irreducible matrix M has a unique largest real eigenvalue, whose corresponding eigenvector has positive entries. The eigenvector is generally referred as the Perron-Frobenius vector of M.
4. The study of Perron-Frobenius vector receives much attention recently, e.g. from the study of graph flows, google page ranks.

Give A_i some weight

1. Let D_α denote a diagonal matrix whose diagonal is the Perron-Frobenius vector α of A.
2. Hence G is regular if $D_\alpha = I$.
3. The matrix $\widetilde{A}_i := D_\alpha A_i D_\alpha$ is called the i-th weighted distance matrix of G.
4. $\widetilde{A}_0, \widetilde{A}_1, \cdots, \widetilde{A}_D$ still form an orthogonal basis of the space they span, which might be different from the space spanned by $A_0, A_1, \ldots, A_D$.
5. Then $\widetilde{A}_0 + \widetilde{A}_1 + \cdots + \widetilde{A}_D = D_\alpha(A_0 + A_1 + \cdots + A_D)D_\alpha = D_\alpha J D_\alpha$.
6. Define $\delta_i := \|\widetilde{A}_i\|^2$, and $\delta_{\geq i} := \delta_i + \delta_{i+1} + \cdots + \delta_D$.
7. Note that δ_i is the "average weights" of vertices at distance i to a vertex.

The space $<A>= \text{Span}(I, A, \cdots, A^d)$

1. Assume the adjacency matrix A has $d+1$ distinct eigenvalues.
2. Then the minimal polynomial of A has degree $d+1$.
3. Thus I, A, $\ldots$, A^d form a basis of the space $<A>$ spanned by I, A, $\ldots$, A^d.
4. We will apply Gram-Schmidt process to the basis I, A, $\ldots$, A^d and obtain an orthogonal basis.

Gram-Schmidt process

1. Set $p'_0(x) = 1$ so that $p'_0(A) = I$.
2. When the polynomial $p'_i(x)$ has been defined with degree$(p'_i(x)) = i$, define

$$p'_{i+1}(A) = A^{i+1} - \sum_{k=0}^{i} \text{Proj}_{p'_k(A)}(A^{i+1})$$

   for $0 \leq i \leq d-1$ recursively.
3. Then $p'_0(A), p'_1(A), \ldots, p'_d(A)$ is an orthogonal basis of the space $<A>$.

Normalization

1. Set
$$p_i(x) = \frac{p'_i(\lambda_0)}{\|p'_i(A)\|^2} p'_i(x). \quad (1)$$
2. Then deg $p_i(x) = i$. and
$$< A >= \text{Span}(p_0(A), p_1(A), \cdots, p_d(A)).$$
3. Note that $p_0(A), p_1(A), \ldots, p_d(A)$ is another orthogonal basis of $< A >$ satisfying
$$\|p_i(A)\|^2 = p_i(\lambda_0)$$
for $0 \leq i \leq d$.
4. The $p_i(x)$ is referred as the i-th predistance polynomial of G.

Orthogonality

The spaces

$$\text{Span } (\widetilde{A}_0, \widetilde{A}_1, \ldots, \widetilde{A}_D)$$

and

$$< A >= \text{Span } (p_0(A), p_1(A), \ldots, p_d(A))$$

are not always equal, but they are connected by the orthogonal property:

$$\widetilde{A}_{\geq i} \perp p_{<i}(A),$$

where

$$p_{<i}(A) = p_0(A) + p_1(A) + \cdots + p_{i-1}(A).$$

This can be proved by using the fact that $(A^j)_{xy}$ counts the number of walks of length j from x to y.

Both spaces have the equal sum $H(A) = D_\alpha J D_\alpha$

It turns out that

$$p_0(A) + p_1(A) + \ldots + p_d(A) = H(A) = D_\alpha J D_\alpha = \widetilde{A}_0 + \widetilde{A}_1 + \cdots + \widetilde{A}_D,$$

where $H(x) = p_0(x) + p_1(x) + \cdots + p_d(x)$ is called the Hoffman polynomial of G.

This follows

$$p_0(\lambda_0) + p_1(\lambda_0) + \ldots + p_d(\lambda_0) = n = \delta_0 + \delta_1 + \cdots + \delta_D.$$

Together with

$$\widetilde{A}_{\geq i} \perp p_{<i}(A)$$

shows a well-known fact that

$$D \leq d.$$

Combining orthogonality and equal sum

Lemma

The projection of $p_{\geq i}(A)$ into $\widetilde{A}_{\geq i}$ is $\widetilde{A}_{\geq i}$.

Proof.

$$\begin{aligned}
\text{Proj}_{\widetilde{A}_{\geq i}} p_{\geq i}(A) &= \frac{\langle \widetilde{A}_{\geq i}, p_{\geq i}(A) \rangle}{\delta_{\geq i}} \widetilde{A}_{\geq i} \\
&= \frac{\langle \widetilde{A}_{\geq i}, H(A) \rangle}{\delta_{\geq i}} \widetilde{A}_{\geq i} \\
&= \frac{\langle \widetilde{A}_{\geq i}, \widetilde{A}_{\geq i} \rangle}{\delta_{\geq i}} \widetilde{A}_{\geq i} \\
&= \widetilde{A}_{\geq i}.
\end{aligned}$$

□

Corollary

$\delta_{\geq i} \leq p_{\geq i}(\lambda_0)$ with equality iff $p_{\geq i}(A) = \widetilde{A}_{\geq i}$.

Proof.

This follows from $\mathrm{Proj}_{\widetilde{A}_{\geq i}} p_{\geq i}(A) = \widetilde{A}_{\geq i}$ and the definitions $\|\widetilde{A}_{\geq i}\|^2 = \delta_{\geq i}$ and $\|p_{\geq i}(A)\|^2 = p_{\geq i}(\lambda_0)$. □

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When $i = D$ the above Corollary is referred as the Spectral Excess Theorem. The original Spectral Excess Theorem only considers the regular graphs with $d = D$ essentially.

In the case $i = d = D$ the above inequality in the last page becomes $\delta_D \leq p_D(\lambda_0)$, and equality hold iff $p_D(A) = \widetilde{A}_D$. Together with $p_{D+1}(A) = 0$,

$$p_0(A) + p_1(A) + \ldots + p_d(A) = H(A) = D_\alpha J D_\alpha = \widetilde{A}_0 + \widetilde{A}_1 + \cdots + \widetilde{A}_D,$$

and using the following three-term relations

Lemma

$$x p_i(x) = c_{i+1} p_{i+1}(x) + a_i p_i(x) + b_{i-1} p_{i-1}(x) \qquad 0 \leq i \leq d$$

for some scalars c_{i+1}, a_i, $b_{i-1} \in \mathbb{R}$ with $b_{-1} = c_{d+1} := 0$,

one can in turns prove

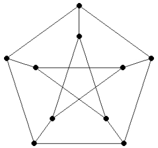
$$p_{D-1}(A) = \widetilde{A}_{D-1}, p_{D-2}(A) = \widetilde{A}_{D-2}, p_{D-3}(A) = \widetilde{A}_{D-3}, \ldots, I = p_0(A) = \widetilde{A}_0.$$

A graph with $D = d$ and all the above equalities is called a distance-regular graph.

As an application we show the following.

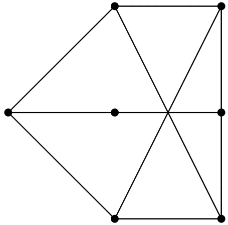
Theorem

A graph whose smallest odd cycle has length $2d+1$ (odd-girth $2d+1$) must be distance-regular. □



Petersen graph has odd-girth

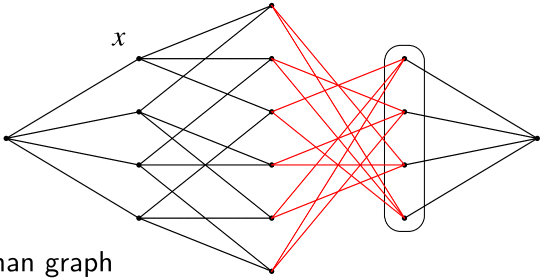
$$5 = 2D+1 = 2d+1.$$



A graph with odd-girth

$$5 = 2D+1 < 2d+1 = 11.$$

Hoffman graph



The Hoffman graph

The Hoffman graph has $d = D = 4$ and $p_i(A) = \widetilde{A}_i$ for $i = 0, 1, 3$, but $p_2(A) \neq \widetilde{A}_2$ and $p_4(A) \neq \widetilde{A}_4$.

The graph P_3

Let G be a path of three vertices. It can be computed that $\lambda_0 = \sqrt{2}$, $d = D = 2$, $\alpha = (\sqrt{3}/2, \sqrt{6}/2, \sqrt{3}/2)^t$, $p_0(x) = 1$, $p_1(x) = 3\sqrt{2}x/4$, $p_2(x) = 3(x^2 - 4/3)/4$, and

$$I + \frac{3\sqrt{2}}{4}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} + \begin{pmatrix} -1/4 & 0 & 3/4 \\ 0 & 1/2 & 0 \\ 3/4 & 0 & -1/4 \end{pmatrix}$$

$$= \begin{pmatrix} 3/4 & 3\sqrt{2}/4 & 3/4 \\ 3\sqrt{2}/4 & 3/2 & 3\sqrt{2}/4 \\ 3/4 & 3\sqrt{2}/4 & 3/4 \end{pmatrix} = \widetilde{A}_0 + \widetilde{A}_1 + \widetilde{A}_2.$$

Hence $I = p_0(A) \neq \widetilde{A}_0$, $p_1(A) = \widetilde{A}_1$, and $p_2(A) \neq \widetilde{A}_2$.

Suppose $D = d$. We are interested in determining the family $\mathscr{S}$ containing the subsets $S \subseteq \{1, 2, \ldots, D\}$ such that $p_i(A) = \widetilde{A}_i$ for $i \in S$ implies the distance-regularity. For example $\{D\} \in \mathscr{S}$ by spectral excess theorem, and $\{D-1\}, \{D-3, D-1\} \notin \mathscr{S}$ from the above two examples.

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By using three-term relations and their variations, we can prove

Theorem

Suppose $D = d$. Then $\{D-2, D-1\} \in \mathscr{S}$.

Theorem

Suppose G is bipartite and $D = d$. Then $\{D-4, D-2\} \in \mathscr{S}$.

Theorem

Suppose $D = d$. Then $\{D-1, D-3, D-5, \ldots\} \notin \mathscr{S}$.

Even though $\{D-1\} \notin \mathscr{S}$, some regularities on G still can be found.

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Theorem

Suppose G is bipartite with $D = d$, and $p_{D-1}(A) = \widetilde{A}_{D-1}$. Then the following holds.

(i) $p_i(A) = \widetilde{A}_i$ for $i = D-3, D-5, \ldots$.

(ii) If D is odd then G is regular.

(iii) If D is even then G is regular or bi-regular.

We are also interested in determining the family $\mathscr{S}'$ containing the subsets $S' \subseteq \{1,2,\ldots,D\}$ such that the assumption

$$p_{>D}(A) + \sum_{i\in S'} p_i(A) = \sum_{i\in S'} \widetilde{A}_i$$

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Theorem

Suppose $D = d$. Then $\{1,2,\ldots,D-1\} \in \mathscr{S}'$.

Theorem

Suppose G is bipartite and $D = d$. Then $\{D-2, D-4, D-6, \ldots\} \in \mathscr{S}'$.

Theorem

Suppose G is bipartite (without assuming $D = d$). Then $\{D-1, D\} \in \mathscr{S}'$.

Back to the inequalities

We have shown that $\delta_{\geq i} \leq p_{\geq i}(\lambda_0)$.

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For the case $i = 0$, we have

$$(\alpha_1^4 + \alpha_2^4 + \cdots + \alpha_n^4)/n = \delta_0 \geq p_0(\lambda_0) = 1,$$

which can be easily proved directly by using Cauchy-Schwarz inequality and using $\alpha_1^2 + \alpha_2^2 + \cdots + \alpha_n^2 = n$.

Questions

1. Is it easy to obtain a direct proof of $\delta_{\leq i-1} \geq p_{\leq i-1}(\lambda_0)$ for $i \geq 1$ as we have deon for $i = 0$ in previous page?

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4. What is the relation among the $(D+1)$-spaces

$$\text{Span}(p_0(A), p_1(A), \ldots, p_{i-1}(A), \widetilde{A}_i, \widetilde{A}_{i+1}, \ldots, \widetilde{A}_D)$$

for $1 \leq i \leq D$.

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Thanks for your attention.