Distance spectral radius of trees

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Let $G = (V, E)$ be a connected simple graph with $n = |V|$ vertices.

- For vertices $u, v \in V$, the distance d_{uv} is defined as the length of the shortest path between u and v in G
- Distance matrix $D = (d_{uv})_{u,v \in V}$ is a symmetric real matrix, with real eigenvalues
- Distance spectral radius of G, denoted as $\rho(G)$, is the largest eigenvalue of the distance matrix $D(G)$.
- Distance energy $DE(G)$ is a newly introduced molecular graph-based analog of the total π-electron energy, and it is defined as the sum of the absolute eigenvalues of distance matrix

$$DE(G) = \sum_{i=1}^{n} |\rho_i|.$$

Let T be a tree with $n > 2$ vertices and let $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$ be the eigenvalues of $D = D(T)$ arranged in a non-increasing order. Merris obtained an interlacing inequality involving the distance and Laplacian eigenvalues of T

$$0 > -\frac{2}{\mu_1} \geq \rho_2 \geq -\frac{2}{\mu_2} \geq \rho_3 \geq \cdots \geq -\frac{2}{\mu_{n-1}} \geq \rho_n,$$

where $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ are the Laplacian eigenvalues of T.

The distance spectra of trees and unicyclic graphs has exactly one positive eigenvalue, and

$$DE(G) = 2\rho(G).$$

We will use Rayleigh quotient inequality for the largest eigenvalue

$$\rho \geq \frac{x^T D x}{x^T x} = \frac{2 \sum_{i<j} x_i x_j d_{ij}}{\sum_{i=1}^{n} x_i^2},$$

with equality if and only if x is the eigenvector corresponding to the largest eigenvalue of D.

Let $e = (u, v)$ be an edge of G such that $G' = G - e$ is also connected, and let D' be the distance matrix of $G - e$. The removal of e may not create shorter paths than the ones in G, and therefore $D_{ij} \leq D'_{ij}$ for all $i, j \in V$. Moreover, $1 = D_{uv} < D'_{uv}$ and by Perron-Frobenius theorem, we conclude that

$$\rho(G) < \rho(G - e).$$

Similarly, we have

$$\rho(G) > \rho(G + e).$$

The complete graph K_n has minimal distance spectral radius among graphs on n vertices,

$$\rho(G) \geq n-1.$$

The star S_n is the unique graph with minimal distance spectral radius among trees on n vertices,

$$\rho(G) \geq \rho(S_n) = n-2+\sqrt{(n-2)^2+(n-1)}.$$

The path P_n is the unique graph with maximal distance spectral radius among trees on n vertices,

$$\rho(G) \leq \rho(P_n) = \frac{n^2}{2a^2} - \frac{2+a^2}{6a^2} + o\left(\frac{1}{n^2}\right),$$

where a is the root of $\tanh a = 1$ ($a \approx 1.99679$).

- Distance energy is a useful molecular descriptor in QSPR modeling, as demonstrated by Consonni and Todeschini;
- Balaban et al. proposed the use of $\rho(G)$ as a molecular structure descriptor in mathematical chemistry;
- It was successfully used to infer the extent of branching and model boiling points of alkanes (Gutman);
- Bapat et al. showed various connections between distance matrix $D(G)$ and Laplacian matrix of a graph;
- Zhou, Trinajstić and Indulal provided upper and lower bounds for $\rho(G)$ in terms of the number of vertices, Wiener index and Zagreb index.

$$W(G) = \sum_{u,v \in V} d_{uv}$$

For $k \geq 1$, we denote by $G(v, k)$ the graph obtained from $G \cup P_k$ by adding an edge between v and the end vertex of P_k.

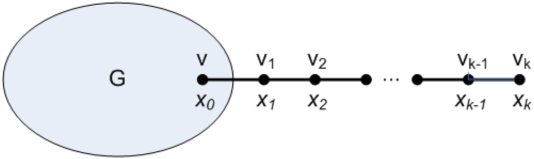

Figure: Principal eigenvector components in $G(v, k)$.

Let x be a positive eigenvector of $G(v, k)$, corresponding to $\rho = \rho(G(v, k))$. Denote by x_0 the component of x at v, and by $x_1, x_2, \ldots, x_k$ the components of x along P_k.

Lemma

Let S be the sum of components of the Perron vector x of $G(v,k)$. Then there exists constants $a_k = a(\rho, S, x_0, k)$ and $b_k = b(\rho, S, x_0, k)$, such that

$$x_i = a_k t_1^i + b_k t_2^i, \qquad 0 \leq i \leq k,$$

where $t_{1,2} = 1 + \frac{1}{\rho} \pm \frac{\sqrt{2\rho+1}}{\rho}$.

From the eigenvalue equation $\rho x = Dx$, written for the components x_{j-1}, x_j and x_{j+1}, for $1 \leq j \leq k-1$, we obtain the recurrence equation

$$2\rho x_j + 2x_j = \rho x_{j-1} + \rho x_{j+1}.$$

For components x_{k-1} and x_k, we have

$$\rho x_{k-1} = x_k + \sum_{u \in G} (d_{uv} + k - 1) x_u + \sum_{i=0}^{k-2} (k - 1 - i) x_i,$$

$$\rho x_k = x_{k-1} + \sum_{u \in G} (d_{uv} + k) x_u + \sum_{i=0}^{k-2} (k - i) x_i,$$

and

$$\rho x_k - \rho x_{k-1} = S - 2x_k.$$

We may use the recurrence equation to formally extend the sequence $x_0, x_1, \ldots, x_k$ with new terms $x_{k+1}, x_{k+2}, \ldots$, so that it represents a particular solution. Finally,

$$a_k = \frac{1}{1 + t_1^{2k+1}} \left(x_0 + \frac{S}{\rho} \frac{t_1^{k+1}}{t_1 - 1} \right),$$

$$b_k = \frac{1}{1 + t_1^{2k+1}} \left(x_0 t_1^{2k+1} - \frac{S}{\rho} \frac{t_1^{k+1}}{t_1 - 1} \right).$$

For $k, l \geq 0$, we denote $G(v, k, l)$ the graph obtained from $G \cup P_k \cup P_l$ by adding edges between v and one of the end vertices in both P_k and P_l.

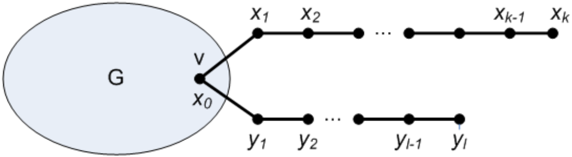

Figure: Principal eigenvector components in $G(v, k, l)$.

Lemma

Let x be a positive eigenvector of $G(v, k, l)$, corresponding to $\rho = \rho(G(v, k, l))$. Denote by x_0 the component of x at v, by $x_1, \ldots, x_k$ the components of x along P_k, starting with the vertex of P_k adjacent to v, and by $y_1, \ldots, y_l$ the components of x along P_l, starting with the vertex of P_l adjacent to v. If $k \geq l$, then

$$\sum_{i=0}^{k} x_i \geq \sum_{j=0}^{l} y_j.$$

Let S denote the sum of components of x, and let $t = 1 + \frac{1}{\rho} + \frac{\sqrt{2\rho+1}}{\rho}$.

$$\begin{aligned}\sum_{i=1}^{k} x_i &= \sum_{i=1}^{k} a_k t^i + b_k / t^i \\ &= a_k \frac{t(t^k-1)}{t-1} + b_k \frac{t^k-1}{t^k(t-1)} \\ &= \frac{1}{1+t^{2k+1}} \left(x_0 \frac{t(t^{2k}-1)}{t-1} + \frac{S}{\rho} \frac{t(t^k-1)(t^{k+1}-1)}{(t-1)^2} \right), \\ &= x_0 f(k) + \frac{S}{\rho} g(k),\end{aligned}$$

where

$$f(x) = \frac{t(t^{2x}-1)}{(1+t^{2x+1})(t-1)} \quad \text{and} \quad g(x) = \frac{t(t^x-1)(t^{x+1}-1)}{(1+t^{2x+1})(t-1)^2}.$$

Furthermore, the functions $f(x)$ and $g(x)$ are monotonically increasing.

Theorem

Let G be a simple graph and v one of its vertices. If $k \geq l \geq 1$, then

$$\rho(G(v,k,l)) < \rho(G(v,k+1,l-1)).$$

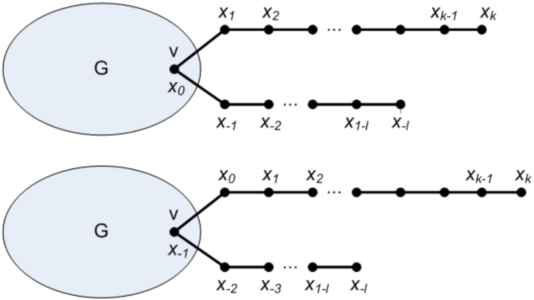

Figure: Graphs $G(v,k,l)$ and $G(v,k+1,l-1)$.

Theorem (Stevanović and Ilić 2010)

Let $T \not\cong B(n, \Delta)$ be an arbitrary tree on n vertices with the maximum vertex degree Δ. Then

$$\rho(B(n, \Delta)) > \rho(T).$$

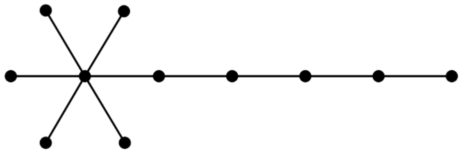

Figure: *The broom tree $B(n, \Delta)$ for $n = 11$ and $\Delta = 6$.*

Among trees on n vertices and maximum degree Δ, the broom $B(n, \Delta)$ uniquely minimizes

- the largest eigenvalue of the adjacency matrix
- the Laplacian coefficients (the Wiener index)
- the graph energy

The linear algorithm for constructing a matching of maximum cardinality in the tree T is greedy and based on mathematical induction:

- take an arbitrary pendent vertex v and match it to its parent w;
- remove both vertices from the tree and solve the resulting problem by induction.

It is easy to prove that a perfect matching of a tree is unique when it exists.

Spur $A(n, m)$ is obtained from the star graph S_{n-m+1} by attaching a pendent edge to each of certain $m-1$ non-central vertices of S_{n-m+1}.

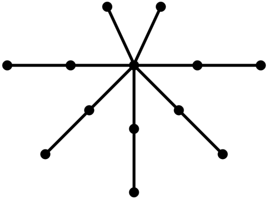

Figure: *The spur* $A(13, 6)$*.*

Among trees on n vertices and matching number m, the spur $A(n, m)$ uniquely minimizes

- the largest eigenvalue of the adjacency matrix
- the Laplacian coefficients (the Wiener index)
- the Hosoya index

Assume there is a pendent path of length $p > 2$ attached at vertex v in the tree T. We can consider new tree T^c that has two pendent paths attached at v, with lengths 2 and $p - 2$. The matching number of trees T and T^c is the same according to the described algorithm and $\rho(T) > \rho(T^c)$.

We can assume that all pendent paths have length one or two.

Let T be an arbitrary tree and let v be a vertex with degree $p + q + 1$. Suppose that w is a parent of v and that there are p paths P_3 (two additional vertices) and q paths P_2 (pendent edges) attached at v. Let G be the maximal subtree of T rooted at w, that does not contain vertex v.

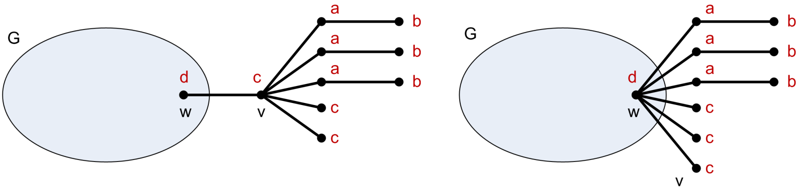

Figure: *Tree T and transformed tree T'.*

After transformation $T \mapsto T'$, the distances from the vertices with the Perron coordinates a, b and c (except v) to all vertices from G decreased by one, while the distances from v to all vertices not in G increased by one. Therefore,

$$\rho(T) > \rho(T').$$

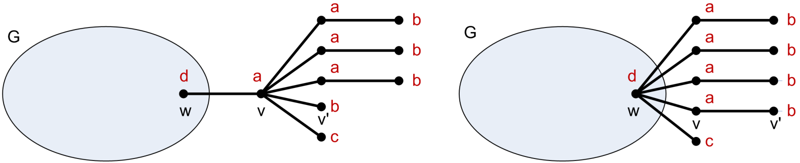

Figure: *Tree T and transformed tree T''.*

After transformation $T \mapsto T''$, the distances from vertices with Perron coordinates a, b and c to all vertices from G decreased by one, except for the vertices v and v', while the distances from v and v' to all vertices not in G increased by one. Therefore,

$$\rho(T) > \rho(T''),$$

if there is at least one vertex u from G, with a pendent path P_3 attached at u; or there are at least three pendent vertices in G.

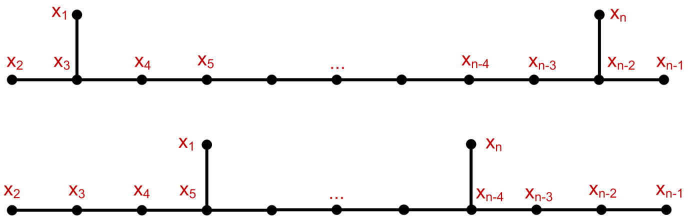

Figure: *Special case – trees T and T^*.*

By direct verification it follows that $\rho(T) > \rho(T^*)$ for $n \geq 9$.

- If $q = 0$, then it follows $m(T') = m(T)$, while $\rho(T') < \rho(T)$.
- If the vertex w is not perfectly matched, there exists a matching M of maximum cardinality, such that no edge from M is incident to w. It follows that

$$m(T') = m(G \setminus \{w\}) + p + 1 = m(G) + p + 1 = m(T).$$

- If the vertex w is perfectly matched and $q > 0$, for every matching M of maximum cardinality, there exists an edge from M incident to w (this edge is not vw). Obviously,

$$m(T'') = m(G) + p + 1 = m(T).$$

Theorem (Ilić 2010)

Let T be an arbitrary tree on $n \geq 4$ vertices with the matching number $1 \leq m \leq \lfloor n/2 \rfloor$. Then,

$$\rho(T) \geq \rho(A(n,m)),$$

with equality if and only if $T \cong A(n,m)$.

Corollary

Among n-vertex trees with matching number m, the spur tree $A(n,m)$ minimizes the distance energy.

Let $C(n, \Delta)$ be a Δ-starlike tree $T(1, n - 2\Delta + 2, 2, 2, \ldots, 2)$ consisting of a central vertex v, one pendent edge attached at v, one pendent path of length $n - 2\Delta + 2$ and $\Delta - 2$ pendent paths of length 2 attached at v.

Theorem

Among trees with perfect matching and maximum degree Δ, the tree $C(n, \Delta)$ has maximal distance spectral radius.

Using the transformation $G(k, l) \mapsto G(k+1, l-1)$, we have chain of inequalities

$$\rho(S_n) = \rho(B(n, n-1)) < \cdots < \rho(B(n, 3)) < \rho(B(n, 2)) = \rho(P_n)$$

$$\rho(S_n) = \rho(A(n, 1)) < \rho(A(n, 2)) < \cdots < \rho(A(n, \lfloor n/2 \rfloor))$$

- $B(n, 3)$ has the second maximum distance spectral radius among trees on n vertices
- $A(n, 2)$ has the second minimum distance spectral radius among trees on n vertices

A complete Δ-ary tree is defined as follows. Start with the root having Δ children. Every vertex different from the root, which is not in one of the last two levels, has exactly $\Delta - 1$ children. While in the last level all nodes need not exist, those that do fill the level consecutively.

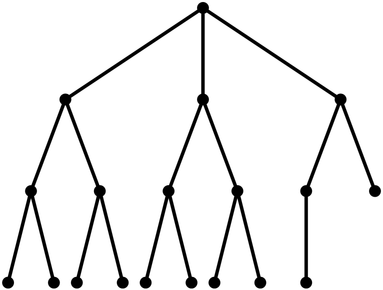

Figure: *The complete 3-ary tree of order* 19.

Volkmann et al. showed that among trees on n vertices with maximum degree Δ, a complete Δ-ary tree minimizes Wiener index.

Based on the computer search among trees with up to 24 vertices and great correlation between the Wiener index and distance spectral radius of trees, we pose the following

Conjecture

A complete Δ-ary tree has the minimum distance spectral radius $\rho(T)$ among trees on n vertices with maximum degree Δ.

The dumbbell $D(n, a, b)$ consists of the path P_{n-a-b} together with a independent vertices adjacent to one pendent vertex of P and b independent vertices adjacent to the other pendent vertex.
Dankelmann showed that

$$W(T) \leq W(D(n, \left\lceil \frac{n+1}{2} \right\rceil - m, \left\lfloor \frac{n+1}{2} \right\rfloor - m)),$$

with equality if and only if $G \cong D(n, \lceil \frac{n+1}{2} \rceil - m, \lfloor \frac{n+1}{2} \rfloor - m)$.

Conjecture

Among trees on n vertices and matching number m, the dumbbell $D(n, \lceil \frac{n+1}{2} \rceil - m, \lfloor \frac{n+1}{2} \rfloor - m)$ is the unique tree that maximizes the distance spectral radius.

Theorem

Among trees on n vertices with diameter d, the caterpillar $C_{n,d}$, obtained from the path P_d with all pendant vertices attached at the center vertex of P_d, has minimal spectral radius.

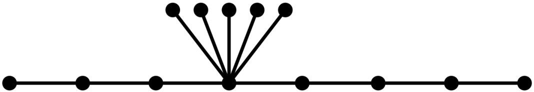

Figure: *Extremal tree $C_{13,7}$.*

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Thank you!