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On the maximal energy among orientations of a tree

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Abstract

The trace norm of a digraph is the trace norm of its adjacency matrix, i.e. the sum of its singular values. Given a bipartite graph G, it is well known that the sink-source orientations have minimal trace norm among all orientations of G. In this paper, we show that the balanced orientations of G attain the maximal trace norm when G is a tree with separated branching vertices, or when G is a double-star tree. We give examples of trees (with adjacent branching vertices) where non-balanced orientations have maximal trace norm. This raises the question in general: Which orientations of a tree have maximal trace norm?

Keywords: Extremal values; digraph; orientation of a tree; trace norm

1. Introduction

One main topic in chemical graph theory is the study of topological indices over graphs (Ali *et al.*, 2016; Abdo *et al.*, 2017). In this work, we are particularly interested in the energy over orientations of a tree. The *energy of a graph* G with n vertices is defined as $\mathcal{E}(G) = \sum_{k=1}^{n} |\lambda_k|$, where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix $A = (a_{jk})$, defined as $a_{jk} = 1$ if there is an edge between j and k and 0 otherwise. The concept of graph energy was proposed by Gutman (1978), and now it is a well-developed theory. For further details on the energy of graphs we refer to Li *et al.* (2012) and the recent papers by Zhu & Yang (2018), Jahanbani (2018), Ashraf (2019) and Ma (2019). Motivated by interesting mathematical results obtained for graph energy, various energy-like quantities have been proposed and studied in the mathematico-chemical literature. These were based on the eigenvalues of other matrices associated to the graph. For instance, the *Laplacian energy* of a graph (Gutman & Zhou, 2016), the *signless Laplacian energy* (So *et al.*, 2010; Abreu *et al.*, 2011), the *normalized Laplacian energy* (Cavers *et al.*, 2010; Allem *et al.*, 2016) and the closely related *Randić energy* (Das *et al.*, 2015; Li *et al.*, 2015; Maden, 2015), the *distance energy* (Indulal *et al.*, 2008; Ramane *et al.*, 2008), the *matching energy* (Gutman & Wagner, 2012) among others (see also (Haemers, 2012; Gutman *et al.*, 2016; Milovanović & Milovanović, 2016)). For more details on energies of graphs, we refer to (Gutman & Li, 2016).

How can we extend the concept of energy to directed graphs? Recall that a *directed graph* (or just a *digraph*) D consists of a non-empty finite set $\mathcal{V}$ of elements called *vertices* and a finite set $\mathcal{A}$ of ordered pairs of distinct vertices called *arcs*. Two vertices are called *adjacent* if they are connected by an arc. If there is an arc from vertex u to vertex v, then we indicate this by writing uv. The *in-degree* (resp. *out-degree*) of a vertex v, denoted by $d^-(v)$ (resp. $d^+(v)$) is the number of arcs of the form uv (resp. vu), where $u \in \mathcal{V}$. A vertex v in D is called a *sink vertex* if $d^+(v) = 0$ and is called a *source vertex* if $d^-(v) = 0$. A vertex v for which $d^+(v) = d^-(v) = 0$ is called an *isolated vertex*.

A digraph D is *symmetric* if, for each $uv \in \mathcal{A}$, $vu \in \mathcal{A}$ too. A one-to-one correspondence between graphs and symmetric digraphs is given by $G \rightsquigarrow \widehat{G}$, where $\widehat{G}$ has the same vertex set as the graph G, and each edge uv of G is replaced by a pair of symmetric arcs uv and vu. Under this correspondence, a graph can be identified with a symmetric digraph. On the other hand, a digraph containing no symmetric pair of arcs is called an *oriented graph*. Thus, an oriented graph D is obtained from a graph G by replacing each edge uv of G by an arc uv or vu, but not both, resulting in an *orientation* of G. We denote by $D^{\top}$ the orientation of G obtained from D by reversing all arrows, which is called the *transpose* of D.

The *adjacency matrix* $A = A(D)$ of a digraph D whose vertex set is $\{v_1, \ldots, v_n\}$ is the $n \times n$ matrix whose entry a_{ij} is defined as

$$a_{ij} = \begin{cases} 1 & \text{if} \quad v_i v_j \in \mathcal{A} \\ 0 & \quad \text{otherwise} \end{cases}.$$

The *characteristic polynomial* of D, denoted by ϕ_D, is the characteristic polynomial $|zI - A|$ of the adjacency matrix A. Likewise, the *eigenvalues* of D are those of A.

One way of extending the concept of energy to digraphs was proposed in (Peña & Rada, 2008) as the sum of the absolute values of the real parts of the eigenvalues of the digraph. Defined so, the Coulson integral formula is applicable. It is a powerful tool to study extrema value problems of the energy in significant classes of digraphs. Another approach to the energy of digraphs was put forward by Adiga *et al.* (2010). They studied the *skew energy* defined as the sum of the absolute values of the eigenvalues of the skew-adjacency matrix. The *skew Laplacian energy* of a digraph was considered in (Adiga & Smitha, 2009). Several other energies of digraphs were studied in (Pirzada & Bhat, 2014; Khan *et al.*, 2017).

However, in this paper, our concern is the approach to the energy of digraphs given by Nikiforov (2007) and Kharaghani & Tayfeh-Rezaie (2008). The *trace norm* of the digraph D, denoted by $\|D\|_*$, is defined as the trace norm of its adjacency matrix. In other words, $\|D\|_* = \sum_{i=1}^{n} \sigma_i$, where $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$ are the singular values of A, i.e. the principal square roots of the eigenvalues of $AA^{\top}$. When D is a symmetric digraph (equivalently, a graph), and $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of A, then $\sigma_i = |\lambda_i|$ for all $i = 1, \ldots, n$ and $\|D\|_* = \sum_{i=1}^{n} |\lambda_i| = \mathcal{E}(D)$, the graph energy introduced by Gutman (1978).

Upper and lower bounds of the trace norm of digraphs were studied in (Agudelo & Rada, 2016; Kharaghani & Tayfeh-Rezaie, 2008). Extrema value problems of the trace norm were determined over oriented trees (Agudelo *et al.*, 2016), oriented unicyclic graphs (Monsalve & Rada, 2019) and oriented bicyclic graphs (Monsalve *et al.*, 2019). In another direction, Monsalve & Rada (2019) showed that among all orientations of a given bipartite graph G, the sink-source orientations of G (i.e. orientations in which all vertices are sink or source vertices) have minimal trace norm. This is a consequence of the following result.

Theorem 1.1 *(Monsalve & Rada, 2019, Theorem 2.5) Let G be a graph. Then*

$$\mathcal{E}(G) \leqslant 2\,\|D\|_* \tag{1}$$

for any orientation D of G. Moreover, equality occurs in Equation (1) if and only if D is a sink-source orientation of G.

A natural question arises:

Problem 1.2 *Among all orientations of a (bipartite) graph, which have the maximal trace norm?*

In the set of trees with separated branching vertices, i.e. trees in which no two branching vertices are adjacent, the *balanced orientations* have the maximal trace norm (Theorem 2.4). This is no longer true when the tree has adjacent branching vertices, as we can see in Example 2.6. However, we show that for double-star trees, or equivalently, the trees with diameter 3 (see Trevisan *et al.* (2011) for results over this class), the balanced orientations again have maximal trace norm (Corollary 3.3). In general, Problem 1.2 remains open even for trees.

The results presented here strongly rely on a theorem of Ky Fan (Day & So, 2007; Fan, 1951). Let us denote by $\sigma_1(M) \geq \sigma_2(M) \geq \cdots \geq \sigma_n(M) \geq 0$ the singular values of the $n \times n$ matrix M.

Theorem 1.3 *(Day & So, 2007; Fan, 1951) Let X, Y and Z be square matrices of order n, such that $Z = X + Y$. Then*

$$\sum_{k=1}^{n} \sigma_i(Z) \leqslant \sum_{k=1}^{n} \sigma_i(X) + \sum_{k=1}^{n} \sigma_i(Y)$$

Equality holds if and only if there exists an orthogonal matrix P, such that PX and PY are both positive semidefinite.

2. Maximal trace norm on orientations of a tree with separated branching vertices

In order to study the problem of maximal trace norm among all orientations of a given tree, we need to generalize Theorem 8 (So *et al.*, 2010). Recall that the coalescence of the digraphs D and E with respect to the vertices $u \in V(D)$ and $v \in V(E)$, denoted by $D \circ E$, is the digraph obtained from D and E by identifying u and v.

Theorem 2.1 *Let $D \circ E$ be the coalescence of the digraphs D and E with respect to the vertices $u \in V(D)$ and $v \in V(E)$. Then*

$$\|D \circ E\|_* \leqslant \|D\|_* + \|E\|_* .$$

Moreover, equality holds if and only if one of the conditions holds:

1. *u is a sink vertex and v is a source vertex (or vice versa);*
2. *u is an isolated vertex;*
3. *v is an isolated vertex.*

Proof. We conveniently label the vertices of $D \circ E$ so that the adjacency matrix $A = A(D \circ E)$ has the form

$$A = \begin{bmatrix} A(D-u) & x & 0 \\ y^\top & 0 & z^\top \\ 0 & w & A(E-v) \end{bmatrix},$$

where x and w are column vectors, $y^\top$ and $z^\top$ are row vectors,

$$A(D) = \begin{bmatrix} A(D-u) & x \\ y^\top & 0 \end{bmatrix},$$

and

$$A(E) = \begin{bmatrix} 0 & z^\top \\ w & A(E-v) \end{bmatrix}.$$

Let

$$B = \begin{bmatrix} A(D-u) & x & 0 \\ y^\top & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

and

$$C = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & z^\top \\ 0 & w & A(E-v) \end{bmatrix}.$$

Note that $A = B + C$, and so by Theorem 1.3

$$\begin{aligned} \|D \circ E\|_* &= \|A\|_* \\ &\leqslant \|B\|_* + \|C\|_* \\ &= \|D\|_* + \|E\|_* . \end{aligned}$$

To see the second part of the theorem, assume that u is a sink vertex and v is a source vertex. Then $y = 0$ and $w = 0$; hence A is a diagonal block matrix

$$A = \left[\begin{array}{cc|c} A(D-u) & x & 0 \\ \hline 0 & 0 & z^\top \\ 0 & 0 & A(E-v) \end{array}\right],$$

which clearly implies $\|D \circ E\|_* = \|D\|_* + \|E\|_*$. This is similarly true if u is a source vertex and v is a sink vertex.

If u is an isolated vertex then $x = y = 0$. Again, A is a block diagonal matrix, then

$$A = \begin{bmatrix} A(D-u) & 0 \\ 0 & A(E) \end{bmatrix}.$$

Since u is an isolated vertex then $\|A(D-u)\|_* = \|A(D)\|_*$ and so $\|D \circ E\|_* = \|D\|_* + \|E\|_*$. Similarly if v is a isolated vertex.

Conversely, assume that $\|D \circ E\|_* = \|D\|_* + \|E\|_*$. Then by Theorem 1.3, there exists an orthogonal matrix

$$P = \begin{bmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{bmatrix}$$

partitioned in blocks according to A, such that PB and PC are positive semidefinite. Then $P^\top P = I$ implies that

$$\begin{aligned} P_{11}^\top P_{11} + P_{21}^\top P_{21} + P_{31}^\top P_{31} &= I \quad (2) \\ P_{13}^\top P_{13} + P_{23}^\top P_{23} + P_{33}^\top P_{33} &= I \quad (3) \\ P_{11}^\top P_{13} + P_{21}^\top P_{23} + P_{31}^\top P_{33} &= 0. \quad (4) \end{aligned}$$

Note that the matrices

$$PB = \begin{bmatrix} P_{11}R + P_{12}y^\top & P_{11}x & 0 \\ P_{21}R + P_{22}y^\top & P_{21}x & 0 \\ P_{31}R + P_{32}y^\top & P_{31}x & 0 \end{bmatrix}$$

and

$$PC = \begin{bmatrix} 0 & P_{13}w & P_{12}z^\top + P_{13}S \\ 0 & P_{23}w & P_{22}z^\top + P_{23}S \\ 0 & P_{33}w & P_{32}z^\top + P_{33}S \end{bmatrix}$$

are positive semidefinite. In particular, PB and PC are symmetric matrices, and so $P_{31}x = 0$ and $P_{13}w = 0$. It follows from Equation 4 that

$$\begin{aligned} 0 =& x^\top P_{11}^\top P_{13}w + x^\top P_{21}^\top P_{23}w + x^\top P_{31}^\top P_{33}w \\ =& (P_{21}x)^\top P_{23}w. \end{aligned}$$

Hence $P_{21}x = 0$ or $P_{23}w = 0$.
Case 1: By (Horn & Johnson, 2013, Exercise 7.1.P2), $P_{21}x = 0$ implies $P_{11}x = P_{31}x = 0$. Then by Equation 2

$$\begin{aligned}&x^\top P_{11}^\top P_{11}x + x^\top P_{21}^\top P_{21}x + x^\top P_{31}^\top P_{31}x \\ =&x^\top x \quad \text{i.e.} \quad x = 0.\end{aligned}$$

And so, u is a source vertex.
Case 2: By (Horn & Johnson, 2013, Exercise 7.1.P2), $P_{23}w = 0$ implies $P_{13}w = P_{33}w = 0$. Then by Equation 3

$$\begin{aligned}&w^\top P_{13}^\top P_{13}w + w^\top P_{23}^\top P_{23}w + w^\top P_{33}^\top P_{33}w \\ =&w^\top w \quad \text{i.e.} \quad w = 0.\end{aligned}$$

And so, v is a source vertex.
A similar argument bearing in mind that

$$\left\|A^\top\right\|_* = \left\|B^\top\right\|_* + \left\|C^\top\right\|_*$$

shows that $y = 0$ or $z = 0$. In other words, u is a sink vertex or v is a sink vertex. ■

A *balanced orientation* X of a graph G is an orientation which satisfies $|d^+(u) - d^-(u)| \leqslant 1$ for all vertices u of X. These types of orientations were considered by Monsalve *et al.* (2019), when studying the maximal trace norm among all orientations of bicyclic graphs. In Monsalve *et al.* (2019), Example 2.2, the orientations of a star tree were completely ordered with respect to the trace norm. In fact, if $\overrightarrow{S}_n(x, y)$ denotes the orientation of the star tree with n vertices S_n (Figure 1), where $x + y = n - 1$ and $x \geq 0, y \geq 0$, then

$$\begin{aligned}&\left\|\overrightarrow{S}_n(x, y)\right\|_* \\ =&\sqrt{x} + \sqrt{y} = \sqrt{x} + \sqrt{n-1-x},\end{aligned} \tag{5}$$

and

$$\begin{aligned}
\left\|\overrightarrow{S}_n(0, n-1)\right\|_* &= \left\|\overrightarrow{S}_n(n-1, 0)\right\|_* \\
&< \\
\left\|\overrightarrow{S}_n(1, n-2)\right\|_* &= \left\|\overrightarrow{S}_n(n-2, 1)\right\|_* \\
&< \\
&\vdots \\
&< \\
\left\|\overrightarrow{S}_n(z, n-1-z)\right\|_* &= \left\|\overrightarrow{S}_n(n-1-z, z)\right\|_*,
\end{aligned} \tag{6}$$

where $z = \lfloor (n-1)/2 \rfloor$. In particular, among all orientations of S_n, the maximal trace norm is attained in balanced orientations of S_n.

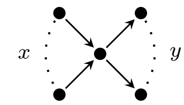

Fig. 1. Orientation of the star

Recall that a *starlike tree* is a tree with a unique branching vertex (i.e. a vertex of degree greater than 2). Now we show that for starlike trees, the balanced orientations attain the maximal trace norm.

Theorem 2.2 *Let T be a starlike tree with branching vertex of degree Δ. Then*

1. For any balanced orientation V of T
$$\begin{aligned}\|V\|_* =&n - 1 - \Delta \\ &+ \sqrt{\left\lfloor \frac{\Delta}{2} \right\rfloor} + \sqrt{\Delta - \left\lfloor \frac{\Delta}{2} \right\rfloor}.\end{aligned}$$
2. The balanced orientations attain the maximal trace norm among all orientations of T.

Proof. 1. Let V be a balanced orientation of T, W the balanced (sub)orientation of the star $S_{\Delta+1}$ induced by V, and let $\overrightarrow{P}_2$ be the orientation of the path P_2. Then clearly $\left\|\overrightarrow{P}_2\right\|_* = 1$ and by Equations 5 and 6

$$\|W\|_* = \sqrt{\left\lfloor \frac{\Delta}{2} \right\rfloor} + \sqrt{\Delta - \left\lfloor \frac{\Delta}{2} \right\rfloor}.$$

Now from the fact that V is a balanced orientation of T, we use the equality condition of Theorem 2.1 to deduce

$$\begin{aligned}\|V\|_* =&(n - 1 - \Delta)\left\|\overrightarrow{P}_2\right\|_* + \|W\|_* \\ =&n - 1 - \Delta \\ &+ \sqrt{\left\lfloor \frac{\Delta}{2} \right\rfloor} + \sqrt{\Delta - \left\lfloor \frac{\Delta}{2} \right\rfloor}.\end{aligned}$$

2. Assume that D is any orientation of T and E is the (sub)orientation of $S_{\Delta+1}$ induced by D. Then again by Theorem 2.1, Equations 5 and 6

$$\begin{aligned}\|D\|_* \leqslant&(n - 1 - \Delta)\left\|\overrightarrow{P}_2\right\|_* + \|E\|_* \\ \leqslant&(n - 1 - \Delta) \\ &+ \left\|\overrightarrow{S}_{\Delta+1}(\lfloor \Delta/2 \rfloor, \Delta - \lfloor \Delta/2 \rfloor)\right\|_* \\ =&n - 1 - \Delta \\ &+ \sqrt{\left\lfloor \frac{\Delta}{2} \right\rfloor} + \sqrt{\Delta - \left\lfloor \frac{\Delta}{2} \right\rfloor}.\end{aligned}$$

■

Let $\mathcal{SL}_n$ denote the set of all starlike trees with n vertices and $\overrightarrow{\mathcal{SL}}_n$ all possible orientations of trees in $\mathcal{SL}_n$. By Agudelo *et al.* (2016), Theorem 2.4, the minimal trace norm over $\overrightarrow{\mathcal{SL}}_n$ is attained in the oriented star trees $\overrightarrow{K}_{1,n-1}$ and $\overrightarrow{K}_{n-1,1}$. We now find the maximal trace norm among all trees in $\overrightarrow{\mathcal{SL}}_n$.

Corollary 2.3 *The balanced orientations of $\overrightarrow{\mathcal{SL}}_n$ with branching vertex of degree 3 have the maximal trace norm over $\overrightarrow{\mathcal{SL}}_n$.*

Proof. This is an immediate consequence of Theorem 2.2, bearing in mind that the function

$$n-1-x+\sqrt{\left\lfloor\frac{x}{2}\right\rfloor}+\sqrt{x-\left\lfloor\frac{x}{2}\right\rfloor}$$

is decreasing for $x \geq 3$. ■

Now based on Theorem 2.2 we find the maximal trace norm among all orientations of a tree T which has separated branching vertices. If v is a vertex of a tree T, we denote by $N(v)$ the set of neighbors of v.

Theorem 2.4 *Let T be a tree with n vertices and k branching vertices $v_1, v_2, \ldots, v_k$ of degree $d_1, \ldots, d_k$, respectively. Suppose that $v_i \notin N(v_j)$ for $1 \leqslant i, j \leqslant k$ and $i \neq j$. Then*

1. For any balanced orientation E of T

$$\begin{aligned}&\|E\|_*\\ &=\left[n-1-\sum_{i=1}^{k} d_i\right]\\ &\quad+\sum_{i=1}^{k}\left[\sqrt{\left\lfloor\frac{d_i}{2}\right\rfloor}+\sqrt{d_i-\left\lfloor\frac{d_i}{2}\right\rfloor}\right].\end{aligned}$$

2. A balanced orientation of T has the maximal trace norm among all orientations of T.

Proof. 1. Let E be a balanced orientation of T. Then each vertex is the coalescence of a sink vertex and a source vertex; hence by the equality condition of Theorem 2.1 and the fact that branching vertices are nonadjacent, we can deduce

$$\begin{aligned}&\|E\|_*\\ &=\left[n-1-\sum_{i=1}^{k} d_i\right]\left\|\overrightarrow{P}_2\right\|_*\\ &\quad+\sum_{i=1}^{k}\left\|\overrightarrow{S}_{d_i+1}(\lfloor d_i/2\rfloor, d_i-\lfloor d_i/2\rfloor)\right\|_*\\ &=\left[n-1-\sum_{i=1}^{k} d_i\right]\\ &\quad+\sum_{i=1}^{k}\left[\sqrt{\left\lfloor\frac{d_i}{2}\right\rfloor}+\sqrt{d_i-\left\lfloor\frac{d_i}{2}\right\rfloor}\right].\end{aligned}$$

2. We use induction on k, the number of branching vertices of T. If $k=1$ then T is a starlike tree and the result follows from Theorem 2.2. Assume that the result holds for trees with less than $k>1$ branching vertices. Let T be a tree with k branching vertices and E an orientation of T. Choose a vertex u of degree 2 between two branching vertices of T. Then E is the coalescence of the two orientations E_1 and E_2 of subtrees T_1 and T_2 of T, with respect to pendant vertices $u_1 \in V(T_1)$ and $u_2 \in V(T_2)$. Then by Theorem 2.1

$$\|E\|_* \leqslant \|E_1\|_* + \|E_2\|_* . \tag{7}$$

Now E_1 and E_2 each have less than k branching vertices, so by induction $\|E_1\|_* \leqslant \|V_1\|_*$ and $\|E_2\|_* \leqslant \|V_2\|_*$, where V_1 and V_2 are balanced orientations of T_1 and T_2, respectively; hence by Equation 7,

$$\|E\|_* \leqslant \|V_1\|_* + \|V_2\|_* .$$

Consider the following cases:

1. u_1 and u_2 are sink vertices (respectively source vertices) of V_1 and V_2, respectively. Then u_1 is a source vertex (respectively a sink vertex) of $V_1^\top$, where $V_1^\top$ is also a balanced orientation of T_1 and by the equality part of Theorem 2.1

$$\begin{aligned}\|V_1\|_* + \|V_2\|_* &= \left\|V_1^\top\right\|_* + \|V_2\|_*\\ &= \left\|V_1^\top \circ V_2\right\|_*,\end{aligned}$$

where $V_1^\top \circ V_2$ is a balanced orientation of T.

2. u_1 is a sink vertex of V_1 and u_2 is a source vertex of V_2 (or viceversa). Then by the equality in Theorem 2.1,

$$\|V_1\|_* + \|V_2\|_* = \|V_1 \circ V_2\|_* ,$$

where $V_1 \circ V_2$ is a balanced orientation of T.

In any case $\|E\|_*$ is less than or equal to the trace norm of a balanced orientation of T. ■

Example 2.5 *In Figure 2 we show some balanced orientations of the given tree T. These have the maximal trace norm among all possible orientations of T by Theorem 2.4.*

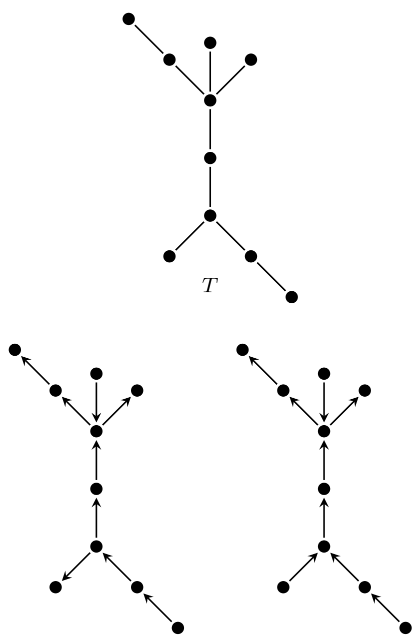

Fig. 2. Some balanced orientations of T

The separation hypothesis of the branching vertices in Theorem 2.4 is necessary, as shown in next example.

Example 2.6 *The non-balanced orientations D and $D^\top$ of the tree T given in the Figure 3 have the maximal trace norm. In fact, we give an algorithm using Wolfram Mathematica (Mathematica, Version 10.0., 2014) to find orientations of T with the maximal trace norm.*

Input 1:= (Function to compute the trace norm of a graph or digraph.)

```
TraceNorm[G_]:=Total[SingularValueList[
  AdjacencyMatrix[G]]] // N
```

Input 2: (The list of all possible orientations of the tree T, this list will have the name X .)

```
X = Map[Graph,Tuples[
   {{1 \[DirectedEdge] 2, 2 \[DirectedEdge] 1},
    {2 \[DirectedEdge] 3, 3 \[DirectedEdge] 2},
    {2 \[DirectedEdge] 4, 4 \[DirectedEdge] 2},
    {4 \[DirectedEdge] 5, 5 \[DirectedEdge] 4},
    {5 \[DirectedEdge] 6, 6 \[DirectedEdge] 5},
    {5 \[DirectedEdge] 7, 7 \[DirectedEdge] 5},
    {4 \[DirectedEdge] 8, 8 \[DirectedEdge] 4},
    {8 \[DirectedEdge] 9, 9 \[DirectedEdge] 8},
    {8 \[DirectedEdge] 10, 10 \[DirectedEdge] 8},
    {4 \[DirectedEdge] 11, 11 \[DirectedEdge] 4}
    }]]
```

Input 3: (The list of the trace norm of the possible orientations of the tree T, this list will have the name Y.)

```
Y = Map[TraceNorm, X]
```

Input 4: (The list of the positions where the maximal value of the list Y appears, this list will have the name Z.)

```
Z = Flatten[ Position[Y, Y // Max]]
```

Input 5: (The list of orientations of T with the maximal trace norm, this list will have the name W.)

```
W = Table[X[[Z[[i]]]], {i, 1, Length[Z]}]
```

Input 6:(The list of orientations that are isomorphic to the first orientation in the list W, this list will have the name A.)

```
A=Select[W, IsomorphicGraphQ[#, W[[1]]] &]
```

Input 7:(Function to compute the transpose orientation of a digraph.)

```
TransposeGraph[G_] := AdjacencyGraph[
Transpose[AdjacencyMatrix[G]]]
```

Input 8:(The list of orientations that are isomorphic to the transpose orientation of the first orientation of W, this orientation will have the name B.)

```
B =Select[W,
IsomorphicGraphQ[#, TransposeGraph[W[[1]]]] &]
```

There are 16 elements in W, so there are 16 elements of T with the maximal trace norm. There are 8 elements in A and 8 elements in B, consequently there are exactly two non-isomorphic orientations of T with the maximal trace norm. These orientations are D and $D^\top$ in Figure 3.

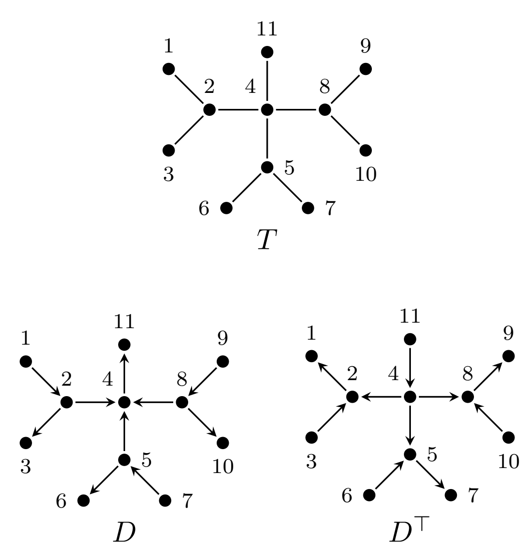

Fig. 3. A non balanced orientation of a graph with the maximal trace norm

So in general the question remains open: For a given tree T (with adjacent branching vertices), which orientations have a maximal trace norm?

3. Maximal trace norm on oriented double-star trees

As we have seen in Example 2.6, if a tree T has adjacent branching vertices, then it is not necessarily true that the balanced orientations have the maximal trace norm. However, we will show in this section that for double-star trees, the maximal trace norm is attained in balanced orientations. The *double-star tree* $S(\alpha,\beta)$ is obtained from the two stars $S_{\alpha+1}$ and $S_{\beta+1}$ by joining with an edge the largest degree vertex of $S_{\alpha+1}$ with the largest degree vertex of $S_{\beta+1}$. Any orientation of $S(\alpha,\beta)$ is of the form $\overrightarrow{S}(a,b;c,d)$, where $\alpha = a+b$ and $\beta = c+d$ (see Figure 4). Consider the forest $B(a,b;c,d)$ together with the orientation $\overrightarrow{B}(a,b;c,d)$ shown in Figure 4. Since $\overrightarrow{B}(a,b;c,d)$ is a sink-source orientation of $B(a,b;c,d)$, it follows from Theorem 1.1 and equality condition of Theorem 2.1 that

$$\begin{aligned}\mathcal{E}\left(B(a,b;c,d)\right) =&2\left\|\overrightarrow{B}(a,b;c,d)\right\|_*\\ =&2\left\|\overrightarrow{S}(a,b;c,d)\right\|_*.\end{aligned}$$

Consequently, the problem of finding the orientation of the maximal trace norm in $S(\alpha,\beta)$ is equivalent to the problem of finding the maximal energy in $B(\alpha,\beta)$, the set of all forests of the form $B(a,b;c,d)$, where $\alpha = a+b$ and $\beta = c+d$. We will use the quasi-order method and graph operations (Li *et al.*, 2012, Chapters 3 and 4) to find the graph with maximal energy in $B(\alpha,\beta)$.

If G is a bipartite graph with n vertices, then its characteristic polynomial is of the form $\sum_{k\geqslant 0}(-1)^k b_{2k}x^{n-2k}$, where $b_{2k} \geqslant 0$ for all k. For two bipartite graphs G_1 and G_2, we define the quasi-order $\preceq$ and write $G_1 \preceq G_2$ (or $G_2 \succeq G_1$) if $b_{2k}(G_1) \leqslant b_{2k}(G_2)$ for all k. Moreover, if at least one of the inequalities $b_{2k}(G_1) \leqslant b_{2k}(G_2)$ is strict, then we can write $G_1 \prec G_2$ (or $G_2 \succ G_1$). Thus, by Coulson's integral formula (Li *et al.*, 2012, Chapters 3 and 4) we have

$$G_1 \prec G_2 \Longrightarrow \mathcal{E}(G_1) < \mathcal{E}(G_2).$$

In other words, the energy increases with respect to the quasi-order defined as above. The following lemma is easy to show and will be useful in the sequel.

Lemma 3.1 *Let T_1 and T_2 be forests with n vertices and assume that*

$$\phi_{T_1}(x) - \phi_{T_2}(x) = \sum_{k=2}^{\lfloor \frac{n}{2}\rfloor} a_k x^{n-2k},$$

where $a_k = (-1)^k(b_{2k}(T_1) - b_{2k}(T_2))$ for $k = 2,\cdots,\lfloor n/2\rfloor$.

(i) If $a_2 \geqslant 0$, $a_3 \leqslant 0$, $a_4 \geqslant 0$, $\cdots$, then $T_1 \succeq T_2$,

(ii) if $a_2 \leqslant 0$, $a_3 \geqslant 0$, $a_4 \leqslant 0$, $\cdots$, then $T_1 \preceq T_2$.

Also, if in (i) or (ii) there is an $a_k \neq 0$, then $T_1 \succ T_2$ or $T_1 \prec T_2$, respectively.

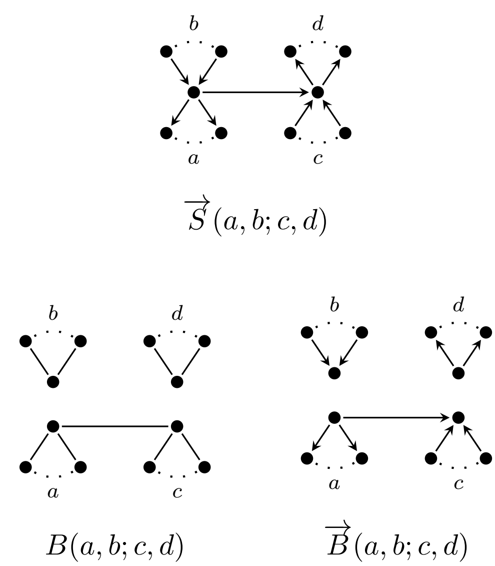

Fig. 4. An orientation of the double-star and the graph $B(a,b;c,d)$

Theorem 3.2

$$B\left(\left\lfloor\frac{\alpha}{2}\right\rfloor, \alpha-\left\lfloor\frac{\alpha}{2}\right\rfloor; \left\lfloor\frac{\beta}{2}\right\rfloor, \beta-\left\lfloor\frac{\beta}{2}\right\rfloor\right)$$

is the unique graph with maximal energy in $B(\alpha,\beta)$.

Proof. By Sachs' Coefficient Theorem (Cvetković *et al.*, 2010, Corollary 2.3.3), the characteristic polynomial of $B(a,b;c,d)$ is

$$x^{n-8}(x^2-b)(x^2-d)(x^4-(a+c+1)x^2+ac),$$

where $n = a+b+c+d+4$. Let $B_1 = B(a+1, b-1; c, d)$ and $B_2 = B(a, b; c, d)$. Then

$$\begin{aligned}&\phi_{B_1}(x) - \phi_{B_2}(x)\\ =&(b-a-2)x^{n-4}\\ &+[(a+1-b)c+(a+2-b)d]x^{n-6}\\ &+[(b-a-1)cd]x^{n-8}.\end{aligned} \tag{8}$$

So, by Lemma 3.1 and Equation 8 it follows that

OP1. $B(a, b; c, d) \prec B(a+1, b-1; c, d)$, if $a+1 < b$,

where OP1 is the operation shown in Figure 5.

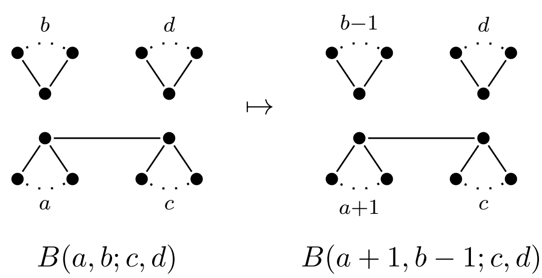

Fig. 5. Operation OP1

Similarly we can show:

OP2. $B(a, b; c, d) \prec B(a-1, b+1; c, d)$, if $b < a$.

OP3. $B(a, b; c, d) \prec B(a, b; c+1, d-1)$, if $c+1 < d$.

OP4. $B(a, b; c, d) \prec B(a, b; c-1, d+1)$, if $d < c$.

Now given

$$\begin{aligned}&B(a, b; c, d)\\ \neq &B\left(\left\lfloor\frac{\alpha}{2}\right\rfloor, \alpha - \left\lfloor\frac{\alpha}{2}\right\rfloor; \left\lfloor\frac{\beta}{2}\right\rfloor, \beta - \left\lfloor\frac{\beta}{2}\right\rfloor\right),\end{aligned}$$

by applying operations OP1-OP4, we obtain a strictly increasing sequence of forests which ends in

$$B\left(\left\lfloor\frac{\alpha}{2}\right\rfloor, \alpha - \left\lfloor\frac{\alpha}{2}\right\rfloor; \left\lfloor\frac{\beta}{2}\right\rfloor, \beta - \left\lfloor\frac{\beta}{2}\right\rfloor\right).$$

The result follows from the increasing property of the energy.

■

Corollary 3.3 *The orientation of the double-star $S(\alpha, \beta)$ that attains the maximal trace norm is the balanced orientation*

$$\overrightarrow{S}\left(\left\lfloor\frac{\alpha}{2}\right\rfloor, \alpha - \left\lfloor\frac{\alpha}{2}\right\rfloor; \left\lfloor\frac{\beta}{2}\right\rfloor, \beta - \left\lfloor\frac{\beta}{2}\right\rfloor\right), \tag{9}$$

or its transpose.

Remark 3.4 *The maximal trace norm over $S(\alpha, \beta)$ is attained in balanced orientations, but not all balanced orientations have the maximal trace norm. For example if α is even, then the orientation*

$$\overrightarrow{S}\left(\frac{\alpha}{2} - 1, \frac{\alpha}{2} + 1; \left\lfloor\frac{\beta}{2}\right\rfloor, \beta - \left\lfloor\frac{\beta}{2}\right\rfloor\right)$$

is balanced, but it does not have the maximal trace norm.

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References

Abdo, H., Dimitrov, D. & **Gutman, I. (2017).** On extremal trees with respect to the F-index. Kuwait Journal of Science, **44**(3): 1-8.

Abreu, N., Cardoso, D.M., Gutman, I., Martins, E.A. & **Robbiano, M. (2011).** Bounds for the signless Laplacian energy. Linear Algebra and its Applications, **435**(11): 2365-2374.

Adiga, C. & **Smitha, M. (2009).** On the skew Laplacian energy of a digraph. International Mathematical Forum, **4**(39): 1907-1914.

Adiga, C., Balakrishnan, R. & **So, W. (2010).** The skew energy of a digraph. Linear Algebra and its Applications, **432**(7): 1825-1835.

Agudelo, N. & **Rada, J. (2016).** Lower bounds of Nikiforov's energy over digraphs. Linear Algebra and its Applications, **496**: 156-164.

Agudelo, N., de la Peña, J.A. & **Rada, J. (2016).** Extremal values of the trace norm over oriented trees. Linear Algebra and its Applications, **505**: 261-268.

Ali, A., Raza, Z. & Bhatti, A.A. (2016). On the augmented Zagreb index. Kuwait Journal of Science, **43**(2): 48-63.

Allem, L.E., Jacobs, D.P. & Trevisan, V. (2016). Normalized Laplacian energy change and edge deletion. MATCH Communications in Mathematical and in Computer Chemistry, **75**(2): 343-353.

Ashraf, F. (2019). On energy of trees with perfect matching. MATCH Communications in Mathematical and in Computer Chemistry, **82**(2): 439-442.

Cavers, M., Fallat, S. & Kirkland, S. (2010). On the normalized Laplacian energy and general Randić index R_{-1} of graphs. Linear Algebra and its Applications, **433**(1): 172-190.

Cvetković, D., Rowlinson, P. & Simić, S. (2010). An Introduction to the Theory of Graph Spectra. Cambridge University Press, Cambridge.

Das, K.C., Sorgun, S. & Gutman, I. (2015). On Randić energy. MATCH Communications in Mathematical and in Computer Chemistry, **73**(1): 81-92.

Day, J. & So, W. (2007). Singular value inequality and graph energy change. ELA The Electronic Journal of Linear Algebra, **16**(1): 291-299.

Fan, K. (1951). Maximum properties and inequalities for the eigenvalues of completely continuous operators. Proceedings of the National Academy of Sciences of the United States of America, **37**(11): 760-766.

Gutman, I. (1978). The energy of a graph. Ber. Math.-Statist. Sekt. Forschungszentrum Graz, **103**: 1-22.

Gutman, I. & Zhou, B. (2016). Laplacian energy of a graph. Linear Algebra and its Applications, **414**(1): 29-37.

Gutman, I. & Wagner, S. (2012). The matching energy of a graph. Discrete Applied Mathematics, **160**(15): 2177-2187.

Gutman, I. & Li, X. (Eds) (2016). Energies of graphs - Theory and Applications. University of Kragujevac, Kragujevac.

Gutman, I., Furtula, B., Zogić, E. & Glogić, E. (2016). Resolvent energy of graphs. MATCH Communications in Mathematical and in Computer Chemistry, **75**(2): 279-290.

Haemers, W.H. (2012). Seidel switching and graph energy. MATCH Communications in Mathematical and in Computer Chemistry, **68**(3): 653-659.

Horn, R. & Johnson, C. (2013). Matrix Analysis. 434. Cambridge University Press, Cambridge.

Indulal, G., Gutman, I. & Vijayakumar, A. (2008). On distance energy of graphs. MATCH Communications in Mathematical and in Computer Chemistry, **60**(2): 461-472.

Jahanbani, A. (2018). Upper bounds for the energy of graphs. MATCH Communications in Mathematical and in Computer Chemistry, **79**(2): 275-286.

Khan, M., Farooq, R. & Rada J. (2017). Complex adjacency matrix and energy of digraphs. Linear and Multilinear Algebra **65**(11): 2170-2186.

Kharaghani, H. & Tayfeh-Rezaie, B. (2008). On the energy of $(0,1)$-matrices. Linear Algebra and its Applications, **429**(8-9): 2046-2051.

Li, J., Guo, J. M. & Shiu, W. C. (2015). A note on Randić energy. MATCH Communications in Mathematical and in Computer Chemistry, **74**(2): 389-398.

Li, X., Shi, Y. & Gutman, I. (2012). Graph energy. Springer-Verlag, New York.

Ma, X. (2019). A low bound on graph energy in terms of minimum degree. MATCH Communications in Mathematical and in Computer Chemistry, **81**(2): 393-404.

Maden, A. D. (2015). New bounds on the incidence energy, Randić energy and Randić Estrada index.MATCH Communications in Mathematical and in Computer Chemistry, **74**(2): 367-387.

Milovanović, I.Ž. & Milovanović, E. I. (2016). Remarks on the energy and the minimum dominating energy of a graph. MATCH Communications in Mathematical and in Computer Chemistry, **75**(2): 305-314.

Monsalve, J. & **Rada, J. (2019).** Oriented bipartite graphs with minimal trace norm. Linear and Multilinear Algebra **67**(6): 1121-1131.

Monsalve, J., Rada, J. & **Shi, Y. (2019).** Extremal values of energy over oriented bicyclic graphs. Applied Mathematics and Computation, **342**: 26-34.

Nikiforov, V. (2007). The energy of graphs and matrices. Journal of Mathematical Analysis and Applications, **326**(2): 1472-1475.

Peña, I. & **Rada, J. (2008).** Energy of digraphs. Linear and Multilinear Algebra, **56**(5): 565-579.

Pirzada, S. & **Bhat, M. (2014).** Energy of signed digraphs. Discrete Applied Mathematics, **169**: 195-205.

Ramane, H.S., Gutman, I. & **Revankar, D.S. (2008).** Distance equienergetic graphs. MATCH Communications in Mathematical and in Computer Chemistry, **60**(2): 473-484.

So, W., Robbiano, M., de Abreu, N.M.M. & **Gutman, I. (2010).** Applications of a theorem by Ky Fan in the theory of graph energy. Linear Algebra and its Applications, **432**(9): 2163-2169.

Trevisan, V., Carvalho, J., Del Vecchio, R. & **Vinagre, C. (2011).** Laplacian energy of diameter 3 trees. Applied Mathematics Letters **24**(6): 918-923.

Wolfram Research, Inc., Mathematica, Version 10.0, Champaign, IL (2014).

Zhu, J. & **Yang, J. (2018).** Minimal energies of trees with three branched vertices. MATCH Communications in Mathematical and in Computer Chemistry, **79**(2): 263-274.

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ملخص

يوضح هذا البحث إن معيار الأثر للرسم المُوَجه هو معيار الأثر للمصفوفة المُجاورة أي مجموعة القيم المُفردة. وفى حال فرضية وجود رسم بياني ثنائي التجزئة ل G، فمن المعروف جيداً ان تشعيبات تدفق التيار يكون لها أدنى معيار أثر بين كل تفريعات G. نوضح في هذا البحث إن تفريعات G المتوازنة تحقق أقصى معيار أثر في حال كون G شجرة ذات رؤوس متشعبة منفصلة أو تكون G شجرة ثنائية الفروع. نقدم في هذا البحث أمثلة لأشجار (ذات رؤوس متفرعة متجاورة) تحقق أقصى معيار أثر للتفريعات غير المتوازنة مما يطرح سؤالاً عاماً: أي التفريعات الشجرية تحقق أقصى معيار أثر؟