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Extremal values of energy over oriented bicyclic graphs

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ABSTRACT

Graph energy can be extended to digraphs via the trace norm. The trace norm of a digraph is the trace norm of its adjacency matrix, i.e. the sum of its singular values. In this work we find the oriented graphs that attain minimal and maximal trace norm over the set of oriented bicyclic graphs.

1. Introduction

A *directed graph* (or just *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 we indicate this by writing uv, in this case we call u the *tail* of the arc uv and v the *head* of the arc 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 $uv \in \mathcal{A}$ then $vu \in \mathcal{A}$, where $u, v \in \mathcal{V}$. 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. In this case D is called an *orientation* of G.

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

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

The characteristic polynomial $|xI - A|$ of the adjacency matrix A of D is called the *characteristic polynomial* of D and it is denoted by $\phi(D, x)$. The eigenvalues of A are called the *eigenvalues* of D.

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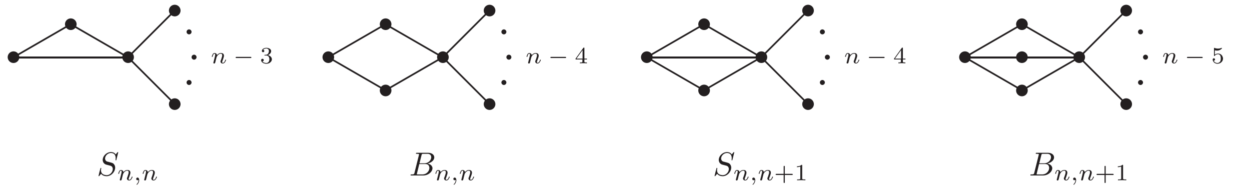

Fig. 1. Graphs in Theorems 1.1, 1.2 and 1.3.

The *energy* of a graph G with n vertices was introduced by Gutman [7] as $\mathcal{E}(G)=\sum_{k=1}^{n}|\lambda_k|$, where $\lambda_1,\dots,\lambda_n$ are the eigenvalues of G. The motivation comes from theoretical chemistry, within the Hückel molecular orbital (HMO) approximation, the energy levels of the π-electrons in molecules of conjugated hydrocarbons are related to the energy of the molecular graphs. Details on the development of the graph energy concept and its associated chemistry applications can be seen in the book [14].

Let G be a graph and $\phi(G,x)=\sum_{i=0}^{n}a_ix^{n-i}$ the characteristic polynomial of G. Then $\mathcal{E}(G)$ can be also expressed as the Coulson integral formula [14],

$$\mathcal{E}(G)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{1}{x^2}\ln\left[\left(\sum_{i=0}^{\lfloor n/2\rfloor}(-1)^i a_{2i}x^{2i}\right)^2+\left(\sum_{i=0}^{\lfloor n/2\rfloor}(-1)^i a_{2i+1}x^{2i+1}\right)^2\right]dx \tag{1}$$

A well-known fact is that the energy is increasing with respect to a quasi-order relation defined over bipartite graphs. More specifically, recall that the characteristic polynomial of a bipartite graph G with n vertices, denoted by $\phi(G, x)$, has the form

$$\phi(G,x)=\sum_{k\geq 0}(-1)^k b_{2k}(G)x^{n-2k},$$

where $b_{2k}(G)\geq 0$ for all k. For two bipartite graphs G_1 and G_2, the *quasi-order* $\preceq$ is defined as $G_1\preceq G_2$ if $b_{2k}(G_1)\leq b_{2k}(G_2)$ for all k. If $b_{2k}(G_1)<b_{2k}(G_2)$ for some k then we write $G_1\prec G_2$. It turns out that the energy is increasing with respect to this quasi-order relation (see [14]):

$$G_1\prec G_2\Longrightarrow \mathcal{E}(G_1)<\mathcal{E}(G_2). \tag{2}$$

The *star tree* on n vertices is the complete bipartite graph $K_{n-1,1}$, it is denoted by S_n and the graphs $S_{n,n}$, $B_{n,n}$, $S_{n,n+1}$ and $B_{n,n+1}$ are shown in Fig. 1.

For unicyclic connected graphs, the graphs with minimal graph energy and second minimal graph energy are determined.

Theorem 1.1 [11]**.** *Let G be a unicyclic graph such that $G\neq S_{n,n}$ and $G\neq B_{n,n}$. Then*

$$\mathcal{E}(S_{n,n})<\mathcal{E}(B_{n,n})<\mathcal{E}(G).$$

For bicyclic graphs it is known the graph with minimal energy.

Theorem 1.2 [19]**.** *Let G be a bicyclic graph such that $G\neq S_{n,n+1}$. Then,*

$$\mathcal{E}(S_{n,n+1})<\mathcal{E}(G).$$

For bicyclic bipartite graphs it is known the graph with minimal energy.

Theorem 1.3 [13]**.** *Let G be a bicyclic bipartite graph such that $G\neq B_{n,n+1}$. Then,*

$$\mathcal{E}(B_{n,n+1})<\mathcal{E}(G).$$

Different generalizations of energy to digraphs appeared in the literature ([1,17], see also [8]). In [16], graph energy is extended to non-symmetric and possibly non-square matrices via the trace norm. Recall that the trace norm $\|B\|_*$ of a matrix B is the sum of its singular values, which for a real symmetric matrix are the moduli of its eigenvalues. Hence if G is a graph with adjacency matrix A, then $\mathcal{E}(G)=\|A\|_*$. This observation motivated the study of the trace norm of the adjacency matrix of digraphs. The *trace norm* of a digraph D, denoted by $\|D\|_*$, is defined as the trace norm of its adjacency matrix. In [2] and [12] bounds for the trace norm of digraphs were discussed. In [3], the extremal values of the trace norm over the set of oriented trees and over the set of oriented paths were found.

Recently, in [15] we considered the following problem: among all orientations of a given bipartite graph, which have minimal trace norm. In order to deal with this problem it was introduced the *sink-source* orientations (i.e. every vertex is a sink vertex or a source vertex). The existence of these type of orientations were characterized in the following result.

Proposition 1.4 [15]**.** *Let G be a graph. The following conditions are equivalent:*

1. *There exists a sink-source orientation of G;*