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Upper Bounds for the Largest Singular Value of Certain Digraph Matrices

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Abstract

In this paper, we consider digraphs with possible loops and the particular case of oriented graphs, i.e. loopless digraphs with at most one oriented edge between every pair of vertices. We provide an upper bound for the largest singular value of the skew Laplacian matrix of an oriented graph, the largest singular value of the skew adjacency matrix of an oriented graph and the largest singular value of the adjacency matrix of a digraph. These bounds are expressed in terms of certain parameters related to vertex degrees. We also consider some bounds for the sums of squares of singular values. As an application, for the skew (Laplacian) adjacency matrix of an oriented graph and the adjacency matrix of a digraph, we derive some upper bounds for the spectral radius and the sums of squares of moduli of eigenvalues.

Keywords Digraph · Oriented graph · (skew) adjacency matrix · Skew Laplacian matrix · Singular value · Eigenvalue · Upper bound

Mathematics Subject Classification 05C20 · 05C50

1 Introduction

A *digraph* G is a pair (V, E), where V denotes the set of vertices with $|V| = n$ and E is the set of *oriented edges* (or *arcs*) consisting of ordered pairs of vertices. The existence of an edge oriented from a vertex i to a vertex j is designated by $i \to j$ (or $j \leftarrow i$). Edges of different orientations between the same vertices are permitted, but multiple edges of the same orientation are not. We also permit the existence of *loops*, i.e. the edges of form $i \to i$.

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The *adjacency matrix* of G is the $n \times n$ (0, 1)-matrix $A_G = (a_{ij})$, such that $a_{ij} = 1$ if there is an arc $i \leftarrow j$, and $a_{ij} = 0$ otherwise. Evidently, the set of adjacency matrices of finite digraphs coincides with the set of finite (0, 1)-matrices.

An *oriented graph* G' is a loopless digraph, such that there is at most one arc between any pair of its vertices. Since an oriented graph is a digraph, it can be represented by the already defined adjacency matrix, but it is often associated with the so-called *skew adjacency matrix*, that is the $n \times n$ $(0, 1, -1)$-matrix $S_{G'} = (s_{ij})$, such that $s_{ij} = 1$ and $s_{ji} = -1$ if there is an arc $i \leftarrow j$, while $s_{ij} = 0$ and $s_{ji} = 0$ if there is no arc between i and j. If $D_{G'}$ is the diagonal matrix of vertex degrees of G', then the *skew Laplacian matrix* of G' is defined by $L_{G'} = D_{G'} - S_{G'}$.

The *singular values* of G and the *skew singular values* of G' are the positive roots of the eigenvalues of $A_G^{\mathsf{T}} A_G$ and $S_{G'}^{\mathsf{T}} S_{G'}$, respectively. In other words, they are identified as the singular values of A_G and $S_{G'}$, respectively. We use the common notation $\sigma_1, \sigma_2, \ldots, \sigma_n$ for the singular values (taken with their repetition) of G and the skew singular values of G'. In particular, the largest one is denoted by σ. Similarly, the *skew Laplacian singular values* of G' are the positive roots of the eigenvalues of $L_{G'}^{\mathsf{T}} L_{G'}$; the largest one is denoted by ς.

For a set $U \subseteq V(G')$, let G'^U be the oriented graph obtained from G' by reversing the orientation of every edge between a vertex in U and a vertex in $V(G') \setminus U$. The oriented graph G'^U is said to be *equivalent* to G'. Equivalent oriented graphs share the same multiset of skew (Laplacian) singular values.

Some bounds for the largest modulus of the eigenvalues of the skew (Laplacian) matrix of an oriented graph can be found in [3,4,8]. Similar results concerning the eigenvalues of the adjacency matrix of digraphs with an emphasis on the largest modulus are given in the expository paper [2]. In this paper, we consider the singular values of the mentioned matrices and then apply the obtained results to derive certain new bounds for moduli of the corresponding eigenvalues.

Here is the contents of the forthcoming sections. Section 2 contains certain additional terminology and notation, mostly used in the next two sections. In Sect. 3, we derive an upper bound for the largest singular value of the skew Laplacian matrix of an oriented graph. The bound is expressed in terms of vertex degrees and some related parameters. On the basis of this result, we derive a similar upper bound for the largest singular value of the skew adjacency matrix, and we do the same for the largest singular value of the adjacency matrix of a digraph. In Sect. 4, we give an upper bound for the sum of the k largest singular values and also a lower bound for the sum of the $k-1$ smallest singular values of the skew adjacency matrix of an oriented graph and the adjacency matrix of a digraph. In Sect. 5, we apply the obtained results to get some bounds concerning the eigenvalues of the mentioned matrices.

2 Terminology and Notation

Formulations of all the forthcoming statements refer to terminology and notation introduced in this short section.

For the particular case of oriented graphs, we use d_i to denote the degree of a vertex i (i.e. the number of edges incident with it regardless of their orientation) and

m_i to denote the average degree of the neighbours of i (so-called the *average* 2*-degree* of i).

For digraphs, the *indegree* r_i of a vertex i is the number of edges oriented to i, while the *outdegree* s_i is the number of edges oriented from i. Accordingly, we denote by R_i and S_i the number of vertices k such that there is an arc $i \leftarrow k$ and the number of vertices k such that there is an arc $i \to k$, respectively.

For the vertices i, j, by c_{ij}^{+} we denote the number of vertices k such that there is an arc $i \leftarrow k$ and there is an arc of any orientation between j and k. By c_{ij}^{++}, we denote the number of vertices k such that there is an arc $i \leftarrow k$ and there is an arc $j \leftarrow k$. We also use the similar notation for all the remaining possibilities. We assume that a loop at i is simultaneously oriented to and from i. For oriented graphs, we do not make a distinction between multiplicative groups $\{+, -\}$ and $\{1, -1\}$, and so for $a, b \in \{1, -1\}$, c_{ij}^{a} denotes the cardinality of the set $\{k \,:\, s_{ik} = a,\ s_{jk} \neq 0\}$ and $c_{ij}^{a,b}$ denotes the cardinality of the set $\{k \,:\, s_{ik} = a,\ s_{jk} = b\}$.

3 Upper Bounds for ς and σ

We first prove the following result.

Theorem 3.1 *For the largest skew Laplacian singular value ς of an oriented graph G',*

$$\varsigma \leq \max\left\{\sqrt{d_i(d_i + m_i) + \sum_{j\sim i}\left(|d_j - d_i| - c_{ij}^{s_{ij}} + \left|c_{ij}^{s_{ij},s_{ji}} - c_{ij}^{s_{ij},s_{ij}}\right|\right)} \,:\, 1 \leq i \leq n\right\}. \tag{1}$$

Proof Let ς^2 be the largest eigenvalue of $L_{G'}^{\mathsf{T}} L_{G'}$, let $\mathbf{x}$ be an eigenvector associated with ς^2, and let x_i be the coordinate that is largest in absolute value. Without loss of generality, we may assume that $x_i > 0$. It holds $\varsigma^2\mathbf{x} = L_{G'}^{\mathsf{T}} L_{G'}\mathbf{x}$, i.e.

$$\varsigma^2\mathbf{x} = (D_{G'} - S_{G'})^{\mathsf{T}}(D_{G'} - S_{G'})\mathbf{x} = (D_{G'}^2 - D_{G'}S_{G'} + S_{G'}D_{G'} - S_{G'}^2)\mathbf{x}, \tag{2}$$

since $S_{G'}^{\mathsf{T}} D_{G'} = -S_{G'}D_{G'}$ and $S_{G'}^{\mathsf{T}} S_{G'} = -S_{G'}^2$. Therefore, we have

$$\begin{aligned}\varsigma^2 x_i &= d_i^2 x_i - d_i\sum_{j\sim i} s_{ij}x_j + \sum_{j\sim i} s_{ij}d_jx_j - \sum_{j\sim i}\sum_{k\sim j} s_{ij}s_{jk}x_k \\ &\leq d_i^2 x_i + \sum_{j\sim i}|d_j - d_i|x_i - \sum_{j\sim i}\sum_{k\sim j} s_{ij}s_{jk}x_k. \end{aligned} \tag{3}$$

Consider now the double summation in more details. We may rewrite it as

$$\sum_{j\sim i}\sum_{k\sim j} s_{ij}s_{jk}x_k = \sum_{i\leftarrow j}\sum_{j\leftarrow k} x_k + \sum_{i\to j}\sum_{j\to k} x_k - \sum_{i\leftarrow j}\sum_{j\to k} x_k - \sum_{i\to j}\sum_{j\leftarrow k} x_k. \tag{4}$$

Extracting the first term on the right-hand side of the previous equality, we get

$$\sum_{i\leftarrow j}\sum_{j\leftarrow k}x_k=\sum_{i\leftarrow j}\sum_{\substack{j\,\leftarrow\,k\\ i\,\leftarrow\,k}}x_k+\sum_{i\leftarrow j}\sum_{\substack{j\,\leftarrow\,k\\ i\,\not\leftarrow\,k}}x_k=\sum_{i\leftarrow j}|R_i\cap S_j|x_j+\sum_{i\leftarrow j}\sum_{\substack{j\,\leftarrow\,k\\ i\,\not\leftarrow\,k}}x_k$$
$$\geq\sum_{i\leftarrow j}|R_i\cap S_j|x_j-\sum_{i\leftarrow j}\big(r_j-|R_i\cap R_j|\big)x_i.$$

Similarly, for the second term, we get

$$\sum_{i\rightarrow j}\sum_{j\rightarrow k}x_k\geq\sum_{i\rightarrow j}|S_i\cap R_j|x_j-\sum_{i\rightarrow j}\big(s_j-|S_i\cap S_j|\big)x_i.$$

The third term gives

$$\sum_{i\leftarrow j}\sum_{j\rightarrow k}x_k=\sum_{i\leftarrow j}\sum_{\substack{j\,\rightarrow\,k\\ i\,\leftarrow\,k}}x_k+\sum_{i\leftarrow j}\sum_{\substack{j\,\rightarrow\,k\\ i\,\not\leftarrow\,k}}x_k$$
$$\leq\sum_{i\leftarrow j}|R_i\cap R_j|x_j+\sum_{i\leftarrow j}\big(s_j-|R_i\cap S_j|\big)x_i.$$

And similarly, for the fourth one, we get

$$\sum_{i\rightarrow j}\sum_{j\leftarrow k}x_k\ \leq\sum_{i\rightarrow j}|S_i\cap S_j|x_j+\sum_{i\rightarrow j}\big(r_j-|S_i\cap R_j|\big)x_i.$$

Returning them into (3), we get

$$\begin{aligned}\Big(\varsigma^2-d_i^2-\sum_{j\sim i}|d_j-d_i|\Big)x_i&\leq\sum_{i\leftarrow j}\big(|R_i\cap S_j|-|R_i\cap R_j|\big)x_j\\&\quad+\sum_{i\rightarrow j}\big(|S_i\cap R_j|-|S_i\cap S_j|\big)x_j\\&\quad+\sum_{i\leftarrow j}\big(r_j+s_j-|R_i\cap R_j|-|R_i\cap S_j|\big)x_i\\&\quad+\sum_{i\rightarrow j}\big(s_j+r_j-|S_i\cap S_j|-|S_i\cap R_j|\big)x_i\\&=\sum_{j\sim i}\big(c_{ij}^{s_{ij},s_{ji}}-c_{ij}^{s_{ij},s_{ij}}\big)x_j+d_im_ix_i-\sum_{j\sim i}c_{ij}^{s_{ij}}x_i\\&\leq\Big(d_im_i-\sum_{j\sim i}\big(c_{ij}^{s_{ij}}-\big|c_{ij}^{s_{ij},s_{ji}}-c_{ij}^{s_{ij},s_{ij}}\big|\big)\Big)x_i,\end{aligned}$$

giving

$$\varsigma^2 \leq \Big(d_i(d_i+m_i) + \sum_{j\sim i}\big(|d_j-d_i| - c_{ij}^{s_{ij}} + \big|c_{ij}^{s_{ij},s_{ji}} - c_{ij}^{s_{ij},s_{ij}}\big|\big)\Big),$$

for the vertex i. Taking the maximum over all vertices, we arrive at (1). □

A similar proof technique can be found in [5].

Observe that if G' is triangle-free (in particular, bipartite), then the inequality (1) reduces to

$$\varsigma \leq \max\left\{\sqrt{d_i(d_i+m_i) + \sum_{j\sim i}|d_j-d_i|}\ :\ 1\leq i\leq n\right\}.$$

Note that for every vertex i of an oriented graph G', there exists an equivalent oriented graph in which $r_i = d_i$ (i.e. all the edges incident with i are oriented to i) – the corresponding oriented graph is obtained by making a switch with respect to the set of neighbours of i such that the corresponding edges are oriented from i to them. On the basis of this observation, we arrive at the following corollary.

Corollary 3.2 *For an oriented graph G', there exists a vertex i and an equivalent oriented graph, such that*

$$\varsigma \leq \sqrt{d_i(d_i+m_i) - 2T_i + \sum_{j\sim i}\big(|d_j-d_i| + |T_{ij}^- - T_{ij}^+|\big)}, \tag{5}$$

where T_i denotes the number of triangles containing i and T_{ij}^- (resp. T_{ij}^+) is the number of triangles containing i, j such that the edge between j and the third vertex is oriented from (resp. to) j.

Proof Let i denote a vertex for which the inequality of (1) holds. Taking the equivalent oriented graph in which $r_i = d_i$, we get the desired upper bound. Indeed, there we have

$$\sum_{j\sim i} c_{ij}^{s_{ij}} = 2T_i \ \text{ and } \ \sum_{j\sim i}\big|c_{ij}^{s_{ij},s_{ji}} - c_{ij}^{s_{ij},s_{ij}}\big| = \sum_{j\sim i}|T_{ij}^- - T_{ij}^+|,$$

and we are done.

Here is another consequence concerning the largest singular value of the skew adjacency matrix.

Corollary 3.3 *For the largest skew singular value σ of an oriented graph G',*

$$\sigma \leq \max\left\{\sqrt{d_i m_i - \sum_{j\sim i}\big(c_{ij}^{s_{ij}} - \big|c_{ij}^{s_{ij},s_{ji}} - c_{ij}^{s_{ij},s_{ij}}\big|\big)}\ :\ 1\leq i\leq n\right\}. \tag{6}$$

Proof The equality (2) reduces to $\sigma^2\mathbf{x} = S_{G'}^{\mathsf{T}} S_{G'}\mathbf{x}$, which further implies

$$\sigma^2 x_i = -\sum_{j\sim i}\sum_{k\sim j} s_{ij}s_{jk}x_k,$$

and now the remainder of the proof follows in the same way as the corresponding part (which starts from (4)) of the proof of Theorem 3.1. □

We now proceed with digraphs.

Theorem 3.4 *For the largest singular value σ of a digraph G,*

$$\sigma \le \max\left\{\sqrt{s_i^{(r)} + \sum_{i\to j}\left(c_{ij}^{--} - c_{ij}^{-+}\right)}\ :\ 1 \le i \le n\right\}, \tag{7}$$

where $s_i^{(r)} = \sum_{i\to j} r_j$.

Proof Acting as in the proof of Theorem 3.1, we get $\sigma^2\mathbf{x} = A_G^{\mathsf{T}} A_G\mathbf{x}$, for a suitable $\mathbf{x} \neq \mathbf{0}$. If $x_i > 0$ is the coordinate that is largest in absolute value, then we compute:

$$\begin{aligned}
\sigma^2 x_i &= \sum_{i\to j}\sum_{j\leftarrow k} x_k = \sum_{i\to j}\sum_{\substack{j\,\leftarrow\,k\\ i\,\to\,k}} x_k + \sum_{i\to j}\sum_{\substack{j\,\leftarrow\,k\\ i\,\not\to\,k}} x_k\\
&\le \sum_{i\to j}|S_i\cap S_j|x_j + \sum_{i\to j}\sum_{\substack{j\,\leftarrow\,k\\ i\,\not\to\,k}} x_k\\
&\le \sum_{i\to j}|S_i\cap S_j|x_i + \sum_{i\to j}(r_j - |S_i\cap R_j|)x_i = \sum_{i\to j}\left(r_j + |S_i\cap S_j| - |S_i\cap R_j|\right)x_i\\
&= \left(s_i^{(r)} + \sum_{i\to j}\left(c_{ij}^{--} - c_{ij}^{-+}\right)\right)x_i.
\end{aligned}$$

Taking the maximum over all vertices, we arrive at the desired result. □

If a digraph is triangle-free and has no loops, then the bound of (7) reduces to

$$\varsigma \le \max\left\{\sqrt{s_i^{(r)}}\ :\ 1 \le i \le n\right\}.$$

In particular case of graphs (i.e. loopless digraphs in which all the edges have both orientations), we have $R_i = S_i$ and $r_i = s_i = d_i$ (the vertex degree), for $1 \le i \le n$. In this way, the upper bound of (7) reduces to $\varsigma \le \max\left\{\sqrt{d_i m_i}\ :\ 1 \le i \le n\right\}$, where m_i is the average degree of neighbours of i. This bound, which for connected graphs attains the equality if and only if the graph is regular or bipartite semiregular, is known (cf. [6] or [7, p. 34]).

4 Sums of Singular Values

Here we extend our consideration to the sums of singular values. For this purpose, we need the following general result due to Bollobás and Nikiforov.

Theorem 4.1 *[1] Let $M = (m_{ij})$ be a Hermitian matrix of size n with eigenvalues $\nu_1, \nu_1, \ldots, \nu_n$ taken with their repetition and indexed non-increasingly. For every vertex set partition $\{1, 2, \ldots, n\} = W_1 \sqcup W_2 \sqcup \cdots \sqcup W_k$ $(2 \leq k \leq n)$, we have*

$$\sum_{p=1}^{k} \nu_p \geq \sum_{p=1}^{k} \frac{1}{|W_p|} \sum_{(i,j):i,j \in W_p} m_{ij}$$

and

$$\sum_{p=n-k+2}^{n} \nu_p \leq \sum_{p=1}^{k} \frac{1}{|W_p|} \sum_{(i,j):i,j \in W_p} m_{ij} - \frac{1}{n} \operatorname{sum}(M),$$

where sum(M) *denotes the sum of the entries of* M.

Here is the result.

Theorem 4.2 *Let $W_1 \sqcup W_2 \sqcup \cdots \sqcup W_k$ $(2 \leq k \leq n)$ denote the vertex set partition of an oriented graph G' or a digraph G with m edges, and let $\sigma_1, \sigma_2, \ldots, \sigma_n$ be non-increasingly indexed singular values of the corresponding graph.*

(i) For G', we have

$$\sum_{p=1}^{k} \sigma_p^2 \geq \sum_{p=1}^{k} \frac{1}{|W_p|} \sum_{(i,j):i,j \in W_p} (w_{ij}^{+} - w_{ij}^{-}) \tag{8}$$

and

$$\sum_{p=n-k+2}^{n} \sigma_p^2 \leq \sum_{p=1}^{k} \frac{1}{|W_p|} \sum_{(i,j):i,j \in W_p} (w_{ij}^{+} - w_{ij}^{-}) - \frac{1}{n}\Big(2m + \sum_{\substack{(i,j)\,:\, i \neq j \\ i,j \in V}} (w_{ij}^{+} - w_{ij}^{-})\Big),$$

where $w_{ij}^{+} = c_{ij}^{++} \cup c_{ij}^{--}$ and $w_{ij}^{-} = c_{ij}^{+-} \cup c_{ij}^{-+}$.

(ii) For G, we have

$$\sum_{p=1}^{k} \sigma_p^2 \geq \sum_{p=1}^{k} \frac{1}{|W_p|} \sum_{(i,j):i,j \in W_p} c_{ij}^{--} \tag{9}$$

and

$$\sum_{p=n-k+2}^{n} \sigma_p^2 \leq \sum_{p=1}^{k} \frac{1}{|W_p|} \sum_{(i,j):i,j \in W_p} c_{ij}^{--} - \frac{1}{n}\Big(m + \sum_{\substack{(i,j)\,:\, i \neq j \\ i,j \in V}} c_{ij}^{--}\Big),$$

Proof If M stands for $S_{G'}$ or A_G, then, for both (i) and (ii), only what we need to do is to check what are the entries of $M^\intercal M$. By direct computation we get that, in the case of $S_{G'}$, the corresponding (i, j)-entry is equal to $w_{ij}^{+} - w_{ij}^{-}$, while in the case of A_G, this entry is equal to c_{ij}^{--}; in both situations the possibility $i = j$ is included. The remainder of the proof follows by Theorem 4.1, as the trace of $M^\intercal M$ is $2m$ in the first case, and m in the second. □

Since $c_{ij}^{--} \geq 0$ and $c_{ii}^{--} = s_i$, one may observe a practical bound (for digraphs) that arises from (ii):

$$\sum_{p=1}^{k} \sigma_p^2 \geq \sum_{i \in W_p} \frac{s_i}{W_p}. \tag{10}$$

Similarly, if W_1 is a set of vertices such that there is no path of length 2 between any two of them, then:

$$\sigma_1^2 + \sigma_2^2 \geq \frac{1}{|W_1|} \sum_{i \in W_1} d_i + \frac{1}{|W_2|} \sum_{(i,j)\,:\,i,j \in W_2} (w_{ij}^{+} - w_{ij}^{-}) \tag{11}$$

holds for an oriented graph and

$$\sigma_1^2 + \sigma_2^2 \geq \frac{1}{|W_1|} \sum_{i \in W_1} s_i + \frac{1}{|W_2|} \sum_{(i,j)\,:\,i,j \in W_2} c_{ij}^{--} \tag{12}$$

holds for a digraph.

Of course, similar inequalities can be derived on the basis of upper bounds given in the previous theorem.

5 Eigenvalues

The eigenvalues of G are identified as the eigenvalues of A_G, while the *skew eigenvalues* and the *skew Laplacian eigenvalues* of G' are identified as the eigenvalues of $S_{G'}$ and $L_{G'}$, respectively. The *spectral radius* of G is the largest modulus of its eigenvalues. The *skew spectral radius* and the *skew Laplacian spectral radius* of G' are defined in the same way.

It is well-known that the singular values of a square matrix dominate its eigenvalues in sense that

$$\sum_{i=1}^{k} \sigma_i \geq \sum_{i=1}^{k} |\lambda_i|, \quad \text{for } 1 \leq k \leq n,$$

where $\sigma_1, \sigma_2, \ldots, \sigma_n$ and $|\lambda_1|, |\lambda_2|, \ldots, |\lambda_n|$ are non-increasingly indexed singular values and non-increasingly indexed moduli of eigenvalues, respectively. Using this result, we conclude that the upper bounds of (1) and (5) remain valid for the skew Laplacian spectral radius of G'. Similarly, (6) holds for the skew spectral radius of G'

and (7) holds for the spectral radius of G. Considering results of Sect. 4, we easily transfer the upper bounds of (8)–(12) to the upper bounds concerning the corresponding moduli of the (skew) eigenvalues.

Since for an oriented graph G', we have $S_{G'}^{\intercal} S_{G'} = -S_{G'}^2$, we deduce that, in this case, $\sigma_i = |\lambda_i|$, for $1 \leq i \leq n$. Consequently, equality in (6), (8) and (11) is attained if and only if it is attained for the corresponding moduli of the skew eigenvalues.

As we pointed out in the introduction, one can find many upper bounds for the skew (Laplacian) spectral radius of an oriented graph and upper bounds for the spectral radius of a digraph. The majority of them is expressed in terms of invariants that differ from those used in this paper. A close situation appears in the case of our bounds (1) (considered as an upper bound for the skew Laplacian spectral radius) and (6) (considered as an upper bound for the skew spectral radius) and the upper bounds established in Theorems 2.3 and 2.4 of [4]. It complicated to derive a general comparison between them, but numerical experiments show that those of the latter reference would often give a finer estimate, although they are more complicated for computation.

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