Analysis of directed networks via partial singular value decomposition and Gauss quadrature

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Abstract

Large-scale networks arise in many applications. It is often of interest to be able to identify the most important nodes of a network or to determine the ease of traveling between them. We are interested in carrying out these tasks for directed networks. These networks have a nonsymmetric adjacency matrix A. Benzi et al. [6] recently proposed that these tasks can be accomplished by studying certain matrix functions, such as hyperbolic cosine and sine, of $\sqrt{A^TA}$ and $\sqrt{AA^T}$. For small to medium-sized networks, the required computations can be easily carried out by first computing the singular value decomposition of A. However, for large networks this is impractical. We propose to first compute a partial singular value decomposition of A, which allows us to determine a subset of nodes that contains the most important nodes or a subset of nodes between which it is easy to travel. We then apply Gauss quadrature to rank the nodes in these subsets. Several computed examples illustrate the performance of the approach proposed.

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1. Introduction

We are interested in studying large unweighted directed networks without multiple edges and loops. This kind of network can be described with a directed graph G. The nodes are represented by vertices of the graph and the connections between adjacent nodes by directed edges. We assume that the number of nodes, n, is large and that the number of edges is much smaller than n^2. Networks that give rise to this kind of graphs arise in many scientific and industrial applications, including genetics, epidemiology, energy distribution, and telecommunications; see, e.g., [8, 11, 15, 17, 19, 29, 38] and references therein. For instance, internet search engines use graphs that describe the connections between web pages.

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The adjacency matrix associated with a directed graph G is a nonsymmetric matrix $A = [A_{ij}] \in \mathbb{R}^{n\times n}$ such that $A_{ij} = 1$ if there is a directed edge from node i to node j, and $A_{ij} = 0$ otherwise. A walk in a directed graph G is a sequence of nodes $v_1, v_2, \ldots, v_k$ such that there is a directed edge from v_i to v_{i+1} for $i = 1, 2, \ldots, k-1$. Nodes and edges may be repeated. A path is a walk with all nodes distinct. A graph is said to be (weakly) connected if every pair of nodes is linked by an undirected path, i.e., by a path where each edge is considered without orientation. We will consider connected graphs in this paper. Disconnected graphs can be studied by treating every connected subgraph separately.

It is often useful to extract numerical quantities that describe interesting global properties of a graph, such as the importance of a particular node or the ease of traveling from one node to another. It is not hard to see that for $m \geq 1$, the entry $[A^m]_{ij}$ of A^m equals the number of walks of length m starting at node i and ending at node j.

For undirected graphs, which have a symmetric adjacency matrix A, Estrada et al. [17, 19, 20, 21] proposed to study matrix-valued functions

$$f(A) = \sum_{m=0}^{\infty} c_m A^m \tag{1.1}$$

with nonnegative coefficients c_m such that the sum converges. The term $c_0 A^0$ is included for convenience and does not have a particular meaning. The diagonal entry $[f(A)]_{ii}$ is referred to as the f-subgraph centrality of node i. A large value indicates that node i is well-connected and therefore important in the graph. The off-diagonal entry $[f(A)]_{ij}$, $i \neq j$, is called the f-subgraph communicability between the nodes i and j. A large value indicates that it is easy to travel from node i to node j; see, e.g., Estrada [17] for insightful discussions on these definitions. The exponential function $f(A) = \exp(A)$, which corresponds to the coefficients $c_m = 1/m!$ in (1.1), has received particular attention in the literature; see [18].

For directed graphs, the size of $[\exp(A)]_{ii}$ is not always a meaningful measure of the importance of node i. Benzi et al. [6] illustrated this with the following example. Let A be a Jordan block

$$A = [A_{ij}] \in \mathbb{R}^{n\times n}, \qquad A_{ij} = \begin{cases} 1, & j = i+1, \\ 0, & j \neq i+1. \end{cases}$$

Then $[\exp(A)]_{ii} = 1$ for all i, and these values do not in an obvious manner correspond to intuition about the importance of the nodes in the associated network; for instance, in many applications it is meaningful to consider the first node less important than the remaining nodes.

To remedy this difficulty, Benzi et al. [6] recently proposed to consider the exponential of the matrix

$$\mathcal{A} = \begin{bmatrix} 0 & A \\ A^T & 0 \end{bmatrix} \tag{1.2}$$

when A is a nonsymmetric adjacency matrix. Here the superscript ^{T} denotes transposition. Using the singular value decomposition (SVD) of A, it is easy to see that

$$\exp(\mathcal{A}) = \begin{bmatrix} \cosh(\sqrt{AA^T}) & A\,\mathrm{s}(\sqrt{AA^T}) \\ \mathrm{s}(\sqrt{AA^T})A^T & \cosh(\sqrt{A^TA}) \end{bmatrix}, \tag{1.3}$$

where

$$\mathrm{s}(t) = \begin{cases} t^{-1}\sinh(t), & t \neq 0, \\ 1, & t = 0; \end{cases} \tag{1.4}$$

see (2.2) below. Let $M^\dagger$ denote the Moore–Penrose pseudoinverse of the matrix M. Then

$$A\,\mathrm{s}(\sqrt{AA^T}) = A(\sqrt{AA^T})^\dagger \sinh(\sqrt{AA^T}).$$

Benzi et al. [6] use the left-hand side of (1.3) in their computations. We find it convenient to use the submatrices in the right-hand side.

The use of the matrix (1.2) is justified by Benzi et al. [6] by its connection to the Hypertext Induced Topics Search (HITS) algorithm by Kleinberg [31]; see also [38, Section 7.5]. Within the framework of this algorithm, there are two

kinds of significant nodes: hubs and authorities. Hubs are distinguished by the fact that they point to many important nodes. The latter are referred to as authorities. Important hubs are nodes that point to many important authorities, important authorities are pointed to by important hubs; see also Blondel et al. [11] for a discussion on this and related network models. We will return to the HITS algorithm in Section 6.

In a directed graph, an alternating walk of length k starting from an out-edge at node v_1 and ending at node v_{k+1} is a list of $k+1$ nodes such that there exists an edge from v_i to v_{i+1} if i is odd and an edge from v_{i+1} to v_i if i is even. Analogously, an alternating walk of length k, starting with an in-edge at node v_1 and ending at node v_{k+1} is a list of $k+1$ nodes such that there exists an edge from v_{i+1} to v_i if i is odd and an edge from v_i to v_{i+1} if i is even; see, e.g., Benzi et al. [6] or Croft et al. [15] for discussions.

The matrix entries $[(AA^T)^k]_{ij}$ and $[(A^TA)^k]_{ij}$ count the number of alternating walks of length $2k$. Following Benzi et al. [6], we refer to

$$[\exp(\mathcal{A})]_{ii} = [\cosh(\sqrt{AA^T})]_{ii}, \qquad 1 \le i \le n,$$

as the hub centrality of node i, and to

$$[\exp(\mathcal{A})]_{n+i,n+i} = [\cosh(\sqrt{A^TA})]_{ii}, \qquad 1 \le i \le n,$$

as the authority centrality of node i. The hub communicability between the nodes i and j, $i \neq j$, is defined as

$$[\exp(\mathcal{A})]_{ij} = [\cosh(\sqrt{AA^T})]_{ij}, \qquad 1 \le i, j \le n,$$

and the authority communicability between the nodes i and j, $i \neq j$, is given by

$$[\exp(\mathcal{A})]_{n+i,n+j} = [\cosh(\sqrt{A^TA})]_{ij}, \qquad 1 \le i, j \le n.$$

Analogously, the hub-authority communicability between the nodes i and j is defined as

$$[\exp(\mathcal{A})]_{i,n+j} = [A\,\mathrm{s}(\sqrt{AA^T})]_{ij} = [\mathrm{s}(\sqrt{AA^T})A^T]_{ji} = \exp(\mathcal{A})_{n+j,i}, \qquad 1 \le i, j \le n.$$

This is also the authority-hub communicability between the nodes j and i.

When the graph G has many nodes and, therefore, the adjacency matrix A is large, direct evaluation of $\exp(\mathcal{A})$ generally is not feasible. Benzi et al. [6] discuss how to apply Gauss-type quadrature rules to determine upper and lower bounds for expressions of the form

$$\mathbf{u}^T \exp(\mathcal{A})\mathbf{v}, \qquad \mathbf{u}, \mathbf{v} \in \mathbb{R}^{2n}. \tag{1.5}$$

Note that the hub and authority centralities as well as the hub-authority communicability can be expressed in the form (1.5) for suitable vectors $\mathbf{u}$ and $\mathbf{v}$. The possibility of determining upper and lower bounds for expressions of the form (1.5) by applying a few steps of the symmetric Lanczos method to $\mathcal{A}$ and interpreting the tridiagonal matrix obtained as a Gauss quadrature rule was first observed by Golub [26]. A simple modification of the tridiagonal matrix gives an associated Gauss–Radau rule with a specified quadrature node. Pairs of a Gauss rule and a suitably chosen Gauss–Radau rule provide upper and lower bounds for (1.5). A detailed description of this approach and many applications can be found in the nice book by Golub and Meurant [28]; see also [27]. Benzi and Boito [5] were the first to apply this technique to studying undirected graphs. We will briefly review this way of determining upper and lower bounds in Section 4, where we also discuss an approach that differs slightly from the one used by Benzi et al. [6].

The application of Gauss-type quadrature rules is attractive when bounds for only a few quantities (1.5) are to be computed. However, when bounds for many hub and authority centralities or hub-authority communicabilities are desired, then the evaluation of all the Gauss and Gauss–Radau rules required can be expensive, because the computational work is proportional to the number of bounds desired. For instance, when we would like to determine one or a few nodes with the largest hub centrality in a large graph, upper and lower bounds for all of the first n diagonal entries of $\exp(\mathcal{A})$ have to be computed in order to be able to ascertain which node(s) have the largest hub centrality. It is even more expensive to determine the node(s) with the largest hub-authority communicability, because this requires

the evaluation of bounds for all the entries of $\exp(\mathcal{A})$ above the diagonal with indices $1 \le i \le n$ and $n+1 \le j \le 2n$, i.e., of $n^2 - 1$ expression of the form (1.5).

To reduce the computational effort, we propose to proceed in two steps. First, we determine a partial SVD of A. Consider for the moment the (full) SVD,

$$A = U\Sigma V^T = \sum_{j=1}^{n} \sigma_j \mathbf{u}_j \mathbf{v}_j^T, \tag{1.6}$$

where the matrices $U = [\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_n] \in \mathbb{R}^{n\times n}$ and $V = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n] \in \mathbb{R}^{n\times n}$ are orthogonal and the diagonal matrix

$$\Sigma = \mathrm{diag}[\sigma_1, \sigma_2, \ldots, \sigma_n] \in \mathbb{R}^{n\times n}, \qquad \sigma_1 \ge \sigma_2 \ge \cdots \ge \sigma_n \ge 0,$$

contains the singular values. We refer to the singular triplets $\{\sigma_i, \mathbf{u}_i, \mathbf{v}_i\}_{i=1}^{N}$ associated with the $N \le n$ largest singular values of A as the N largest singular triplets. The numerical examples of Section 6 illustrate that many adjacency matrices can be approximated fairly accurately by a matrix of low rank $N \ll n$ made up of the N largest singular triplets. We use this rank-N approximation to identify a subset of nodes that contains the desired nodes, such as the five nodes with the largest hub centrality, and then compute improved bounds with the aid of Gauss-type quadrature rules for the nodes in the determined subset. This hybrid approach can be much cheaper for large graphs than only using Gauss quadrature. The latter approach, in turn, is much cheaper than evaluating the matrix exponential $\exp(\mathcal{A})$. This is illustrated in Section 6. Our hybrid method generalizes the scheme proposed in [22] for undirected graphs to directed ones.

This paper is organized as follows. Section 2 describes how upper and lower bounds for all the entries of certain functions of the matrix $\mathcal{A}$ can be determined via partial SVD of A. The particular application of determining upper and lower bounds for hub and authority centralities is considered in Section 3. Several methods are available for computing a partial SVD of a large matrix; see, e.g., [2, 3, 4, 30, 39] and references therein. We apply the augmented implicitly restarted Golub–Kahan bidiagonalization[4] method described in [2] in our computed examples. A brief outline of this method is provided in Section 3. The application of Gauss-type quadrature rules to compute upper and lower bounds for the entries of a matrix function $f(\mathcal{A})$ is reviewed in Section 4, and we describe our hybrid method based on first computing a partial SVD and then bounding quantities of interest using Gauss-type rules in Section 5. Numerical examples reported in Section 6 illustrate the competitiveness of the hybrid approach. Section 7 contains concluding remarks.

2. Bounds via partial singular value decomposition

In this section, we derive bounds for expressions of the form

$$\mathbf{z}^T \exp(\mathcal{A})\mathbf{w}, \qquad \mathbf{z} = \begin{bmatrix}\mathbf{z}_1\\ \mathbf{z}_2\end{bmatrix}, \qquad \mathbf{w} = \begin{bmatrix}\mathbf{w}_1\\ \mathbf{w}_2\end{bmatrix}, \qquad \mathbf{z}_1, \mathbf{z}_2, \mathbf{w}_1, \mathbf{w}_2 \in \mathbb{R}^n, \tag{2.1}$$

that are computable with a partial SVD of the adjacency matrix A. Using the SVD of A (1.6), we obtain

$$\mathcal{A} = \begin{bmatrix} U & 0\\ 0 & V\end{bmatrix}\begin{bmatrix} 0 & \Sigma\\ \Sigma & 0\end{bmatrix}\begin{bmatrix} U^T & 0\\ 0 & V^T\end{bmatrix}$$

and

$$\begin{aligned}\exp(\mathcal{A}) &= \begin{bmatrix} U & 0\\ 0 & V\end{bmatrix}\exp\left(\begin{bmatrix} 0 & \Sigma\\ \Sigma & 0\end{bmatrix}\right)\begin{bmatrix} U^T & 0\\ 0 & V^T\end{bmatrix}\\ &= \begin{bmatrix} U & 0\\ 0 & V\end{bmatrix}\begin{bmatrix} \cosh(\Sigma) & \sinh(\Sigma)\\ \sinh(\Sigma) & \cosh(\Sigma)\end{bmatrix}\begin{bmatrix} U^T & 0\\ 0 & V^T\end{bmatrix}\\ &= \begin{bmatrix} \sum_{k=1}^{n}\cosh(\sigma_k)\mathbf{u}_k\mathbf{u}_k^T & \sum_{k=1}^{n}\sinh(\sigma_k)\mathbf{u}_k\mathbf{v}_k^T\\ \sum_{k=1}^{n}\sinh(\sigma_k)\mathbf{v}_k\mathbf{u}_k^T & \sum_{k=1}^{n}\cosh(\sigma_k)\mathbf{v}_k\mathbf{v}_k^T\end{bmatrix}.\end{aligned} \tag{2.2}$$

[4] In older literature, Golub–Kahan bidiagonalization is commonly referred to as Lanczos bidiagonalization.

It follows that

$$\mathbf{z}^T \exp(\mathcal{A})\mathbf{w} = \sum_{k=1}^{n} \cosh(\sigma_k)\left[\bar{z}_k \bar{w}_k + \tilde{z}_k \tilde{w}_k\right] + \sinh(\sigma_k)\left[\bar{z}_k \tilde{w}_k + \tilde{z}_k \bar{w}_k\right], \tag{2.3}$$

where

$$\begin{aligned} \bar{z}_k &= \mathbf{z}_1^T \mathbf{u}_k, \qquad & \tilde{z}_k &= \mathbf{z}_2^T \mathbf{v}_k, \\ \bar{w}_k &= \mathbf{w}_1^T \mathbf{u}_k, \qquad & \tilde{w}_k &= \mathbf{w}_2^T \mathbf{v}_k. \end{aligned} \tag{2.4}$$

Using the N largest singular triplets, we can approximate the bilinear form (2.3) by

$$F_{\mathbf{z},\mathbf{w}}^{(N)} := \sum_{k=1}^{N} \cosh(\sigma_k)\left[\bar{z}_k \bar{w}_k + \tilde{z}_k \tilde{w}_k\right] + \sinh(\sigma_k)\left[\bar{z}_k \tilde{w}_k + \tilde{z}_k \bar{w}_k\right]. \tag{2.5}$$

Throughout this paper $\|\cdot\|$ denotes the Euclidean vector norm.

Theorem 2.1. *Let $\{\sigma_i, \mathbf{u}_i, \mathbf{v}_i\}_{i=1}^N$ denote the N largest singular triplets of A. Let the vectors $\mathbf{z}$ and $\mathbf{w}$ be split according to (2.1). Then we have the bounds*

$$L_{\mathbf{z},\mathbf{w}}^{(N)} \le \mathbf{z}^T \exp(\mathcal{A})\mathbf{w} \le U_{\mathbf{z},\mathbf{w}}^{(N)}, \tag{2.6}$$

with

$$\begin{aligned} L_{\mathbf{z},\mathbf{w}}^{(N)} &:= F_{\mathbf{z},\mathbf{w}}^{(N)} - G_{\mathbf{z},\mathbf{w}}^{(N)}, \\ U_{\mathbf{z},\mathbf{w}}^{(N)} &:= F_{\mathbf{z},\mathbf{w}}^{(N)} + G_{\mathbf{z},\mathbf{w}}^{(N)}, \end{aligned} \tag{2.7}$$

where $F_{\mathbf{z},\mathbf{w}}^{(N)}$ is defined by (2.5) *and*

$$\begin{aligned} G_{\mathbf{z},\mathbf{w}}^{(N)} = \cosh(\sigma_N)&\left[\|\bar{\mathbf{z}}^{(N)}\|\,\|\bar{\mathbf{w}}^{(N)}\| + \|\tilde{\mathbf{z}}^{(N)}\|\,\|\tilde{\mathbf{w}}^{(N)}\|\right] \\ + \sinh(\sigma_N)&\left[\|\bar{\mathbf{z}}^{(N)}\|\,\|\tilde{\mathbf{w}}^{(N)}\| + \|\tilde{\mathbf{z}}^{(N)}\|\,\|\bar{\mathbf{w}}^{(N)}\|\right]. \end{aligned} \tag{2.8}$$

Here we use the notation

$$\mathbf{x}^{(N)} = [x_{N+1}, \ldots, x_n]^T$$

for any $\mathbf{x} \in \mathbb{R}^n$. The entries $\bar{z}_k$, $\tilde{z}_k$, $\bar{w}_k$, $\tilde{w}_k$ of the vectors $\bar{\mathbf{z}}^{(N)}$, $\tilde{\mathbf{z}}^{(N)}$, $\bar{\mathbf{w}}^{(N)}$, $\tilde{\mathbf{w}}^{(N)}$ are given by (2.4).

Proof. Let $c_k = \cosh(\sigma_k)$ and $s_k = \sinh(\sigma_k)$. The functions $\cosh(x)$ and $\sinh(x)$ are nondecreasing and nonnegative for $x \ge 0$. Therefore the Cauchy and triangle inequalities yield

$$\begin{aligned} \left|\mathbf{z}^T \exp(\mathcal{A})\mathbf{w} - F_{\mathbf{z},\mathbf{w}}^{(N)}\right| &= \left|\sum_{k=N+1}^{n} c_k\left[\bar{z}_k \bar{w}_k + \tilde{z}_k \tilde{w}_k\right] + s_k\left[\bar{z}_k \tilde{w}_k + \tilde{z}_k \bar{w}_k\right]\right| \\ &\le c_N \sum_{k=N+1}^{n} \left(|\bar{z}_k|\,|\bar{w}_k| + |\tilde{z}_k|\,|\tilde{w}_k|\right) + s_N \sum_{k=N+1}^{n} \left(|\bar{z}_k|\,|\tilde{w}_k| + |\tilde{z}_k|\,|\bar{w}_k|\right) \\ &\le c_N \left[\left(\sum_{k=N+1}^{n} \bar{z}_k^2\right)^{\frac{1}{2}} \left(\sum_{k=N+1}^{n} \bar{w}_k^2\right)^{\frac{1}{2}} + \left(\sum_{k=N+1}^{n} \tilde{z}_k^2\right)^{\frac{1}{2}} \left(\sum_{k=N+1}^{n} \tilde{w}_k^2\right)^{\frac{1}{2}}\right] \\ &\quad + s_N \left[\left(\sum_{k=N+1}^{n} \bar{z}_k^2\right)^{\frac{1}{2}} \left(\sum_{k=N+1}^{n} \tilde{w}_k^2\right)^{\frac{1}{2}} + \left(\sum_{k=N+1}^{n} \tilde{z}_k^2\right)^{\frac{1}{2}} \left(\sum_{k=N+1}^{n} \bar{w}_k^2\right)^{\frac{1}{2}}\right], \end{aligned}$$

from which (2.6) follows.

We have formulated the bounds (2.6) so that they can be evaluated when the N largest singular triplets of A are known; see below. It is possible to sharpen the bounds by replacing σ_N by σ_{N+1} in (2.8), but then knowledge of the N largest singular triplets of A is not sufficient to compute the bounds.

Corollary 2.2. *Let the norm of the vectors* $\mathbf{z}_1$, $\mathbf{z}_2$, $\mathbf{w}_1$, $\mathbf{w}_2$ *and the* N *largest singular triplets of* A *be known. Then the bounds (2.6) can be evaluated.*

Proof. It follows from (2.4) that $\|\overline{\mathbf{z}}\| = \|\mathbf{z}_1\|$ and $\|\tilde{\mathbf{z}}\| = \|\mathbf{z}_2\|$. Therefore,

$$\|\overline{\mathbf{z}}^{(N)}\| = \left(\|\mathbf{z}_1\|^2 - \sum_{k=1}^{N} \overline{z}_k^2 \right)^{\frac{1}{2}}, \qquad \|\tilde{\mathbf{z}}^{(N)}\| = \left(\|\mathbf{z}_2\|^2 - \sum_{k=1}^{N} \tilde{z}_k^2 \right)^{\frac{1}{2}},$$

and similarly for the vectors $\|\overline{\mathbf{w}}^{(N)}\|$ and $\|\tilde{\mathbf{w}}^{(N)}\|$. Substituting these expressions into the right-hand side of (2.8) shows the desired result.

Remark 2.3. If either one of the two halves $\mathbf{z}_1$ or $\mathbf{z}_2$ of the vector $\mathbf{z}$ vanish, then the bounds of Theorem 2.1 simplify. The same is true for the vector $\mathbf{w}$. For example, if $\mathbf{z}_2 = \mathbf{0}$, then

$$G_{\mathbf{z},\mathbf{w}}^{(N)} = \cosh(\sigma_N)\, \|\overline{\mathbf{z}}^{(N)}\|\, \|\overline{\mathbf{w}}^{(N)}\| + \sinh(\sigma_N)\, \|\overline{\mathbf{z}}^{(N)}\|\, \|\tilde{\mathbf{w}}^{(N)}\|.$$

Corollary 2.4. *Assume that the conditions of Theorem 2.1 hold. Then*

$$F_{\mathbf{z},\mathbf{z}}^{(N)} \leq \mathbf{z}^T \exp(\mathcal{A})\mathbf{z} \leq U_{\mathbf{z},\mathbf{z}}^{(N)}. \tag{2.9}$$

Proof. For each k every pair of terms in the right-hand side of (2.3) is nonnegative. This is a consequence of $\cosh(\sigma) > \sinh(\sigma) \geq 0$ for $\sigma \geq 0$ and $\overline{z}_k^2 + \tilde{z}_k^2 + 2\overline{z}_k\tilde{z}_k = (\overline{z}_k + \tilde{z}_k)^2$. Therefore $F_{\mathbf{z},\mathbf{z}}^{(N)}$ is a lower bound. The upper bound is established by Theorem 2.1.

Corollary 2.5. *Let the conditions of Theorem 2.1 hold. Then the bounds* (2.6) *satisfy*

$$\begin{array}{rcl} L_{\mathbf{z},\mathbf{w}}^{(N)} - F_{\mathbf{z},\mathbf{w}}^{(N)} & \leq & L_{\mathbf{z},\mathbf{w}}^{(N+1)} - F_{\mathbf{z},\mathbf{w}}^{(N+1)} \leq 0, \\ U_{\mathbf{z},\mathbf{w}}^{(N)} - F_{\mathbf{z},\mathbf{w}}^{(N)} & \geq & U_{\mathbf{z},\mathbf{w}}^{(N+1)} - F_{\mathbf{z},\mathbf{w}}^{(N+1)} \geq 0, \end{array} \tag{2.10}$$

for $1 \leq N < n$. *Under the assumptions of Corollary 2.4, the bounds* (2.9) *satisfy*

$$F_{\mathbf{z},\mathbf{w}}^{(N)} \leq F_{\mathbf{z},\mathbf{w}}^{(N+1)}, \qquad U_{\mathbf{z},\mathbf{w}}^{(N)} \geq U_{\mathbf{z},\mathbf{w}}^{(N+1)}, \qquad 1 \leq N < n. \tag{2.11}$$

Proof. The inequality $\|\mathbf{x}^{(N)}\| \geq \|\mathbf{x}^{(N+1)}\|$ yields

$$\begin{aligned} G_{\mathbf{z},\mathbf{w}}^{(N)} &= F_{\mathbf{z},\mathbf{w}}^{(N)} - L_{\mathbf{z},\mathbf{w}}^{(N)} \\ &= \cosh(\sigma_N) \left[\|\overline{\mathbf{z}}^{(N)}\|\, \|\overline{\mathbf{w}}^{(N)}\| + \|\tilde{\mathbf{z}}^{(N)}\|\, \|\tilde{\mathbf{w}}^{(N)}\| \right] \\ &\quad + \sinh(\sigma_N) \left[\|\overline{\mathbf{z}}^{(N)}\|\, \|\tilde{\mathbf{w}}^{(N)}\| + \|\tilde{\mathbf{z}}^{(N)}\|\, \|\overline{\mathbf{w}}^{(N)}\| \right] \\ &\geq \cosh(\sigma_{N+1}) \left[\|\overline{\mathbf{z}}^{(N+1)}\|\, \|\overline{\mathbf{w}}^{(N+1)}\| + \|\tilde{\mathbf{z}}^{(N+1)}\|\, \|\tilde{\mathbf{w}}^{(N+1)}\| \right] \\ &\quad + \sinh(\sigma_{N+1}) \left[\|\overline{\mathbf{z}}^{(N+1)}\|\, \|\tilde{\mathbf{w}}^{(N+1)}\| + \|\tilde{\mathbf{z}}^{(N+1)}\|\, \|\overline{\mathbf{w}}^{(N+1)}\| \right] = G_{\mathbf{z},\mathbf{w}}^{(N+1)}. \end{aligned}$$

The inequalities (2.10) are a consequence of $F_{\mathbf{z},\mathbf{w}}^{(N)} - L_{\mathbf{z},\mathbf{w}}^{(N)} = U_{\mathbf{z},\mathbf{w}}^{(N)} - F_{\mathbf{z},\mathbf{w}}^{(N)}$, and the inequalities (2.11) follow from the fact that $\cosh(x)$ and $\sinh(x)$ are nonnegative and nondecreasing functions for $x \geq 0$.

The above bounds are of particular interest when the vectors $\mathbf{z}$ and $\mathbf{w}$ are axis vectors. We therefore provide expressions for this situation. Also, the case when $\mathbf{w}_1$ has all entries equal is considered. Let $\mathbf{e}_i = [0, \ldots, 0, 1, 0, \ldots, 0]^T$ denote the ith axis vector of appropriate dimension. When $\mathbf{z} = \mathbf{e}_i$ and $\mathbf{w} = \mathbf{e}_j$, we can write

$$[\exp(\mathcal{A})]_{ij} = \begin{cases} \sum_{k=1}^{n} \cosh(\sigma_k) u_{ik} u_{jk}, & 1 \leq i, j \leq n, \\ \sum_{k=1}^{n} \sinh(\sigma_k) u_{ik} v_{j-n,k}, & 1 \leq i \leq n,\ n+1 \leq j \leq 2n, \\ \sum_{k=1}^{n} \sinh(\sigma_k) v_{i-n,k} u_{j,k}, & n+1 \leq i \leq 2n,\ 1 \leq j \leq n, \\ \sum_{k=1}^{n} \cosh(\sigma_k) v_{i-n,k} v_{j-n,k}, & n+1 \leq i, j \leq 2n, \end{cases}$$

where $\mathbf{u}_k = [u_{1k}, u_{2k}, \ldots, u_{nk}]^T$ and $\mathbf{v}_k = [v_{1k}, v_{2k}, \ldots, v_{nk}]^T$ are the kth left and right singular vectors of A, respectively.

Letting $\mathbf{z} = \mathbf{w} = \mathbf{e}_i$, $i = 1, \ldots, n$, yields hub centralities, and $\mathbf{z} = \mathbf{w} = \mathbf{e}_i$, $i = n+1, \ldots, 2n$, gives authority centralities. We obtain the bounds

$$F_{ii}^{(N)} \leq \left[e^{\mathcal{A}}\right]_{ii} \leq U_{ii}^{(N)}, \qquad 1 \leq i \leq 2n, \tag{2.12}$$

where

$$F_{ii}^{(N)} := \begin{cases} \sum_{k=1}^{N} \cosh(\sigma_k) u_{ik}^2, & 1 \leq i \leq n, \\ \sum_{k=1}^{N} \cosh(\sigma_k) v_{i-n,k}^2, & n+1 \leq i \leq 2n, \end{cases}$$

$$U_{ii}^{(N)} := F_{ii}^{(N)} + \begin{cases} \cosh(\sigma_N) \left(\mathcal{U}_i^{(N)}\right)^2, & 1 \leq i \leq n, \\ \cosh(\sigma_N) \left(\mathcal{V}_{i-n}^{(N)}\right)^2, & n+1 \leq i \leq 2n, \end{cases}$$

and

$$\mathcal{U}_r^{(N)} = \left(1 - \sum_{k=1}^{N} u_{rk}^2\right)^{\frac{1}{2}}, \qquad \mathcal{V}_r^{(N)} = \left(1 - \sum_{k=1}^{N} v_{rk}^2\right)^{\frac{1}{2}}.$$

Letting $\mathbf{z} = \mathbf{e}_i$ and $\mathbf{w} = \mathbf{e}_j$, $i, j = 1, \ldots, n$, $i \neq j$, determines hub communicabilities, and the choice $\mathbf{z} = \mathbf{e}_i$ and $\mathbf{w} = \mathbf{e}_j$, $i, j = n+1, \ldots, 2n$, $i \neq j$, gives authority communicabilities. We have the bounds

$$L_{ij}^{(N)} \leq [\exp(\mathcal{A})]_{ij} \leq U_{ij}^{(N)}, \qquad i \neq j, \tag{2.13}$$

where $L_{ij}^{(N)} = F_{ij}^{(N)} - G_{ij}^{(N)}$ and $U_{ij}^{(N)} = F_{ij}^{(N)} + G_{ij}^{(N)}$, with

$$F_{ij}^{(N)} := \begin{cases} \sum_{k=1}^{N} \cosh(\sigma_k) u_{ik} u_{jk}, & 1 \leq i, j \leq n, \\ \sum_{k=1}^{N} \cosh(\sigma_k) v_{i-n,k} v_{j-n,k}, & n+1 \leq i, j \leq 2n, \end{cases}$$

$$G_{ij}^{(N)} := \begin{cases} \cosh(\sigma_N)\, \mathcal{U}_i^{(N)} \mathcal{U}_j^{(N)}, & 1 \leq i, j \leq n, \\ \cosh(\sigma_N)\, \mathcal{V}_{i-n}^{(N)} \mathcal{V}_{j-n}^{(N)}, & n+1 \leq i, j \leq 2n. \end{cases}$$

Setting $\mathbf{z} = \mathbf{e}_i$, $i = 1, \ldots, n$, $\mathbf{w}_1 = n^{-\frac{1}{2}}[1, \ldots, 1]^T$, and $\mathbf{w}_2 = \mathbf{0}$, we can write

$$n^{-\frac{1}{2}} \sum_{j=1}^{n} [\exp(\mathcal{A})]_{ij} = n^{-\frac{1}{2}} \sum_{k=1}^{n} \cosh(\sigma_k)\, u_{ik} \sum_{j=1}^{n} u_{jk}, \qquad i = 1, \ldots, n, \tag{2.14}$$

which is a measure of the importance of a node as a hub. This concept is connected to the *total subgraph communicability* for a node of an undirected network, defined in [7], and to the *f-starting convenience* for a node of a directed network, introduced in [23]. We have

$$L_{\mathbf{z},\mathbf{w}}^{(N)} \leq n^{-\frac{1}{2}} \sum_{j=1}^{n} [\exp(\mathcal{A})]_{ij} \leq U_{\mathbf{z},\mathbf{w}}^{(N)}, \tag{2.15}$$

where the bounds are given by (2.7), with

$$F_{\mathbf{z},\mathbf{w}}^{(N)} := n^{-\frac{1}{2}} \sum_{k=1}^{N} \cosh(\sigma_k)\, u_{ik} \sum_{j=1}^{n} u_{jk},$$

$$G_{\mathbf{z},\mathbf{w}}^{(N)} := n^{-\frac{1}{2}} \cosh(\sigma_N)\, \mathcal{U}_i^{(N)} \left(n - \sum_{k=1}^{N} \left(\sum_{j=1}^{n} u_{jk}\right)^2\right)^{\frac{1}{2}}.$$

Analogously, setting $\mathbf{z}_1 = \mathbf{0}$, $\mathbf{z}_2 = n^{-\frac{1}{2}}[1, \ldots, 1]^T$, and $\mathbf{w} = \mathbf{e}_j$, $j = n+1, \ldots, 2n$, we obtain

$$n^{-\frac{1}{2}} \sum_{i=n+1}^{2n} [\exp(\mathcal{A})]_{ij} = n^{-\frac{1}{2}} \sum_{k=1}^{n} \cosh(\sigma_k) v_{j-n,k} \sum_{i=1}^{n} v_{ik}, \qquad j = n+1, \ldots, 2n,$$

which is a measure of the importance of a node as an authority; see also the definition of f*-ending convenience* in [23]. We have

$$L_{\mathbf{z},\mathbf{w}}^{(N)} \leq n^{-\frac{1}{2}} \sum_{i=n+1}^{2n} [\exp(\mathcal{A})]_{ij} \leq U_{\mathbf{z},\mathbf{w}}^{(N)},$$

where the bounds are given by (2.7), with

$$F_{\mathbf{z},\mathbf{w}}^{(N)} := n^{-\frac{1}{2}} \sum_{k=1}^{N} \cosh(\sigma_k) v_{j-n,k} \sum_{i=1}^{N} v_{ik},$$

$$G_{\mathbf{z},\mathbf{w}}^{(N)} := n^{-\frac{1}{2}} \cosh(\sigma_N)\, \mathcal{V}_{j-n}^{(N)} \left(n - \sum_{k=1}^{N} \left(\sum_{i=1}^{n} v_{ik} \right)^2 \right)^{\frac{1}{2}}.$$

We conclude this section with two observations. It suffices that the function f be nondecreasing and nonnegative on the spectrum of $\mathcal{A}$ in order to establish upper and lower bounds for $\mathbf{z}^T f(\mathcal{A})\mathbf{w}$ for given vectors $\mathbf{z}$ and $\mathbf{w}$. This is discussed in [22]. The fact that f is the exponential function yields the particular structure exhibited in (2.2). Moreover, the situation $\mathbf{z} \neq \mathbf{w}$ also can be dealt with by using the relation

$$\mathbf{z}^T \exp(\mathcal{A})\mathbf{w} = \frac{1}{4}(\mathbf{z}+\mathbf{w})^T \exp(\mathcal{A})(\mathbf{z}+\mathbf{w}) - \frac{1}{4}(\mathbf{z}-\mathbf{w})^T \exp(\mathcal{A})(\mathbf{z}-\mathbf{w}). \tag{2.16}$$

Thus, we can apply Corollary 2.4 to determine upper and lower bounds for the left-hand side expression. Computed examples of Section 6 illustrate the performance of the bounds of this section.

3. Determining important nodes by partial singular value decomposition

This section describes how knowledge of the N leading singular triplets $\{\sigma_k, \mathbf{u}_k, \mathbf{v}_k\}_{k=1}^{N}$ of A and the bounds (2.12) can be used to determine two subsets of nodes that contain the nodes with the largest hub centrality $[\cosh(\sqrt{AA^T})]_{ii}$ and the nodes with the largest authority centrality $[\cosh(\sqrt{A^TA})]_{ii}$, respectively. An approach analogous to the one of this paper was applied in [22] to determine a low-rank approximant of a large symmetric adjacency matrix. However, several aspects of the method of the present paper are different, because the adjacency matrices considered in this paper are not symmetric.

Let $F_{ii}^{(N)}$ and $U_{ii}^{(N)}$ be the lower and upper bounds (2.12), respectively, and let $\mathcal{L}_{H,m}^{(N)}$ denote the mth largest lower bound $F_{ii}^{(N)}$ for $1 \leq i \leq n$. Introduce the index sets

$$S_{H,m}^{(N)} = \left\{ i \ : \ 1 \leq i \leq n \text{ and } U_{ii}^{(N)} \geq \mathcal{L}_{H,m}^{(N)} \right\}, \qquad N = 1, 2, \ldots, n. \tag{3.1}$$

This set is of interest when ranking nodes according to their hub centrality.

Let $\mathcal{L}_{A,m}^{(N)}$ denote the mth largest lower bound $F_{ii}^{(N)}$ for $n+1 \leq i \leq 2n$ and consider the index sets

$$S_{A,m}^{(N)} = \left\{ i \ : \ n+1 \leq i \leq 2n \text{ and } U_{ii}^{(N)} \geq \mathcal{L}_{A,m}^{(N)} \right\}, \qquad N = 1, 2, \ldots, n. \tag{3.2}$$

We use this set to determine nodes with the largest authority centrality.

The computations required to determine the most important hubs and the most important authorities are similar. We therefore can treat both computations simultaneously and omit the subscripts H and A for the sets (3.1) and (3.2). It is not hard to see that if $i \notin S_m^{(N)}$, then node i cannot be in the subset of the m nodes with the largest centrality. Moreover, any node whose index is an element of $S_m^{(N)}$ can be in this subset. Let $|S_m^{(N)}|$ denote the cardinality of $S_m^{(N)}$. The following inequalities are useful in our computations.

Corollary 3.1.

$$S_m^{(n)} \subseteq S_m^{(n-1)} \subseteq \cdots \subseteq S_m^{(1)} \quad \textit{and} \quad |S_m^{(n)}| \geq m. \tag{3.3}$$

The set $S_m^{(N)}$ contains the indices for a subset of nodes that contains the set of the m most important nodes. In particular, when $|S_m^{(N)}| = m$, the set $S_m^{(N)}$ contains the indices for the m most important nodes.

Proof. By the definition of the sets $S_m^{(N)}$, each set contains at least m indices. The relations (3.3) now follow from (2.11) and (2.12). The observation about the situation when $|S_m^{(N)}| = m$ is a consequence of the fact that the set $S_m^{(N)}$ contains the indices for the m nodes with the largest centrality.

Remark 3.2. The lower bound $F_{ii}^{(N)}$ of (2.12) usually converges to $[\exp(\mathcal{A})]_{ii}$ much faster than the upper bound $U_{ii}^{(N)}$ as N increases. Therefore, for N fixed, $F_{ii}^{(N)}$ typically is a better approximation of $[\exp(\mathcal{A})]_{ii}$ than $\frac{1}{2}(F_{ii}^{(N)} + U_{ii}^{(N)})$.

Remark 3.3. The ordering of the lower bounds $F_{ii}^{(N)}$, $i \in S_m^{(N)}$, may be different from the ordering of the centralities $[\exp(\mathcal{A})]_{ii}$.

We turn to some computational issues. Evaluation of the bounds (2.12) and (2.13) requires the computation of $f(\sigma_N)$. This may result in overflow when the graph contains many nodes and f is the hyperbolic sine or cosine function. For instance, when the computations are carried out in double precision arithmetic, i.e., with about 16 significant decimal digits, we obtain overflow when evaluating $\cosh(x)$ for $x \gtrsim 710$. This difficulty can be circumvented by replacing $\cosh(x)$ by

$$\exp(-\mu)\cosh(x) = \frac{1}{2}(\exp(x-\mu) + \exp(-x-\mu)),$$

for an appropriate value of μ. Since the largest singular triplet $\{\sigma_1, \mathbf{u}_1, \mathbf{v}_1\}$ of A is available, we use $\mu = \sigma_1$ in the computed examples reported in Section 6.

Another computational difficulty to overcome is that we do not know in advance how many of the largest singular triplets $\{\sigma_k, \mathbf{u}_k, \mathbf{v}_k\}_{k=1}^N$ of A have to be computed to obtain useful bounds (2.12) or (2.13). Assume for definiteness that we would like to determine the m nodes with the largest hub centrality. We use the augmented implicitly restarted Golub–Kahan bidiagonalization method described in [2] to compute the largest triplets in the examples of Section 6. Our implementation of this method is a slight modification of the MATLAB function irlba described in [2]. It differs in that it can be restarted with singular triplets produced by previous calls to the function as input. This modification, which we also refer to as irlba, makes it possible to compute new singular triplets without recomputing already known triplets. In the examples of Section 6, we determine the $q = 5$ largest singular triplets that have not yet been computed by repeated calls of irlba. Thus, the first call of irlba yields the singular triplets $\{\sigma_k, \mathbf{u}_k, \mathbf{v}_k\}_{k=1}^q$. If $|S_m^{(q)}| > m$, then we call irlba again to determine the next q singular triplets $\{\sigma_k, \mathbf{u}_k, \mathbf{v}_k\}_{k=q+1}^{2q}$. If $|S_m^{(N)}| = m$ for some $N \leq 2q$, then we are done; otherwise we compute the next q singular triplets $\{\sigma_k, \mathbf{u}_k, \mathbf{v}_k\}_{k=2q+1}^{3q}$ of A with irlba, and so on. This approach to computing the N largest singular triplets of A only requires storage of the already computed triplets and a residual vector when the next batch of q singular triplets is to be computed.

The above method for determining singular triplets is attractive when the computer at hand allows storage of all already computed singular triplets. However, when the adjacency matrix is very large and fairly many singular triplets $\{\sigma_k, \mathbf{u}_k, \mathbf{v}_k\}_{k=1}^N$ are required for $|S_m^{(N)}| = m$ to hold, the use of a method that requires less computer storage may be preferable. We now outline such a method. Note that the bounds (2.12) and (2.13) can be updated when a new batch of q singular triplets has been computed. Therefore, the evaluation of the bounds (2.12) and (2.13) does not require simultaneous access to all computed singular triplets. Hence, we may reduce the storage demand by using an augmented implicitly restarted Golub–Kahan bidiagonalization method that does not require access to all already computed singular triplets to determine the next batch of q singular triplets. The algorithm irblb described in [4] has this property. It uses Leja shifts to determine an acceleration polynomial that dampens singular values outside a region of interest. When calling irblb, the smallest computed singular value σ_N is passed as a parameter. The algorithm then seeks to determine the q singular values that are closest to σ_N and the corresponding singular vectors. This method requires fairly little temporary storage. The memory requirement therefore is much smaller than for the irlba-based computations described above when a large number, N, of singular triplets is needed to secure that $|S_m^{(N)}| = m$. We remark that the use of irblb may require more matrix-vector product evaluations with A and A^T than irlba, because a few of the already computed singular triplets might be recomputed at a subsequent call of irblb. Our computational experience indicates that for many real-world networks the required size of N is quite small and, therefore, irlba generally can be used also for large networks.

In the above discussion, we determined more and more singular triplets of A until their number N is such that

$$|S_m^{(N)}| = m. \tag{3.4}$$

We refer to this stopping rule as the *strong convergence criterion*. By Corollary 3.1, the set $S_m^{(N)}$ contains the indices of the m nodes with the largest centrality.

The criterion (3.4) for choosing N is useful if the required value of N is not too large. We introduce the *weak convergence criterion* to be used for problems for which the large size of N required to satisfy (3.4) makes it impractical to compute the associated bounds (2.12). The weak convergence criterion is well suited for use with the hybrid algorithm described in Section 5 for determining the most important nodes. This criterion is designed to stop increasing N when the lower bounds $F_{ii}^{(N)}$ do not increase significantly with N. Specifically, in the case of hub centrality, we stop increasing N when the average increment of the lower bounds $F_{ii}^{(N)}$, $1 \le i \le n$, is small when including the Nth singular triplet $\{\sigma_N, \mathbf{u}_N, \mathbf{v}_N\}$ in the bounds. The average contribution of this singular triplet to the bounds $F_{ii}^{(N)}$, $1 \le i \le n$, is

$$\frac{1}{n}\sum_{i=1}^{n} f(\sigma_N) u_{i,N}^2 = \frac{1}{n} f(\sigma_N),$$

and we stop increasing N when

$$\frac{1}{n} f(\sigma_N) \le \tau \cdot \mathcal{L}_{H,m}^{(N)} \tag{3.5}$$

for a user-specified tolerance τ. We use $\tau = 10^{-3}$ in the computed examples. Note that when this criterion is satisfied, but not (3.4), the m nodes with indices in $S_m^{(N)} = S_{H,m}^{(N)}$ with the largest lower bounds $F_{ii}^{(N)}$ are not guaranteed to be the nodes with the largest hub centrality.

The weak convergence criterion (3.5) might yield a set $S_{H,m}^{(N)}$ with many more indices than m, and we may not want to compute accurate bounds for the hub centrality using the approach of Section 4 for all nodes with index in $S_{H,m}^{(N)}$. We therefore describe how to determine a smaller index set $\mathcal{J}$, which is likely to contain the indices of the m nodes with the largest hub centrality. In view of that $F_{ii}^{(N)}$ generally is a better approximation of $[f(A)]_{ii}$ than $U_{ii}^{(N)}$ (cf. Remark 3.2), we discard from the set $S_{H,m}^{(N)}$ indices for which $F_{ii}^{(N)}$ is much smaller than $\mathcal{L}_{H,m}^{(N)}$. Thus, for a user-chosen parameter $\rho > 0$, we include in the set $\mathcal{J}$ all indices $i \in S_{H,m}^{(N)}$ such that

$$\mathcal{L}_{H,m}^{(N)} - F_{ii}^{(N)} < \rho \cdot \mathcal{L}_{H,m}^{(N)}. \tag{3.6}$$

In the computed examples, we use $\rho = 10^{-1}$. We may proceed similarly to prune the set $S_{A,m}^{(N)}$.

Algorithms 1 and 2 describe the computation of the index sets $S_{H,m}^{(N)}$ and $S_{A,m}^{(N)}$, as well as the determination of a suitable value of N. The singular triplets are computed either with the slightly modified MATLAB function irlba from [2] or with algorithm irblb from [4]. The function f is the exponential function (1.3); it may be replaced by some other nonnegative nondecreasing function.

The algorithm requires functions for the evaluation of matrix-vector products with the adjacency matrix A and its transpose, its order n, and the desired number of nodes m with the largest hub centrality and authority centrality. In addition, the following parameters have to be provided:

- $N_{\max}$, maximum number of iterations performed;
- q, number of singular triplets computed at each irlba call;
- $M_{\max}$, maximum number of singular vectors kept in memory;
- τ, tolerance used to detect *weak* convergence;
- ρ, tolerance used to construct an extended list of nodes in case of weak convergence; cf. (3.6).

Algorithm 1 first initializes the vectors $\boldsymbol{\ell}^H$, $\mathbf{z}^H$, and $\mathbf{s}^H$, whose components at each iteration N are given by

$$\ell_i^H = F_{ii}^{(N)}, \quad z_i^H = U_{ii}^{(N)}, \quad s_i^H = \sum_{k=1}^{N} u_{ik}^2, \quad i = 1, \ldots, n.$$

The vectors $\boldsymbol{\ell}^A$, $\mathbf{z}^A$, and $\mathbf{s}^A$ for authority centrality, are initialized similarly. Then, irlba is called to compute the first batch of q singular triplets and the main loop is entered. The Boolean variable "flag" is used to signal whether the

Algorithm 1 Low-rank approximation, part 1

Input: matrix A of size n, number m of nodes to be identified,
  tuning constants: $N_{\max}$, q, $M_{\max}$, τ, ρ
for $i = 1$ **to** n **do** $\ell_i^H, \ell_i^A, s_i^H, s_i^A = 0$ **end**
call irlba to compute $\{\sigma_i, \mathbf{u}_i, \mathbf{v}_i\}_{i=1}^q$ such that $\sigma_i \geq \sigma_{i+1}$
if shift is active **then** $\mu = \sigma_1$ **else** $\mu = 0$ **end**
$N = 0$, $\overline{N} = 0$, flag = **true** , flag^H = **true** , flag^A = **true**
while flag **and** $(N < \min\{N_{\max}, n\})$ **and** $(\overline{N} < q)$
  $N = N + 1$, $\overline{N} = \overline{N} + 1$
  $f_\sigma = (\exp(\sigma_N - \mu) + \exp(-\sigma_N - \mu))/2$
  if flag^H
    for $i = 1$ **to** n **do** $t_i = u_{iN}^2$ **end**
    $\mathbf{s}^H = \mathbf{s}^H + \mathbf{t}$
    $\boldsymbol{\ell}^H = \boldsymbol{\ell}^H + f_\sigma \cdot \mathbf{t}$
    $\mathbf{z}^H = \boldsymbol{\ell}^H + f_\sigma(1 - \mathbf{s}^H)$
    let $\boldsymbol{\psi} = [\psi_1, \ldots, \psi_n]$ be an index permutation such that $\ell_{\psi_i}^H \geq \ell_{\psi_{i+1}}^H$
    $L_{\max}^H = \ell_{\psi_m}^H$
    $S_{H,m}^{(N)} = \{i \,:\, z_i^H \geq L_{\max}^H\}$
    flag^H = $(|S_{H,m}^{(N)}| > m)$ **and** $(\frac{1}{n} f_\sigma > \tau \cdot L_{\max}^H)$
  end if
  if flag^A
    for $i = 1$ **to** n **do** $w_i = v_{iN}^2$ **end**
    $\mathbf{s}^A = \mathbf{s}^A + \mathbf{w}$
    $\boldsymbol{\ell}^A = \boldsymbol{\ell}^A + f_\sigma \cdot \mathbf{w}$
    $\mathbf{z}^A = \boldsymbol{\ell}^A + f_\sigma(1 - \mathbf{s}^A)$
    let $\boldsymbol{\phi} = [\phi_1, \ldots, \phi_n]$ be an index permutation such that $\ell_{\phi_i}^A \geq \ell_{\phi_{i+1}}^A$
    $L_{\max}^A = \ell_{\phi_m}^A$
    $S_{A,m}^{(N)} = \{i \,:\, z_i^A \geq L_{\max}^A\}$
    flag^A = $(|S_{A,m}^{(N)}| > m)$ **and** $(\frac{1}{n} f_\sigma > \tau \cdot L_{\max}^A)$
  end if
  flag = flag^H **or** flag^A
  if flag **and** $\overline{N} = q$
    if $N < M_{\max}$
      call irlba to compute $\{\sigma_k, \mathbf{u}_k, \mathbf{v}_k\}_{i=N+1}^{N+q}$ such that $\sigma_{N+i} \geq \sigma_{N+i+1}$
      $\overline{N} = 0$
    else
      call irblb to compute sing. values $\nu_1 \geq \cdots \geq \nu_q$ closest to σ_N
      $r = \arg\min_i |\nu_i - \sigma_N|$
      $\sigma_{N+i} = \nu_{r+i}$, $i = 1, \ldots, q - r$; $\{\mathbf{u}_{N+i}, \mathbf{v}_{N+i}\}$ associated sing. vectors
      $\overline{N} = r$
    end if
  end if
end while

strong or weak convergence criterion is satisfied. The parameter $N_{\max}$ specifies the maximum number of iterations, i.e., the maximum number of times the loop comprised of lines 7–42 is executed. We found it beneficial to introduce the auxiliary parameter $\overline{N}$ to keep track of how many singular triplets from the current batch are being used. When $\overline{N} = q$, a new batch of singular triplets is computed.

The bounds (2.12) are computed in lines 12–14 and 22–24. The vector of indices $\boldsymbol{\psi}$ contains a permutation which yields the lower bounds ℓ_i^H in decreasing order. The set $S_{H,m}^{(N)}$ is constructed at line 17, while the set $S_{A,m}^{(N)}$ is constructed in lines 20–29. Subsequently the exit condition is checked. Lines 31–41 give a new batch of singular triplets. Either one of the two kinds of restarts discussed above may be applied. If $\overline{N}$ is smaller than $M_{\max}$, then we compute the next q singular triplets. If, instead, $\overline{N} \geq M_{\max}$, then we seek to determine the q singular values close to the smallest available singular value σ_N, and we select those singular triplets that have singular values smaller than σ_N; see lines 37–38.

Algorithm 2 Low-rank approximation, part 2

43: **if** flag^H
44: $\quad j = |S_{H,m}^{(N)}| - m$
45: $\quad$ info = 2 *% no convergence*
46: **else**
47: $\quad$ **if** $|S_{H,m}^{(N)}| > m$
48: $\quad\quad \mathcal{J} = \{i \,:\, i > m,\ L_{\max}^H - \ell_{\psi_i}^H < \rho \cdot L_{\max}^H\}$
49: $\quad\quad j = \min(|\mathcal{J}|, 100),\ j = \max(j, 5)$
50: $\quad\quad$ info = 1 *% weak convergence*
51: $\quad$ **else**
52: $\quad\quad j = 0$
53: $\quad\quad$ info = 0 *% strong convergence*
54: $\quad$ **end if**
55: **end if**
56: **for** $i = 1$ **to** $m + j$
57: $\quad \mathcal{N}_i^H = \psi_i$
58: $\quad \mathcal{V}_i^H = \mathrm{e}^{\mu} \cdot \ell_{\psi_i}^H$
59: **end if**
60: **Output:** list of nodes $\mathcal{N}^H$, hub centralities $\mathcal{V}^H$,
61: $\quad$ spectrum shift μ, iterations N, info

Algorithm 2 describes the continued computations when the m nodes with the largest hub centrality are desired. The m nodes with the largest authority centrality can be computed in a similar way. Lines 43–55 of the algorithm determine whether the strong or weak convergence criterion is satisfied. The variable "info" contains this information. A list of the desired nodes $\mathcal{N}^H$ is formed in lines 56–59, where the hub centralities also are updated, keeping in mind the spectrum shift at line 9 of Algorithm 1. We remark that the MATLAB implementation of Algorithms 1 and 2 contains some features not described here. For instance, we only apply the correction due to the spectrum shift when this does not cause overflow.

This section described how to determine the m nodes with the largest hub centrality and authority centrality of a large network by using the bounds (2.6) and (2.9) with $\mathbf{w} = \mathbf{z}$. These bounds can be used in a similar way with $\mathbf{w} \neq \mathbf{z}$ to compute upper and lower bounds for hub and authority communicability. This allows us to determine subsets of nodes with the largest hub or authority communicability; see [6, 23] for other approaches to determine hub and authority communicability.

4. Bounds via Gauss quadrature

This section discusses how to compute upper and lower bounds for the entries of the submatrices of the matrix (1.3) with the aid of Gauss quadrature rules. This technique is applied by Benzi et al. [6] to the expressions (1.5).

Our approach is based on partial Golub–Kahan bidiagonalization of the matrix A and requires less storage than the approach in [6], which computes a partial Lanczos tridiagonalization of the matrix (1.2). A nice overview of Gauss quadrature-based methods for computing bounds for matrix functionals has recently been presented by Golub and Meurant [28]; see also [27]. A thorough discussion of how Golub–Kahan bidiagonalization can be applied to computing upper and lower bounds for certain matrix functional can be found in [14]. Other applications of quadrature rules to bound quantities of interest in network analysis are discussed in [5, 13, 23].

We first consider the computation of upper and lower bounds for the ith diagonal entry of the matrix $\cosh(\sqrt{AA^T})$. Application of ℓ Golub–Kahan bidiagonalization steps to the matrix A with initial vector $\mathbf{e}_i$ yields the decompositions

$$AP_\ell = Q_{\ell+1}B_{\ell+1,\ell}, \qquad A^T Q_\ell = P_\ell B_\ell^T, \tag{4.1}$$

where the matrices $P_\ell \in \mathbb{R}^{n\times\ell}$ and $Q_{\ell+1} \in \mathbb{R}^{n\times(\ell+1)}$ have orthonormal columns, $Q_\ell \in \mathbb{R}^{n\times\ell}$ consists of the first ℓ columns of $Q_{\ell+1}$ and $Q_{\ell+1}\mathbf{e}_1 = \mathbf{e}_i$, the matrix $B_{\ell+1,\ell} = [\beta_{jk}] \in \mathbb{R}^{(\ell+1)\times\ell}$ is lower bidiagonal with leading $\ell \times \ell$ submatrix B_ℓ. All diagonal and subdiagonal entries of $B_{\ell+1,\ell}$ may be assumed to be nonvanishing, otherwise the recursions break down and the discussion simplifies; see below. A detailed discussion on Golub–Kahan bidiagonalization is provided, e.g., by Björck [10].

Combining the equations (4.1) gives

$$AA^T Q_\ell = Q_\ell B_\ell B_\ell^T + \beta_{\ell+1,\ell}\beta_{\ell,\ell}\mathbf{q}_{\ell+1}\mathbf{e}_\ell^T, \tag{4.2}$$

where $\mathbf{q}_{\ell+1}$ denotes the last column of $Q_{\ell+1}$. The matrix

$$T_\ell = B_\ell B_\ell^T \tag{4.3}$$

is symmetric and tridiagonal. Therefore, the expression (4.2) is a partial symmetric Lanczos tridiagonalization of the symmetric positive semidefinite matrix AA^T.

Following Golub and Meurant [27, 28], we write the ith diagonal entry of the matrix $\cosh(\sqrt{AA^T})$ as a Stieltjes integral

$$\mathbf{e}_i^T \cosh(\sqrt{AA^T})\mathbf{e}_i = \int \cosh(\sqrt{t})d\omega(t), \tag{4.4}$$

where ω is a piecewise constant step function with jumps at the eigenvalues σ_j^2 of AA^T. The integral is over the support of the measure, i.e., over the interval $[\sigma_n^2, \sigma_1^2]$. The identity (4.4) is obtained by substituting the spectral factorization of AA^T into the left-hand side. It is natural to approximate (4.4) by using the small tridiagonal matrix (4.3). Golub and Meurant [27, 28] observed that $\mathbf{e}_1^T \cosh(\sqrt{T_\ell})\mathbf{e}_1$ is an ℓ-point Gauss quadrature rule for the approximation of (4.4); see also [14]. The remainder term for Gauss quadrature yields

$$\mathbf{e}_i^T \cosh(\sqrt{AA^T})\mathbf{e}_i - \mathbf{e}_1^T \cosh(\sqrt{T_\ell})\mathbf{e}_1 = \frac{1}{(2\ell)!}\left(\frac{d^{2\ell}}{dt^{2\ell}}\cosh(\sqrt{\theta})\right)\int \prod_{j=1}^{\ell}(t-\theta_j^{(\ell)})^2 d\omega(t), \tag{4.5}$$

where $\sigma_n^2 < \theta_1^{(\ell)} < \theta_2^{(\ell)} < \cdots < \theta_\ell^{(\ell)} < \sigma_1^2$ are the nodes of the quadrature rule and $\sigma_n^2 < \theta < \sigma_1^2$; see, e.g., Gautschi [24]. It follows for instance from the Taylor expansion of $\cosh(\sqrt{t})$ that all derivatives of this function are positive for $t \geq 0$. This fact is required in the derivation of the right-hand side of (4.5) and shows that

$$\mathbf{e}_i^T \cosh(\sqrt{AA^T})\mathbf{e}_i - \mathbf{e}_1^T \cosh(\sqrt{T_\ell})\mathbf{e}_1 > 0.$$

Consequently, the Gauss rule provides a lower bound for (4.4). Moreover, it is fairly easy to show that the lower bound is strictly increasing with ℓ; see [36] for details.

The remainder term for an $(\ell+1)$-point Gauss–Radau quadrature rule with ℓ "free" nodes and one fixed node at σ_1^2 is given by

$$\frac{1}{(2\ell+1)!}\left(\frac{d^{2\ell+1}}{dt^{2\ell+1}}\cosh(\sqrt{\theta})\right)\int (t-\sigma_1^2)\prod_{j=1}^{\ell}(t-\hat{\theta}_j^{(\ell)})^2 d\omega(t),$$

where $\sigma_n^2 < \hat{\theta}_1^{(\ell)} < \hat{\theta}_2^{(\ell)} < \cdots < \hat{\theta}_\ell^{(\ell)} < \sigma_1^2$ denote the free nodes and $\sigma_n^2 < \theta < \sigma_1^2$; see [24]. It is clear that the remainder term is negative, i.e.,

$$\mathbf{e}_i^T \cosh(\sqrt{AA^T})\mathbf{e}_i - \mathbf{e}_1^T \cosh(\sqrt{\hat{T}_{\ell+1}})\mathbf{e}_1 < 0.$$

It follows that the Gauss–Radau rule with a fixed node at σ_1^2 provides an upper bound for (4.4). The singular value σ_1 is known from the computations required to evaluate the bounds of Section 2. It can be shown that the upper bound is strictly decreasing with ℓ; see [36].

The $(\ell+1)$-point Gauss–Radau quadrature rule with a fixed node at σ_1^2 can be expressed with a symmetric tridiagonal matrix $\hat{T}_{\ell+1} \in \mathbb{R}^{(\ell+1)\times(\ell+1)}$, whose elements, except for the last diagonal entry, are those of $B_{\ell+1,\ell}B_{\ell+1,\ell}^T$. The last diagonal entry of $\hat{T}_{\ell+1}$ is determined so that the matrix has the eigenvalue σ_1^2. This entry can be computed in only $\mathcal{O}(\ell)$ arithmetic floating point operations; see [27, 28] for details.

The above discussion carries over to expressions of the form $\mathbf{w}^T \cosh(\sqrt{AA^T})\mathbf{w}$, where $\mathbf{w}$ is a unit vector. The only change required is that Golub–Kahan bidiagonalization has to be started with the vector $\mathbf{w}$ instead of with $\mathbf{e}_i$. Then the first column of the matrix $Q_{\ell+1}$ is $\mathbf{w}$.

Let $\mathbf{w}_1$ and $\mathbf{w}_2$ be linearly independent vectors in $\mathbb{R}^n$. Then

$$\begin{aligned}\mathbf{w}_1^T \cosh(\sqrt{AA^T})\mathbf{w}_2 = &\ \frac{1}{4}(\mathbf{w}_1+\mathbf{w}_2)^T \cosh(\sqrt{AA^T})(\mathbf{w}_1+\mathbf{w}_2)\\ &- \frac{1}{4}(\mathbf{w}_1-\mathbf{w}_2)^T \cosh(\sqrt{AA^T})(\mathbf{w}_1-\mathbf{w}_2).\end{aligned} \tag{4.6}$$

This identity, which is analogous to (2.16), allows us to compute bounds for the entry in row i and column j of the matrix $\cosh(\sqrt{AA^T})$ by choosing $\mathbf{w}_1 = \mathbf{e}_i$ and $\mathbf{w}_2 = \mathbf{e}_j$. Hence, we are able to compute bounds for all the entries in the leading principal $n\times n$ submatrix of (1.3). Bounds for the trailing principal $n\times n$ submatrix of (1.3) can be determined analogously by interchanging A and A^T in the partial Golub–Kahan bidiagonalization (4.1). Finally, bounds for the entries in the off-diagonal $n\times n$ blocks of (1.3) can be obtained by replacing $\cosh(\sqrt{AA^T})$ by the function $A\,\mathrm{s}(\sqrt{AA^T})$ defined by (1.4) and choosing suitable vectors $\mathbf{w}_1$ and $\mathbf{w}_2$ in (4.6). The Taylor expansion of (1.4) shows that all derivatives are positive on the nonnegative real axis.

In the rare event that the recursion formulas for Golub–Kahan bidiagonalization break down, the Gauss quadrature rule gives the exact value (in the absence of round-off errors).

5. The hybrid method

The computations with our hybrid method already have been commented on. The method first evaluates a partial singular value decomposition of the adjacency matrix A and applies it to determine which nodes might be the most interesting ones with respect to the criterion chosen. This is described in Section 3 for the situation when we would like to determine the nodes of a large network with the largest hub and authority centrality. More accurate upper and lower bounds for expressions of the form (2.1) for the nodes singled out are then determined with the aid of Gauss quadrature rules. This allows us to compute the node with the largest hub and authority centrality of a large graph without evaluating pairs of Gauss and Gauss–Radau rules for every node of the network, i.e., for every diagonal entry of the matrix (1.2). The evaluation of Gauss-type rules for every diagonal entry can be expensive for large graphs. The computations with our hybrid method typically are considerably cheaper. This is illustrated in the following section.

6. Computed examples

This section presents a few examples that illustrate the performance of the methods discussed in the paper. All computations were carried out in MATLAB version 8.1 (R2013a) 64-bit for Linux, in double precision arithmetic, on an Intel Core i7-860 computer, with 8 Gb RAM. The function f is the exponential function (1.3). We applied the methods discussed in the paper to eight directed unweighted networks coming from the following real-world applications:

Airlines (235 nodes, 2101 edges) represents air traffic and is available at [25]. The nodes represent airports and the directed edges represent flights between them.

Celegans (306 nodes, 2345 edges) is the metabolic network of *Caenorhabditis elegans* [16], a small nematode (roundworm). The data set is available at [1].

Air500 (500 nodes, 24009 edges) is a network of worldwide flight connections between the top 500 airports based on total passenger volume [9] during the time from July 1, 2007, to June 30, 2008 [37].

Twitter (3556 nodes, 188712 edges) is part of the Twitter network [25]. The nodes are users and the directed edges are mentions and re-tweets between users.

Wikivote (8297 nodes, 103689 edges) is the network of administrator elections and vote history data: a directed edge from node i to node j indicates that user i voted for user j [32, 33]. The data set is available at SNAP (Stanford Network Analysis Platform) Network Data Sets [40].

PGP (10680 nodes, 24316 edges) represents the giant component of the network of users of the Pretty-Good-Privacy algorithm for secure information interchange [12]. The data set is available at [1].

Wikipedia (49728 nodes, 941425 edges) represents the Italian Wikipedia. In this graph the nodes are articles and the links represent references to other articles. This data set can be downloaded from [35].

Slashdot (82168 nodes, 948464 edges) represents the Slashdot social network (February 2009). A directed edge from node i to node j indicates that user i tagged user j as a friend or a foe [34]. The data set is available at SNAP (Stanford Network Analysis Platform) Network Data Sets [40].

Figure 1 displays the singular values of the Celegans and Air500 test matrices, both in decimal and semilogarithmic scales. These matrices are small enough to allow the computation of all singular values by the MATLAB function svd. The graphs are typical for many adjacency matrices that arise in real applications in the sense that they are numerically rank deficient and all but a fairly small number of singular values can be ignored when evaluating the exponential of the adjacency matrix. The leading 100 singular values of the three largest complex networks considered in the experiments are plotted in Figure 2. The singular values are computed by the irlba routine from [2].

Table 1 shows for each of the above networks the results obtained by the low-rank approximation, either with the strong or the weak convergence criterion (labeled LR strong and LR weak, respectively), when identifying the 5 most important hubs and the 5 most important authorities in the order of importance. At each iteration we have two sets of candidate nodes, namely $S_{H,5}^{(N)}$ and $S_{A,5}^{(N)}$, which contain the indices of the nodes with the largest hub centrality and the indices of the nodes with the largest authority centrality, respectively. We terminate the computations when $|S_{H,5}^{(N)}| = 5$ for the hub nodes and when $|S_{A,5}^{(N)}| = 5$ for the authority nodes. By Corollary 3.1, the set $S_{H,5}^{(N)}$ ($S_{A,5}^{(N)}$) contains the indices of the 5 nodes with the largest hub centrality (authority centrality). The entry of the column labeled "fail" is set to "1" when the relative sizes of the lower bounds $F_{ii}^{(N)}$ (2.12) are not in agreement with the exact relative sizes of the hub centralities of the nodes; the entry is "0" when ordering of the lower bounds agrees with the ordering of the exact hub centralities. The exact values of the hub centralities are computed with the MATLAB function expm when $n \leq 5 \cdot 10^3$ and by Gauss quadrature rules when $n > 5 \cdot 10^3$. Column 4 of Table 1 shows the number N of singular triplets required to satisfy the strong convergence criterion. The convergence tolerance for the irlba and irblb routines is set to $1 \cdot 10^{-3}$ for all computations of this section.

Columns 5–6 of Table 1 are obtained when terminating the low-rank approximation method with the weak convergence criterion (3.5). The columns display the number of singular triplets needed to reach convergence and the number of candidate nodes included in the resulting index set $S_{H,5}^{(N)}$. The table shows that for hub nodes, the strong convergence criterion requires the computation of at most the 5 largest singular triplets. The weak convergence criterion results in index sets with at most 10 nodes. The results for authority nodes, reported in columns 7–10, are very similar. The table shows that no more than 4 triplets are needed to satisfy the strong convergence criterion and the maximum number of candidate nodes obtained with the weak convergence criterion is 15.

Table 2 reports the number of matrix-vector product evaluations (mvp) required when determining the 5 nodes with the largest hub centrality and the 5 nodes with the largest authority centrality. Column 3 shows the number of

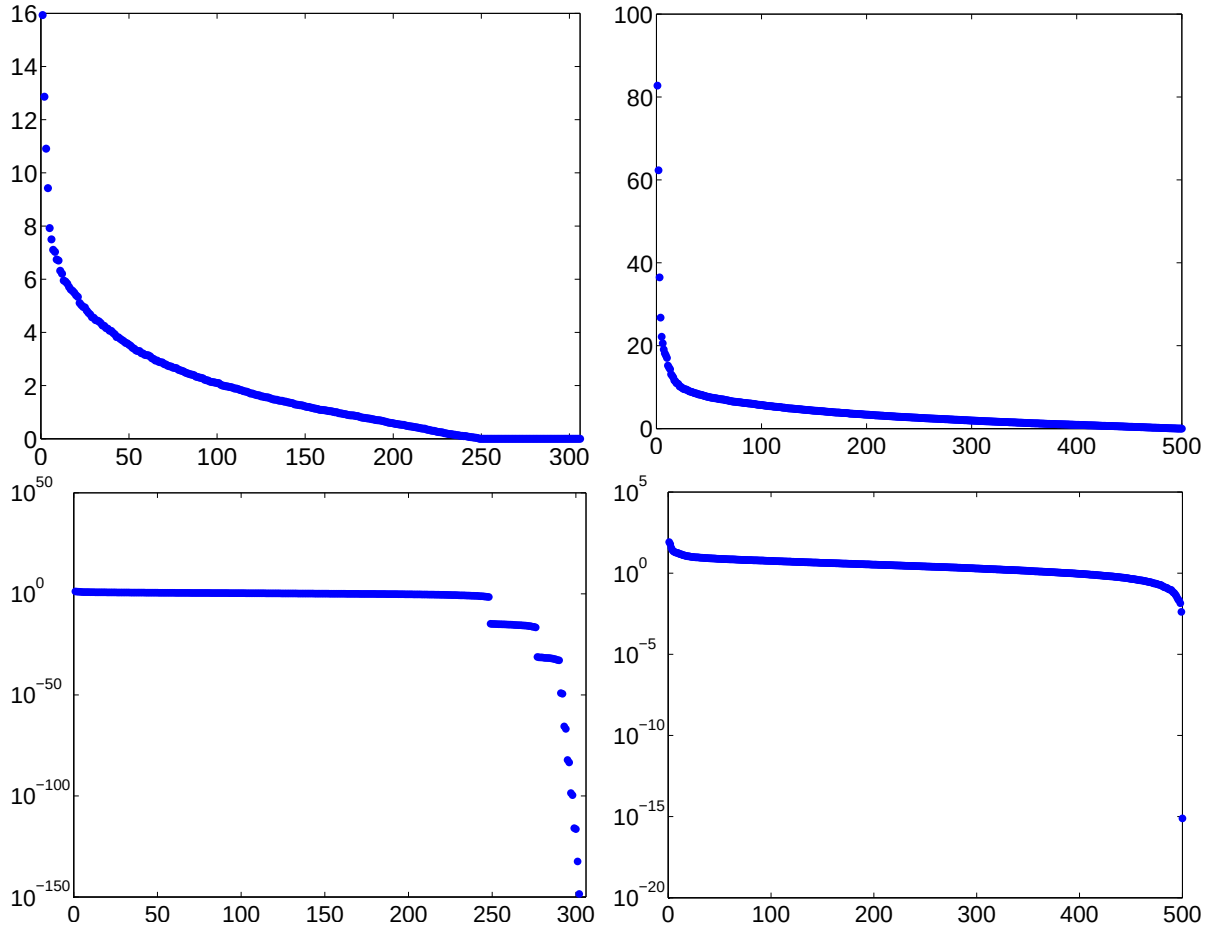

Figure 1: Singular values of the Celegans (left) and Air500 (right) test matrices. The graphs in the top row are in decimal scale, while the ones at the bottom are plotted using a semilogarithmic scale.

mvps needed for the evaluation of pairs of Gauss and Gauss–Radau quadrature rules as described in Section 4. The number of mvps required for computing low-rank approximations using the strong and weak convergence criteria, as described in Section 3, are displayed in columns 4–5, and the total number of mvps demanded by the hybrid method of Section 5 is shown in column 7. All methods compared in Table 2 correctly identify the 5 most important nodes of each network. The hybrid method can be seen to require fewer matrix-vector product evaluation than the use of Gauss quadrature rules only.

Table 3 compares the execution times for the approaches of Table 2 with the evaluation of the matrix exponential by the MATLAB function expm, which is based on Padé approximation. The table shows the Gauss quadrature approach to be faster than expm, which is too slow to be practical to use for matrices of size larger than 5000×5000. The Gauss quadrature approach is slower than the methods that compute low-rank approximation with a partial singular value decomposition. Moreover, Gauss quadrature and the methods that use low-rank approximations require far less storage space than the expm function, which needs to allocate storage for up to six matrices of the same size as the input matrix.

We note that even though low-rank approximation with the strong convergence criterion successfully identified the most important nodes in all of our experiments, the ordering of the lower bounds for nodes with indices in the sets $S_{H,m}^{(N)}$ and $S_{A,m}^{(N)}$ is not guaranteed to agree with the ordering of the exact values of the hub or authority centralities; cf. Remark 3.3. To secure that the correct order is determined, we apply Gauss quadrature to refine the bounds in

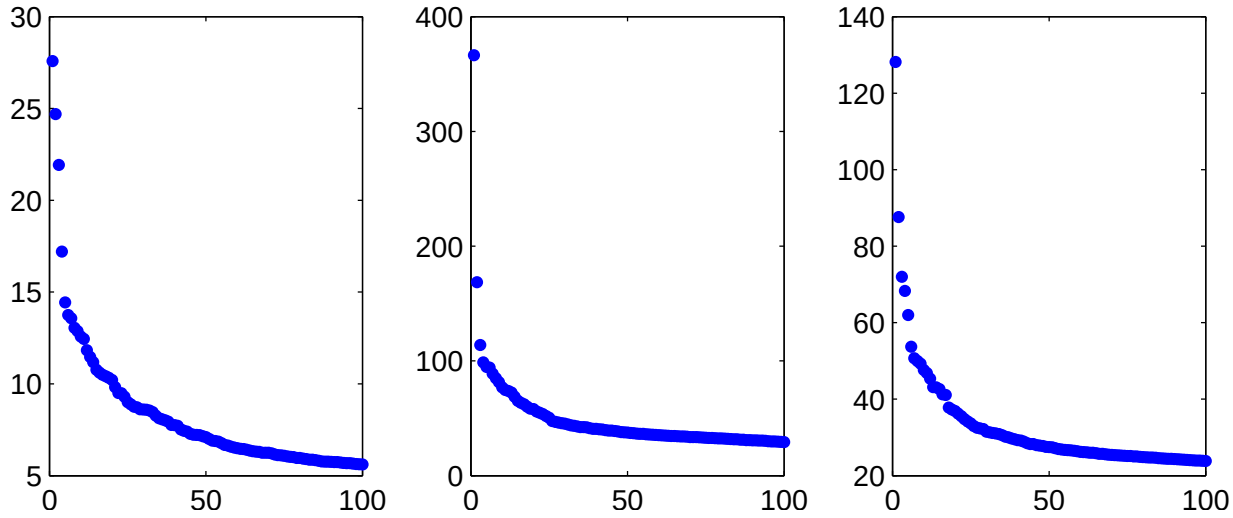

Figure 2: Graph of the first 100 singular values of the adjacency matrices of the three largest networks considered in the experiments. From left to right: PGP, Wikipedia, and Slashdot.

the hybrid method. Table 3 shows that the computation time is not much larger for the hybrid method than for just computing low-rank approximations.

Table 4 investigates the performance of our low-rank approximation methods when more than 5 hubs or authorities are to be identified. Specifically, we seek to identify the m most important hubs and authorities of the four largest networks in our set of test problems and choose m to be 1%, 5%, and 10% of the number of nodes in the network. It is interesting to note that in most cases the number N of singular triplets necessary to meet the strong and week convergence criteria does not increase with m. In fact, the number of terms in (2.5) required to identify a set of nodes does not depend on the number of nodes in the group, but on the topology of the network. The PGP network is the only one for which the strong convergence criterion fails when m is large. The reason for the failure is that the maximum number of terms allowed in (2.5) by our code is exceeded. This may depend on many nodes having close values of the hub or authority centralities. However, note that application of the weak convergence criterion produces useful results. Our hybrid algorithm based on the weak convergence criterion yields the correct ordering of the m nodes with the largest hub centrality and of the m nodes with the largest authority centrality for all values of m. This experiment indicates that the computing time required to construct the lists $S_{H,m}^{(N)}$ and $S_{A,m}^{(N)}$ does not vary much with m. Of course, the execution time for the refinement phase, in which Gauss quadrature is applied to each node in the lists $S_{H,m}^{(N)}$ and $S_{A,m}^{(N)}$ to improve the bounds, grows linearly with m.

Our next example compares the performance of the bounds (2.15) and (2.16) in the case when $\mathbf{z} \neq \mathbf{w}$. Specifically, we considered the problem of ranking the hubs of a network according to their starting convenience; see (2.14). Table 5 is determined by applying Algorithm 1-2 in conjunction with the bounds (2.15) or with bounds derived from (2.16) to identify the 5 most important hubs in a network according to starting convenience. For each network we report the number N of singular triplets required to satisfy the strong convergence criterion and the number of matrix-vector product evaluations. It turns out that the use of the bounds (2.15) and those derived from (2.16) is essentially equivalent, provided that the evaluation of the two expressions in the right-hand side of (2.16) is implemented efficiently, that is, by bounding both expressions simultaneously by using the computed singular triplets. The alternative approach of applying the symmetric Lanczos process to bound each one of the two expressions in the right-hand side of (2.16) separately requires more matrix-vector product evaluations with A and A^T. For two of the networks, the bounds obtained from (2.16) are less tight and therefore require a larger number of matrix-vector product evaluations. Since we compute the singular triplets in batches of 5, this is only noticeable for the Celegans network in Table 5. We illustrate the tightness of the bounds for this network in Figure 3. The left-hand side displays the differences between the upper and lower bounds (2.15) for all the 306 nodes of the network for the first 5 steps of the algorithm. The top graph on the left-hand side of the figure shows the differences of the upper and lower bounds (2.15) for each one of

Table 1: Results obtained by the low-rank approximation algorithm, with both strong and weak convergence criteria, when determining the 5 most important hubs and authorities. The table reports the number of failures, the number N of triplets required to reach convergence, and, in case of weak convergence, the cardinality of the lists $S_{H,5}^{(N)}$ and $S_{A,5}^{(N)}$ of candidate nodes.

		hubs				authorities			
		LR strong		LR weak		LR strong		LR weak	
matrix	nodes	fail	N	N	$\lvert S_{H,5}^{(N)}\rvert$	fail	N	N	$\lvert S_{A,5}^{(N)}\rvert$
Airlines	235	0	2	2	5	0	2	2	5
Celegans	306	0	5	3	10	0	3	3	5
Air500	500	0	2	2	5	0	2	2	5
Twitter	3656	0	2	2	5	0	2	2	5
Wikivote	8297	0	2	2	5	0	2	2	5
PGP	10680	0	4	2	10	0	4	2	10
Wikipedia	49728	0	2	2	5	0	2	1	15
Slashdot	82168	0	2	2	5	0	2	2	5

Table 2: Comparison of Gauss quadrature, low rank approximations and the hybrid algorithm. For each adjacency matrix, we report the number of matrix-vector product evaluations required (mvp).

		Gauss	LR strong	LR weak	hybrid	
matrix	nodes	mvp	mvp	mvp	fail	mvp
Airlines	235	1895	30	44	0	84
Celegans	306	2722	44	44	0	104
Air500	500	4914	30	30	0	73
Twitter	3656	38105	30	30	0	84
Wikivote	8297	52871	44	30	0	74
PGP	10680	69012	44	44	0	143
Wikipedia	49728	471917	44	44	0	110
Slashdot	82168	960760	30	44	0	80

the nodes after one step of the algorithm, the next graph depicts the corresponding differences after two steps, and so on. The bottom graph shows the differences of the upper and lower bounds (2.15) for each node after 5 steps of the algorithm. The graphs on the right-hand side display the analogous bounds obtained from (2.16). It is clear that the bounds (2.15) are tighter than the bounds obtained from (2.16).

We conclude this section with a comparison of our approach to the HITS algorithm by Kleinberg [31], which is a popular method for ranking nodes in a directed network. This algorithm gives nodes a large hub score if they point to many important nodes (authorities), and a large authority score if they are pointed to by many important nodes (hubs). It is easy to see that the HITS method is equivalent to only considering the first singular triplet in (1.6) and rank the nodes according to the values of the entries of the singular vectors $\mathbf{u}_1$ (hub score) and $\mathbf{v}_1$ (authority score). Therefore, the HITS algorithm may produce rankings that are different from those obtained by evaluating hub and authority centralities. However, Table 1 illustrated that only a few singular triplets suffice to identify the most important nodes by using hub and authority centralities. It is therefore interesting to investigate how different the orderings determined by the HITS algorithm and by our approach are. To gain some insight into the orderings produced, we determine the 100 nodes with the largest hub and authority centralities, and compute the 100 most important hubs and authorities with the HITS algorithm for our test networks. We found that the identification and ordering of the 100 most important hubs and authorities obtained by these methods for the networks Airlines, Air500, Twitter, and Wikivote are the same. The orderings differ for the networks of Table 6. The second and fourth columns of the table show how many nodes among the 100 nodes in each list differ; the third and fifth columns show the index of the first node that differs in each list. The table illustrates that the HITS algorithm does not always yield the nodes with the largest hub/authority

Table 3: Comparison of expm, Gauss quadrature, low rank approximations and the hybrid algorithm. For each adjacency matrix, we report the execution time in seconds.

matrix	nodes	expm	Gauss	LR strong	LR weak	hybrid
Airlines	235	5.0e-01	1.0	7.5e-02	6.1e-03	6.1e-02
Celegans	306	5.8e-01	1.3	6.2e-03	5.9e-03	3.4e-02
Air500	500	1.3	5.2	1.1e-01	8.5e-03	1.0e-01
Twitter	3656	1.2e+03	5.9e+01	2.2e-02	2.1e-02	1.0e-01
Wikivote	8297	–	8.0e+01	4.3e-02	2.8e-02	9.1e-02
PGP	10680	–	7.9e+01	5.5e-02	4.2e-02	1.5e-01
Wikipedia	49728	–	5.0e+03	3.1e-01	2.9e-01	1.2
Slashdot	82168	–	1.1e+04	2.7e-01	4.0e-01	8.8e-01

Table 4: Results obtained by the low-rank approximation algorithm, with both strong and weak convergence criteria, when determining the m most important hubs and authorities with m = 1%, 5%, and 10% of the number of nodes in the network. The table reports the number of failures, the number N of singular triplets required to reach convergence, and, in case of weak convergence, the cardinality of the lists $S_{H,m}^{(N)}$ and $S_{A,m}^{(N)}$ of candidate nodes.

		hubs				authorities			
		LR strong		LR weak		LR strong		LR weak	
matrix	m	fail	N	N	$\lvert S_{H,m}^{(N)}\rvert$	fail	N	N	$\lvert S_{A,m}^{(N)}\rvert$
Wikivote	83	0	2	2	83	0	2	2	83
	415	0	2	2	415	0	2	2	415
	830	0	2	2	830	0	2	2	830
PGP	107	0	5	3	112	0	4	3	115
	534	2	26	4	553	8	17	5	542
	1068	124	143	7	1084	248	143	9	1087
Wikipedia	497	0	2	2	497	0	2	2	497
	2486	0	2	2	2486	0	2	2	2486
	4973	0	2	2	4973	0	2	2	4973
Slashdot	822	0	2	2	822	0	2	2	822
	4108	0	2	2	4108	0	2	2	4108
	8217	0	2	2	8217	0	2	2	8217

centrality. Moreover, when a few singular triplets of the adjacency matrix are sufficient to determine an accurate ordering of the nodes hub and authority centralities, the HITS algorithm does not have a significant advantage in terms of complexity over our method.

7. Conclusion

This paper proposes a new computational method, based on low rank approximation of the adjacency matrix, to rank the nodes of a directed network, and in particular to determine the most important hubs and authorities of the network. This methods extends the approach originally presented in [22] for undirected networks. The numerical examples illustrate the competitiveness of the hybrid approach when applied to the analysis of large directed networks, and show that it produces accurate results in a reasonable time. Hybrid methods may be the only feasible approach for determining the most important nodes in terms of hub and authority subgraph centrality of a large directed graph.

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Table 5: Computation of starting conveniences by Algorithm 1-2 with the aid of the strong convergence criterion using the bounds (2.15) or (2.16). We report the number of singular triplets required to satisfy the strong convergence criterion and the number of matrix-vector product evaluations.

		bounds (2.15)		bounds (2.16)	
matrix	nodes	N	mvp	N	mvp
Airlines	235	2	44	2	44
Celegans	306	5	44	6	112
Air500	500	2	30	2	30
Twitter	3656	2	44	2	44
Wikivote	8297	2	30	2	30
PGP	10680	4	44	5	44
Wikipedia	49728	2	44	2	44
Slashdot	82168	2	30	2	30

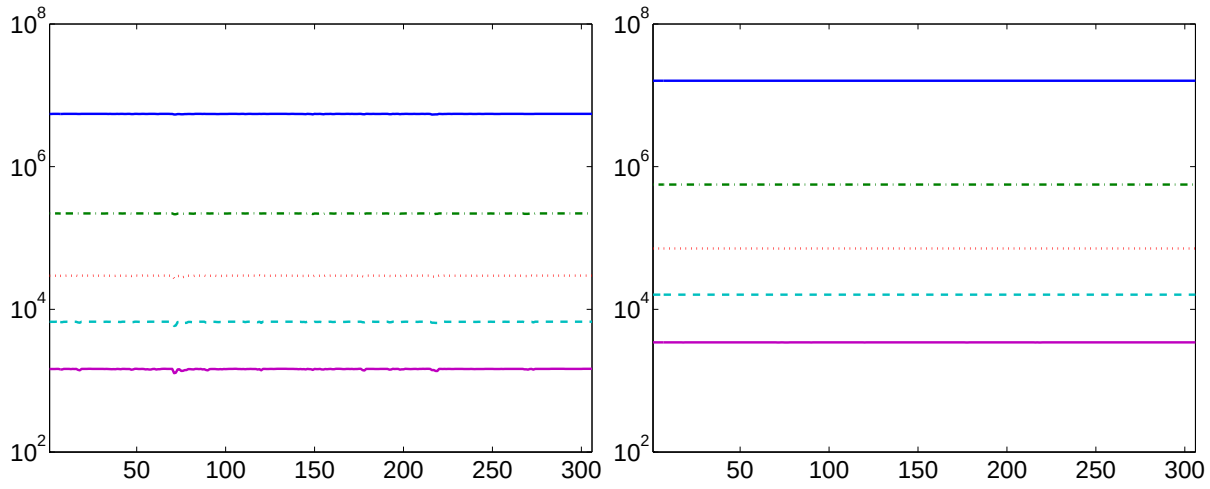

Figure 3: Differences between upper and lower bounds during the first 5 steps of Algorithm 1–2. On the left, we report the differences for the bounds (2.15), on the right those resulting from (2.16).

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Table 6: Differences between the ranking produced by the hub/authority centrality and by the HITS algorithm. We report the number of nodes, among the first 100, which are placed in a different position by the two methods, and the index of the first different node in each ranking list.

	HITS-hubs		HITS-auth	
matrix	fail	index	fail	index
Celegans	62	12	56	15
PGP	54	35	54	41
Wikipedia	5	34	0	0
Slashdot	6	33	0	0

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