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Quadrature rule-based bounds for functions of adjacency matrices ☆

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ABSTRACT

Bounds for entries of matrix functions based on Gauss-type quadrature rules are applied to adjacency matrices associated with graphs. This technique allows to develop inexpensive and accurate upper and lower bounds for certain quantities (Estrada index, subgraph centrality, communicability) that describe properties of networks.

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1. Introduction

Complex networks represent interaction models that characterize physical, biological or social systems. Examples include molecular structure, protein interaction, food webs, social networks, and so forth. Since networks can be described by graphs and by the associated adjacency matrices, graph theory and linear algebra naturally take an important place among the tools used in the study of network properties. Recent work has often focused on the definition and evaluation of computable quantities that describe interesting characteristics of a given network or of its parts. For instance, one may wish to quantify the importance of a single entity in the network (e.g., the popularity of a member of a social community), or examine the way information spreads along the network.

Some of these quantities are expressed in terms of adjacency matrices; in particular, we will use here the notions of *Estrada index*, *subgraph centrality* and *communicability*, which are presented in detail in [5,8–16]; see also the discussion in [20].

Relevant definitions are briefly recalled in the next section. In the context of a general discussion, however, it suffices to say that such quantities can be seen as entries of certain functions (e.g., exponential and resolvent) of adjacency matrices; therefore, their explicit computation is often expensive. Moreover, the exact value of these quantities may not be required in practical applications: accurate bounds are often equally useful. For this reason, we are interested in formulating upper and lower bounds that can be inexpensively computed and possibly refined until the desired degree of accuracy is reached. We refer to the book [19] for a general reference on functions of matrices.

The main purpose of the present work is to specialize known quadrature-based bounds for entries of matrix functions to the case of adjacency matrices, and therefore to subgraph centrality, Estrada index and communicability. The general idea [2,17,18] consists in applying Gauss-type quadrature rules and evaluating them via the Lanczos algorithm. One may obtain *a priori* upper and lower bounds by employing one Lanczos step, or carry out explicitly several Lanczos steps to compute more accurate bounds. We derive such bounds and test their effectiveness on a number of examples. We also suggest an application of known bounds on the exponential decay behavior of a class of matrix functions.

2. Definitions

Let G be a simple graph (i.e., unweighted, undirected, with no loops or multiple edges) with N nodes; without loss of generality, we will also assume that G is connected. Let $A \in \mathbb{R}^{N\times N}$ be the associated adjacency matrix, which has $A_{ij} = 1$ if the nodes i and j are connected, and $A_{ij} = 0$ otherwise. Observe that A is symmetric and that $A_{ii} = 0$ for $i = 1, \ldots, N$. The eigenvalues of A are denoted in non-decreasing order as $\lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_N$.

Here is a list of some useful quantities that describe the connectivity properties of G (see [5–16]):

- *Degree* of a node i (number of neighbors): it is defined as $d_i = \sum_{k=1}^{N} A_{ik}$, that is, the number of nodes connected to i. It gives a rough measure of how important is the node i in the graph.
- *Subgraph centrality* of a node i: it is defined as $[\mathrm{e}^A]_{ii}$ and gives a more refined measure of the importance of the node i.
- *Estrada index*: it is defined as $EE(G) = \sum_{k=1}^{N} \mathrm{e}^{\lambda_k} = \sum_{k=1}^{N} [\mathrm{e}^A]_{kk}$.
- *Communicability* between nodes i and j: it is defined as $[\mathrm{e}^A]_{ij}$ and it quantifies how long it takes to pass a message (or disease, computer virus, drug needle…) from i to j.
- *Communicability betweenness* of a node r: it is defined as

$$\frac{1}{(N-1)^2-(N-1)} \sum \sum_{i\neq j, i\neq r, j\neq r} \frac{[\mathrm{e}^A]_{ij} - [\mathrm{e}^{A-E(r)}]_{ij}}{[\mathrm{e}^A]_{ij}},$$

  where $E(r)$ is the adjacency matrix associated with the graph obtained from G by removing all edges involving node r. Communicability betweenness measures how much communication passes through node r.

The degree certainly looks like a very natural notion when trying to define the "popularity" of a node: a node is very popular if it has many adjacent nodes. However, this idea does not take into account the importance of the adjacent nodes. A better approach consists in counting closed walks based at the selected node. Recall that a *walk* on a graph is an ordered list of nodes such that successive nodes in the list are connected. The nodes need not be distinct; in other words, some nodes may be revisited along the way (compare to the notion of *path*, where nodes are required to be distinct). A *closed walk* is a walk whose starting and ending nodes coincide.

A suitable weight should be assigned to each walk, so that longer walks are penalized. For instance, one may choose the weight $1/k!$ for walks of length k; this is why the exponential function comes up in the definition of subgraph centrality.

A similar argument holds for communicability. If we seek to define "how easy" it is to go from node i to node j, we can count the number of walks that start at i and end at j, with weights that penalize long walks. Factorial weights are again a common choice.

Some generalizations proposed in the literature include:

- weighted graphs, where $0 \leqslant A_{ij} \leqslant 1$; it is suggested in [5] that in this case communicability should be defined as $\left[\exp(D^{-\frac{1}{2}}AD^{-\frac{1}{2}})\right]_{ij}$, where $D = \mathrm{diag}(d_1, d_2, \ldots, d_n)$ is the degree matrix;
- use of a general set of weights for longer walks (so that subgraph centrality and communicability are no longer defined by exponentials). An example is given by resolvent-based subgraph centrality and communicability; see Section 5.

3. Bounds via quadrature formulas

Gauss-type quadrature rules can be used to obtain bounds on the entries of a function of a matrix (see [2,17]). Here we specialize the results of [2,17] to the case of adjacency matrices.

Recall that a real function $f(x)$ is *strictly completely monotonic* (s.c.m.) on an interval $I \subset \mathbb{R}$ if $f^{(2j)}(x) > 0$ and $f^{(2j+1)}(x) < 0$ on I for all $j \geqslant 0$, where $f^{(k)}$ denotes the kth derivative of f and $f^{(0)} \equiv f$. For instance, the inverse function $f(x) = 1/x$ is s.c.m. on the set of positive real numbers. Moreover, observe that the exponential function e^x is not s.c.m., whereas the negative exponential e^{-x} is s.c.m. on $\mathbb{R}$.

Now, consider the eigendecompositions $A = Q\Lambda Q^T$ and $f(A) = Qf(\Lambda)Q^T$. For $u, v \in \mathbb{R}^N$ we have

$$u^T f(A)v = u^T Qf(\Lambda)Q^T v = p^T f(\Lambda)q = \sum_{i=1}^{N} f(\lambda_i)p_i q_i, \tag{1}$$

where $p = Q^T u$ and $q = Q^T v$. One motivation for using (1) comes from the fact that $[f(A)]_{ij} = e_i^T f(A)e_j$, where $\{e_k\}_{k=1}^N$ is the canonical basis of $\mathbb{R}^N$.

Let us rewrite (1) as a Riemann–Stieltjes integral with respect to the spectral measure:

$$u^T f(A)v = \int_a^b f(\lambda)d\mu(\lambda), \quad \mu(\lambda) = \begin{cases} 0, & \text{if } \lambda < a = \lambda_1, \\ \sum_{j=1}^{i} p_j q_j, & \text{if } \lambda_i \leqslant \lambda < \lambda_{i+1}, \\ \sum_{j=1}^{N} p_j q_j, & \text{if } b = \lambda_N \leqslant \lambda. \end{cases}$$

The general Gauss-type quadrature rule gives in this case:

$$\int_a^b f(\lambda)d\mu(\lambda) = \sum_{j=1}^{n} w_j f(s_j) + \sum_{k=1}^{M} v_k f(z_k) + R[f], \tag{2}$$

where the nodes $\{s_j\}_{j=1}^n$ and the weights $\{w_j\}_{j=1}^n$ are unknown, whereas the nodes $\{z_k\}_{k=1}^M$ are prescribed. We have

- $M = 0$ for the Gauss rule,
- $M = 1, z_1 = a$ or $z_1 = b$ for the Gauss–Radau rule,
- $M = 2, z_1 = a$ and $z_2 = b$ for the Gauss–Lobatto rule.

Also recall that, for the case $u = v$, the remainder in (2) can be written as

$$R[f] = \frac{f^{(2n+M)}(\eta)}{(2n+M)!}\int_a^b \prod_{k=1}^{M}(\lambda - z_k)\left[\prod_{j=1}^{n}(\lambda - s_j)\right]^2 d\mu(\lambda), \tag{3}$$

for some $a < \eta < b$. It can be proved that, if $f(x)$ is s.c.m. on an interval containing the spectrum of A, then quadrature rules applied to (2) give bounds on $u^T f(A)v$. More precisely, the Gauss rule gives a lower bound, the Gauss–Lobatto rule gives an upper bound, whereas the Gauss–Radau rule can be used to obtain both a lower and an upper bound. The evaluation of these quadrature rules is reduced to the computation of orthogonal polynomials via three-term recurrence, or, equivalently, to the computation of entries and spectral information on a certain tridiagonal matrix via the Lanczos algorithm. Let us briefly recall how this can be done for the case of the Gauss quadrature rule, when we wish to estimate the ith diagonal entry of $f(A)$. It follows from (2) that the quantity we seek to compute has the form $\sum_{j=1}^{n} w_j f(s_j)$. However, it is not necessary to explicitly compute the Gauss nodes and weights. Instead, we can use the following relation (Theorem 3.4 in [17]):

$$\sum_{j=1}^{n} w_j f(s_j) = e_1^T f(J_n) e_1,$$

where

$$J_n = \begin{pmatrix} \omega_1 & \gamma_1 & & & \\ \gamma_1 & \omega_2 & \gamma_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \gamma_{n-2} & \omega_{n-1} & \gamma_{n-1} \\ & & & \gamma_{n-1} & \omega_n \end{pmatrix}$$

is a tridiagonal matrix whose eigenvalues are the Gauss nodes, whereas the Gauss weights are given by the squares of the first entries of the normalized eigenvectors of J_n. The entries of J_n are computed using the symmetric Lanczos algorithm. The initial vectors are $x_{-1} = 0$ and $x_0 = e_i$; the iteration goes as follows:

$$\begin{aligned} \gamma_j x_j &= r_j = (A - \omega_j I)x_{j-1} - \gamma_{j-1}x_{j-2}, \qquad j = 1, \ldots \\ \omega_j &= x_{j-1}^T A x_{j-1}, \\ \gamma_j &= \|r_j\|. \end{aligned} \tag{4}$$

Before we proceed, we mention a couple of technical details:

- Since the quadrature-based bounds we use here are designed for s.c.m. functions, we will need to write the exponential of a matrix as $e^A = e^{-(-A)}$.
- The paper [17] assumes that A is positive definite in order to ensure that certain functions (namely $f(x) = 1/x$) are s.c.m. on an interval containing the spectrum of A. This hypothesis is not needed when giving bounds for the entries of e^A.

4. *A priori* bounds

In this section we present upper and lower bounds on entries of functions of adjacency matrices (such as the notions of subgraph centrality, Estrada index and communicability), that can be inexpensively computed in terms of some basic properties of the given graph or adjacency matrix.

Such bounds can be obtained by taking a single Lanczos step when evaluating (2). The paper [2] gives bounds on the entries of $f(A)$ based on the Gauss, Gauss–Lobatto and Gauss–Radau quadrature rules, under the hypothesis that A is a symmetric matrix and $f(x)$ is s.c.m. on an interval containing the spectrum of A.

The following results are obtained for the particular case of adjacency matrices. We derive bounds for diagonal entries (subgraph centrality), for the trace (Estrada index) and for off-diagonal entries (communicability) of $f(A)$, with particular attention to the case $f(x) = \mathrm{e}^x$.

4.1. Diagonal entries (Gauss)

The Gauss quadrature rule allows to obtain a lower bound on the diagonal entries of $f(A)$. Let d_i be the degree of the ith node and let t_i be the number of triangles in G with a vertex on node i, i.e., one half of the number of closed walks of length three beginning and ending at node i; we may equivalently write $t_i = \frac{1}{2}\sum_{k\neq i}\sum_{\ell\neq i} A_{ki}A_{k\ell}A_{\ell i}$. We have

$$[f(A)]_{ii} \geqslant \frac{(\mu_2)_i f((\mu_1)_i) - (\mu_1)_i f((\mu_2)_i)}{\delta_i},$$

where

$$\delta_i = \frac{1}{d_i}\sqrt{4t_i^3 + 4d_i^3},$$

$$(\mu_1)_i = \frac{1}{d_i}\left(-t_i - \sqrt{t_i^2 + d_i^3}\right), \qquad (\mu_2)_i = \frac{1}{d_i}\left(-t_i + \sqrt{t_i^2 + d_i^3}\right).$$

In the particular case where f is the exponential function, as discussed above, we obtain:

$$[\mathrm{e}^A]_{ii} \geqslant \frac{\mathrm{e}^{\frac{t_i}{d_i}}}{\sqrt{t_i^3 + d_i^3}}\left(\sqrt{t_i^3 + d_i^3}\cosh\frac{\sqrt{t_i^3 + d_i^3}}{d_i} - t_i \sinh\frac{\sqrt{t_i^3 + d_i^3}}{d_i}\right). \tag{5}$$

4.2. Diagonal entries (Gauss–Radau)

The Gauss–Radau quadrature rule is used to obtain upper and lower bounds on the diagonal entries of $f(A)$. Let $a, b \in \mathbb{R}$ be such that the spectrum of A is contained in $[a, b]$. Ideally, we would like to choose $a = \lambda_1$ and $b = \lambda_N$, but in order to avoid explicit eigenvalue computations we may resort to estimates. For instance, it follows from Gershgorin's theorem that we may choose $a = -\max\{d_i\}$ and $b = \max\{d_i\}$ if more refined bounds are not available.[1] We have:

$$\frac{b^2 f(-d_i/b) + d_i f(b)}{b^2 + d_i} \leqslant [f(A)]_{ii} \leqslant \frac{a^2 f(-d_i/a) + d_i f(a)}{a^2 + d_i} \tag{6}$$

and in particular:

$$\frac{b^2\mathrm{e}^{\frac{d_i}{b}} + d_i\mathrm{e}^{-b}}{b^2 + d_i} \leqslant [\mathrm{e}^A]_{ii} \leqslant \frac{a^2\mathrm{e}^{\frac{d_i}{a}} + d_i\mathrm{e}^{-a}}{a^2 + d_i}. \tag{7}$$

Note that (7) is obtained from (6) in the particular case where the function $f(x) = \mathrm{e}^{-x}$ is applied to the matrix $-A$. Therefore, the parameters a and b in (7) are a lower and an upper bound, respectively, for the spectrum of $-A$.

If desired, the bounds for $[\mathrm{e}^A]_{ii}$ can be simplified further by choosing $a = 1 - N$ and $b = N - 1$:

$$\frac{(N-1)^2\mathrm{e}^{\frac{1}{N-1}} + \mathrm{e}^{1-N}}{N(N-1)} \leqslant [\mathrm{e}^A]_{ii} \leqslant \frac{N-1}{\mathrm{e}} \cdot \frac{N-1+\mathrm{e}^N}{N^2 - 2N}. \tag{8}$$

[1] These estimates are used throughout all the numerical experiments, unless otherwise noted.

4.3. Diagonal entries (Gauss–Lobatto)

The Gauss–Lobatto quadrature rule allows to obtain an upper bound on the diagonal entries of $f(A)$. We have:

$$[f(A)]_{ii} \leqslant \frac{af(b) - bf(a)}{a - b}$$

and in particular:

$$[\mathrm{e}^A]_{ii} \leqslant \frac{a\mathrm{e}^{-b} - b\mathrm{e}^{-a}}{a - b}. \tag{9}$$

4.4. Estrada index (Gauss–Radau)

The inequalities (7) and (8) can be used to compute lower and upper bounds for the Estrada index $EE(G)$:

$$\sum_{i=1}^{N} \frac{b^2 \mathrm{e}^{\frac{d_i}{b}} + d_i \mathrm{e}^{-b}}{b^2 + d_i} \leqslant EE(G) \leqslant \sum_{i=1}^{N} \frac{a^2 \mathrm{e}^{\frac{d_i}{a}} + d_i \mathrm{e}^{-a}}{a^2 + d_i}, \tag{10}$$

$$\frac{(N-1)^2 \mathrm{e}^{\frac{1}{N-1}} + \mathrm{e}^{1-N}}{N-1} \leqslant EE(G) \leqslant \frac{N-1}{\mathrm{e}} \cdot \frac{N-1+\mathrm{e}^N}{N-2}. \tag{11}$$

A priori bounds for $EE(G)$ are also given in the paper [6]; they require knowledge of the number N of nodes and the number m of edges and they are sharp bounds (equality on both sides is attained for edgeless graphs):

$$\sqrt{N^2 + 4m} \leqslant EE(G) \leqslant N - 1 + \mathrm{e}^{\sqrt{2m}}.$$

See the section on numerical experiments for comparisons.

4.5. Off-diagonal entries (Gauss–Radau)

Quadrature rules provide bounds for $[f(A)]_{ii} + [f(A)]_{ij}$, from which we can derive bounds for off-diagonal entries of $f(A)$. For these bounds to hold, however, the following condition on the entries of A must be satisfied (see [17] for details):

$$\tau_{ij} := \sum_{k \neq i} A_{ki}(A_{ki} + A_{kj}) - A_{ij}(A_{ij} + A_{ii}) \geqslant 0.$$

When $A_{ii} = 0$, as it is the case for adjacency matrices, this condition becomes

$$\tau_{ij} = \sum_{k \neq i} A_{ki}(A_{ki} + A_{kj}) - (A_{ij})^2 \geqslant 0. \tag{12}$$

Observe that (12) is always true for adjacency matrices. Indeed, $(A_{ij})^2$ is either 1 or 0 and the sum over k is $\geqslant 1$ because the graph is connected. In view of the quadrature bounds, one should consider $-A$ here instead of A; but each term of τ_{ij} is a product of two entries of $-A$, so we can equivalently compute τ_{ij} using the elements of A.

The bounds given by the Gauss–Radau rule for the exponential function (and therefore for subgraph centrality) are:

$$\frac{b^2 \mathrm{e}^{\frac{\tau_{ij}}{b}} + \tau_{ij} \mathrm{e}^{-b}}{b^2 + \tau_{ij}} - \frac{a^2 \mathrm{e}^{\frac{d_i}{a}} + d_i \mathrm{e}^{-a}}{a^2 + d_i} \leqslant [\mathrm{e}^A]_{ij} \leqslant \frac{a^2 \mathrm{e}^{\frac{\tau_{ij}}{a}} + \tau_{ij} \mathrm{e}^{-a}}{a^2 + \tau_{ij}} - \frac{b^2 \mathrm{e}^{\frac{d_i}{b}} + d_i \mathrm{e}^{-b}}{b^2 + d_i}. \tag{13}$$

5. Resolvent subgraph centrality and communicability

Estrada and Higham propose in [13] the notions of *resolvent subgraph centrality*, *resolvent communicability* and *resolvent betweenness*, which are based on the function

$$f(x) = \left(1 - \frac{x}{N-1}\right)^{-1}$$

exactly in the same way as the classic subgraph centrality, communicability and communicability betweenness are based on the exponential function. For instance:

- the resolvent subgraph centrality of node i is $\left[\left(I - \frac{A}{N-1}\right)^{-1}\right]_{ii}$,
- the resolvent Estrada index is the trace of $\left(I - \frac{A}{N-1}\right)^{-1}$,
- the resolvent communicability between nodes i and j is $\left[\left(I - \frac{x}{N-1}\right)^{-1}\right]_{ij}$.

These definitions are designed to be applied to sparse networks, so that one may assume $d_i \leqslant N-2$ for all $i = 1, \ldots, N$. This implies that the spectrum of the adjacency matrix A is contained in the interval $[-(N-2), N-2]$; as a consequence, the matrix $B = I - A/(N-1)$ is nonsingular (indeed, positive definite), so $f(A)$ is well defined. Also observe that B is an irreducible M-matrix and therefore $B^{-1} > 0$; see [4].

Since B is positive definite, we may apply the quadrature bounds of [17] for inverse matrices. Let a and b be real numbers such that the spectrum of B is contained in $[a, b]$. For diagonal entries we have:

$$\text{(Gauss)} \qquad \frac{\sum_{k\neq i}\sum_{\ell\neq i} B_{ki}B_{k\ell}B_{\ell i}}{\sum_{k\neq i}\sum_{\ell\neq i} B_{ki}B_{k\ell}B_{\ell i} - \frac{d_i^2}{(N-1)^4}} \leqslant [B^{-1}]_{ii}, \tag{14}$$

$$\text{(Radau)} \qquad \frac{1 - b + \frac{d_i}{b(N-1)^2}}{1 - b + \frac{d_i}{(N-1)^2}} \leqslant [B^{-1}]_{ii} \leqslant \frac{1 - a + \frac{d_i}{a(N-1)^2}}{1 - a + \frac{d_i}{(N-1)^2}}, \tag{15}$$

$$\text{(Lobatto)} \qquad \left[B^{-1}\right]_{ii} \leqslant \frac{a+b-1}{ab}. \tag{16}$$

Experiments suggest that in many cases the best lower/upper bounds are given by the Gauss and Radau rules, respectively.

As a consequence of Gershgorin's theorem, possible choices for a and b include

$$a = 1 - \frac{1}{N-1}\max_{1\leqslant i\leqslant N}\{d_i\}, \qquad b = 1 + \frac{1}{N-1}\max_{1\leqslant i\leqslant N}\{d_i\},$$

therefore we have

$$a \geqslant \frac{1}{N-1}, \qquad b \leqslant 1 + \frac{N-2}{N-1}.$$

By substituting the latter formulas for a and b in the Radau bounds and recalling that $1 \leqslant d_i \leqslant N-2$ as assumed above, one may compute bounds that only require knowledge of N. Moreover, it follows from the Gauss bound that $1 \leqslant [B^{-1}]_{ii}$ for all i.

In order to estimate $EE_r(G)$, one may also use existing bounds on the trace of the inverse matrix (see e.g. [1,21]). For instance, the bounds given by Bai and Golub in [1] become in our case:

$$\begin{pmatrix} N & N \end{pmatrix} \begin{pmatrix} N + \frac{2m}{(N-1)^2} & N \\ b^2 & b \end{pmatrix}^{-1} \begin{pmatrix} N \\ 1 \end{pmatrix} \leqslant EE_r(G), \tag{17}$$

$$EE_r(G) \leqslant \begin{pmatrix} N & N \end{pmatrix} \begin{pmatrix} N + \frac{2m}{(N-1)^2} & N \\ a^2 & a \end{pmatrix}^{-1} \begin{pmatrix} N \\ 1 \end{pmatrix}. \tag{18}$$

See Section 8 for comparisons.

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6. MMQ bounds

More accurate *a posteriori* bounds and estimates on the entries of $f(A)$ can be computed by carrying out explicitly several Lanczos steps applied to the quadrature formula (2). Bounds on $[f(A)]_{ii}$ are obtained using symmetric Lanczos, whereas bounds for $[f(A)]_{ij}$, with $i \neq j$, come from the application of unsymmetric or block Lanczos. These techniques are implemented in Gérard Meurant's MMQ toolbox for Matlab [22]; they prove to be quite efficient when estimating exponential or resolvent based subgraph centrality, Estrada index and communicability.

6.1. Convergence and conditioning

Bounds computed by carrying out several explicit iterations of Lanczos' algorithm generally display a fast convergence to the exact values of subgraph centrality and communicability. Moreover, the number of iterations required to reach a given accuracy (or, equivalently, the accuracy reached using a fixed number of iterations) seems to be quite insensitive to the size of the matrix; see Section 8 for experiments supporting these claims.

An explanation for this favorable behavior can be formulated as follows. Consider a sequence $\{A_j\}_{j=1}^{\infty}$ of adjacency matrices of increasing sizes $\{N_j\}_{j=1}^{\infty}$. We can also reasonably assume that there exists a uniform upper bound d on the node degrees. As pointed out earlier, it follows from Gershgorin's theorem that there exists an interval $[a, b]$ such that the spectrum of A_j is contained in $[a, b]$ for all values of j; for instance, we may choose $a = -d$ and $b = d$. As a consequence, matrix size does not play a role in the convergence rate of the Lanczos iteration that approximates the entries of e^A. In particular, observe that the quadrature approximation error (3) does not depend on matrix size under our hypotheses, although it may depend on the eigenvalue distribution.

A similar argument applies to the case of resolvent based subgraph centrality, Estrada index and communicability. Indeed, there exists an interval $[a_r, b_r]$, with $a_r > 0$, such that the spectrum of $B_j = (I_{N_j} - A_j/(N_j - 1))^{-1}$ is contained in $[a_r, b_r]$ for all values of j. In fact, the situation is even more favorable here, because the spectrum of B_j is contained in $[1 - d/(N_j - 1), 1 + d/(N_j - 1)]$ for all j. Note that the uniform boundedness of the spectra away from 0 is crucial in this case, where we are dealing with the inverse function. Finally, recall that the MMQ algorithm requires to compute the $(1, 1)$ entry of the inverse of the symmetric tridiagonal matrix J_n; the conditioning of this problem is again uniformly bounded with respect to j, because the eigenvalues of J_n belong to the interval $[a_r, b_r]$.

6.2. Computational cost and adaptation to sparse matrices

For a general matrix A, the computational effort required by the Lanczos iteration (4) is dominated by matrix-vector products of the type $A \cdot x$. When A is an adjacency matrix, however, such products are considerably simplified and amount essentially to sums of selected entries of x. The computational cost for each iteration is then dominated by vector norm and dot product computations and, in the worst case, it grows linearly with respect to the matrix size. Typically, however, x is a sparse vector during the first few iterations, so the computational cost is often less than $\mathcal{O}(N)$ per iteration in practice. Note also that individual entries of $f(A)$ can be estimated largely independent of one another, hence a high degree of parallelism is in principle possible.

The functions in the MMQ Matlab package can also accept matrices in sparse format as input: this helps to improve computational speed when working on adjacency matrices.

7. Decay bounds

Let A be a symmetric banded matrix and f be a smooth function defined on an interval containing the spectrum of A. Then the entries of $f(A)$ are bounded in an exponentially decaying way away from the main diagonal [2]. More precisely, there exist constants $C > 0$ and $0 < \rho < 1$ such that:

$$|[f(A)]_{ij}| \leqslant C\rho^{|i-j|}, \qquad i \neq j. \tag{19}$$

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Note that C and ρ can be computed explicitly; see [2] for details. This result can be generalized to the nonsymmetric case and to the case where A is not necessarily banded but displays a general sparsity pattern [3,23]. In the latter case, the exponent $|i-j|$ is replaced by the graph distance between i and j, that is, the length of the shortest path connecting nodes i and j in the unweighted graph associated with A.

The property of exponential decay may be employed to compute bounds on communicability for large networks. If the adjacency matrix under consideration is banded, or becomes banded after reordering (e.g., via reverse Cuthill–McKee, see [7]), then (19) with $f(x) = e^x$ shows that the communicability becomes negligible outside a certain bandwidth s. The same property holds for resolvent-based communicability.

Observe that reordering the adjacency matrix merely corresponds to relabeling the nodes of the network and does not change the network structure.

The decay bound (19) may prove particularly useful when one has to deal with networks of increasing size. If the bandwidth of the (possibly reordered) adjacency matrix is independent of the matrix size N, then s is also independent of N. Therefore the number of node pairs whose communicability should be computed explicitly grows linearly in N, rather than quadratically. See Section 8 for a numerical example.

8. Numerical experiments

The adjacency matrices used in these examples have been generated using the CONTEST toolbox for Matlab [24,25]; see the CONTEST documentation for references and for a detailed description of the models that motivate the choice of such matrices. The classes of matrices used here include:

- Small world matrices, generated by the command `smallw`. These are matrices associated with a modified Watts–Strogatz model, which interpolates between a regular lattice and a random graph. In order to build such a model, one begins with a k-nearest-neighbor ring, i.e., a graph where nodes i and j are connected if and only if $|i-j| \leqslant k$ or $N - |i-j| \leqslant k$, for a certain parameter k. Then, for each node, an extra edge is added, with probability p, which connects said node to another node chosen uniformly at random. Self-links and repeated links, if they occur, are removed at the end of the process. The required parameters are the size N of the matrix, the number k of nearest neighbors to connect and the probability p of adding a shortcut in a given row. The parameter p should be chosen quite small in order to capture the typical small-world behavior characterized by short average distance and large clustering; see [26,25] for further details.

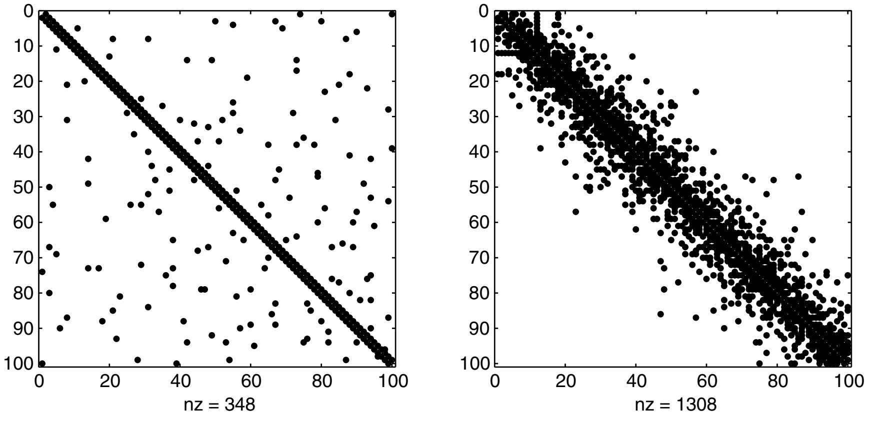

Fig. 1. Sparsity pattern for a 100 × 100 small world matrix (left) and a range-dependent matrix (right) used in the experiments.

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Table 1
MMQ bounds for the Estrada index $EE(A) = 425.0661$ of a 100×100 range-dependent matrix A with parameters $\alpha = 1$, $\lambda = 0.85$.

# it	1	2	3	4	5
Gauss	348.9706	416.3091	424.4671	425.0413	425.0655
Radau (lower)	378.9460	420.6532	424.8102	425.0570	425.0659
Radau (upper)	652.8555	437.7018	425.6054	425.0828	425.0664
Lobatto	2117.9233	531.1509	430.3970	425.2707	425.0718

Table 2
MMQ Radau bounds for $[e^A]_{1,5} = 0.396425$, with A as in Table 1.

# it	1	2	3	4	5
Radau (lower)	−2.37728	0.213316	0.388791	0.396141	0.396420
Radau (upper)	4.35461	0.595155	0.404905	0.396626	0.396431

Table 3
Relative errors for MMQ Radau bounds for Erdös–Rényi matrices associated with graphs with N vertices and $4N$ edges; five iterations. For each value of N, we compute average errors on 10 matrices. Columns 2 and 3 show relative errors on the Estrada index; columns 4 and 5 show relative errors on subgraph centrality, averaged along the matrix diagonal.

N	Err. on $EE(G)$ (upper)	Err. on $EE(G)$ (lower)	Av. err. u.	Av. err. l.
50	2.66e−4	2.60e−5	2.66e−4	3.52e−5
100	1.09e−3	1.02e−4	1.48e−3	1.37e−4
150	3.64e−3	1.92e−4	4.85e−3	2.55e−4
200	3.81e−3	2.56e−4	4.90e−3	3.27e−4
250	5.63e−3	3.26e−4	7.04e−2	4.01e−4
300	6.76e−3	3.99e−4	8.81e−3	8.18e−4
350	9.34e−3	4.57e−4	1.13e−2	5.58e−4
400	6.70e−3	4.96e−4	8.41e−3	1.07e−3
450	8.65e−3	5.57e−4	1.06e−2	1.08e−3
500	1.41e−2	6.41e−4	1.70e−2	1.14e−3

Table 4
Relative error for MMQ Radau bounds for the Estrada index of small world matrices of parameters (4,0.1); averaged over 10 matrices; five iterations.

N	Error (upper bound)	Error (lower bound)
50	4.87e−5	4.35e−5
100	5.05e−5	4.09e−5
150	5.31e−5	3.98e−5
200	5.05e−5	3.57e−5
250	5.57e−5	3.84e−5
300	5.63e−5	3.73e−5

Table 5
Relative error for MMQ Radau bounds for the Estrada index of small world matrices of parameters $(4 \cdot 10^{-3})$; averaged over 10 matrices; five iterations.

N	Error (upper bound)	Error (lower bound)
50	1.3893e−5	2.5634e−5
100	1.2126e−5	2.4678e−5
150	1.2171e−5	2.4705e−5
200	1.5277e−5	2.5024e−5
250	1.5266e−5	2.5021e−5

- Erdös–Rényi matrices, generated by the command `erdrey`. Given N and m, the function computes the adjacency matrix associated with a graph chosen uniformly at random from the set of graphs with N nodes and m edges.
- Range-dependent matrices, generated by the command `renga`. These are adjacency matrices associated with range-dependent random graphs. The required parameters are the size of the

Table 6
Relative errors for MMQ bounds on the resolvent subgraph centrality of node 10 for Erdös–Rényi matrices associated with graphs with N vertices and $4N$ edges; averaged on 10 matrices; two iterations.

N	Cond. number	Gauss	Radau (lower)	Radau (upper)	Lobatto
100	1.16	3.00e−9	1.29e−11	1.84e−9	2.70e−9
200	1.08	3.02e−11	4.65e−14	6.99e−12	2.79e−11
300	1.05	2.51e−12	8.35e−15	1.21e−12	2.38e−12
400	1.04	3.15e−13	5.55e−16	1.67e−14	2.85e−13

matrix and two numbers $0 < \lambda < 1$ and $\alpha > 0$. The probability for two nodes to be connected is $\alpha \cdot \lambda^{d-1}$, where d is the distance between the nodes.

Fig. 1 shows the sparsity patterns of the small world and range-dependent matrices used in the experiments.

The effectiveness of the quadrature-based bounds has been tested in the following experiments.

1. Convergence rate of MMQ approximations. Tables 1 and 2 show examples of convergence to the Estrada index and communicability of a 100×100 range-dependent matrix.
2. Accuracy of MMQ approximations with a fixed number of iterations: see Tables 3–6 for relative errors on Estrada index, subgraph centrality and resolvent subgraph centrality for Erdös-Rényi and small world matrices. The matrices used in these experiments have a random component; for this reason the displayed data are computed as averages over 10 matrices defined by the same parameters.
3. Estrada index. Fig. 2 compares bounds (10) and (11) with those of de la Peña et al. for the Estrada index of small world matrices of increasing size. Table 7 shows bounds on the Estrada index for a 100×100 range-dependent matrix with parameters $\alpha = 1$ and $\lambda = 0.85$.
4. Communicability with MMQ Gauss–Radau bounds: see Fig. 3.

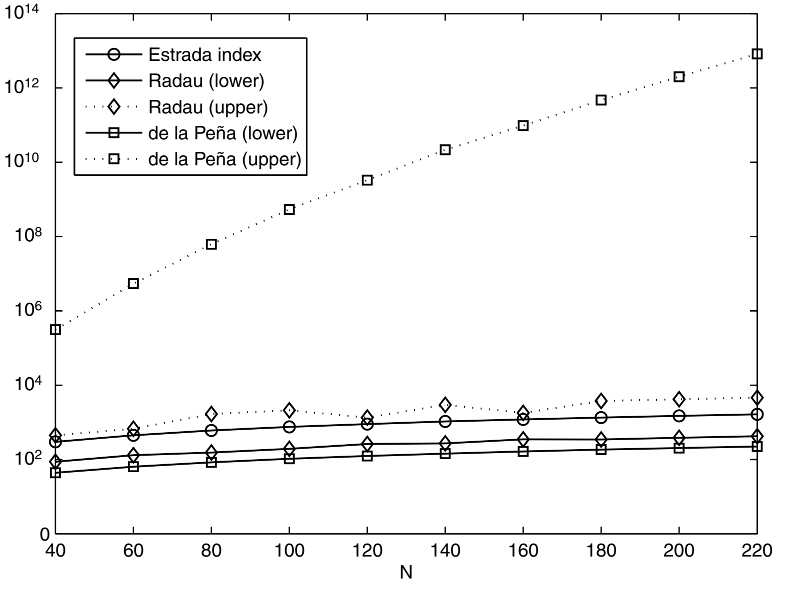

Fig. 2. Logarithmic plot of the Estrada index, of the bounds given by the Gauss–Radau rule and of the bounds given by de la Peña et al. for matrices of increasing size. The test matrices are small world matrices defined by parameters $k = 2$ and $p = 0.01$.

Table 7
Bounds for the Estrada index.

de la Peña	Radau	Gauss	$EE(G)$
$1.1134 \cdot 10^3$	$1.8931 \cdot 10^3$	$1.8457 \cdot 10^4$	$5.4802 \cdot 10^5$
$EE(G)$	Radau	Lobatto	de la Peña
$5.4802 \cdot 10^5$	$2.3373 \cdot 10^8$	$1.3379 \cdot 10^7$	$1.0761 \cdot 10^{15}$

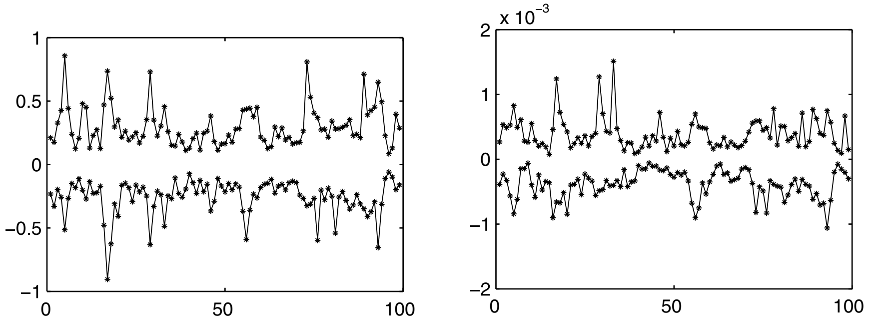

Fig. 3. MMQ Gauss–Radau bounds for off-diagonal entries of the exponential of a 100×100 small world matrix. The plots show the approximation error (first row of the exponential matrix minus bounds). The number of iterations is 2 for the plot on the left and 4 for the plot on the right.

Table 8
Bounds for the resolvent-based Estrada index.

Bai–Golub	Radau	Gauss	$EE_r(G)$	Radau	Lobatto	Bai–Golub
100.0706	100.0707	100.0823	100.0824	100.0968	102.6820	100.0969

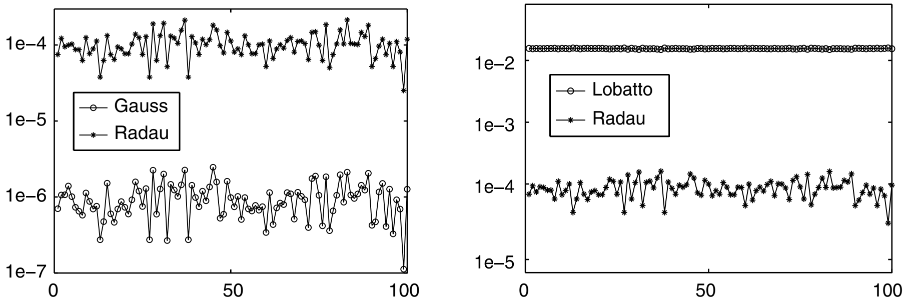

Fig. 4. Left: Logarithmic plot of the difference between the resolvent-based subgraph centrality of a Erdös–Rényi matrix ($N = 100$, $m = 400$) and the lower bounds given by the Gauss and the Gauss–Radau rules. Right: Logarithmic plot of the difference between resolvent-based subgraph centrality and bounds given by Gauss–Radau and Gauss–Lobatto rules.

5. Resolvent-based Estrada index. Table 8 compares bounds (17), (18) and the bounds obtained from (14), (15) and (16) with the resolvent-based Estrada index of an Erdös–Rényi matrix ($N = 100, m = 400$).
6. Resolvent-based subgraph centrality. Fig. 4 compares the bounds (14), (15) and (16) with the resolvent based subgraph centrality of an Erdös–Rényi matrix ($N = 100, m = 400$).

Experiments 1 and 2 aim to verify experimentally the effectiveness of the MMQ method, which usually gives good approximations of Estrada index and subgraph centrality with few Lanczos iterations. Moreover, the number of iterations required to reach a given accuracy does not depend on matrix size. We also to point out that, in experiments with matrices where the random component plays little or no role, the error quickly tends to stabilize when the matrix size increases (see Tables 4 and 5).

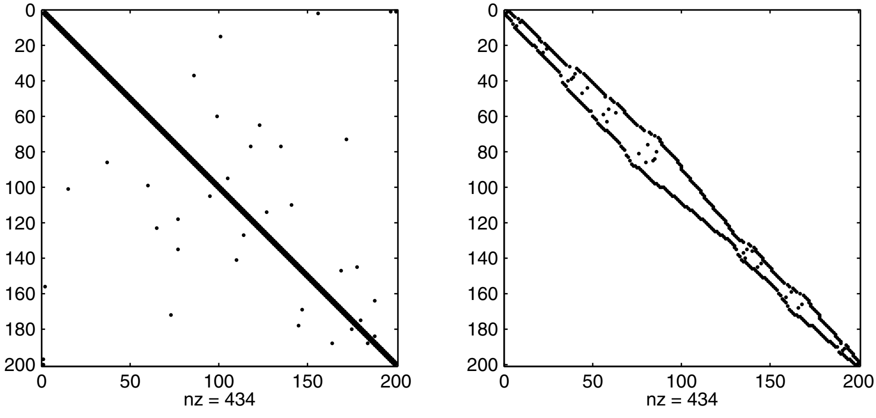

Fig. 5. Sparsity pattern of a 200 × 200 small world matrix (left) and of the correspondent reordered matrix (right).

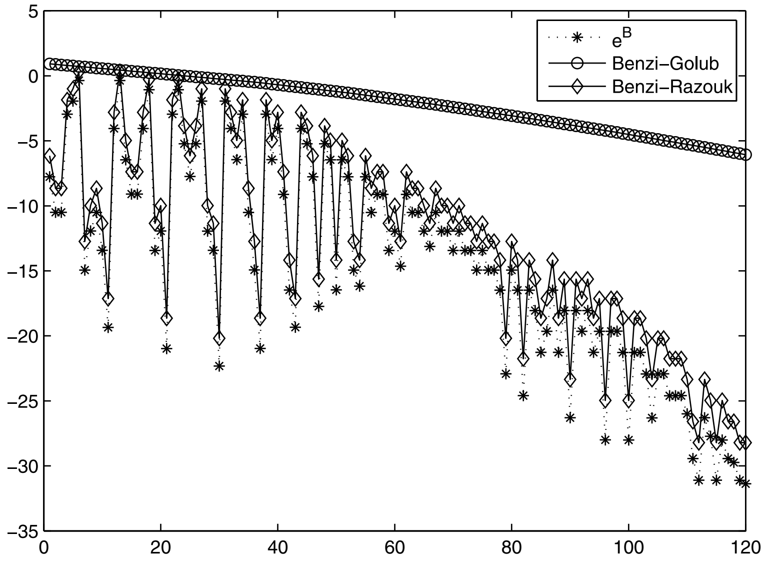

Fig. 6. Logarithmic plot of decay bounds (solid line) and of the absolute values of the 80th row of e^B (dotted line), as defined in Section 7.

A priori bounds for the Estrada index follow quite closely the computed values of $EE(G)$ and show a remarkable improvement with respect to known bounds presented in [6]. Moreover, *a priori* bounds for resolvent-based subgraph centrality and Estrada index prove to be particularly effective. Observe, for instance, that in the proposed example the upper and lower Gauss–Radau bounds for resolvent-based subgraph centrality have an average distance of about 10^{-4} from the exact values. As for MMQ bounds, experiment 4 shows that good approximations can be computed using a very small number of Lanczos iterations.

So far we have only used examples of sparse networks, where all nodes generally have low degree. In some applications, however, models containing a few high-degree nodes are employed. For this reason, we have briefly examined the behavior of our bounds for the Estrada index when a node of maximum degree is added to an otherwise sparse network (a small world model with $N = 200$, $k = 2$ and $p = 0.01$). *A priori* bounds, especially upper bounds, deteriorate to the point of being useless when

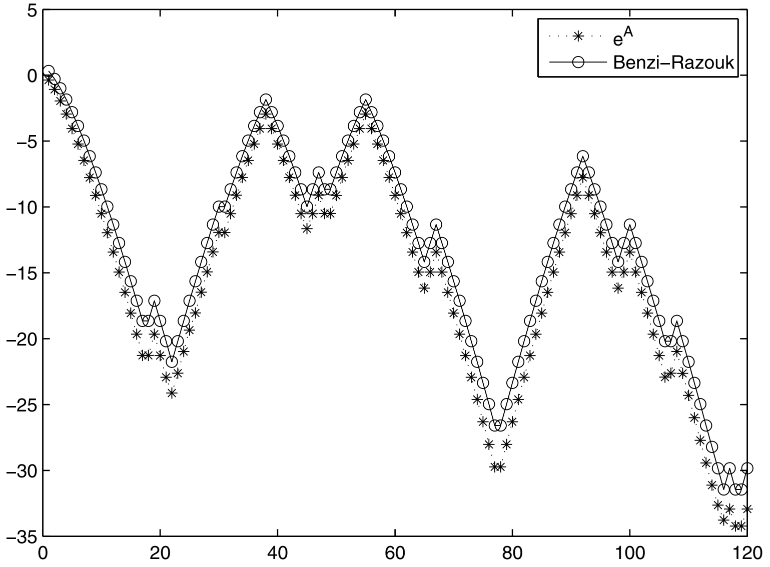

Fig. 7. Logarithmic plot of decay bounds (solid line) and of the absolute values of the 80th row of e^A (dotted line), as defined in Section 7.

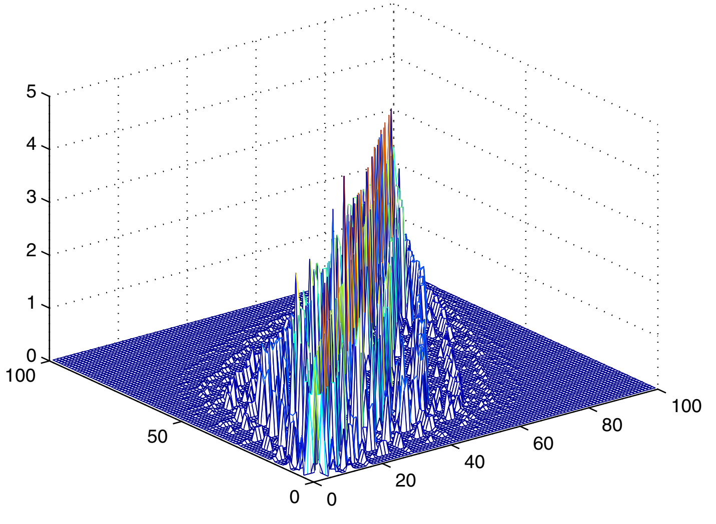

Fig. 8. City plot for the exponential of a reordered small world matrix with parameters $k = 1$ and $p = 0.1$.

Gershgorin estimates are applied, since in this case Gershgorin's theorem considerably overestimates the maximum eigenvalue. The bounds' accuracy becomes acceptable, however, when a better estimate of the extreme eigenvalues is available. MMQ bounds still work with Gershgorin eigenvalue estimates, at the price of increasing the number of iterations. In this case, too, the bounds become much more effective when the maximum and minimum eigenvalue are known, thus suggesting that, in general, poor results for the extended network are a consequence of bad eigenvalue estimates, rather than an inadequacy of the methods used.

We also consider the application of decay bounds for functions of matrices to the computation of network communicability, as suggested in Section 7. Here A is a 200×200 small world matrix defined

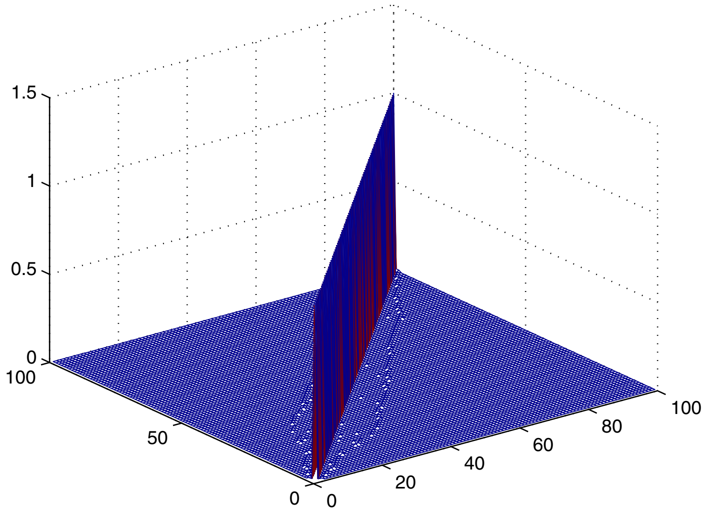

Fig. 9. City plot for the resolvent of a reordered small world matrix with parameters $k = 1$ and $p = 0.1$ (same matrix as in Fig. 8).

by parameters $k = 1$ and $p = 0.1$, normalized so that $\|A\|_2 = 1$. Fig. 5 shows the sparsity patterns of A and of the matrix B obtained by reordering A via reverse Cuthill–McKee; observe that B can be seen as a banded matrix of bandwidth 15. The behavior of the decay bounds (19) for e^B is shown in Fig. 6. In particular, for a tolerance $\epsilon = 10^{-4}$, the bounds tell us that $|[e^B]_{ij}| \leqslant \epsilon$ whenever $|i - j| \geqslant 93$, thus identifying *a priori* a fairly large set of pairs of nodes for which the communicability is negligible. Note that this is independent of N, hence as N increases the fraction of non-negligible communicabilities tends to zero. One may also employ a variant of the bounds (19) where the exponent $|i - j|$ is replaced by the graph distance between nodes i and j (see [3,23]). This allows to better capture the decay properties of B and e^B and obtain tighter bounds for rows where the actual bandwidth is narrower. Moreover, this variant can be applied to sparse matrices that do not have a band structure, such as the non reordered matrix A itself. Bounds for a row of e^A are shown in Fig. 7.

Figs. 8 and 9 are 'city-plots' showing the magnitude of the entries in the exponential and in the resolvent. Note the extremely fast off-diagonal decay in the resolvent, suggesting that the resolvent-based communicability may not be a useful measure in the case of very sparse networks with high locality (that is, small bandwidth).

9. Conclusions

We have used methods based on Gauss-type quadrature rules to develop upper and lower bounds for certain functions (Estrada index, subgraph centrality, communicability) of adjacency matrices, which give useful information on the connectivity properties of associated networks. Such results are especially interesting for large networks, and therefore for adjacency matrices of large size, for which the explicit computation of matrix exponentials and resolvents is computationally very expensive.

More precisely, we have proposed two types of bounds:

- *A priori* bounds, which only require knowledge of some fundamental properties of the graph under study, such as the number and degrees of nodes; the computational cost is $\mathcal{O}(1)$ and numerical tests show that these bounds can give a fairly good approximation of the exact values, significantly more accurate than previously known bounds;
- Bounds obtained via explicit computation of a few Lanczos iterations applied to quadrature rules (MMQ bounds). The cost per iteration grows linearly with respect to matrix size and the number

of iterations can be chosen so as to reach any desired approximation accuracy. Numerical tests and theoretical considerations show that, under mildly restrictive hypotheses, the convergence of these bounds to the exact values is quite fast and the number of iterations required to reach a given accuracy is independent of matrix size.

It also is interesting to point out that the computation of MMQ bounds for the Estrada index is easily parallelized, as the subgraph centrality of each node can be computed independently.

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