Orthogonal Expansion of Network Functions

Mohammed Al Mugahwi* Omar De la Cruz Cabrera*
Lothar Reichel*

Dedicated to Volker Mehrmann
on the occasion of his 65th birthday

Abstract

The power series expansion of functions of the adjacency matrix for a network can be interpreted in terms of walks in the network. This makes matrix functions, such as the exponential or resolvent, useful for the analysis of graphs. For instance, these functions shed light on the relative importance of the nodes of the graph and on the overall connectivity. However, the power series expansions may converge slowly, and the coefficients of these expansions typically are not helpful in assessing how important longer walks are in the network. Expansions of matrix functions in terms of orthogonal or bi-orthogonal polynomials make it possible to determine scaling parameters so that a given network has a specified effective diameter (the length after which walks become essentially irrelevant for the connectivity of the network). We describe several approaches for generating orthogonal and bi-orthogonal polynomial expansions, and discuss their relative merits for network analysis.

1 Introduction

Many complex systems that describe the interaction between entities can be modeled by networks. For mathematical and statistical modeling, as well as for analysis, networks are usually represented by a graph $G = \{V, E\}$, which consist of a set of vertices $V = \{v_j\}_{j=1}^{n}$ and a set of edges $E = \{e_k\}_{k=1}^{\ell}$, the latter being the links between the vertices. A graph may be *undirected*, in which case each edge e_k represents a "two-way street" between a pair of vertices $\{v_i, v_j\}$, or *directed*, in which case at least one of the edges is a "one-way street" between a pair of nodes. Examples of networks include:

- Flight networks, with airports represented by vertices and flights by directed edges.

*Department of Mathematical Sciences, Kent State University, Kent, OH 44242, USA. Email: malmugah@kent.edu (M. Al Mugahwi), odelacru@kent.edu (O. De la Cruz Cabrera), reichel@math.kent.edu (L. Reichel)

- Social networking services, such as Facebook, Twitter, and Snapchat, with members or accounts represented by vertices, and interactions between any two accounts by edges, which can be undirected (e.g., a "friendship") or directed (e.g., "follow" or "like").

- Phone networks can be modeled by directed graphs, in which phone numbers are represented by vertices, and text messages or calls that occur in a fixed span of time by edges from the originator to the receiver.

Numerous applications of networks and associated directed or undirected graphs are described in [12, 14, 17, 19, 31].

We consider unweighted graphs $G = \{V, E\}$ with n vertices v_j and ℓ edges e_k, without self-loops or multiple edges. For a *directed* graph G, the associated adjacency matrix $A = [a_{ij}]_{i,j=1}^{n} \in \mathbb{R}^{n\times n}$ has the entry $a_{ij} = 1$ if there is an edge emerging from vertex v_i and pointing to vertex v_j; otherwise $a_{ij} = 0$. Thus, A has vanishing diagonal entries and ℓ non-vanishing entries. Typically, $1 \leq \ell \ll n^2$, which makes the matrix A sparse. The adjacency matrix for an *undirected* graph is symmetric and has 2ℓ entries $a_{ij} = 1$. Adjacency matrices associated with weighted graphs can easily be defined by allowing the non-vanishing entries to be arbitrary positive real numbers. The discussion of this paper can be extended to weighted graphs. This is illustrated in Subsection 5.2.

A common task in network analysis is to determine which vertices of an associated graph are the most important ones by measuring how well-connected a vertex is to other vertices in the graph. This kind of importance measure, which often is referred to as a *centrality measure*, ignores intrinsic properties of the vertices but often provides vital information about the vertices just from network connections. Simple centrality measures for a vertex v_k of a directed graph are its *in-degree* and *out-degree*, which count the number of edges that point directly to v_k and the number of edges that emerge from v_k, respectively. In undirected graphs, every edge from vertex v_j to vertex v_k also is an edge from vertex v_k to vertex v_j. The number of distinct edges that connect a vertex v_k to other vertices of the graph is referred to as the *degree* of v_k.

The in-degree, out-degree, or degree of a vertex v_k are centrality measures that are easily computable. However, these measures may be unsatisfactory measures of importance of a vertex v_k, because they do not take into account the importance of the vertices that are connected to v_k. This shortcoming has spurred the introduction of several alternative centrality measures. Of particular interest are centrality measures derived from the application of matrix functions to the adjacency matrix A of G. A nice introduction to matrix functions in network analysis is provided by Estrada and Higham [21]; see also [9, 10, 11, 15, 16, 19, 20] for discussions and examples.

We will need the notion of a walk in a graph. A walk of length k is a sequence of $k+1$ vertices $v_{i_1}, v_{i_2}, \ldots, v_{i_{k+1}}$ and a sequence of k edges $e_{j_1}, e_{j_2}, \ldots, e_{j_k}$ such that e_{j_ℓ} points from v_{i_ℓ} to $v_{i_{\ell+1}}$ for $j = 1, 2, \ldots, k$. The vertices in a walk do not have to be distinct.

A fundamental property of A is that for any positive integer k, the entry $[A^k]_{ij}$ of A^k gives the number of walks of length k that start at the vertex v_i and

end at the vertex v_j; see, e.g., [21]. This suggests the use of linear combinations of powers of A to measure the centrality of vertices of a graph. Commonly used matrix functions for measuring the centrality of the vertices of a graph include the exponential function $\exp(\gamma_e A)$ and the resolvent $(I-\gamma_r A)^{-1}$, where γ_e and γ_r are positive user-chosen parameters; see, e.g., [21]. The power series expansions of these functions are given by

$$\exp(\gamma_e A) = I + \gamma_e A + \frac{1}{2!}(\gamma_e A)^2 + \frac{1}{3!}(\gamma_e A)^3 + \dots , \tag{1.1}$$

$$(I - \gamma_r A)^{-1} = I + \gamma_r A + (\gamma_r A)^2 + (\gamma_r A)^3 + \dots . \tag{1.2}$$

For the resolvent, the parameter γ_r has to be chosen small enough so that the power series (1.2) converges, that is, γ_r should be strictly smaller than $1/\rho(A)$, where $\rho(A)$ denotes the spectral radius of A.

Long walks are considered less important than short walks. Therefore, the coefficients for high powers of A are chosen to be smaller than the coefficients for low powers. For instance, the coefficients for A^k are $\gamma_e^k/(k!)$ for the exponential and γ_r^k for the resolvent.

The diagonal entries $[\exp(\gamma_e A)]_{ii}$ and $[(I - \gamma_r A)^{-1}]_{ii}$ measure how easy it is to return from the vertex v_i back to itself via available edges. These entries are commonly referred to as *subgraph centralities* of the vertex v_i, and are used as centrality measures for the vertex. Similarly, the entries $[\exp(\gamma_e A)]_{ij}$ and $[(I - \gamma_r A)^{-1}]_{ij}$, for $i \neq j$, measure how easy communication is between the vertices v_i and v_j. These entries are referred to as the *communicability* between the vertices v_i and v_j; see, e.g., [21] for further details.

The subgraph centralities and communicabilities depend on the choice of the parameters γ_e and γ_r in (1.1) and (1.2). However, the choices of these parameters have not received much attention in the literature. Insightful discussions are provided by Estrada et al. [20], who interpret γ_e in (1.1) as reciprocal temperature in a system of oscillators, by Benzi and Klymko [11], who analyze the behavior of the subgraph centrality and communicability as the parameter γ_e in (1.1) goes to zero or infinity, or the parameter γ_r in (1.2) increases to $1/\rho(A)$ or decreases to zero, and by Aprahamian et al. [3] who examine how the parameters γ_e and γ_r can be related.

We seek to shed some light on the choices of γ_e and γ_r by expanding the matrix functions (1.1) and (1.2) in terms of orthogonal and bi-orthogonal polynomials. These expansions help us define the *effective diameter* of a graph, which is the maximum length of walks that contribute substantially to the communication within the network. The effective diameter depends on the choices of the parameters γ_e and γ_r. In particular, these parameters can be chosen to achieve a desired effective diameter. Our analysis complements that of Benzi and Klymko [11].

The expansion of a matrix function as a power series, like (1.1) and (1.2), is not always "efficient", in the sense that many terms may be required to approximate the function to desired accuracy. Often expansions in terms of suitably defined orthogonal polynomials require fewer terms to approximate the matrix

function to a specified accuracy. This means that an expansion in terms of orthogonal polynomials gives a better idea of how important long walks are in the network than a power series expansion. This paper investigates three approaches for generating orthogonal polynomial bases, and evaluates their strengths and weaknesses as tools for network analysis.

The three methods considered might seem quite different at first sight, but they can be seen as particular cases of a general construction. Let $\mathcal{A}$ be an algebra, with an algebra product $\mathcal{A} \times \mathcal{A} \to \mathcal{A}$, and assume that $\mathcal{A}$ also has an inner product $\langle \cdot, \cdot \rangle_{\mathcal{A}}$. Let $\mathbb{P}_n$ denote the set of polynomials of degree at most n. For $a_0 \in \mathcal{A}$, define a linear map $\mathbb{P}_n \to \mathcal{A}$ by $p \mapsto p(a_0)$. Then we can pull back the inner product in $\mathcal{A}$ to $\mathbb{P}_n$ by $\langle p, q \rangle = \langle p(a_0), q(a_0) \rangle_{\mathcal{A}}$ (this is an inner product in $\mathbb{P}_n$ as long as $p(a_0) \neq 0$ for all non-zero $p \in \mathbb{P}_n$ and n is sufficiently small). Using this inner product, we can define a basis $\{p_0, p_1, \ldots, p_n\}$ of orthogonal polynomials for $\mathbb{P}_n$. As particular cases, we have:

1. $\mathcal{A} = \mathcal{C}([a, b])$ (continuous functions on $[a, b]$), with the algebra product given by point-wise multiplication, and the inner product given by $\langle f, g \rangle_{\mathcal{A}} = \int_a^b f(x)g(x)W(x)dx$ with an appropriate weight function $W(x)$. We take a_0 to be the identity function $a_0(x) = x$ on $[a, b]$. Then we obtain, for instance, the orthogonal Chebyshev polynomials for the interval $[a, b]$; see Section 2.

2. $\mathcal{A} = \mathbb{R}^{m \times m}$, with matrix multiplication, and inner product given by $\langle A, B \rangle_{\mathcal{A}} = \text{trace}(A^T B)$. Here and throughout this paper the superscript ^{T} denotes transposition. Let a_0 be the given, fixed, adjacency matrix A. Then we obtain the global Arnoldi (or nonsymmetric Lanczos) orthogonal (or bi-orthogonal) polynomials; see Section 3.

3. $\mathcal{A} = \mathbb{R}^{m \times m}$, like above, but now with the inner product given by $\langle A, B \rangle_{\mathcal{A}} = 1^T A^T B 1$. Taking a_0 again to be A, we obtain the standard Arnoldi (or nonsymmetric Lanczos) orthogonal (or bi-orthogonal) polynomials; see Section 4.

This paper is organized as follows: Section 2 reviews the approximation of analytic functions by expansions in terms of orthogonal polynomials. Expansions in terms of Chebyshev polynomials, as well as in terms of orthogonal polynomials associated with inner products defined by the adjacency matrix A are considered. Section 3 focuses on orthogonal and bi-orthogonal polynomials determined by the global Arnoldi and nonsymmetric Lanczos methods, respectively. These are block iterative methods introduced by Jbilou et al. [27, 28] for the solution of matrix equations and linear systems of equations with multiple right-hand sides. Section 4 discusses the computation of orthogonal and bi-orthogonal polynomials associated with the "standard" Arnoldi and nonsymmetric Lanczos methods, respectively, and Section 5 presents a few numerical examples. Concluding remarks can be found in Section 6.

2 Expansion of functions in terms of orthogonal polynomials

We review a few results from Trefethen [34]. Related results also can be found in, e.g., [24, 35]. Let $\rho > 1$ and $i = \sqrt{-1}$. Following Trefethen [34, Chapter 8], we refer to the open interior of the set

$$\left\{ \frac{1}{2} \left(\rho \exp(i\theta) + \rho^{-1} \exp(-i\theta) \right) : \ 0 \le \theta < 2\pi \right\}$$

as a *Bernstein ellipse*, which we denote by $\mathbb{E}_\rho$. This ellipse has foci at ± 1 and contains the real interval $[-1, 1]$. The closer the interval $[-1, 1]$ is to the boundary of $\mathbb{E}_\rho$, the closer $\rho > 1$ is to unity. Moreover, $\mathbb{E}_{\rho_1} \subsetneqq \mathbb{E}_{\rho_2}$ for $1 < \rho_1 < \rho_2$.

Proposition 1. *([34, Theorem 8.1]) Let a function f, analytic on $[-1, 1]$, be analytically continuable to the open Bernstein ellipse $\mathbb{E}_\rho$, where it satisfies $|f(x)| \le M_f$ for some constant M_f independent of x in $\mathbb{E}_\rho$. Consider the expansion of f in terms of orthogonal Chebyshev polynomials of the first kind,*

$$T_j(x) = \cos(j \arccos(x)), \quad -1 \le x \le 1, \quad j = 0, 1, \dots \ , \tag{2.1}$$

with regard to the inner product

$$(g, h) = \frac{2}{\pi} \int_{-1}^{1} g(x) h(x) \frac{1}{\sqrt{1 - x^2}} dx$$

for sufficiently smooth functions g and h on the interval $[-1, 1]$. Thus,

$$f(x) = \sum_{j=0}^{\infty} c_j T_j(x), \qquad c_j = (f, T_j). \tag{2.2}$$

Then the expansion coefficients satisfy $|c_0| \le M_f$ and

$$|c_j| \le 2 M_f \rho^{-j}, \qquad j = 1, 2, \dots \ . \tag{2.3}$$

Thus, the larger the Bernstein ellipse $\mathbb{E}_\rho$ can be chosen, i.e., the larger ρ can be chosen, the faster the bound for the coefficients c_j decreases to zero with increasing j. The following result can be shown by using the bounds of Proposition 1.

Proposition 2. *([34, Theorem 8.2]) Let f satisfy the conditions of Proposition 1. Define the Chebyshev projection*

$$f_n(x) = \sum_{j=0}^{n} c_j T_j(x) \tag{2.4}$$

with the coefficients c_j given by (2.2). Then

$$\max_{-1 \le x \le 1} |f(x) - f_n(x)| \le \frac{2 M_f \rho^{-n}}{\rho - 1}, \qquad n = 0, 1, 2, \dots \ . \tag{2.5}$$

Thus, the bound for the approximation error (2.5) decreases to zero at the same rate as the bound (2.3) for the highest order coefficient in (2.4).

The converse of Proposition 2 also holds.

Proposition 3. *([34, Theorem 8.3]) Let the function f be defined on the real interval $[-1,1]$. Suppose that there is a sequence of polynomials $q_0, q_1, q_2, \ldots$, with q_j of degree at most j, such that*

$$\max_{-1\leq x\leq 1} |f(x) - q_n(x)| \leq C\rho^{-n}, \qquad n = 0, 1, 2, \ldots ,$$

for some constants $C > 0$ and $\rho > 1$ independent of n. Then f can be analytically continued to an analytic function in the open Bernstein ellipse $\mathbb{E}_\rho$.

Example 2.1. Consider the Runge function

$$f(x) = \frac{1}{1+25x^2}.$$

The power series expansion of f at the origin does not converge to f on the interval $[-1,1]$. However, the expansion (2.4) converges to f on $[-1,1]$ according to (2.5) as n increases with $\rho = 1.22$. □

Example 2.2. We are particularly interested in the entire function $f(x) = \exp(x)$. The expansion (2.4) of f converges to f on $[-1,1]$ faster than (2.5) for any $\rho > 1$ as n increases. We therefore can expect the magnitude of the coefficients c_j to decrease to zero quite rapidly with increasing index j. □

The fact that the magnitude of the terms of an expansion of an analytic function in terms of suitably scaled orthogonal polynomials decays at least exponentially with the degree of the polynomials holds for more general sets than the interval $[-1,1]$. Let $\mathbb{S}$ be a Jordan domain in the complex plane $\mathbb{C}$, i.e., the boundary of $\mathbb{S}$ is a Jordan curve. Let ψ denote the conformal mapping from the exterior of the unit disc $\mathbb{D}_c = \{w \in \mathbb{C} : |w| > 1\}$ to the exterior of $\mathbb{S}$ with a pole at infinity. Then $\psi(w)$ has an expansion of the form

$$z = \psi(w) = dw + d_0 + d_1 w^{-1} + d_2 w^{-2} + \ldots ,$$

with $d_j \in \mathbb{C}$ for $j = 0, 1, \ldots$, and $d > 0$ for $|w|$ sufficiently large. Let $\mathbb{S}_\rho$ for some $\rho > 1$ denote the open set that is bounded by the curve

$$\{z \in \mathbb{C} : z = \psi(w),\ w = \rho\exp(i\theta),\ 0 \leq \theta < 2\pi\}, \qquad i = \sqrt{-1}.$$

Introduce the orthogonal polynomials $p_0, p_1, p_2, \ldots$ with respect to some inner product on $\mathbb{S}$, i.e., p_i is of degree i and

$$\langle p_i, p_j\rangle = \int_{\mathbb{S}} p_i(x)\overline{p_j(x)}d\omega(x) = \begin{cases} 1, & i = j, \\ 0, & i \neq j, \end{cases} \tag{2.6}$$

where $d\omega$ is a positive measure with support on $\mathbb{S}$ and the bar denotes complex conjugation. Define the finite expansion

$$f_n(z) = \sum_{j=0}^{n} c_j p_j(z), \qquad c_j = \langle f, p_j\rangle, \qquad j = 0, 1, \ldots, n. \tag{2.7}$$

Then

$$\limsup_{j\to\infty} |c_j|^{1/j} = \rho^{-1}$$

and

$$\limsup_{n\to\infty} \left(\max_{z\in\mathbb{S}} |f(z) - f_n(z)| \right)^{1/n} = \rho^{-1}; \tag{2.8}$$

see Gaier [24, Chapter 1] or Walsh [35, Chapter 6] for details. In particular, when $\mathbb{S} = [-1, 1]$, we can choose

$$\psi(w) = \frac{1}{2}(w + w^{-1}),$$

and the set $\mathbb{S}_\rho$ for some $\rho > 1$ is the Bernstein ellipse $\mathbb{E}_\rho$.

We are concerned with the expansion of the matrix functions (1.1) and (1.2) in terms of the orthogonal polynomials p_k. Let A be the adjacency matrix associated with the graph G, and consider the expansion

$$\exp(\gamma_e A) = \sum_{k=0}^{\infty} c_k^{(\gamma_e)} p_k(A).$$

Since the polynomial $p_k(A)$ is a linear combination of the powers A^j, $j = 0, 1, \ldots, k$, it only depends on walks of length at most k. The polynomials p_k are independent of the parameter γ_e, but the coefficients $c_k^{(\gamma_e)}$ are functions of this parameter.

Example 2.3. Let $A \in \mathbb{R}^{n\times n}$ be an adjacency matrix that is associated with an undirected graph, and assume that its spectrum is contained in the interval $[a, b]$, with $-\infty < a < b < \infty$. The identity

$$\exp(\gamma x) = I_0(\gamma) + 2\sum_{j=1}^{\infty} I_j(\gamma) T_j(x), \qquad -1 \le x \le 1, \tag{2.9}$$

where the

$$I_j(\gamma) = \sum_{\ell=0}^{\infty} \frac{(\frac{\gamma}{2})^{j+2\ell}}{\ell!(\ell + j)!}, \qquad j = 0, 1, \ldots\ , \tag{2.10}$$

are modified Bessel functions of the first kind, the T_j are defined by (2.1), and γ is a real constant, is a consequence of [1, Eq. (9.6.34)]. Since the spectrum of A is in $[a, b]$, it is appropriate to expand $\exp(\gamma_e A)$ in terms of Chebyshev polynomials for the interval $[a, b]$. They are given by

$$T_j^{[a,b]}(z) = T_j(x(z)), \qquad x(z) = \frac{2}{b-a} z - \frac{b+a}{b-a}, \qquad j = 1, 2, \ldots\ ,$$

for $a \le z \le b$. We obtain from (2.9) that

$$\begin{aligned} \exp(\gamma z) &= \exp(\frac{\gamma}{2}(b-a)x) \exp(\frac{\gamma}{2}(b+a)) \qquad (2.11) \\ &= \exp(\frac{\gamma}{2}(b+a)) \left(I_0(\frac{\gamma}{2}(b-a)) + 2\sum_{j=1}^{\infty} I_j(\frac{\gamma}{2}(b-a)) T_j^{[a,b]}(z) \right). \end{aligned}$$

Introduce the spectral factorization

$$A = S\Lambda S^{-1}, \quad \Lambda = \mathrm{diag}[\lambda_1, \lambda_2, \ldots, \lambda_n], \tag{2.12}$$

where the matrix S can be chosen to be real and orthogonal. Then

$$\exp(\gamma_e A) = S\,\mathrm{diag}[\exp(\gamma_e\lambda_1), \exp(\gamma_e\lambda_2), \ldots, \exp(\gamma_e\lambda_n)]\,S^{-1}$$

and, by (2.11),

$$\exp(\gamma_e\lambda_k) = \exp(\frac{\gamma_e}{2}(b+a))\left(I_0(\frac{\gamma_e}{2}(b-a)) + 2\sum_{j=1}^{\infty} I_j(\frac{\gamma_e}{2}(b-a))T_j^{[a,b]}(\lambda_k)\right).$$

This yields the expansion

$$\exp(\gamma_e A) = \sum_{k=0}^{\infty} c_k^{(\gamma_e)} p_k(A), \tag{2.13}$$

where

$$\begin{aligned} p_k(A) &= T_k^{[a,b]}(A), \quad k = 0, 1, \ldots\ , \\ c_0^{(\gamma_e)} &= \exp(\frac{\gamma_e}{2}(b+a))I_0(\frac{\gamma_e}{2}(b-a)), \\ c_k^{(\gamma_e)} &= 2\exp(\frac{\gamma_e}{2}(b+a))I_k(\frac{\gamma_e}{2}(b-a)), \quad k = 1, 2, \ldots\ . \end{aligned}$$

It is clear from (2.10) that the functions $t \to I_j(t)$, $j = 0, 1, \ldots$, are increasing for $t \geq 0$ and, therefore, the coefficients $c_k^{(\gamma_e)}$ for, $k = 0, 1, \ldots$, are increasing functions of $\gamma_e > 0$, while the polynomials p_k are independent of γ_e. The larger γ_e is chosen, the more terms in the expansion (2.13) should be included in an approximation of $\exp(\gamma_e A)$. $\square$

Assume that the first $\ell+1$ terms $c_0^{(\gamma_e)}p_0(A), c_1^{(\gamma_e)}p_1(A), \ldots, c_\ell^{(\gamma_e)}p_\ell(A)$ in the expansion (2.13) are significant, and that the remaining terms are of comparatively small norm. Then this suggests that only walks of length smaller than or equal to ℓ have to be considered when analyzing the network represented by the matrix A. In particular, $\exp(\gamma_e A)$ may be approximated well by a polynomial in A of degree at most ℓ. We will say that ℓ is the *effective diameter* of the graph G. The effective diameter depends on the parameter γ_e; the smaller $\gamma_e > 0$ is, the fewer terms are required. Thus, if we know that in our network all walks of length larger than j_0 may be ignored, then γ_e can be chosen so that the terms $c_j^{(\gamma_e)}p_j(A)$ for $j > j_0$ are negligible. We will provide a more precise definition of the effective diameter below. The parameter γ_r in the resolvent can be chosen in a similar fashion.

Definition 1. *Let the c_j be coefficients in an expansion of a function of an adjacency matrix in terms of orthogonal or bi-orthogonal polynomials. We refer to the smallest integer $k \geq 1$ such that*

$$\frac{|c_{k+1}|}{\max_{0\leq j\leq k}|c_j|} \leq \delta$$

as the δ-effective diameter *of the graph.*

The intuition is that the matrix function under consideration can be well approximated, when evaluated at A, by a polynomial of degree k, and therefore walks or multi-step connections of length greater than k are mostly irrelevant for the communication within the network. The δ-effective diameter depends on the matrix function and the expansion used.

The determination of the expansion (2.13) requires that estimates of the largest and smallest eigenvalues of A be known, so that the interval $[a, b]$ can be chosen large enough to contain the spectrum of A. Then the polynomials $p_k(A)$ in (2.13) are of about unit norm and the magnitude of each term in the expansion depends primarily on the size of the coefficients $c_k^{(\gamma_e)}$. In this paper, we will use expansions in terms of orthogonal matrix polynomials, whose computation does not require a priori knowledge of the spectrum of A. When the matrix A is symmetric, these orthogonal matrix polynomials are generated with the symmetric Lanczos process equipped with the matrix inner product

$$\langle M_1, M_2 \rangle_F = \mathrm{trace}(M_1^T M_2), \tag{2.14}$$

where $M_1, M_2 \in \mathbb{R}^{n\times n}$. The associated matrix norm

$$\|M\|_F = \sqrt{\langle M, M \rangle_F} \tag{2.15}$$

is the Frobenius norm. For a nonsymmetric matrix A, orthogonal matrix polynomials $p_k(A)$ of degree k, for $k = 0, 1, 2, \ldots$, can be generated by the Arnoldi process furnished with the inner product (2.14) and norm (2.15). Alternatively, families of bi-orthogonal polynomials can be generated with the aid of the nonsymmetric Lanczos process. Arnoldi and Lanczos processes using inner products of the form (2.14) have been studied in the context of solving matrix equations and linear systems of equations with several right-hand sides, see Jbilou et al. [27, 28], who refer to the Arnoldi and Lanczos processes so defined as global Arnoldi and Lanczos processes, respectively. The approximation of matrix functions using this kind of inner product has recently been discussed by Bellalij et al. [7], Bentbib et al. [8], and Frommer et al. [23].

The approximation of the matrix functions (1.1) and (1.2) in terms of orthogonal matrix polynomials that are determined by global Lanczos or Arnoldi processes is described in Section 3. These expansions can be applied to determine suitable values of the parameters γ_e or γ_r. The computation of this kind of polynomial expansions requires the explicit evaluation of the matrix exponential or resolvent and, therefore, can be applied to adjacency matrices A of small to moderate size. However, they cannot be used when the matrix A is large. This situation is considered in Section 4, where we discuss expansions of the form

$$\exp(\gamma_e A)v = \sum_{k=0}^{\infty} c_k^{(\gamma_e)} p_k(A)v, \qquad (I - \gamma_r A)^{-1}v = \sum_{k=0}^{\infty} c_k^{(\gamma_r)} p_k(A)v, \tag{2.16}$$

for some vector $v \in \mathbb{R}^n$. These kinds of matrix functions have been discussed in, e.g., [10, 15, 30]. In the computed examples, we let $v = [1, 1, \ldots, 1]^T$, but

other choices of v also are possible. The expansions (2.16) can be computed with the "standard" symmetric or nonsymmetric Lanczos processes, or with the "standard" Arnoldi process. The computation of these expansions does not require the evaluation of the matrix exponential or resolvent. We note that the expansions (2.16) also are of interest when A is replaced by A^T; see, e.g., [15].

3 The computation of orthogonal and bi-orthogonal matrix polynomials

The algorithms of this section determine expansions of a matrix function in terms of orthogonal and bi-orthogonal matrix polynomials. This allows for the computation of the δ-effective diameter of a graph without having to explicitly define a measure $d\omega$, like in (2.6). The computation of the effective diameter in this manner provides insight into properties of the graph, but is expensive when the adjacency matrix A is large. A cheaper approach is described in Section 4.

Let $A \in \mathbb{R}^{n\times n}$ be the adjacency matrix for a graph G, and let f be a function such that $f(A)$ is defined. It suffices that f is analytic in a simply connected region in the complex plane that contains the spectrum of A in its interior; see, e.g., [25, 26] for details. Let $\mathbb{P}_k$ denote the set of polynomials of degree at most k, and consider the approximation of $f(A)$ by a polynomial $p \in \mathbb{P}_k$ using the Frobenius norm (2.15). Thus, we would like to solve

$$\min_{p\in\mathbb{P}_k} \|f(A) - p(A)\|_F. \tag{3.1}$$

The meaning of this norm is most transparent when the matrix A is normal, such as symmetric or skew-symmetric. Then the eigenvector matrix S in (2.12) can be chosen to be orthogonal or unitary. Substituting (2.12) into (3.1) gives the equivalent minimization problem

$$\min_{p\in\mathbb{P}_k} \sum_{j=1}^{n} |f(\lambda_j) - p(\lambda_j)|^2. \tag{3.2}$$

Thus, the minimization problem (3.1) is a polynomial least-squares approximation problem in the complex plane. We assume that the number of distinct eigenvalues λ_j is strictly larger than the degree k. Then the problem (3.1) has a unique solution. For adjacency matrices for "real" networks, this requirement on k generally is satisfied. In the rare events when it is not, we can reduce k suitably.

The polynomial least squares problem (2.6)-(2.8) differs from the least-squares problem (3.2) in that the integral in (2.6) is replaced by a sum over the n eigenvalues of A. If n is much larger than the degree k of the polynomial approximant and the eigenvalues λ_j are distributed fairly uniformly over a set $\mathbb{S}$, then we can expect the solution of the discrete approximation problem (3.2) to behave similarly as the solution of the approximation problem (2.6)-(2.8). In

particular, the solutions p of (3.2) typically converge quite rapidly to f as the degree k of the solutions increases. This is illustrated in Section 5.

When the graph G is directed, the associated adjacency matrix $A \in \mathbb{R}^{n\times n}$ is nonsymmetric. Assume for the moment that A has a spectral factorization (2.12) with a nonsingular matrix S made up of unit eigenvectors. We then obtain the bound

$$\min_{p\in\mathbb{P}_k} \|f(A) - p(A)\|_F \leq \|S\|_2\|S^{-1}\|_2 \left(\min_{p\in\mathbb{P}_k} \sum_{j=1}^{n} |f(\lambda_j) - p(\lambda_j)|^2 \right)^{1/2}, \quad (3.3)$$

where $\|\cdot\|_2$ denotes the spectral matrix norm. The derivation of the above bound uses the fact that $\|M_1M_2\|_F \leq \|M_1\|_2\|M_2\|_F$ for any pair of compatible matrices M_1 and M_2. The sum in (3.3) is analogous to (3.2). We therefore expect fast reduction of the approximation error when the degree k of the polynomial p increases and $\|S\|_2\|S^{-1}\|_2$ is not very large. In any case, the polynomial expansion computed minimizes the left-hand side of (3.3). Computed examples that illustrate the convergence of the left-hand side can be found in Section 5. We remark that in the rare event that a spectral factorization of the form (2.12) does not exist, the Jordan normal form can be used; see [26]. The sum in the right-hand side of (3.3) then also contains terms with the magnitude of differences of derivative values of f and p at eigenvalues of A associated with nontrivial Jordan blocks; see [26] for details.

Algorithm 1 The global Arnoldi process for approximating $\exp(\gamma_e A)$, $A \in \mathbb{R}^{n\times n}$.

1. Let $V_1 = I/\sqrt{n}$, where I denotes the identity matrix of order n. Then $||V_1||_F = 1$. Let m denote the number of steps of the algorithm.
2. For $j = 1, 2, \ldots, m$ Do:
3. $c_{j-1} = \langle \exp(\gamma_e A), V_j\rangle_F$
4. $W = AV_j$
5. For $i = 1, 2, \ldots, j$ Do:
6. $h_{ij} = \langle W, V_i\rangle_F$
7. $W = W - h_{ij}V_i$
8. EndDo
9. $h_{j+1,j} = ||W||_F$. If $h_{j+1,j} = 0$ Then Stop
10. $V_{j+1} = W/h_{j+1,j}$
11. EndDo

We turn to the computation of orthogonal matrix polynomials with respect to the inner product (2.14) and associated norm (2.15). When A is nonsymmetric, such polynomials can be computed with the global Arnoldi process [27, 28], described by Algorithm 1. The matrices $V_1, V_2, \ldots, V_{m+1}$ generated by the algorithm satisfy

$$\langle V_j, V_k\rangle_F = \begin{cases} 1, & j = k, \\ 0, & j \neq k, \end{cases}$$

and it follows from the recursion formulas of the algorithm that $V_j = p_{j-1}(A)$ for some polynomial $p_{j-1} \in \mathbb{P}_{j-1}$ for $j = 1, 2, \ldots, m+1$. Hence,

$$\langle p_j(A), p_k(A) \rangle_F = \begin{cases} 1, & j = k, \\ 0, & j \neq k. \end{cases}$$

Thus, the p_j are the desired orthogonal polynomials. The scalars c_j determined in line 3 of Algorithm 1 are the expansion coefficients for

$$\exp(\gamma_e A) \approx \sum_{j=0}^{m-1} c_j p_j(A). \tag{3.4}$$

The polynomial in the right-hand side solves the minimization problem in the left-hand side of (3.3) for $k = m-1$ and $f(A) = \exp(\gamma_e A)$. The polynomials $p_j(A)$ are independent of the parameter γ_e, but the coefficients c_{j-1} computed in line 3 are not. The exponential function may be replaced by the resolvent.

The main computational cost of Algorithm 1 is the evaluation of the matrix function $\exp(\gamma_e A)$ used in line 3 of the algorithm. The scalars h_{ij} determined by Algorithm 1 yield the nontrivial entries of an upper Hessenberg matrix

$$H_m := \begin{bmatrix} h_{1,1} & h_{1,2} & h_{1,3} & \cdots & h_{1,m} \\ h_{2,1} & h_{2,2} & h_{2,3} & \cdots & h_{2,m} \\ & \ddots & \ddots & \ddots & \\ & & h_{m-1,m-2} & h_{m-1,m-1} & h_{m-1,m} \\ 0 & & & h_{m,m-1} & h_{m,m} \end{bmatrix} \in \mathbb{R}^{m \times m} \tag{3.5}$$

When the matrix A is symmetric, the recursion relations of Algorithm 1 simplify to give the global symmetric Lanczos process for approximating $\exp(\gamma_e A)$. In particular, the matrix (3.5) becomes symmetric and tridiagonal. We refer to [27] for details on and properties of the global symmetric Lanczos process.

Algorithm 2 The global nonsymmetric Lanczos process for approximating $\exp(\gamma_e A)$.

1. Let $V_1 = I_n, W_1 = I_n/n$. Choose number of steps m.
2. $\beta_1 = \delta_1 = 0 \in \mathbb{R}$, $V_0 = W_0 = 0 \in \mathbb{R}^{n \times n}$
3. For $j = 1, 2, \ldots, m$ Do:
4. $\quad c_{j-1} = \langle \exp(\gamma_e A), W_j \rangle_F$
5. $\quad \alpha_j = \langle AV_j, W_j \rangle_F$
6. $\quad \hat{V} = AV_j - \alpha_j V_j - \beta_j V_{j-1}$
7. $\quad \hat{W} = A^T W_j - \alpha_j W_j - \delta_j W_{j-1}$
8. $\quad \delta_{j+1} = |\langle \hat{V}, \hat{W} \rangle_F|^{1/2}$. If $\delta_{j+1} = 0$ Then Stop
9. $\quad \beta_{j+1} = \langle \hat{V}, \hat{W} \rangle_F / \delta_{j+1}$
10. $\quad W_{j+1} = \hat{W}/\beta_{j+1}$
11. $\quad V_{j+1} = \hat{V}/\delta_{j+1}$
12. EndDo

When the matrix $A \in \mathbb{R}^{n\times n}$ is nonsymmetric, approximations of functions of A also can be determined with the aid of the global nonsymmetric Lanczos process described by Algorithm 2. We assume that m is small enough so that the computations of the algorithm can be carried out without breakdown. Algorithm 2 was first introduced by Jbilou et al. [28].

The recursion formulas of Algorithm 2 show that $V_j = p_{j-1}(A)$ and $W_j = q_{j-1}(A)$ for some polynomials $p_{j-1}, q_{j-1} \in \mathbb{P}_{j-1}$ for $j = 1, 2, \ldots, m+1$. The matrices V_j and W_j are bi-orthogonal, i.e., they satisfy

$$\langle W_j, V_k \rangle_F = \begin{cases} 1, & j = k, \\ 0, & j \neq k. \end{cases}$$

It follows that the polynomials p_j and q_k are bi-orthogonal with respect to the bilinear form (2.14), i.e.,

$$\langle q_j(A), p_k(A) \rangle_F = \begin{cases} 1, & j = k, \\ 0, & j \neq k. \end{cases}$$

Moreover, the polynomials p_j and q_j satisfy three-term recurrence relations. This follows from the recursion relations of Algorithm 2.

4 The standard Arnoldi and Lanczos processes

This section discusses the approximation of $\exp(\gamma_e A)v$ for some vector $v \neq 0$ by application of the standard Arnoldi or Lanczos processes. In our computed examples in Section 5, we let $v = [1, 1, \ldots, 1]^T \in \mathbb{R}^n$, but other vectors also are of interest in applications; see [15]. The methods described also can be applied to the approximation of the matrix resolvent. As usual, we let $A \in \mathbb{R}^{n\times n}$ be an adjacency matrix.

We would like to approximate $\exp(\gamma_e A)v$ by $p(\gamma_e A)v$, where p is a polynomial determined with the aid of the standard Arnoldi or Lanczos processes. The former is described by Algorithm 3. The inner product used in the algorithm is the standard inner product in $\mathbb{R}^n$.

Algorithm 3 The standard Arnoldi process, $A \in \mathbb{R}^{n\times n}$.

1. Let $v_1 = v/||v||_2$. Let m denote the number of steps of the algorithm.
2. For $j = 1, 2, \ldots, m$ Do:
3. $\quad w = Av_j$
4. $\quad$ For $i = 1, 2, \ldots, j$ Do:
5. $\quad\quad h_{ij} = \langle w, v_i \rangle$
6. $\quad\quad w = w - h_{ij}v_i$
7. $\quad$ EndDo
8. $\quad h_{j+1,j} = ||w||_2$. If $h_{j+1,j} = 0$ Then Stop
9. $\quad v_{j+1} = w/h_{j+1,j}$
10. EndDo

Each iteration with Algorithm 3 generates a unit vector v_{j+1} that is orthogonal to the previously computed vectors $v_1, v_2, \ldots, v_j$. It follows from the recursion formulas of the algorithm that $v_{j+1} = p_j(A)v$, $j = 0, 1, 2, \ldots, m$, for certain polynomials $p_j \in \mathbb{P}_j$. These polynomials are orthogonal with respect to the inner product

$$\langle p_j, p_k \rangle = v^T (p_j(A))^T p_k(A) v.$$

We have

$$\langle p_j, p_k \rangle = \begin{cases} 1, & j = k, \\ 0, & j \neq k. \end{cases}$$

The scalars h_{ij} determined by Algorithm 3 define the nontrivial entries of an upper Hessenberg matrix $H_m \in \mathbb{R}^{m \times m}$, which is analogous to the matrix (3.5). The recursion formulas of Algorithm 3 can be expressed as

$$AV_m = V_m H_m + h_{j+1,j} v_{m+1} e_m^T,$$

where e_j denotes the jth axis vector of appropriate dimension and $V_m = [v_1, v_2, \ldots, v_m] \in \mathbb{R}^{n \times m}$. It can be verified by induction that

$$p(A)v = \|v\| p(H_m) e_1$$

for any polynomial $p \in \mathbb{P}_{m-1}$. This suggests the polynomial approximation

$$\exp(\gamma_e A)v \approx \|v\| V_m \exp(\gamma_e H_m) e_1; \tag{4.1}$$

see, e.g., [6] for error bounds. Note that the right-hand side is a linear combination of $p_0(A)v, p_1(A)v, \ldots, p_{m-1}(A)v$. This leads us to expect that for a general vector v, the convergence behavior of the right-hand side (4.1) towards the left-hand side as m increases is similar to the convergence for the problems considered in Section 2. In particular, we expect the coefficients of these polynomials, i.e., the coefficients of the columns v_j in the right-hand side of (4.1) to decrease in magnitude quite rapidly with increasing index number.

Similarly, as in Section 3, Algorithm 3 can be simplified to the standard Lanczos process when the matrix A is symmetric. In this case, the Hessenberg matrix H_m in (4.1) is symmetric and tridiagonal. Moreover, a more accurate approximation of $\exp(\gamma_e A)v$ can be computed by using the subdiagonal element $h_{m+1,m}$ of H_{m+1} generated by Algorithm 3 as described in [18].

Algorithm 4 The standard nonsymmetric Lanczos process, $A \in \mathbb{R}^{n\times n}$.

1. Let $v_1 = w_1 = v/||v||_2$. Choose number of steps m.
2. $\beta_1 = \delta_1 = 0 \in \mathbb{R}$, $v_0 = w_0 = 0 \in \mathbb{R}^{n\times n}$
3. For $j = 1, 2, \ldots, m$ Do:
4. $\quad \alpha_j = \langle Av_j, w_j \rangle$
5. $\quad \hat{v} = Av_j - \alpha_j v_j - \beta_j v_{j-1}$
6. $\quad \hat{w} = A^T w_j - \alpha_j w_j - \delta_j w_{j-1}$
7. $\quad \delta_{j+1} = |\langle \hat{v}, \hat{w} \rangle|^{1/2}$. If $\delta_{j+1} = 0$ Then Stop
8. $\quad \beta_{j+1} = \langle \hat{v}, \hat{w} \rangle / \delta_{j+1}$
9. $\quad w_{j+1} = \hat{w}/\beta_{j+1}$
10. $\quad v_{j+1} = \hat{v}/\delta_{j+1}$
11. EndDo

A nonsymmetric matrix A can be reduced to a small nonsymmetric tridiagonal matrix

$$T_m := \begin{bmatrix} \alpha_1 & \beta_2 & & & 0 \\ \delta_2 & \alpha_2 & \beta_3 & & \\ & \ddots & \ddots & \ddots & \\ & & \delta_{m-1} & \alpha_{m-1} & \beta_m \\ 0 & & & \delta_m & \alpha_m \end{bmatrix} \in \mathbb{R}^{m\times m}, \tag{4.2}$$

whose entries are determined by Algorithm 4. It follows from the recursion formulas of Algorithm 4 that $v_j = p_{j-1}(A)v_1$ and $w_j = q_{j-1}(A)w_1$ for some polynomials $p_{j-1}, q_{j-1} \in \mathbb{P}_{j-1}$. The vectors v_j are bi-orthogonal to the vectors w_j, i.e.,

$$\langle v_j, w_k \rangle = \begin{cases} 1, & j = k, \\ 0, & j \neq k. \end{cases}$$

and therefore the polynomials p_j and q_k are bi-orthogonal. We have

$$\langle q_j(A), p_k(A) \rangle = \begin{cases} 1, & j = k, \\ 0, & j \neq k. \end{cases}$$

We assume for simplicity that the computations with Algorithm 4 can be carried out without breakdown. A recent discussion of breakdowns is provided by Pozza et al. [32].

The matrix (4.2) furnishes the following polynomial approximation

$$\exp(\gamma_e A)v \approx \exp(\gamma_e T_m)e_1\|v\|.$$

5 Computed examples

This section shows expansions of the functions (1.1) and (1.2) for several networks and values of the parameters γ_e and γ_r.

5.1 Expanding $\exp(\gamma_e A)$ for a protein-protein interaction network

We illustrate the convergence of the coefficients of the expansions (3.4) and

$$\exp(\gamma_e A) = I + \gamma_e \|A\|_F \frac{A}{\|A\|_F} + \frac{\gamma_e^2 \|A\|_F^2}{2!} \frac{A^2}{\|A\|_F^2} + \cdots , \tag{5.1}$$

when applied to an undirected network that models protein-protein interaction in yeast. Specifically, we use part of the NDyeast network. Each edge represents an interaction between two proteins [29]. The data set is available at [5] and has 2114 nodes. There are 74 self-loops (nodes connected only to themselves) and 268 isolated nodes. The adjacency matrix obtained by removing the self-loops and isolated nodes is of order $n = 1846$. It has 149 connected components, which can be identified with the MATLAB function `getconcomp` from the PQser toolbox [13]. Most of the connected components have very few nodes. We will use the only connected component with more than 10 nodes. It has 1458 nodes and yields a symmetric adjacency matrix $A \in \mathbb{R}^{1458\times 1458}$. Since the adjacency matrix is not very large, $\exp(\gamma_e A)$ easily can be evaluated by using the MATLAB function `expm`.

We use the normalization of (5.1) because the normalized matrix $A/\|A\|_F$ is of unit norm, and each coefficient $\gamma_e^j \|A\|_F^j / j!$ provides the norm of the corresponding term. Note that the coefficients $\gamma_e^j \|A\|_F^j / j!$ might not depend monotonically on j; this is illustrated below.

Figure 1(a) displays for $\gamma_e = 1$ the magnitude of the coefficients in the expansion (3.4) of the exponential function $\exp(\gamma_e A)$ in terms of orthogonal polynomials in A determined by the global Lanczos method (blue dashed curve), as well as the coefficients $\gamma_e^k \|A\|_F^k/(k!)$, $k = 0, 1, 2, \ldots$ in (5.1) (black continuous curve). The coefficients in the expansion of orthogonal polynomials are seen to converge to zero much faster with increasing index than the coefficients in the power series expansion. Figure 1(b) is analogous to Figure 1(a) for $\gamma_e = 0.5$. The coefficients in Figure 1(b) converge to zero faster than the corresponding coefficients in Figure 1(a).

Figure 1(c) depicts for $\gamma_e = 1$ the norm of the approximation errors in terms of the degree of the approximating polynomials for expansions of orthogonal polynomials (blue dashed curve) and for the power series expansion (black continuous curve). The error, measured with the Frobenius norm (3.1), in the orthogonal polynomial expansion is seen to converge to zero much faster with increasing degree than the error in the power series expansion. Thus, the polynomial p in (3.1) is either the right-hand side of (3.4) for increasing degree, or the first terms in the power series expansion in the right-hand side of (5.1). Figure 1(d) is analogous to Figure 1(c) for $\gamma_e = 0.5$.

Let c_j, $j = 0, 1, 2, \ldots$ denote the expansion coefficients in (3.4). Table 1(a) shows the ratio of $|c_k|$ and $\max_{0\leq j\leq k} |c_j|$ for $k = 5$ and several values of γ_e. The ratio is seen to decrease quite rapidly when γ_e decreases. Table 1(b) is analogous to Table 1(a) for $k = 10$. Table 1 and Figure 1 suggest that one can approximate $\exp(\gamma_e A)$ quite accurately with fairly few terms in the expansion

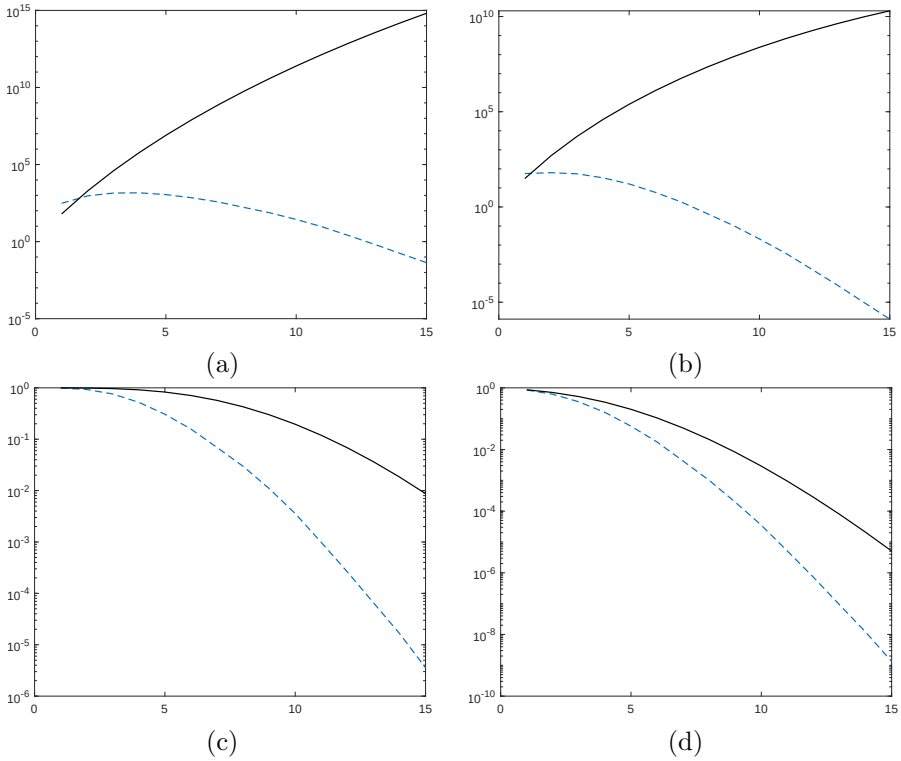


Figure 1: Yeast: (a) The magnitude of the coefficients in expansions of $\exp(\gamma_e A)$ in terms of orthogonal polynomials (blue dashed curve) and in a power series expansion (black continuous curve) for $\gamma_e = 1$, (b) Curves are analogous to those in (a) for $\gamma_e = 0.5$, (c) Norm of approximation error furnished by expansion in terms of orthogonal polynomials (blue dashed curve) and by power series expansion as a function of the degree of the approximating polynomial for $\gamma_e = 1$, (d) The curves are analogous to those in (c) for $\gamma_e = 0.5$. $\|A\|_F = 62.42$

(3.4). The number of large terms in the expansion increases with γ_e. The parameter $\gamma_e > 0$ can be chosen so that a given graph has a desired δ-effective diameter.

5.2 Expanding $(I - \gamma_r A)^{-1}$ for a neural network

The neural network of the worm *Caenorhabditis elegans* has 306 individual neurons (vertices) and 2345 edges. The edges are directed and most of them are unweighted: 14 edges have weight 2 and the remaining edges have weight 1; see [2, 4, 22]. Thus, the adjacency matrix associated with this graph is nonsymmetric. This example illustrates the role of the parameter γ_r in expansions of the resolvent. If longer walks are important, then we should choose a larger value of

γ_e	$\lvert c_k\rvert / \max_{0\le j\le k} \lvert c_j\rvert$
1.0	7.7e-01
0.9	7.0e-01
0.8	6.0e-01
0.7	5.0e-01
0.6	4.0e-01
0.5	2.6e-01
0.4	1.1e-01
0.3	3.4e-02
0.2	6.5e-03
0.1	4.0e-04

(a) $k = 5$

γ_e	$\lvert c_k\rvert / \max_{0\le j\le k} \lvert c_j\rvert$
1.0	1.9e-02
0.9	1.2e-02
0.8	6.2e-03
0.7	2.9e-03
0.6	1.2e-03
0.5	3.3e-04
0.4	5.1e-05
0.3	3.4e-06
0.2	1.0e-07
0.1	1.9e-10

(b) $k = 10$

Table 1: Yeast: The ratio of the orthogonal expansion coefficient $|c_k|$ and the largest of the $k + 1$ first coefficients for $k = 5$ and $k = 10$ for several values of γ_e.

	Arnoldi	Nonsymmetric Lanczos
γ_r	$\lvert c_5\rvert / \max_{0\le j\le 5} \lvert c_j\rvert$	$\lvert c_5\rvert / \max_{0\le j\le 5} \lvert c_j\rvert$
0.10	4.3e-01	9.3e-02
0.09	1.6e-01	2.7e-02
0.08	6.4e-02	1.0e-02
0.07	2.7e-02	4.1e-03
0.06	1.1e-02	1.6e-03
0.05	4.3e-03	6.2e-04
0.04	1.5e-03	2.0e-04
0.03	3.9e-04	5.3e-05
0.02	6.6e-05	8.9e-06
0.01	3.6e-06	4.8e-07

Table 2: Celegans: The ratio of the orthogonal expansion coefficient $|c_5|$ and the largest of the 6 first coefficients for several values of γ_e.

γ_r. For example, if walks of length 5 and shorter are important, then we should choose γ_r large enough to make the coefficients $c_0, c_1, \ldots, c_5$ in the expansion in terms of orthogonal polynomials

$$(I - \gamma_r A)^{-1} \approx \sum_{j=0}^{m-1} c_j p_j(A) \tag{5.2}$$

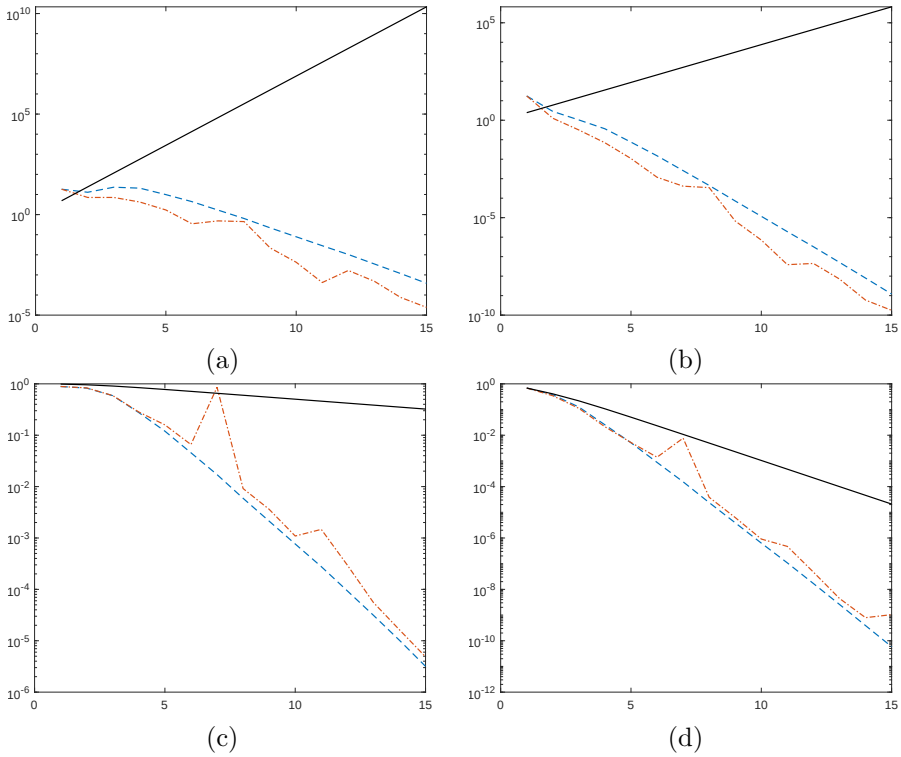


Figure 2: Celegans: (a) The magnitude of the coefficients in expansions of $(I-\gamma_r A)^{-1}$ in terms of orthogonal and bi-orthogonal polynomials determined by the global Arnoldi method (blue dashed curve) and the global nonsymmetric Lanczos method (orange dash-dotted curve), as well as in a power series expansion (black continuous curve) for $\gamma_r = 0.1$, (b) The curves are analogous to those in (a) for $\gamma_r = 0.05$, (c) Norm of approximation error furnished by expansions in terms of orthogonal and bi-orthogonal polynomials determined by the global Arnoldi method (blue dashed curve) and the global nonsymmetric Lanczos method (orange dash-dotted curve), respectively, and by power series expansion as functions of the degree of the approximating polynomial for $\gamma_r = 0.1$, (d) The curves are analogous to those in (c) for $\gamma_r = 0.05$. $\|A\|_F = 48.86$

significant. We require $0 < \gamma_r < 1/\rho(A)$; see the discussion following (1.2). For the present network, $\rho(A) = 9.15$. As γ_r decreases, the coefficients in the expansion (5.2) decrease faster in magnitude with increasing index j.

Figure 2 compares the coefficients in the expansion (5.2) with the coefficients in the power series expansion

$$(I-\gamma_r A)^{-1} = I + \gamma_r \|A\|_F \frac{A}{\|A\|_F} + \gamma_r^2 \|A\|_F^2 \frac{A^2}{\|A\|_F^2} + \gamma_r^3 \|A\|_F^3 \frac{A^3}{\|A\|_F^3} + \cdots . \quad (5.3)$$

	Arnoldi	Nonsymmetric Lanczos
γ_r	$\lvert c_{10}\rvert / \max_{0\le j\le 10} \lvert c_j\rvert$	$\lvert c_{10}\rvert / \max_{0\le j\le 10} \lvert c_j\rvert$
0.10	3.4e-03	2.3e-04
0.09	6.9e-04	3.8e-05
0.08	1.3e-04	7.7e-06
0.07	2.6e-05	1.5e-06
0.06	4.6e-06	2.8e-07
0.05	6.7e-07	4.0e-08
0.04	7.0e-08	4.2e-09
0.03	4.1e-09	2.6e-10
0.02	8.9e-11	5.3e-12
0.01	1.4e-13	9.7e-14

Table 3: Celegans: The ratio of the orthogonal expansion coefficient $|c_{10}|$ and the largest of the 11 first coefficients for several values of γ_e.

This expansion is analogous to the expansion (5.1). Clearly, the coefficients $\gamma_r^j \|A\|_F^j$ converge to zero faster as j increases, the smaller $\gamma_r > 0$ is.

Table 2 shows for the global Arnoldi and global Lanczos methods, the ratio of the magnitude of the coefficient c_5 in the expansions (5.2) and $\max_{0\le j\le 5} |c_j|$ as a function of γ_r. The ratio is seen to decrease quite rapidly when γ_r decreases. Table 3 is analogous to Table 2 for the 10th coefficients. Based on the tables and Figure 2, we may approximate $(I-\gamma_r A)^{-1}$ with fairly few terms in the expansion (5.2). The number of terms depends on the size of γ_r. We remark that since the matrix A in this example is fairly small, the evaluation of $(I - \gamma_r A)^{-1}$ can easily be carried out with the MATLAB function `inv`.

5.3 Expanding $\exp(\gamma_e A)v$ for an air traffic network

Air500 is a directed network with 500 nodes and 24009 edges [22, 33]. This example illustrates the convergence of the expansions on the left-hand side of (2.16) and of

$$\exp(\gamma_e A)v = v + \gamma_e \|A\|_F \frac{A}{\|A\|_F} v + \frac{\gamma_e^2 \|A\|_F^2}{2!} \frac{A^2}{\|A\|_F^2} v + \cdots \ .$$

We let $v = [1, 1, \ldots, 1]^T$, but other choices of v also are possible. Figure 3(a) compares for $\gamma_e = 1$ the magnitude of the coefficients in the left-hand side expansion (2.16) of the exponential function $\exp(\gamma_e A)$ in terms of orthogonal and bi-orthogonal polynomials in A determined by the standard Arnoldi method (blue dashed curve) and the standard nonsymmetric Lanczos method (orange dash-dotted curve), respectively. The magnitude of the coefficients $\gamma_e^k \|A\|_F^k/(k!)$, for $k = 0, 1, 2, \ldots$, in the power series expansion also is shown (black continuous

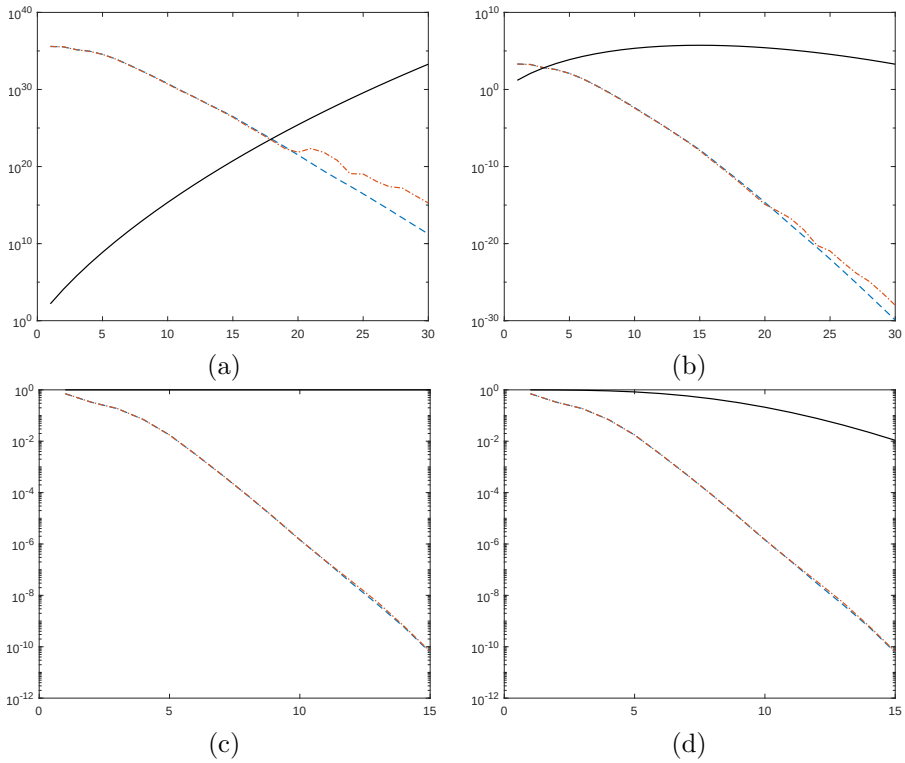


Figure 3: Air500: (a) The magnitude of the coefficients in expansions of $\exp(\gamma_e A)$ in terms of orthogonal polynomials determined by the standard Arnoldi method (blue dashed curve), the standard nonsymmetric Lanczos method (orange dash-dotted curve), and in a power series expansion (black continuous curve) for $\gamma_e = 1$, (b) The curves are analogous to those in (a) for $\gamma_e = 0.1$, (c) Norms of the approximation errors in expansions in terms of orthogonal polynomials determined by the standard Arnoldi method (blue dashed curve) and the standard nonsymmetric Lanczos method (orange dash-dotted curve), respectively, as well as by the power series expansion as functions of the degree of the approximating polynomial for $\gamma_e = 1$, (d) The curves are analogous to those in (c) for $\gamma_e = 0.1$. $\|A\|_F = 154.95$

curve). The coefficients in the expansions of orthogonal and bi-orthogonal polynomials converge to zero much faster than the coefficients in the power series expansion. Figure 3(b) is analogous to Figure 3(a) for $\gamma_e = 0.1$. The coefficients in Figure 3(b) converge to zero faster than the corresponding coefficients in Figure 3(a).

Figure 3(c) displays for $\gamma_e = 1$ the relative error when approximating the matrix function $\exp(\gamma_e A)v$ by orthogonal and bi-orthogonal polynomial expan-

	Arnoldi	Nonsymmetric Lanczos
k	$\lvert c_k\rvert / \max_{0\le j\le k} \lvert c_j\rvert$	$\lvert c_k\rvert / \max_{0\le j\le k} \lvert c_j\rvert$
1	1.0	1.0
2	8.8e-01	8.7e-01
3	3.8e-01	3.7e-01
4	2.4e-01	2.3e-01
5	9.5e-02	9.3e-02
6	2.4e-02	2.3e-02
7	4.3e-03	4.0e-03
8	7.0e-04	6.4e-04
9	1.1e-04	9.7e-05
10	1.5e-05	1.2e-05

Table 4: Air500: The ratio of the orthogonal expansion coefficients $|c_k|$ and $\max_{0\le j\le k} |c_j|$ for several values of k and $\gamma_e = 1$.

	Arnoldi	Nonsymmetric Lanczos
k	$\lvert c_k\rvert / \max_{0\le j\le k} \lvert c_j\rvert$	$\lvert c_k\rvert / \max_{0\le j\le k} \lvert c_j\rvert$
1	1.0	1.0
2	8.7e-01	8.6e-01
3	3.4e-01	3.3e-01
4	1.9e-01	1.8e-01
5	6.1e-02	6.0e-02
6	1.3e-02	1.3e-02
7	1.8e-03	1.7e-03
8	2.2e-04	2.0e-04
9	2.4e-05	2.1e-05
10	2.3e-06	1.9e-06

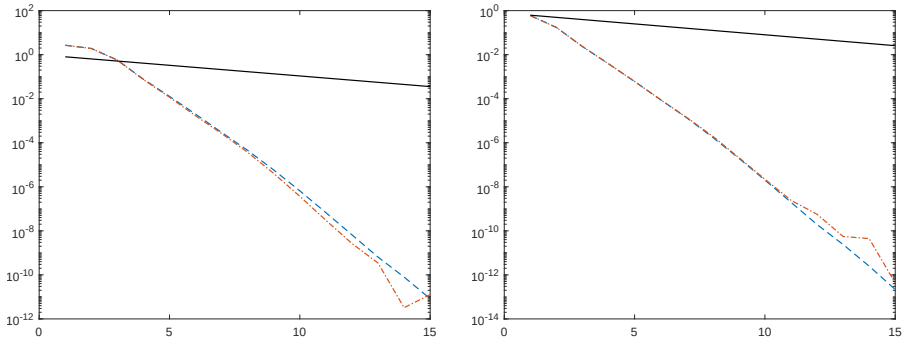
Table 5: Air500: The ratio of the orthogonal expansion coefficients $|c_k|$ and $\max_{0\le j\le k} |c_j|$ for several values of k and $\gamma_e = 0.1$.

sions determined by the standard Arnoldi method (blue dashed curve) and the standard nonsymmetric Lanczos method (orange dash-dotted curve), respectively. The relative error of the power series expansion also is displayed (black continuous curve). The errors in the orthogonal and bi-orthogonal polynomial expansions are seen to converge to zero much faster than the error in the power series expansion. Figure 3(d) is analogous to Figure 3 for $\gamma_e = 0.1$.

Table 4 displays the ratio of the kth to largest coefficients in magnitude for

$k = 1, 2, \ldots, 10$ and $\gamma_e = 1$. The ratio is seen to decrease rapidly as k increases. Table 5 is analogous for $\gamma_e = 0.1$. Since k represents the maximum length of walks in the network, we can determine the length of the longest significant walks, and based on that, we can decide how many terms are needed in our orthogonal and bi-orthogonal polynomial expansions to approximate $\exp(\gamma_e A v)$ sufficiently accurately for some $\gamma_e > 0$. Conversely, we may adjust γ_e to obtain a network with significant walks of desired lengths.

5.4 Expanding $(I - \gamma_r A)^{-1} v$ (Airlines)



(a) (b)

Figure 4: Airlines: (a) The magnitude of the coefficients in expansions of $(I - \gamma_r A)^{-1}$ in terms of orthogonal and bi-orthogonal polynomials determined by the global Arnoldi method (blue dashed curve) and the global nonsymmetric Lanczos method (orange dash-dotted curve), respectively, as well as in a power series expansion (black continuous curve) for $\gamma_r = 0.03$, (b) Norms of approximation errors in expansions in terms of orthogonal polynomials determined by the global Arnoldi method (blue dashed curve) and the global nonsymmetric Lanczos method (orange dash-dotted curve), respectively, and by the power series expansion as a function of the degree of the approximating polynomial for $\gamma_r = 0.03$. $\|A\|_F = 45.84$

The network Airlines represents air traffic. It has 235 airports (vertices) and 2101 directed flights (edges) between them; see [22, 33]. This example illustrates the relationship between the parameter γ_r in the expansions of the resolvent and the length of the longest significant walks. As γ_r gets larger, the importance of longer walks increases. We require $|\gamma_r| < 1/\rho(A)$ to make sure that the resolvent exists. In this example, $\rho(A) = 26.54$. Therefore, we should choose $0 < \gamma_r < 0.0377$

Figure 4 compares the coefficients in the expansion in the right-hand side of

	Arnoldi	Nonsymmetric Lanczos
k	$\lvert c_k\rvert / \max_{0\le j\le k}\lvert c_j\rvert$	$\lvert c_k\rvert / \max_{0\le j\le k}\lvert c_j\rvert$
1	1.0	1.0
2	1.8e-01	1.8e-01
3	1.9e-02	1.8e-02
4	8.4e-04	8.0e-04
5	4.5e-05	4.1e-05
6	2.2e-06	1.9e-06
7	1.1e-07	9.7e-08
8	5.3e-09	4.2e-09
9	2.2e-10	1.5e-10
10	8.2e-12	4.6e-12

Table 6: Airlines: The ratio of the orthogonal expansion coefficients $|c_k|$ and $\max_{0\le j\le k}|c_j|$ for several values of k and $\gamma_e = 0.03$.

(2.16) with the coefficients in the power series expansion

$$(I-\gamma_r A)^{-1}v = v + \gamma_r\|A\|_F\frac{A}{\|A\|_F}v + \gamma_r^2\|A\|_F^2\frac{A^2}{\|A\|_F^2}v + \gamma_r^3\|A\|_F^3\frac{A^3}{\|A\|_F^3}v + \cdots .$$

Figure 4(a) shows the magnitude of the coefficients in the expansions (2.16) for $\gamma_r = 0.03$. The coefficients are determined by the standard Arnoldi method (blue dashed curve) and the standard nonsymmetric Lanczos method (orange dash-dotted curve). We also display the coefficients $\gamma_r^k\|A\|_F^k$ for $k = 0, 1, 2, \ldots$ (black continuous curve). The coefficients in the expansions in terms of orthogonal and bi-orthogonal polynomials are seen to converge to zero faster than the coefficients in the power series expansion. Figure 4(b) depicts the relative error when approximating the resolvent by orthogonal and bi-orthogonal polynomials determined by the standard Arnoldi method (blue dashed curve) and the standard nonsymmetric Lanczos method (orange dash-dotted curve), respectively. Also the relative error when approximating the resolvent by a finite power series is shown (black continuous curve).

Table 6 illustrates the decrease in magnitude of the coefficients in the expansions considered for $\gamma_r = 0.03$. The magnitude is seen to decrease rapidly as k increases. Figure 4 and the table suggest that we can approximate the resolvent $(I-\gamma_r A)^{-1}$ with fairly few terms in the right-hand side expansion (2.16). The number of terms depends on the size of γ_r.

6 Conclusion

This paper illustrates the fast convergence to zero of the magnitude of the coefficients of expansions of matrix functions in terms of orthogonal and bi-orthogonal polynomials; the convergence is much faster than the convergence to zero of the coefficients of the power series that defines the function. The fast convergence has important implications for the understanding of the structure of the network. Fast decay indicates that a polynomial expansion of low degree suffices to approximate the desired matrix function of the adjacency matrix, suggesting that the important interactions in the network are only those of fairly short length. This insight can be used in at least two ways.

First, if we know *a priori* the value of γ_e in (1.1) or γ_r in (1.2) (through previous theoretical or empirical work), the orthogonal and bi-orthogonal polynomial expansions described in this article can be used to determine the δ-effective diameter of the network, at the scale implied by γ_e, for a suitably small $\delta > 0$, and conclude that multi-step connections of length greater than the δ-effective diameter are essentially irrelevant for the global structure of the network.

Second, and perhaps more interestingly, the effective diameter of the network might be known through previous theoretical or empirical work (for example, a modeler might put an upper limit on the number of connections in each itinerary for the air traffic network example). In this case, one can use the orthogonal and bi-orthogonal polynomial expansions in this paper to find the value of γ_e and γ_r that yields that effective diameter. This provides an objective criterion for the choices of γ_e and γ_r, an issue that is often overlooked in the discussion of matrix function methods for network analysis.

In any case, the observation that most important interactions in many networks have fairly short length makes it possible to approximate functions of the adjacency matrix, such as the exponential and the resolvent, accurately by polynomials of fairly low degree.

Acknowledgments

The authors would like the referees for comments that improved the presentation. They also would like to thank Giuseppe Rodriguez for providing the adjacency matrix of Subsection 5.1. This work was supported in part by NSF grants DMS-1720259 and DMS-1729509.

References

[1] M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions, Dover, New York, 1970.

[2] L. A. N. Amaral, A. Scala, M. Barthelemy, and H. E. Stanley. Classes of small-world networks, PNAS, 97 (2000), pp. 11149–11152.

[3] M. Aprahamian, D. J. Higham, and N. J. Higham, Matching exponential-based and resolvent-based centrality measures, J. Complex Networks, 4 (2016), pp 157–176.

[4] Alex Arena's data sets, http://deim.urv.cat/∼aarenas/data/welcome.htm

[5] V. Batagelj and A. Mrvar, Pajek data sets (2006). Available at http://vlado.fmf.uni-lj.si/pub/networks/data/

[6] B. Beckermann and L. Reichel, Error estimates and evaluation of matrix functions via the Faber transform, SIAM J. Numer. Anal., 47 (2009), pp. 3849–3883.

[7] M. Bellalij, L. Reichel, G. Rodriguez, and H. Sadok, Bounding matrix functionals via partial global block Lanczos decomposition, Appl. Numer. Math., 94 (2015), pp. 127–139.

[8] A. H. Bentbib, M. El Ghomari, C. Jagels, K. Jbilou, and L. Reichel, The extended global Lanczos method for matrix function approximation, Electron. Trans. Numer. Anal., 50 (2018), pp. 144–163.

[9] M. Benzi, E. Estrada, and C. Klymko, Ranking hubs and authorities using matrix functions, Linear Algebra Appl., 438 (2013), pp. 2447–2474.

[10] M. Benzi and C. Klymko, Total communicability as a centrality measure, J. Complex Networks, 1 (2013), pp. 124–149.

[11] M. Benzi and C. Klymko, On the limiting behavior of parameter-dependent network centrality measures, SIAM J. Matrix Anal. Appl., 36 (2015), pp. 686–706.

[12] S. Cipolla, M. Redivo-Zaglia, and F. Tudisco, Shifted and extrapolated power methods for tensor ℓ^p-eigenpairs, Electron. Trans. Numer. Anal., 53 (2020), pp. 1–27.

[13] A. Concas, C. Fenu, and G. Rodriguez, PQser: A Matlab package for spectral seriation, Numer. Algorithms, 80 (2019), pp. 879–902.

[14] J. J. Crofts, E. Estrada, D. J. Higham, and A. Taylor, Mapping directed networks, Electron. Trans. Numer. Anal., 37 (2010), pp. 337–350.

[15] O. De la Cruz Cabrera, M. Matar, and L. Reichel, Analysis of directed networks via the matrix exponential, J. Comput. Appl. Math., 355 (2019), pp. 182–192.

[16] O. De la Cruz Cabrera, M. Matar, and L. Reichel, Edge importance in a network via line graphs and the matrix exponential, Numer. Algorithms, 83 (2020), pp. 807–832.

[17] P. Domschke, A. Dua, J. J. Stolwijk, J. Lang, and V. Mehrmann, Adaptive refinement strategies for the simulation of gas flow in networks using a model hierarchy, Electron. Trans. Numer. Anal., 48 (2018), pp. 97–113.

[18] N. Eshghi, L. Reichel, and M. M. Spalević, Enhanced matrix function approximation, Electron. Trans. Numer. Anal., 47 (2017), pp. 197–205.

[19] E. Estrada, The Structure of Complex Networks, Oxford University Press, Oxford, 2012.

[20] E. Estrada, N. Hatano, and M. Benzi, The physics of communicability in complex networks, Physics Reports, 514 (2012), pp. 89–119.

[21] E. Estrada and D. J. Higham, Network properties revealed through matrix functions, SIAM Rev., 52 (2010), pp. 696–714.

[22] C. Fenu, D. Martin, L. Reichel, and G. Rodriguez, Block Gauss and anti-Gauss quadrature with application to networks, SIAM J. Matrix Anal. Appl., 34 (2013), pp. 1655–1684.

[23] A. Frommer, K. Lund, and D. B. Szyld, Block Krylov subspace methods for functions of matrices, Electron. Trans. Numer. Anal., 47 (2017), pp. 100–126.

[24] D. Gaier, Lectures on Complex Approximation, Birkhäuser, Boston. 1987.

[25] G. H. Golub and C. F. Van Loan, Matrix Computations, 4th ed, Johns Hopkins Unviversity Press, Baltimore, 2013.

[26] N. J. Higham, Functions of Matrices: Theory and Computation, SIAM, Philadelphia, 2008.

[27] K. Jbilou, A. Messaoudi, and H. Sadok, Global FOM and GMRES algorithms for matrix equations, Appl. Numer. Math., 31 (1999), pp. 49–63.

[28] K. Jbilou, H. Sadok, and A. Tinzefte, Oblique projection methods for linear systems with multiple right-hand sides, Electron. Trans. Numer. Anal., 20 (2005), pp. 119–138.

[29] H. Jeong, S. Mason, A.-L. Barabási, and Z. N. Oltvai, Lethality and centrality in protein networks, Nature, 411 (2001), pp. 41–42.

[30] L. Katz, A new status index derived from sociometric data analysis, Psychometrika, 18 (1953), pp. 39–43.

[31] M. E. J. Newman, Networks: An Introduction, Oxford University Press, Oxford, 2010.

[32] S. Pozza, M. S. Pranić, and Z. Strakoš, The Lanczos algorithm and complex Gauss quadrature, Electron. Trans. Numer. Anal., 50 (2018), pp. 1–19.

[33] G. Rodriguez's software, http://bugs.unica.it/∼gppe/

[34] L. N. Trefethen, Approximation Theory and Approximation Practice, SIAM, Philadelphia, 2013.

[35] J. L. Walsh, Interpolation and Approximation by Rational Functions in the Complex Domain, 4th ed., Amer. Math. Soc., Providence, 1969.