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New block quadrature rules for the approximation of matrix functions

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ABSTRACT

Golub and Meurant have shown how to use the symmetric block Lanczos algorithm to compute block Gauss quadrature rules for the approximation of certain matrix functions. We describe new block quadrature rules that can be computed by the symmetric or nonsymmetric block Lanczos algorithms and yield higher accuracy than standard block Gauss rules after the same number of steps of the symmetric or nonsymmetric block Lanczos algorithms. The new rules are block generalizations of the generalized averaged Gauss rules introduced by Spalević. Applications to network analysis are presented.

1. Introduction

The aim of this paper is to describe new methods for the approximation of expressions of the form

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$$W^T f(A)W, \tag{1.1}$$

where $A \in \mathbb{R}^{m\times m}$ is a large symmetric matrix, $W \in \mathbb{R}^{m\times k}$ has a few orthonormal columns, i.e., $1 \leq k \ll m$, and f is a function such that $f(A)$ is well defined. The superscript ^{T} denotes transposition. We also consider expressions of the type

$$W^T f(A)V, \tag{1.2}$$

in which $A \in \mathbb{R}^{m\times m}$ is a large possibly nonsymmetric matrix and the matrices $W, V \in \mathbb{R}^{m\times k}$, with $1 \leq k \ll m$, are biorthogonal, i.e., $W^T V = I_k$. Throughout this paper I_k denotes the identity matrix of order k.

The matrix function $f(A)$ can be defined, e.g., by the spectral factorization of A, assuming that it exists; see, e.g., [22,24] for discussions on several possible definitions of matrix functions. In the present paper, we assume that the matrix A is so large that it is unfeasible or impractical to evaluate its spectral factorization.

For symmetric matrices A, Golub and Meurant [20,21] show how approximations of (1.1) can be conveniently computed by first carrying out $\ell \ll m/k$ steps with the symmetric block Lanczos algorithm applied to A with initial block vector W. This algorithm produces the decomposition

$$A[W_1, \dots, W_\ell] = [W_1, \dots, W_\ell]J_\ell + W_{\ell+1}\Gamma_\ell E_\ell^T, \tag{1.3}$$

where the block vectors $W_j \in \mathbb{R}^{m\times k}$ are orthonormal, i.e.,

$$W_i^T W_j = \begin{cases} I_k, & i = j, \\ O_k, & i \neq j, \end{cases}$$

with $W_1 = W$. Here and below O_k denotes the zero matrix of order k. Moreover, $E_\ell = [O_k, \dots, O_k, I_k]^T \in \mathbb{R}^{k\ell\times k}$ and the matrix

$$J_\ell = \begin{bmatrix} \Omega_1 & \Gamma_1^T & & & O \\ \Gamma_1 & \Omega_2 & \Gamma_2^T & & \\ & \ddots & \ddots & \ddots & \\ & & \Gamma_{\ell-2} & \Omega_{\ell-1} & \Gamma_{\ell-1}^T \\ O & & & \Gamma_{\ell-1} & \Omega_\ell \end{bmatrix} \in \mathbb{R}^{k\ell\times k\ell} \tag{1.4}$$

is block tridiagonal with symmetric diagonal blocks $\Omega_i \in \mathbb{R}^{k\times k}$. The subdiagonal blocks $\Gamma_i \in \mathbb{R}^{k\times k}$ may be chosen to be upper triangular, but this is not necessary. The remainder term in (1.3) contains the matrix Γ_ℓ, which is the last subdiagonal block in the symmetric block tridiagonal matrix $J_{\ell+1} \in \mathbb{R}^{k(\ell+1)\times k(\ell+1)}$ that would have been obtained if $\ell + 1$ steps with the symmetric block Lanczos algorithm were carried out. We assume that ℓ is chosen small enough so that the recursion relations of the symmetric block Lanczos method do not break down. Remedies for breakdown are commented on in Section 2.