ARTICLE IN PRESS

Computers and Mathematics with Applications ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa

Inverse subspace bi-iteration and bi-Newton methods for computing spectral projectors

Kirill V. Demyanko [a], Yuri M. Nechepurenko [b], Miloud Sadkane [c,*]

[a] Keldysh Institute of Applied Mathematics, Russian Academy of Sciences, Miusskaya sq. 4, Moscow, 125047, Russia

[b] Institute of Numerical Mathematics, Russian Academy of Sciences, ul. Gubkina 8, Moscow, 119333, Russia

[c] Université de Brest. CNRS - UMR 6205, Laboratoire de Mathématiques de Bretagne Atlantique, 6 avenue Victor Le Gorgeu, CS 93837, 29285 Brest Cedex 3, France

ARTICLE INFO

Article history:
Received 5 September 2014
Received in revised form 11 January 2015
Accepted 3 February 2015
Available online xxxx

Keywords:
Inverse subspace iteration
Newton method
Invariant subspace
Spectral projector

ABSTRACT

Efficient inverse subspace bi-iteration and bi-Newton methods for computing the spectral projector associated with a group of eigenvalues near a specified shift of a large sparse matrix is proposed and justified. Numerical experiments with a discrete analogue of a non-Hermitian elliptic operator are discussed to illustrate the theory.

© 2015 Elsevier Ltd. All rights reserved.

1. Introduction

This work is devoted to the computation of the spectral projector onto the invariant subspace associated with a group of eigenvalues of a large-scale sparse matrix $A \in \mathbb{C}^{n\times n}$. It is assumed that the target group is near a given complex value and is well separated from the rest of the spectrum. We can assume without loss of generality that A is nonsingular and the desired projector corresponds to the $p \ll n$ eigenvalues of smallest magnitude (taking multiplicities into account), since otherwise we may replace A with $A - \sigma I$, where σ is some shift and I denotes the identity matrix.

Let $\mathcal{X}_1$ and $\mathcal{X}_2$ be respectively the right and left invariant subspaces of A associated with the p eigenvalues of smallest magnitude, and let $X_1, X_2 \in \mathbb{C}^{n\times p}$ be matrices whose columns form biorthogonal bases of $\mathcal{X}_1$ and $\mathcal{X}_2$. That is, $\mathcal{X}_l = \mathrm{span}(X_l)$ and

$$X_2^* X_1 = I. \tag{1}$$

Then

$$AX_1 = X_1\Lambda, \qquad A^*X_2 = X_2\Lambda^*,$$

where $\Lambda = X_2^* A X_1 \in \mathbb{C}^{p\times p}$ is a matrix whose spectrum consists of the p target eigenvalues, and the corresponding spectral projector is given by

$$\mathcal{P} = X_1 X_2^*. \tag{2}$$

* Corresponding author.
E-mail addresses: kirill.demyanko@yandex.ru (K.V. Demyanko), yumn@inm.ras.ru (Y.M. Nechepurenko), sadkane@univ-brest.fr (M. Sadkane).

http://dx.doi.org/10.1016/j.camwa.2015.02.002
0898-1221/© 2015 Elsevier Ltd. All rights reserved.

Please cite this article in press as: K.V. Demyanko, et al., Inverse subspace bi-iteration and bi-Newton methods for computing spectral projectors, Computers and Mathematics with Applications (2015), http://dx.doi.org/10.1016/j.camwa.2015.02.002

Usually the projector is not formed explicitly but computed and used in the low-rank form (2) as two rectangular matrices. It may be useful, for example, in model order reduction, stability analysis and spectral dichotomy [1–3].

For brevity we will refer to the matrices X_1 and X_2, which satisfy (1), as biorthogonal. Biorthogonal bases for the subspaces $\mathcal{X}_1$ and $\mathcal{X}_2$ are not unique, but the projector (2) does not depend on the choice of the bases. However, for reasons of numerical stability it is preferable to choose X_1 and X_2 so that the condition

$$X_2^* X_2 = X_1^* X_1 \tag{3}$$

is satisfied, together with (1). This guarantees that

$$\|\mathcal{P}\|_2 = \|X_1\|_2^2 = \|X_2\|_2^2. \tag{4}$$

Matrices which satisfy (1) and (3) will be referred to as balanced biorthogonal.

To compute the matrices X_1 and X_2 we propose to use a combination of an inverse subspace bi-iteration and a bi-Newton method. The first one is described in Section 2. Starting with biorthogonal matrices $X_{1,0}, X_{2,0} \in \mathbb{C}^{n\times p}$, it constructs two sequences of matrices $X_{1,k}$ and $X_{2,k}$, $k = 1, 2, \ldots$, by solving inexactly, at each iteration k, systems with multiple right-hand sides of the form $AX_{1,k+1} = X_{1,k}$ and $A^*X_{2,k+1} = X_{2,k}$. These systems are solved by GMRES [4] with a right preconditioner tuned in a way similar to [5], see also [6,7]. A biorthogonalization of the computed matrices $X_{1,k+1}$ and $X_{2,k+1}$ is carried out afterwards.

After a few iterations of this method, the computed approximate invariant subspaces are used to start a bi-Newton iteration described in Section 3. This is an extension of the Newton iteration described in [8,9]. Results of numerical experiments with the proposed algorithms are discussed in Section 4.

Note that the right and left invariant subspaces of the matrix A, which are necessary for computing the spectral projector, can also be computed by applying to A and A^* methods such as Arnoldi or Jacobi–Davidson [10,2]. However, a block version with a deflation procedure is often needed. The proposed bi-Newton method has the advantage of being easy to implement, requires less storage space, and has an ultimately quadratic rate of convergence.

To describe the proposed algorithms we will use some auxiliary procedures. The first one performs a column orthonormalization of a full rank matrix $W \in \mathbb{C}^{n\times r}$ by means of QR-decomposition [11]: $W = QR$, where $Q \in \mathbb{C}^{n\times r}$ has orthonormal columns and $R \in \mathbb{C}^{r\times r}$ is upper triangular. A result of this procedure will be written as $(Q, R) = \mathrm{ort}(W)$ or $Q = \mathrm{ort}(W)$ if R is not needed.

The second procedure performs a column biorthogonalization of two full rank matrices $W_1, W_2 \in \mathbb{C}^{n\times r}$ using the singular value decomposition $W_2^*W_1 = UDV^*$ [11], where U and V are unitary and D is positive semidefinite diagonal of order r whose diagonal entries are ordered in a non-increasing order. From U, V and D, this procedure computes the biorthogonal matrices

$$V_1 = W_1 V D^{-1/2}, \qquad V_2 = W_2 U D^{-1/2}$$

if D is nonsingular, and otherwise states that the biorthogonalization is infeasible. A successful result of the procedure will be written as $(V_1, V_2) = \mathrm{biort}\,(W_1, W_2)$.

To obtain balanced biorthogonal matrices from W_1 and W_2, it is sufficient to perform the column-orthonormalization of each matrix before the column biorthogonalization:

$$(V_1, V_2) = \mathrm{biort}\,(\mathrm{ort}(W_1), \mathrm{ort}(W_2))\,.$$

The matrices V_1 and V_2 obtained this way satisfy the following properties:

$$\mathrm{span}(V_l) = \mathrm{span}(W_l), \qquad V_l^* V_l = D^{-1}, \qquad V_2^* V_1 = I.$$

In addition to the above two procedures we will use the Schur decomposition $B = QTQ^*$ of a given matrix $B \in \mathbb{C}^{n\times n}$, where $Q \in \mathbb{C}^{n\times n}$ is unitary and $T \in \mathbb{C}^{n\times n}$ is upper triangular. A result of this procedure will be written as $(Q, T) = \mathrm{schur}\,(B)$. The Schur decomposition is usually computed with the QR-algorithm [11]. The diagonal entries of T form the spectrum of B (accurate within rounding errors) and are arranged in an unpredictable order. To obtain the Schur decomposition with the diagonal entries of T arranged in a desired order, a reordering procedure is applied to Q and T. The reordering in a non-decreasing order of magnitude and in a non-increasing order of magnitude will be written respectively as

$$(Q, T) = \mathrm{reord}\,(Q, T, \preceq)\,, \qquad (Q, T) = \mathrm{reord}\,(Q, T, \succeq)\,.$$

Let X_1 and X_2 be biorthogonal matrices. Then $\mathcal{P} = X_1 X_2^*$ is a spectral projector, associated with a subset of eigenvalues of the matrix A, if and only if it commutes with A. This leads us to use the norm of the commutator

$$E = A\mathcal{P} - \mathcal{P}A \tag{5}$$

as a stopping criterion in the proposed algorithms. Another stopping criterion can be based on the residuals

$$R_1 = AX_1 - X_1\Lambda, \qquad R_2 = A^*X_2 - X_2\Lambda^*, \tag{6}$$

where $\Lambda = X_2^*AX_1$. The matrices E, R_1 and R_2 are related as follows:

$$E = R_1X_2^* - X_1R_2^*, \qquad R_1 = EX_1, \qquad R_2 = -E^*X_2. \tag{7}$$

Please cite this article in press as: K.V. Demyanko, et al., Inverse subspace bi-iteration and bi-Newton methods for computing spectral projectors, Computers and Mathematics with Applications (2015), http://dx.doi.org/10.1016/j.camwa.2015.02.002

Download English Version:

https://daneshyari.com/en/article/471589

Download Persian Version:

https://daneshyari.com/article/471589

Daneshyari.com