Linear Algebra and its Applications 522 (2017) 51–70

Contents lists available at ScienceDirect

Linear Algebra and its Applications

www.elsevier.com/locate/laa

On the correction equation of the Jacobi–Davidson method

Gang Wu [a,1], Hong-Kui Pang [b,*,2]

[a] *School of Mathematics, China University of Mining and Technology, Xuzhou, 221116, Jiangsu, PR China*
[b] *School of Mathematics and Statistics, Jiangsu Normal University, Xuzhou, 221116, Jiangsu, PR China*

A R T I C L E I N F O

Article history:
Received 9 February 2016
Accepted 3 February 2017
Submitted by V. Mehrmann

MSC:
65F15
65F10

Keywords:
Large eigenproblem
Jacobi–Davidson method
Jacobi–Davidson correction equation
Stagnation
Two-sided Jacobi–Davidson method

A B S T R A C T

The Jacobi–Davidson method is one of the most popular approaches for iteratively computing a few eigenvalues and their associated eigenvectors of a large matrix. The key of this method is to expand the search subspace via solving the Jacobi–Davidson correction equation, whose coefficient matrix is singular. It is believed by scholars that the Jacobi–Davidson correction equation is consistent and has a unique solution. In this paper, however, we point out that the correction equation either has a unique solution or has no solution, and we derive a computable necessary and sufficient condition for cheaply judging the existence and uniqueness of the solution. Furthermore, we consider the problem of stagnation and verify that if the Jacobi–Davidson method stagnates, then the corresponding Ritz value is a defective eigenvalue of the projection matrix. Finally, we provide a computable criterion for expanding the search subspace successfully. The properties

* Corresponding author.
E-mail addresses: gangwu76@126.com, gangwu@cumt.edu.cn (G. Wu), panghongkui@163.com (H.-K. Pang).

[1] This author is supported by the National Science Foundation of China under grant 11371176, and the Talent Introduction Program of China University of Mining and Technology.
[2] This author is supported by the National Science Foundation of China under grant 11201192, the Natural Science Foundation of Jiangsu Province under grant BK2012577, Jiangsu Key Laboratory of Education Big Data Science and Engineering, and a Project Funded by the Priority Academic Program Development of Jiangsu Higher Education Institutions.

http://dx.doi.org/10.1016/j.laa.2017.02.007
0024-3795/

of some alternative Jacobi–Davidson correction equations are also discussed.

1. Introduction

We are interested in computing a few eigenvalues and the corresponding eigenvectors of an n-by-n large matrix A. The Jacobi–Davidson method is one of the most popular approaches for this type of problem, see [1,4,7,10–16] and the references therein. In essence, this method can be understood as a Newton-based method [15]. The Jacobi–Davidson method relies on two principles [11,12]: Given a subspace $\mathcal{V}_k$ and let $V_k = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_k]$ be an orthonormal basis for $\mathcal{V}_k$ with $k \ll n$, the first principle is to apply a Ritz–Galerkin approach [15] on the large eigenproblem $A\mathbf{x} = \lambda\mathbf{x}$, i.e.,

$$AV_k\mathbf{y}_k - \widetilde{\lambda}_k V_k\mathbf{y}_k \perp \mathcal{V}_k,$$

which reduces to a k-by-k eigenproblem

$$V_k^{\mathrm{H}} AV_k\mathbf{y}_k = \widetilde{\lambda}_k\mathbf{y}_k,$$

with $V_k^{\mathrm{H}} AV_k$ being the projection matrix of A in $\mathcal{V}_k$. Then this method makes use of $(\widetilde{\lambda}_k, \mathbf{u}_k = V_k\mathbf{y}_k)$ as an approximate eigenpair, called Ritz pair of A in the subspace spanned by the columns of V_k.

The second principle is to modify the approximation from solving the Jacobi–Davidson correction equation for expanding $\mathcal{V}_k$. More precisely, for the approximate eigenvector $\mathbf{u}_k$, the Jacobi–Davidson method computes an *orthogonal* correction $\mathbf{v}_*$ for $\mathbf{u}_k$, such that

$$A(\mathbf{u}_k + \mathbf{v}_*) = \lambda(\mathbf{u}_k + \mathbf{v}_*).$$

As $\mathbf{v}_* \perp \mathbf{u}_k$, we focus on the subspace orthogonal to $\mathbf{u}_k$. Let $\mathbf{r}_k = (A - \widetilde{\lambda}_k I)\mathbf{u}_k$ be the residual, then $\mathbf{r}_k \perp \mathbf{u}_k$, and the orthogonal projection of A onto the subspace range$\{\mathbf{u_k}\}^\perp$ is $(I - \mathbf{u}_k\mathbf{u}_k^{\mathrm{H}})A(I - \mathbf{u}_k\mathbf{u}_k^{\mathrm{H}})$, where range$\{\mathbf{u_k}\}$ denotes the range or the subspace spanned by $\mathbf{u_k}$, range$\{\mathbf{u_k}\}^\perp$ represents the orthogonal complement of range$\{\mathbf{u_k}\}$, and $(\cdot)^{\mathrm{H}}$ stands for the conjugate transpose of a matrix or vector. It is easy to check that the vector $\mathbf{v}_*$ satisfies

$$(I - \mathbf{u}_k\mathbf{u}_k^{\mathrm{H}})(A - \lambda I)(I - \mathbf{u}_k\mathbf{u}_k^{\mathrm{H}})\mathbf{v}_* = -\mathbf{r}_k.$$

Since the eigenvalue λ is unknown, we replace it by $\widetilde{\lambda}_k$, which yields the famous *Jacobi–Davidson correction equation* [11,12]

$$(I - \mathbf{u}_k\mathbf{u}_k^{\mathrm{H}})(A - \widetilde{\lambda}_k I)(I - \mathbf{u}_k\mathbf{u}_k^{\mathrm{H}})\mathbf{v} = -\mathbf{r}_k. \tag{1.1}$$