# EFFICIENTLY PRECONDITIONED INEXACT NEWTON METHODS FOR LARGE SYMMETRIC EIGENVALUE PROBLEMS 

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#### Abstract

In this paper we propose an efficiently preconditioned Newton method for the computation of the leftmost eigenpairs of large and sparse symmetric positive definite matrices. A sequence of preconditioners based on the BFGS update formula is proposed, for the Preconditioned Conjugate Gradient solution of the linearized Newton system to solve $A \boldsymbol{u}=q(\boldsymbol{u}) \boldsymbol{u}, q(\boldsymbol{u})$ being the Rayleigh Quotient. We give theoretical evidence that the sequence of preconditioned Jacobians remains close to the identity matrix if the initial preconditioned Jacobian is so. Numerical results onto matrices arising from various realistic problems with size up to one million unknowns account for the efficiency of the proposed algorithm which reveals competitive with the Jacobi-Davidson method on all the test problems.


Key words. Eigenvalues, SPD matrix, Newton method, BFGS update, Incomplete Cholesky preconditioner

AMS subject classifications. 65F05, 65F15, 65H17

1. Introduction. Consider a symmetric positive definite (SPD) matrix $A$, which is also assumed to be large and sparse. We will denote as

$$
\lambda_{1}<\lambda_{2}<\ldots<\lambda_{p}<\ldots<\lambda_{n}
$$

the eigenvalues of $A$ and

$$
\boldsymbol{v}_{1}, \boldsymbol{v}_{2}, \ldots, \boldsymbol{v}_{p}, \ldots, \boldsymbol{v}_{n}
$$

the corresponding (normalized) eigenvectors.
The computation of the $p \ll n$ leftmost eigenpairs of $A$ is a common task in many scientific applications. Typical examples are offered by the vibrational analysis of mechanical structures [2], the lightwave technology [39], electronic structure calculations [32], and the spectral superposition approach for the solution of large sets of 1 st order linear differential equations [24]. Computation of a few eigenpairs is also crucial in the approximation of the generalized inverse of the graph Laplacian $[16,5]$.

In this paper we propose to use an efficiently preconditioned Newton method for the nonlinear system of equations:

$$
\begin{equation*}
A \boldsymbol{u}-q(\boldsymbol{u}) \boldsymbol{u}=0 \quad \text { where } \quad q(\boldsymbol{u})=\frac{\boldsymbol{u}^{\top} A \boldsymbol{u}}{\boldsymbol{u}^{\top} \boldsymbol{u}} \tag{1.1}
\end{equation*}
$$

is the Rayleigh Quotient. The idea of employing the Newton method for this nonlinear system is obviously not new: among the others we mention Davidson ([18]) who approximated the Jacobian of (1.1) with $\operatorname{diag}(A-q(\boldsymbol{u}) I)$ and combined this system solution with a Rayleigh-Ritz procedure.

The Newton method in the unit sphere [33, 22] or Newton-Grassman method, constructs a sequence of vectors $\left\{\boldsymbol{u}_{k}\right\}$ by solving the linear systems

$$
\begin{equation*}
\left(I-\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}\right)\left(A-\theta_{k} I\right)\left(I-\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}\right) \boldsymbol{s}=-\left(A \boldsymbol{u}_{k}-\theta_{k} \boldsymbol{u}_{k}\right), \quad \theta_{k}=\frac{\boldsymbol{u}_{k}^{\top} A \boldsymbol{u}_{k}}{\boldsymbol{u}_{k}^{\top} \boldsymbol{u}_{k}} \tag{1.2}
\end{equation*}
$$

[^0]ensuring that the correction $\boldsymbol{s}$ be orthogonal to $\boldsymbol{u}_{k}$. Then the next approximation is set as $\boldsymbol{u}_{k+1}=\boldsymbol{t}\|\boldsymbol{t}\|^{-1}$ where $\boldsymbol{t}=\boldsymbol{u}_{k}+\boldsymbol{s}$. Linear system (1.2) is shown to be better conditioned than the one with $A-\theta_{k} I$. The same linear system represents the correction equation in the well-known Jacobi-Davidson method [34], which in its turn can be viewed as an accelerated Inexact Newton method [19]. When $A$ is SPD and the leftmost eigenpairs are being sought, it has been proved in [29] that the Preconditioned Conjugate Gradient (PCG) method can be employed in the solution of the correction equation.

There are still a number of drawbacks that advises against using pure Newton method: first, the choice of an initial vector. In the Jacobi-Davidson algorithm the Rayleigh-Ritz procedure implements a sort of restart that in part solves this problem. Second, even the projected Jacobian $\left(I-\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}\right)\left(A-\theta_{k} I\right)\left(I-\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}\right)$ in the correction equation is ill-conditioned, or at least more illconditioned than the original matrix $A$, being its smallest eigenvalue smaller than $\lambda_{j+1}-\lambda_{j}$ when seeking the $j$-th eigenpair (see Lemma 3.1). In [37] the problem of finding a "well-conditioned" Jacobian matrix for the Newton method is considered by the authors, who describe some low-rank variants of the Jacobian of (1.1) and perform a large set of numerical experiments showing that the best choice is problem dependent. Many authors have also tried to find a good preconditioner for matrix $A-\theta_{k} I$ since it is the key for efficient iterative solution of the correction equation. This remains an open problem (see for example [26]).

Starting from the findings in [8] and [6], the main contribution of this paper is the development of a sequence of preconditioners $\left\{P_{k}\right\}$ for the PCG solution of the Newton correction equation (1.2), based on the BFGS update of a given initial preconditioner for the coefficient matrix $A$. We will theoretically prove that the sequence of the preconditioned Jacobians will remain close to the identity matrix if the first preconditioned Jacobian is so. A similar approach has been used in [38] where a rank-two modification of a given preconditioner is used to accelerated MINRES in the framework of the Inexact Rayleigh Quotient Iteration.

The BFGS formula as used in this paper is one more example of the strict connection between two overlapping worlds: numerical linear algebra and optimization. Many papers have discussed this relationship. Among the others we refer to [17] and the references therein. Also the problem of finding efficient preconditioners for the linearized systems has become a crucial issue for the efficient implementation of the interior point method in constrained optimization, see e.g. [1, 36, 11, 10]. Often, the coefficient matrices of the linear systems to be solved at each Newton iteration are very close in structure and this motivates a number of works which study the possibility of updating a given preconditioner to obtain with small computational effort a new preconditioner [3, 4].

To overcome the problem of the starting point, we also propose to start the Newton process after a small number of iterations of a Conjugate Gradient procedure for the minimization of the Rayleigh Quotient (DACG, [9]) to yield a good initial vector.

The combined DACG-Newton algorithm is used in the approximation of $p \in[10,20]$ eigenpairs of a number of matrices arising from various realistic applications of size up to $10^{6}$ and number of nonzeros up to $4 \times 10^{7}$. Numerical results show that, in the solution of the correction equation, the PCG method preconditioned by BFGS displays much faster convergence than the same method when the preconditioner is kept fixed during the Newton process, in every test case. Moreover, the proposed approach is shown to be competitive with the Jacobi-Davidson method.

The remaining of the paper proceeds as follows: in Section 2 we introduce the preconditioner; Section 3 is devoted to the proof of the main theorem which states the closeness of the preconditioned matrix to the identity matrix. In Section 4 we describe implementation details while Section 5 reports some numerical results of the proposed method for the eigensolution of the test matrices. Section 6 reports comparisons against the Jacobi-Davidson method and Section 7 draws the conclusions.
2. BFGS update of an initial preconditioner. Following the idea described in [6], we propose a sequence of preconditioners for the Newton systems using the BFGS rank-two update.

To precondition the initial Newton system $J_{0} s_{0}=-\boldsymbol{r}$, where

$$
J_{0}=\left(I-\boldsymbol{u}_{0} \boldsymbol{u}_{0}^{\top}\right)\left(A-\theta_{0} I\right)\left(I-\boldsymbol{u}_{0} \boldsymbol{u}_{0}^{\top}\right), \quad \boldsymbol{r}=-\left(A \boldsymbol{u}_{0}-\theta_{0} \boldsymbol{u}_{0}\right), \quad \theta_{0}=\boldsymbol{u}_{0}^{\top} A \boldsymbol{u}_{0}
$$

we chose to use a projected incomplete Cholesky preconditioner with partial fill-in [30]: $P_{0}=\left(I-\boldsymbol{u}_{0} \boldsymbol{u}_{0}^{\top}\right) \widehat{P}_{0}\left(I-\boldsymbol{u}_{0} \boldsymbol{u}_{0}^{\top}\right) \quad$ with $\quad \widehat{P}_{0}=\left(L L^{\top}\right)^{-1}$ being $L=I C\left(\right.$ LFIL, $\left.\tau_{I C}, A\right)$ an incomplete triangular Cholesky factor of $A$, with parameters lfil, maximum fill-in of a row in $L$, and $\tau_{I C}$ the threshold for dropping small elements in the factorization. Then a sequence of projected preconditioners for the subsequent linear systems $J_{k} s_{k}=-\boldsymbol{r}_{k}$ may be defined by using the BFGS formula as:

$$
\begin{align*}
& P_{k+1}=\left(I-\boldsymbol{u}_{k+1} \boldsymbol{u}_{k+1}^{\top}\right) \widehat{P}_{k+1}\left(I-\boldsymbol{u}_{k+1} \boldsymbol{u}_{k+1}^{\top}\right), \quad \text { where } \\
& \widehat{P}_{k+1}=\frac{\boldsymbol{s} \boldsymbol{s}^{\top}}{\boldsymbol{s}^{\top} \boldsymbol{y}}+\left(I-\frac{\boldsymbol{s} \boldsymbol{y}^{\top}}{\boldsymbol{s}^{\top} \boldsymbol{y}}\right) \widehat{P}_{k}\left(I-\frac{\boldsymbol{y} \boldsymbol{s}^{\top}}{\boldsymbol{s}^{\top} \boldsymbol{y}}\right) \tag{2.1}
\end{align*}
$$

and $\boldsymbol{s} \equiv \boldsymbol{s}_{k}$ is the solution of the $k$-th Newton system whereas $\boldsymbol{y} \equiv \boldsymbol{y}_{k}=\boldsymbol{r}_{k+1}-\boldsymbol{r}_{k}$.
We propose here a simplification of the preconditioner update formula based on the wellknown cubic convergence of the Newton method which implies that $\left\|e_{k+1}\right\| \ll\left\|e_{k}\right\|$, in a suitable neighborhood of the solution (i.e. for a suitable $\delta$ s.t. $\left\|e_{k}\right\|<\delta$ ). As a consequence also the residual norm satisfies $\left\|\boldsymbol{r}_{k+1}\right\| \ll\left\|\boldsymbol{r}_{k}\right\|$. We can then approximate $\boldsymbol{y}_{k}$ with $-\boldsymbol{r}_{k}$ and write the preconditioner at level $k+1$ as (with $\boldsymbol{r} \equiv \boldsymbol{r}_{k}$ ):

$$
\begin{equation*}
\widehat{P}_{k+1}=-\frac{s^{\top}}{\boldsymbol{s}^{\top} \boldsymbol{r}}+\left(I-\frac{\boldsymbol{s} \boldsymbol{r}^{\top}}{\boldsymbol{s}^{\top} \boldsymbol{r}}\right) \widehat{P}_{k}\left(I-\frac{\boldsymbol{r} \boldsymbol{s}^{\top}}{\boldsymbol{s}^{\top} \boldsymbol{r}}\right) \tag{2.2}
\end{equation*}
$$

Theorem 3.2 of next Section will prove that the preconditioner defined in (2.2) is SPD if $\widehat{P}_{k}$ is so.

## 3. Theoretical analysis of the preconditioner.

3.1. Finding the smallest eigenpair. The idea of the BFGS preconditioner is taken from the general analysis in $[6,7]$ where a sequence of preconditioners is devised in order to precondition the sequence of Newton systems for a general nonlinear problem. One of the "Standard Assumptions" made in these papers was the nonsingularity of the Jacobian in the solution of the nonlinear system. Here the situation is different, the Jacobian in the correction equation $J(\boldsymbol{u})=\left(I-\boldsymbol{u} \boldsymbol{u}^{\top}\right)(A-q(\boldsymbol{u}) I)\left(I-\boldsymbol{u} \boldsymbol{u}^{\top}\right)$ is singular whatever $\boldsymbol{u}$, in particular it is singular when $\boldsymbol{u}$ is equal to the exact eigenvector. The theoretical analysis of the goodness of the preconditioner will be therefore completely different, though obtaining similar results, than that proposed in $[6,7]$.

We start by recalling some known results about convergence of the Newton method for eigenproblems. At every step of our Newton method we approximately solve

$$
\left(I-\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}\right)\left(A-\theta_{k} I\right)\left(I-\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}\right) \boldsymbol{s}=-\left(A \boldsymbol{u}_{k}-\theta_{k} \boldsymbol{u}_{k}\right)
$$

where $\theta_{k}=\boldsymbol{u}_{k}^{\top} A \boldsymbol{u}_{k}$, in the space orthogonal to $\boldsymbol{u}_{k}$. Then we set

$$
\begin{equation*}
\boldsymbol{u}_{k+1}=\frac{\boldsymbol{u}_{k}+\boldsymbol{s}}{\left\|\boldsymbol{u}_{k}+\boldsymbol{s}\right\|}=\frac{\boldsymbol{u}_{k}+\boldsymbol{s}}{\sqrt{1+\|\boldsymbol{s}\|^{2}}}=\frac{\boldsymbol{u}_{k}+\boldsymbol{s}}{\beta} \tag{3.1}
\end{equation*}
$$

in view of $\boldsymbol{u}_{k}^{\top} \boldsymbol{s}=0$ and $\left\|\boldsymbol{u}_{k}\right\|=1$, where we have defined $\beta=\sqrt{1+\|\boldsymbol{s}\|^{2}}$.
The above mentioned Newton iteration is shown to converge cubically if the correction equation is solved exactly. Since this is not the case when it is iteratively solved, we simply assume convergence, namely that for a suitable $\delta>0$ such that $\left\|\boldsymbol{e}_{0}\right\|<\delta$ there is a constant $r<1$ such that

$$
\begin{equation*}
\left\|\boldsymbol{e}_{k+1}\right\|<r\left\|\boldsymbol{e}_{k}\right\|, \quad k=0, \ldots \tag{3.2}
\end{equation*}
$$

## Notation.

In the sequel we will indicate as $\boldsymbol{v}_{1}$ the exact eigenvector corresponding to the smallest exact eigenvalue $\lambda_{1}$. The error vector at step $k$ is denoted by $\boldsymbol{e}_{k}=\boldsymbol{u}_{k}-\boldsymbol{v}_{1}$, while the error in the eigenvalue approximation is $\varepsilon_{k}=\theta_{k}-\lambda_{1}(>0)$. It is easily proved that there is a constant $M$ independent of $k$ such that

$$
\begin{equation*}
\varepsilon_{k} \leq M\left\|\boldsymbol{e}_{k}\right\|^{2} \tag{3.3}
\end{equation*}
$$

With $\rho(A)$ we mean the largest modulus eigenvalue of $A$ while $\lambda(A)$ refers to a generic eigenvalue of matrix $A$. As the matrix norm of a symmetric matrix $A$ we will use the Euclidean norm $\|A\| \equiv\|A\|_{2}=\rho(A)=\sup _{\boldsymbol{x} \in \mathcal{R}^{n}, \boldsymbol{x} \neq 0} \frac{\boldsymbol{x}^{\top} A \boldsymbol{x}}{\boldsymbol{x}^{\top} \boldsymbol{x}}$.

REMARK 3.1. At first sight the Jacobian matrix in the correction equation is singular, but this does not matter since the PCG algorithm is run within the subspace of vectors orthogonal to $\boldsymbol{u}_{k}$ (in fact also $\boldsymbol{r}^{\top} \boldsymbol{u}_{k}=0$ ). Thus, notion of positive definiteness, eigenvalue distribution, condition number, norms, etc, apply as usual but with respect to matrices restricted to this subspace.
The following Lemma will bound the extremal eigenvalues of $J_{k}$ in the subspace orthogonal to $\boldsymbol{u}_{k}$.

Lemma 3.1. There is a positive number $\delta$ such that if $\left\|\boldsymbol{e}_{k}\right\|<\delta$ then

$$
J_{k}=\left(I-\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}\right)\left(A-\theta_{k} I\right)\left(I-\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}\right)
$$

is SPD in the subspace orthogonal to $\boldsymbol{u}_{k}$. Moreover the following bounds hold:

$$
\frac{\lambda_{2}-\lambda_{1}}{2}<\boldsymbol{z}^{\top} J_{k} \boldsymbol{z}<\lambda_{n}
$$

for every unit norm vector $\boldsymbol{z}$ orthogonal to $\boldsymbol{u}_{k}$.
Proof. From Lemma 3.1 in [29] and the definition of $\varepsilon_{k}$, we have that $\min _{\boldsymbol{z} \perp \boldsymbol{u},\|\boldsymbol{z}\|=1} \boldsymbol{z}^{\top} J_{k} \boldsymbol{z} \geq$ $\lambda_{1}+\lambda_{2}-2 \theta_{k}=\lambda_{2}-\lambda_{1}-2 \varepsilon_{k}$. Now using (3.3),
$\lambda_{2}-\lambda_{1}-2 \varepsilon_{k} \geq \lambda_{2}-\lambda_{1}-2 M\left\|\boldsymbol{e}_{k}\right\|^{2} \geq \lambda_{2}-\lambda_{1}-2 M \delta^{2}>\frac{\lambda_{2}-\lambda_{1}}{2}>0 \quad\left(\right.$ if $\left.\delta<\sqrt{\frac{\lambda_{2}-\lambda_{1}}{4 M}}\right)$,
showing that $J_{k}$ is SPD. The upper bound for the eigenvalues of $J_{k}$ is straightforward. The previous Lemma allows us to prove that the preconditioner defined in (2.2) is SPD, as stated in the following Theorem.

ThEOREM 3.2. If the correction equation is solved exactly, then any matrix $\widehat{P}_{k}$ defined by (2.2) is $S P D$ and hence $P_{k}$ is $S P D$ in the subspace orthogonal to $\boldsymbol{u}_{k}$.

Proof. The proof is carried out by induction. $\widehat{P}_{0}$ is SPD being an incomplete Cholesky factorization of the SPD matrix $A$, then from $J_{k} \boldsymbol{s}=-\boldsymbol{r}$, we can write

$$
\begin{equation*}
\widehat{P}_{k+1}=-\frac{\boldsymbol{s}^{\top}}{\boldsymbol{s}^{\top} \boldsymbol{r}}+\left(I-\frac{\boldsymbol{s} \boldsymbol{r}^{\top}}{\boldsymbol{s}^{\top} \boldsymbol{r}}\right) \widehat{P}_{k}\left(I-\frac{\boldsymbol{r} \boldsymbol{s}^{\top}}{\boldsymbol{s}^{\top} \boldsymbol{r}}\right)=\frac{\boldsymbol{s} \boldsymbol{s}^{\top}}{\boldsymbol{s}^{\top} J_{k} \boldsymbol{s}}+\left(I-\frac{\boldsymbol{s} \boldsymbol{s}^{\top} J_{k}}{\boldsymbol{s}^{\top} J_{k} \boldsymbol{s}}\right) \widehat{P}_{k}\left(I-\frac{J_{k} \boldsymbol{s} \boldsymbol{s}^{\top}}{\boldsymbol{s}^{\top} J_{k} \boldsymbol{s}}\right) \tag{3.4}
\end{equation*}
$$

We define $F=\left(I-\frac{J_{k} \boldsymbol{s}^{\top}}{\boldsymbol{s}^{\top} J_{k} \boldsymbol{s}}\right)$ and note that, by previous Lemma, $\alpha=\boldsymbol{s}^{\top} J_{k} \boldsymbol{s}>0$ since $\boldsymbol{s}^{\top} \boldsymbol{u}_{k}=0$. Let now $\widehat{P}_{k}$ be SPD by induction hypothesis, then for every $\boldsymbol{z} \neq 0$,

$$
\boldsymbol{z}^{\top} \widehat{P}_{k+1} \boldsymbol{z}=\frac{\left(\boldsymbol{z}^{\top} \boldsymbol{s}\right)^{2}}{\alpha}+\boldsymbol{z}^{\top} F^{\top} \widehat{P}_{k} F \boldsymbol{z}= \begin{cases}\boldsymbol{z}^{\top} \widehat{P}_{k} \boldsymbol{z}>0 & \left(\text { if } \boldsymbol{z}^{\top} \boldsymbol{s}=0\right) \\ \frac{\left(\boldsymbol{z}^{\top} \boldsymbol{s}\right)^{2}}{\alpha}+(F \boldsymbol{z})^{\top} \widehat{P}_{k}(F \boldsymbol{z}) \geq \frac{\left(\boldsymbol{z}^{\top} \boldsymbol{s}\right)^{2}}{\alpha}>0, & \left(\text { if } \boldsymbol{z}^{\top} \boldsymbol{s} \neq 0\right)\end{cases}
$$

which proves that $\widehat{P}_{k+1}$ is SPD. If we now take $\boldsymbol{z} \perp \boldsymbol{u}_{k+1}$, we have

$$
\boldsymbol{z}^{\top} P_{k+1} \boldsymbol{z}=\boldsymbol{z}^{\top}\left(I-\boldsymbol{u}_{k+1} \boldsymbol{u}_{k+1}^{\top}\right) \widehat{P}_{k+1}\left(I-\boldsymbol{u}_{k+1} \boldsymbol{u}_{k+1}^{\top}\right) \boldsymbol{z}=\boldsymbol{z}^{\top} \widehat{P}_{k+1} \boldsymbol{z}>0
$$

which completes the proof.
Let us define the difference between the preconditioned Jacobian and the identity matrix as

$$
E_{k}=I-J_{k}^{1 / 2} P_{k} J_{k}^{1 / 2}
$$

Since by definition we have $J_{k} \boldsymbol{u}_{k}=0$ then $\boldsymbol{u}_{k}$ is the eigenvector of $J_{k}$ corresponding to the zero eigenvalue. Hence, since also $J_{k}^{1 / 2} \boldsymbol{u}_{k}=0$ the error $E_{k}$ can also be defined as

$$
E_{k}=I-J_{k}^{1 / 2} P_{k} J_{k}^{1 / 2}=I-J_{k}^{1 / 2}\left(I-\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}\right) \widehat{P}_{k}\left(I-\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}\right) J_{k}^{1 / 2}=I-J_{k}^{1 / 2} \widehat{P}_{k} J_{k}^{1 / 2}
$$

The following technical lemma will bound the norm of $\widehat{P}_{k}$ in terms of that of $E_{k}$. Being $\widehat{P}_{k}$ SPD we can define its norm in the space orthogonal to $\boldsymbol{u}_{k}$ as

$$
\left\|\widehat{P}_{k}\right\|=\sup _{\boldsymbol{w} \perp \boldsymbol{u}_{k}, \boldsymbol{w} \neq 0} \frac{\boldsymbol{w}^{\top} \widehat{P}_{k} \boldsymbol{w}}{\boldsymbol{w}^{\top} \boldsymbol{w}}
$$

Lemma 3.3. There is a positive number $\delta$ such that if $\left\|\boldsymbol{e}_{k}\right\|<\delta$ then

$$
\left\|\widehat{P}_{k}\right\| \leq \frac{2}{\lambda_{2}-\lambda_{1}}\left(1+\left\|E_{k}\right\|\right)
$$

Proof. Let $\boldsymbol{w} \in \mathcal{R}^{n}, \boldsymbol{w}^{\top} \boldsymbol{u}_{k}=0, \boldsymbol{w} \neq 0$. Then since $J_{k}$ (and thus $J_{k}^{1 / 2}$ ) is SPD in the subspace orthogonal to $\boldsymbol{u}_{k}$ the linear system $J_{k}^{1 / 2} \boldsymbol{z}=\boldsymbol{w}$ has a unique solution $\boldsymbol{z}$ such that $\boldsymbol{z}^{\top} \boldsymbol{u}_{k}=0$. Therefore

$$
\begin{aligned}
0 & <\frac{\boldsymbol{w}^{\top} \widehat{P}_{k} \boldsymbol{w}}{\boldsymbol{w}^{\top} \boldsymbol{w}}=\frac{\boldsymbol{z}^{\top} J^{1 / 2} \widehat{P}_{k} J^{1 / 2} \boldsymbol{z}}{\boldsymbol{z}^{\top} J_{k} \boldsymbol{z}}=\frac{\boldsymbol{z}^{\top}\left(I-E_{k}\right) \boldsymbol{z}}{\boldsymbol{z}^{\top} J_{k} \boldsymbol{z}}=\frac{\boldsymbol{z}^{\top} \boldsymbol{z}}{\boldsymbol{z}^{\top} J_{k} \boldsymbol{z}}\left(1-\frac{\boldsymbol{z}^{\top} E_{k} \boldsymbol{z}}{\boldsymbol{z}^{\top} \boldsymbol{z}}\right) \leq \text { (by Lemma 3.1) } \\
& \leq \frac{2}{\lambda_{2}-\lambda_{1}}\left(1-\frac{\boldsymbol{z}^{\top} E_{k} \boldsymbol{z}}{\boldsymbol{z}^{\top} \boldsymbol{z}}\right) \leq \frac{2}{\lambda_{2}-\lambda_{1}}\left(1+\left|\frac{\boldsymbol{z}^{\top} E_{k} \boldsymbol{z}}{\boldsymbol{z}^{\top} \boldsymbol{z}}\right|\right) \leq \frac{2}{\lambda_{2}-\lambda_{1}}\left(1+\left\|E_{k}\right\|\right)
\end{aligned}
$$

The next lemma will relate the norms of the difference $\boldsymbol{s}$ and of the norm of the error vector $\boldsymbol{e}_{k}$ :
Lemma 3.4. There exists a positive number $\delta$ s.t. if $\left\|\boldsymbol{e}_{k}\right\|<\delta$ then

$$
\|\boldsymbol{s}\| \leq 3\left\|\boldsymbol{e}_{k}\right\|
$$

Proof. From (3.1) we have

$$
\begin{equation*}
\boldsymbol{s}=\beta \boldsymbol{u}_{k+1}-\boldsymbol{u}_{k}=\beta \boldsymbol{u}_{k+1}-\beta \boldsymbol{v}_{1}+\beta \boldsymbol{v}_{1}-\boldsymbol{v}_{1}+\boldsymbol{v}_{1}-\boldsymbol{u}_{k}=\beta \boldsymbol{e}_{k+1}+(\beta-1) \boldsymbol{v}_{1}-\boldsymbol{e}_{k} . \tag{3.5}
\end{equation*}
$$

Hence, taking norms and using (3.2),

$$
\begin{align*}
\|\boldsymbol{s}\| & \leq \sqrt{1+\|\boldsymbol{s}\|^{2}}\left\|\boldsymbol{e}_{k+1}\right\|+\sqrt{1+\|\boldsymbol{s}\|^{2}}-1+\left\|\boldsymbol{e}_{k}\right\| \\
& \leq(1+\|\boldsymbol{s}\|)\left\|\boldsymbol{e}_{k+1}\right\|+\frac{\|\boldsymbol{s}\|^{2}}{2}+\left\|\boldsymbol{e}_{k}\right\| \\
& \leq(2+\|\boldsymbol{s}\|)\left\|\boldsymbol{e}_{k}\right\|+\frac{\|\boldsymbol{s}\|^{2}}{2} . \tag{3.6}
\end{align*}
$$

The last 2nd order inequality, when solved for $\|\boldsymbol{s}\|$ gives

$$
\begin{equation*}
\|\boldsymbol{s}\| \leq 1-\left\|\boldsymbol{e}_{k}\right\|-\sqrt{1-6\left\|\boldsymbol{e}_{k}\right\|+\left\|\boldsymbol{e}_{k}\right\|^{2}} \tag{3.7}
\end{equation*}
$$

Choosing $\delta<\frac{2}{15}$ implies $\sqrt{1-6\left\|e_{k}\right\|+\left\|\boldsymbol{e}_{k}\right\|^{2}} \geq 1-4\left\|\boldsymbol{e}_{k}\right\|$, which, combined with (3.7) provides the desired result.

Now we need to prove that the distance between two consecutive Jacobians is bounded by a constant times the error vector:

Lemma 3.5. There exists a positive number $\delta$ s.t. if $\left\|\boldsymbol{e}_{k}\right\|<\delta$ then

$$
\left\|J_{k+1}-J_{k}\right\| \leq c_{1}\left\|\boldsymbol{e}_{k}\right\|
$$

for a suitable constant $c_{1}$.
Proof.

$$
\begin{align*}
\Delta_{k}= & J_{k+1}-J_{k}= \\
= & \left(I-\boldsymbol{u}_{k+1} \boldsymbol{u}_{k+1}^{\top}\right)\left(A-\theta_{k+1} I\right)\left(I-\boldsymbol{u}_{k+1} \boldsymbol{u}_{k+1}^{\top}\right)-\left(I-\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}\right)\left(A-\theta_{k} I\right)\left(I-\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}\right) \\
= & \left(\theta_{k}-\theta_{k+1}\right) I+\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}\left(A-\theta_{k} I\right)-\boldsymbol{u}_{k+1} \boldsymbol{u}_{k+1}^{\top}\left(A-\theta_{k+1} I\right) \\
& \quad+\left(A-\theta_{k} I\right) \boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}-\left(A-\theta_{k+1} I\right) \boldsymbol{u}_{k+1} \boldsymbol{u}_{k+1}^{\top}= \\
= & \left(\theta_{k}-\theta_{k+1}\right) I+G+G^{\top} \tag{3.8}
\end{align*}
$$

where we set $G=\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}\left(A-\theta_{k} I\right)-\boldsymbol{u}_{k+1} \boldsymbol{u}_{k+1}^{\top}\left(A-\theta_{k+1} I\right)$. The first term in (3.8) can be bounded, using (3.3), as

$$
\begin{equation*}
\left\|\left(\theta_{k}-\theta_{k+1}\right) I\right\|=\theta_{k}-\theta_{k+1}=\varepsilon_{k}-\varepsilon_{k+1} \leq \varepsilon_{k} \leq M\left\|\boldsymbol{e}_{k}\right\|^{2} \leq\left\|\boldsymbol{e}_{k}\right\| \quad\left(\text { if } \quad \delta<\frac{1}{M}\right) \tag{3.9}
\end{equation*}
$$

To bound $\|G\|$ recall that $\boldsymbol{u}_{k+1}=\frac{\boldsymbol{u}_{k}+\boldsymbol{s}}{\beta}$ therefore

$$
\boldsymbol{u}_{k+1} \boldsymbol{u}_{k+1}^{\top}=\frac{\boldsymbol{u}_{k}+\boldsymbol{s}}{\beta} \frac{\boldsymbol{u}_{k}^{\top}+\boldsymbol{s}^{\top}}{\beta}=\frac{1}{1+\|\boldsymbol{s}\|^{2}}\left(\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}+\boldsymbol{u}_{k} \boldsymbol{s}^{\top}+\boldsymbol{s} \boldsymbol{u}_{k}^{\top}+\boldsymbol{s} \boldsymbol{s}^{\top}\right)=\frac{1}{\beta^{2}} \boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}+H
$$

with $\|H\| \leq\|\boldsymbol{s}\|\left(2+\frac{\|\boldsymbol{s}\|}{1+\|\boldsymbol{s}\|^{2}}\right) \leq \frac{5}{2}\|\boldsymbol{s}\| \leq \frac{15}{2} \boldsymbol{e}_{k}$, by Lemma 3.4, then

$$
\begin{align*}
G & =-\frac{\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}}{1+\|\boldsymbol{s}\|^{2}}\left(A-\theta_{k+1} I\right)-H\left(A-\theta_{k+1} I\right)+\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}\left(A-\theta_{k} I\right) \\
& =-\frac{\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}}{1+\|\boldsymbol{s}\|^{2}}\left(\theta_{k}-\theta_{k+1}\right) I+\frac{\|\boldsymbol{s}\|^{2}}{1+\|\boldsymbol{s}\|^{2}}\left(\boldsymbol{u}_{k} \boldsymbol{u}_{k}^{\top}\right)\left(A-\theta_{k} I\right)-H\left(A-\theta_{k+1} I\right), \tag{3.10}
\end{align*}
$$

whence, using (3.9) and again Lemma 3.4,

$$
\begin{equation*}
\|G\| \leq\left\|\boldsymbol{e}_{k}\right\|+9\left\|\boldsymbol{e}_{k}\right\|^{2} \lambda_{n}+\frac{15}{2}\left\|\boldsymbol{e}_{k}\right\| \lambda_{n} \leq\left(1+9 \delta \lambda_{n}+\frac{15}{2} \lambda_{n}\right)\left\|\boldsymbol{e}_{k}\right\|=c_{2}\left\|\boldsymbol{e}_{k}\right\| \tag{3.11}
\end{equation*}
$$

Combining (3.8), (3.9) and (3.11) we have:

$$
\left\|\Delta_{k}\right\| \leq\left\|\boldsymbol{e}_{k}\right\|+2\|G\| \leq\left(1+2 c_{2}\right)\left\|\boldsymbol{e}_{k}\right\|
$$

Setting $c_{1}=1+2 c_{2}$ completes the proof.

Before stating Theorem 3.7 we need to prove as a last preliminary result that also the difference between the square root of two consecutive Jacobians is bounded in terms of the norm of the error vector:

LEMMA 3.6. Let $S_{k}=J_{k+1}^{1 / 2}-J_{k}^{1 / 2}$. Then there is a positive number $\delta$ s.t. if $\left\|\boldsymbol{e}_{k}\right\|<\delta$ then

$$
\left\|S_{k}\right\| \leq c_{3} \sqrt{\left\|\boldsymbol{e}_{k}\right\|}
$$

for a suitable constant $c_{3}$.
Proof. By squaring the equation $S_{k}+J_{k}^{1 / 2}=\sqrt{J_{k}+\Delta_{k}}$ we obtain

$$
\begin{equation*}
S_{k}^{2}+J_{k}^{1 / 2} S_{k}+S_{k} J_{k}^{1 / 2}-\Delta_{k}=0 \tag{3.12}
\end{equation*}
$$

Let now $\boldsymbol{x}$ be a normalized eigenvector of the symmetric matrix $S$ such that $S \boldsymbol{x}=\eta \boldsymbol{x}$. Premultiplying by $\boldsymbol{x}^{\top}$ and postmultiplying by $\boldsymbol{x}$ equation (3.12) yields

$$
\begin{equation*}
\eta^{2}+2\left(\boldsymbol{x}^{\top} J_{k}^{1 / 2} \boldsymbol{x}\right) \eta-\boldsymbol{x}^{\top} \Delta_{k} \boldsymbol{x}=0 \tag{3.13}
\end{equation*}
$$

This quadratic equation has two solutions:

$$
\begin{equation*}
\eta_{12}=-\boldsymbol{x}^{\top} J_{k}^{1 / 2} \boldsymbol{x} \pm \sqrt{\left(\boldsymbol{x}^{\top} J_{k}^{1 / 2} \boldsymbol{x}\right)^{2}+\boldsymbol{x}^{\top} \Delta_{k} \boldsymbol{x}} \tag{3.14}
\end{equation*}
$$

The smallest solution is not an eigenvalue of $S_{k}$ since from the definition of $S_{k}$, an eigenvalue $\eta$ of $S_{k}$ would satisfy

$$
\eta=\eta \boldsymbol{x}^{\top} \boldsymbol{x}=\boldsymbol{x}^{\top} S_{k} \boldsymbol{x}=\boldsymbol{x}^{\top} J_{k+1}^{1 / 2} \boldsymbol{x}-\boldsymbol{x}^{\top} J_{k}^{1 / 2} \boldsymbol{x} \geq-\boldsymbol{x}^{\top} J_{k}^{1 / 2} \boldsymbol{x}
$$

Then, considering the largest solution of (3.14)

$$
\begin{aligned}
\eta & =-\boldsymbol{x}^{\top} J_{k}^{1 / 2} \boldsymbol{x}+\sqrt{\left(\boldsymbol{x}^{\top} J_{k}^{1 / 2} \boldsymbol{x}\right)^{2}+\boldsymbol{x}^{\top} \Delta_{k} \boldsymbol{x}} \\
& =\frac{\boldsymbol{x}^{\top} \Delta_{k} \boldsymbol{x}}{\boldsymbol{x}^{\top} J_{k}^{1 / 2} \boldsymbol{x}+\sqrt{\left(\boldsymbol{x}^{\top} J_{k}^{1 / 2} \boldsymbol{x}\right)^{2}+\boldsymbol{x}^{\top} \Delta_{k} \boldsymbol{x}}} \leq \sqrt{\left|\boldsymbol{x}^{\top} \Delta_{k} \boldsymbol{x}\right|}
\end{aligned}
$$

Let $(\bar{\eta}, \overline{\boldsymbol{x}})$ be the eigenpair corresponding to the largest modulus eigenvalue of $S$. Then

$$
\left\|S_{k}\right\|=|\bar{\eta}| \leq \sqrt{\left|\overline{\boldsymbol{x}}^{\top} \Delta_{k} \overline{\boldsymbol{x}}\right|} \leq \sqrt{c_{1}\left\|\boldsymbol{e}_{k}\right\|}=c_{3} \sqrt{\left\|\boldsymbol{e}_{k}\right\|}
$$

We are finally ready to prove the main results of this Section. The following theorem will state the so called bounded deterioration [25] of the preconditioner at step $k+1$ with respect to that of step $k$, namely that the distance of the preconditioned matrix from the identity matrix at step $k+1$ is less or equal than that at step $k$ plus a constant that may be small as desired, depending on the closeness of $\boldsymbol{u}_{0}$ to the exact solution.

Theorem 3.7. Let $\delta_{0}$ be such that $\left\|E_{0}\right\|<\delta_{0}$, there is a positive number $\delta$ s.t. if $\left\|\boldsymbol{e}_{0}\right\|<\delta$ then

$$
\left\|E_{k+1}\right\| \leq\left\|E_{k}\right\|+K \sqrt{\left\|\boldsymbol{e}_{k}\right\|}
$$

for a suitable constant $K$.

Proof. The distance of the preconditioned Jacobian from the identity matrix can be written as follows, where we have defined $N=S_{k} \widehat{P}_{k+1} J_{k+1}^{1 / 2}+J_{k+1}^{1 / 2} \widehat{P}_{k+1} S_{k}+S_{k} \widehat{P}_{k+1} S_{k}$ :

$$
\begin{align*}
E_{k+1} & =I-J_{k+1}^{1 / 2} \widehat{P}_{k+1} J_{k+1}^{1 / 2}= \\
& =I-\left(J_{k}^{1 / 2}+S_{k}\right) \widehat{P}_{k+1}\left(J_{k}^{1 / 2}+S_{k}\right)= \\
& =I-J_{k}^{1 / 2} \widehat{P}_{k+1} J_{k}^{1 / 2}-N= \\
& =I-J_{k}^{1 / 2} \frac{\boldsymbol{s} \boldsymbol{s}^{\top}}{\boldsymbol{s}^{\top} J_{k} \boldsymbol{s}} J_{k}^{1 / 2}-J_{k}^{1 / 2}\left(I-\frac{\boldsymbol{s} \boldsymbol{s}^{\top} J_{k}}{\boldsymbol{s}^{\top} J_{k} \boldsymbol{s}}\right) \widehat{P}_{k}\left(I-\frac{J_{k} \boldsymbol{s} \boldsymbol{s}^{\top}}{\boldsymbol{s}^{\top} J_{k} \boldsymbol{s}}\right) J_{k}^{1 / 2}-N= \\
& =I-\frac{J_{k}^{1 / 2} \boldsymbol{s} \boldsymbol{s}^{\top} J_{k}^{1 / 2}}{\boldsymbol{s}^{\top} J_{k} \boldsymbol{s}}-\left(I-\frac{J_{k}^{1 / 2} \boldsymbol{s} \boldsymbol{s}^{\top} J_{k}^{1 / 2}}{\boldsymbol{s}^{\top} J_{k} \boldsymbol{s}}\right) J_{k}^{1 / 2} \widehat{P}_{k} J_{k}^{1 / 2}\left(I-\frac{J_{k}^{1 / 2} \boldsymbol{s} \boldsymbol{s}^{\top} J_{k}^{1 / 2}}{\boldsymbol{s}^{\top} J_{k} \boldsymbol{s}}\right)-N . \tag{3.15}
\end{align*}
$$

Now set $\boldsymbol{w}=\frac{J_{k}^{1 / 2} \boldsymbol{s}}{\left\|J_{k}^{1 / 2} \boldsymbol{s}\right\|}$ and $W=I-\boldsymbol{w} \boldsymbol{w}^{\top} ; W$ is an orthogonal projector since $\|\boldsymbol{w}\|=1$. Then

$$
\begin{align*}
E_{k+1} & =W-W J_{k}^{1 / 2} \widehat{P}_{k} J_{k}^{1 / 2} W-N \\
& =W+W\left(E_{k}-I\right) W-N=W E_{k} W-N \tag{3.16}
\end{align*}
$$

To bound $\|N\|$ we will use Lemma 3.3 and Lemma 3.6:

$$
\|N\| \leq \frac{2}{\lambda_{2}-\lambda_{1}}\left(1+\left\|E_{k+1}\right\|\right)\left(2 c_{3} \sqrt{\left\|\boldsymbol{e}_{k}\right\|} \sqrt{\lambda_{n}}+c_{3}^{2} \sqrt{\delta} \sqrt{\left\|\boldsymbol{e}_{k}\right\|}\right)=c_{4}\left(1+\left\|E_{k+1}\right\|\right) \sqrt{\left\|\boldsymbol{e}_{k}\right\|} .
$$

Now taking norms in (3.16) yields

$$
\left\|E_{k+1}\right\| \leq\left\|E_{k}\right\|+c_{4}\left(1+\left\|E_{k+1}\right\|\right) \sqrt{\left\|e_{k}\right\|}
$$

which can be rewritten as

$$
\begin{equation*}
\left\|E_{k+1}\right\|\left(1-c_{4} \sqrt{\left\|\boldsymbol{e}_{k}\right\|}\right) \leq\left\|E_{k}\right\|+c_{4} \sqrt{\left\|\boldsymbol{e}_{k}\right\|} \tag{3.17}
\end{equation*}
$$

From (3.17), we derive a bound for $\left\|E_{k}\right\|$. If $\sqrt{\delta}<\frac{1}{2 c_{4}}$ then

$$
\begin{equation*}
\left\|E_{k}\right\| \leq 2\left\|E_{k-1}\right\|+1 \leq \ldots \leq 2^{k}\left\|E_{0}\right\|+2^{k}-1 \leq 2^{k}\left(\delta_{0}+1\right)=c_{5} \tag{3.18}
\end{equation*}
$$

Again from (3.17) and using the bound (3.18) we finally have

$$
\begin{aligned}
\left\|E_{k+1}\right\| & \leq \frac{\left\|E_{k}\right\|+c_{4} \sqrt{\left\|\boldsymbol{e}_{k}\right\|}}{1-c_{4} \sqrt{\left\|\boldsymbol{e}_{k}\right\|}} \\
& \leq\left(\left\|E_{k}\right\|+c_{4} \sqrt{\left\|\boldsymbol{e}_{k}\right\|}\right) \cdot\left(1+2 c_{4} \sqrt{\left\|\boldsymbol{e}_{k}\right\|}\right) \\
& \leq\left\|E_{k}\right\|+2 c_{4} \sqrt{\left\|\boldsymbol{e}_{k}\right\|} c_{5}+c_{4}\left(1+2 c_{4} \delta\right) \sqrt{\left\|\boldsymbol{e}_{k}\right\|}=\left\|E_{k}\right\|+c_{4}\left(2 c_{5}+1+2 c_{4} \delta\right) \sqrt{\left\|\boldsymbol{e}_{k}\right\|} .
\end{aligned}
$$

Setting $K=c_{4}\left(2 c_{5}+1+2 c_{4} \delta\right)$ completes the proof.
REmARK 3.2. It is more usual to evaluate the goodness of a preconditioner by bounding the extremal eigenvalues of the preconditioned matrix (if SPD) instead of using norms. However, it is worth observing that the initial preconditioner can be selected so as to give $\rho\left(J_{0}^{1 / 2} P_{0} J_{0}^{1 / 2}\right)<2$. In such case, in the most common situation we would have

$$
\left\|E_{k}\right\|=\max \left\{\left|\lambda\left(E_{k}\right)\right|\right\}=1-\min \left\{\lambda\left(J_{k}^{1 / 2} P_{k} J_{k}^{1 / 2}\right)\right\}
$$

so that minimizing $\left\|E_{k}\right\|$ is the same as maximizing the smallest eigenvalue of the preconditioned matrix.
3.2. Computing several eigenpairs. When seeking an eigenvalue different from $\lambda_{1}$, say $\lambda_{j}$, the Jacobian matrix changes as

$$
J_{k}=\left(I-Q Q^{\top}\right)\left(A-\theta_{k} I\right)\left(I-Q Q^{\top}\right)
$$

where $Q=\left[\boldsymbol{v}_{1} \boldsymbol{v}_{2} \ldots \boldsymbol{v}_{j} \boldsymbol{u}_{k}\right]$ is the matrix whose first $j$ columns are the previously computed eigenvectors. Analogously, also the preconditioner must be chosen orthogonal to $Q$ as

$$
\begin{equation*}
P_{k+1}=\left(I-Q Q^{\top}\right) \widehat{P}_{k+1}\left(I-Q Q^{\top}\right) \tag{3.19}
\end{equation*}
$$

The theoretical analysis developed in the previous Section applies with small technical variants also in this case since it is readily proved that $J_{k+1}^{1 / 2} P_{k+1} J_{k+1}^{1 / 2}=J_{k+1}^{1 / 2} \widehat{P}_{k+1} J_{k+1}^{1 / 2}$. The most significant changes regard the definition of $\varepsilon_{k}=\theta_{k}-\lambda_{j}, \boldsymbol{e}_{k}=\boldsymbol{u}_{k}-\boldsymbol{v}_{j}$ and the statement of Lemma 3.1 (and the proof of Lemma 3.5 that uses its results), namely the bound for the smallest eigenvalue of $J_{k}$ which in the general case becomes:

$$
\boldsymbol{z}^{\top} J_{k} \boldsymbol{z}>\frac{\lambda_{j+1}-\lambda_{j}}{2}
$$

for every unit norm vector $\boldsymbol{z}$ such that $Q^{\top} \boldsymbol{z}=0$.

## 4. Implementation.

4.1. Choosing an initial eigenvector guess. As mentioned in Section 1, another important issue in the efficiency of the Newton approach for eigenvalue computation is represented by the appropriate choice of the initial guess. We propose here to perform some preliminary iterations of another eigenvalue solver, in order to start the Newton iteration 'sufficiently' close to the exact eigenvector. We chose as the 'preliminary' eigenvalue solver DACG [9, 14, 15], which is based on the preconditioned conjugate gradient (nonlinear) minimization of the Rayleigh Quotient. This method has proven very robust, and not particularly sensitive to the initial vector, in the computation of a few eigenpairs of large SPD matrices.
4.2. Implementation of the BFGS preconditioner update. In this section we give the main lines of the implementation of the product of our preconditioner times a vector, which is needed when using a preconditioned Krylov method. At a certain nonlinear iteration level, $k$, we need to compute $\boldsymbol{c}=P_{k} \boldsymbol{g}_{l}$, where $\boldsymbol{g}_{l}$ is the residual of the linear system at iteration $l$. Let us suppose we compute an initial preconditioner $P_{0}$. Then, at the initial nonlinear iteration $k=0$, we simply have $\boldsymbol{c}=P_{0} \boldsymbol{z}_{l}$. At step $k+1$ the preconditioner $\widehat{P}_{k+1}$ is defined recursively by (2.2) while $P_{k+1}$ using (3.19) can be written as

$$
\begin{align*}
P_{k+1} & =\left(I-Q Q^{\top}\right) \widehat{P}_{k+1}\left(I-Q Q^{\top}\right)= \\
& =\left(I-Q Q^{\top}\right)\left\{\left(I-\frac{\boldsymbol{s} \boldsymbol{r}^{\top}}{\boldsymbol{s}^{\top} \boldsymbol{r}}\right) \widehat{P}_{k}\left(I-\frac{\boldsymbol{r} \boldsymbol{s}^{\top}}{\boldsymbol{s}^{\top} \boldsymbol{r}}\right)-\frac{\boldsymbol{s}^{\top}}{\boldsymbol{s}^{\top} \boldsymbol{r}}\right\}\left(I-Q Q^{\top}\right) . \tag{4.1}
\end{align*}
$$

To compute vector $\boldsymbol{c}$ first we observe that $\boldsymbol{g}_{l}$ is orthogonal to $Q$ so there is no need to apply matrix $I-Q Q^{\top}$ on the right of (4.1). Application of preconditioner $\widehat{P}_{k+1}$ to the vector $\boldsymbol{g}_{l}$ can be performed at the price of $2 k$ dot products and $2 k$ daxpys as described in Algorithm 1. The scalar products $\alpha_{k}=\boldsymbol{s}_{k}^{\top} \boldsymbol{r}_{k}$, which appear at the denominator of $\widehat{P}_{k+1}$, can be computed once and for all before starting the solution of the $(k+1)$-th linear system. Last, the obtained vector $\boldsymbol{c}$ must be orthogonalized against the columns of $Q$ by a classical Gram-Schimdt procedure.
4.3. PCG solution of the correction equation. As a Krylov subspace solver for the correction equation we chose the Preconditioned Conjugate gradient (PCG) method since the Jacobian $J_{k}$ has been shown to be SPD in the subspace orthogonal to $\boldsymbol{u}_{k}$. Regarding the implementation of PCG, we mainly refer to the work [29], where the author shows that it is possible to

```
Algorithm 1 Computation of \(\boldsymbol{c}=P_{k} \boldsymbol{g}_{l}\) for the BFGS preconditioner.
    Input: Vector \(\boldsymbol{g}_{l}\), scalar products \(\alpha_{s}=\boldsymbol{s}_{s}^{\top} \boldsymbol{r}_{s}, s=0, \ldots, k-1\).
    \(\boldsymbol{w}:=\boldsymbol{g}_{l}\)
    FOR \(s:=k-1\) TO 0
        1. \(a_{s}:=\boldsymbol{s}_{s}^{\top} \boldsymbol{w} / \alpha_{s}\)
        2. \(\boldsymbol{w}:=\boldsymbol{w}-a_{s} \boldsymbol{r}_{s}\)
    END FOR
    \(\boldsymbol{c}:=\widehat{P}_{0} \boldsymbol{w}\)
    FOR \(s:=0\) TO \(k-1\)
            1. \(b:=\boldsymbol{r}_{s}^{\top} \boldsymbol{c} / \alpha_{s}\)
            2. \(\boldsymbol{c}:=\boldsymbol{c}-\left(a_{s}+b\right) \boldsymbol{s}_{s}\)
        END FOR
        \(\boldsymbol{z}:=Q^{\top} \boldsymbol{c}\)
        \(c:=\boldsymbol{c}-Q \boldsymbol{z}\)
```

solve the linear system in the subspace orthogonal to $\boldsymbol{u}_{k}$ and hence the projection step needed in the application of $J_{k}$ can be skipped. Moreover, we adopted the exit strategy for the linear system solution described in the above paper, which allows for stopping the PCG iteration, in addition to the classical exit test based on a tolerance on the relative residual and on the maximum number of iterations, whenever the current solution $\boldsymbol{x}_{l}$ satisfies

$$
\begin{equation*}
\left\|\boldsymbol{r}_{k, l}\right\|=\left\|A \boldsymbol{x}_{l}-\frac{\boldsymbol{x}_{l}^{\top} A \boldsymbol{x}_{l}}{\boldsymbol{x}_{l}^{\top} \boldsymbol{x}_{l}} \boldsymbol{x}_{l}\right\|<\tau\left(\boldsymbol{x}_{l}^{\top} A \boldsymbol{x}_{l}\right) \tag{4.2}
\end{equation*}
$$

or when the decrease of $\left\|\boldsymbol{r}_{k, l}\right\|$ is slower than the decrease of $\left\|\boldsymbol{g}_{l}\right\|$, because in this case further iterating does not improve the accuracy of the eigenvector. Note that this dynamic exit strategy implicitly defines an Inexact Newton method since the correction equation is not solved "exactly" i.e. up to machine precision.

We have implemented the PCG method as described in Algorithm 5.1 of [29] with the obvious difference in the application of the preconditioner which is described here in Algorithm 1.
4.4. Implementation of the DACG-Newton method. The BFGS preconditioner defined in Algorithm 1 suffers from two main drawbacks, namely increasing costs of memory for storing $s$ and $r$, and the increasing cost of preconditioner application with the iteration index $k$. Note that these drawbacks are common to many iterative schemes, such as for example sparse (Limited Memory) Broyden implementations [28], GMRES [31] and Arnoldi method for eigenvalue problems [27]. There are different ways to overcome these difficulties, all based on variations of a restart procedure, that is, the iteration scheme is reset after a fixed number of iterations. If the number of nonlinear iterations is high (e.g. more than ten iterations), the application of BFGS preconditioner may be too heavy to be counterbalanced by a reduction in the iteration number. To this aim we define $k_{\max }$ the maximum number of rank two corrections we allow. When the nonlinear iteration counter $k$ is larger than $k_{\max }$, the vectors $s_{i}, \boldsymbol{r}_{i}, i=k-k_{\max }$ are substituted with the last computed $\boldsymbol{s}_{k}, \boldsymbol{r}_{k}$. Vectors $\left\{\boldsymbol{s}_{i}, \boldsymbol{r}_{i}\right\}$ are stored in a matrix $V$ with $n$ rows and $2 \times k_{\text {max }}$ columns.

The implementation of our DACG-Newton method for computing the leftmost eigenpairs of large SPD matrices is described in Algorithm 2.

The above described implementation is well suited to parallelization provided that an efficient matrix-vector product routine is available. The bottleneck is represented by the high number of

```
Algorithm 2 DACG-Newton Algorithm.
    - Input:
    1. Matrix \(A\);
    2. number of sought eigenpairs \(n_{\text {eig }}\);
    3. tolerance and maximum number of its for the outer iteration: \(\tau\), ITMAX;
    4. tolerance for the initial eigenvector guess \(\tau_{D A C G}\);
    5. tolerance and maximum number of its for the inner iteration: \(\tau_{P C G}\), ITMAX \(_{P C G}\);
    6. parameters for the IC preconditioner:, LFIL and \(\tau_{I C}\);
    7. maximum allowed rank-two updates in the BFGS preconditioner: \(k_{\max }\).
    - \(\widetilde{Q}:=[]\).
    - Compute an incomplete Cholesky factorization of \(A\) : \(\widehat{P}_{0}\) with parameters LFIL and \(\tau_{I C}\).
    - FOR \(j:=1\) TO \(n_{\text {eig }}\)
            1. Choose \(\boldsymbol{x}_{0}\) such that \(\widetilde{Q}^{\top} \boldsymbol{x}_{0}=0\).
            2. Compute \(\boldsymbol{u}_{0}\), an approximation to \(\boldsymbol{v}_{j}\) by the DACG procedure with initial vector
                \(\boldsymbol{x}_{0}\), preconditioner \(\widehat{P}_{0}\) and tolerance \(\tau_{D A C G}\).
            3. \(k:=0, \theta_{k}:=\boldsymbol{u}_{k}^{\top} A \boldsymbol{u}_{k}\).
            4. WHILE \(\left\|A \boldsymbol{u}_{k}-\theta_{k} \boldsymbol{u}_{k}\right\|>\tau \theta_{k} \quad\) AND \(k<\operatorname{IMAX}\) DO
                    1. \(Q:=\left[\begin{array}{ll}\widetilde{Q} & \boldsymbol{u}_{k}\end{array}\right]\).
                    2. Solve \(J_{k} \boldsymbol{s}_{k}=-\boldsymbol{r}_{k}\) for \(\boldsymbol{s}_{k} \perp Q\) by the PCG method with preconditioner \(P_{k}\)
                    and tolerance \(\tau_{P C G}\).
                    3. \(\boldsymbol{u}_{k+1}:=\frac{\boldsymbol{u}_{k}+\boldsymbol{s}_{k}}{\left\|\boldsymbol{u}_{k}+\boldsymbol{s}_{k}\right\|}, \quad \theta_{k+1}=\boldsymbol{u}_{k+1}^{\top} A \boldsymbol{u}_{k+1}\).
                    4. \(k_{1}=k \operatorname{MOD} k_{\max } ; V\left(*, 2 k_{1}+1\right):=\boldsymbol{s}_{k}, V\left(*, 2 k_{1}+2\right):=\boldsymbol{r}_{k}\),
                    5. \(k:=k+1\)
            6. END WHILE
            7. Assume \(\boldsymbol{v}_{j}=\boldsymbol{u}_{k}\) and \(\lambda_{j}=\theta_{k}\). Set \(\widetilde{Q}:=\left[\widetilde{Q} \boldsymbol{v}_{j}\right]\)
    - END FOR
```

scalar products which may worsen the parallel efficiency when a very large number of processor is employed. Preliminary numerical results are encouraging as documented in [12].
5. Numerical Results. In this Section we provide numerical results which compare the performance of the DACG-Newton algorithm for various $k_{\max }$ values. We tested the proposed algorithm in the computation of the 20 smallest eigenpairs of a number of small to very large matrices arising from various realistic applications.

The list of the selected problems together with their size $n$, and nonzero number $n z$ is reported in Table 5, where (M)FE stands for (Mixed) Finite Elements.

TABLE 5.1
Main characteristics of the matrices used in the tests.

| Matrix | where it comes from | $n$ | $n z$ |
| :--- | :--- | ---: | ---: |
| TRINO | 3D-FE elasticity problem | 4560 | 604030 |
| HYB2D | 2D-MFE groundwater flow | 28600 | 142204 |
| MONTE-CARLO | 2D-MFE stochastic PDE | 77120 | 384320 |
| EMILIA-923 | 3D-FE elasticity problem | 923136 | 41005206 |
| DBLP | network connected graph | 928498 | 8628378 |

In most of the runs, unless differently specified, we selected the values of the parameters as reported in Table 5.

Table 5.2
Default values of parameters.

| Number of eigenpairs to compute | $n_{\text {eig }}=20$ |
| :--- | :--- |
| Parameters for the outer iteration | $\tau=10^{-8}, \quad$ ITMAX $=100$ |
| Tolerance for the initial eigenvector guess | $\tau_{D A C G}=10^{-2}$ |
| Parameters for the PCG iteration | $\tau_{P C G}=10^{-2}, \quad$ ITMAX $_{P C G}=20$ |
| Parameters for the initial preconditioner | LFIL $=30, \quad \tau_{I C}=10^{-2}$. |

We will also compute the fill-in $\sigma$ of the initial preconditioner defined as

$$
\sigma=\frac{\text { nonzeros of } L}{\text { nonzeros of lower triangular part of } A}
$$

The CPU times (in seconds) refer to running a Fortran 90 code on an IBM Power6 at 4.7 GHz and with up to 64 Gb of RAM.
5.1. Condition number of the preconditioned matrix. We consider first the small TRINO problem, for which we were able to compute all the eigenvalues of $\widetilde{J}_{k}=J_{k}^{1 / 2} P_{k} J_{k}^{1 / 2}$. In Table 5.1 we report for each eigenvalue level $\tilde{\widetilde{J}}^{j}$, the smallest eigenvalue of $\widetilde{J}_{0}$ and of $\widetilde{J}_{5}$, together with the ratio between condition numbers $\frac{\kappa\left(\widetilde{J}_{0}\right)}{\kappa\left(\widetilde{J}_{5}\right)}$ where

$$
\kappa\left(\widetilde{J}_{k}\right)=\frac{\max \left\{\lambda\left(\widetilde{J}_{k}\right)\right\}}{\min \left\{\lambda\left(\widetilde{J}_{k}\right)>0\right\}},
$$

and the reciprocal of the relative separation between consecutive eigenvalues, $\xi_{j}=\frac{\lambda_{j}}{\lambda_{j+1}-\lambda_{j}}$ which is indicative of the ill-conditioning of $\widetilde{J}_{0}[9,13]$.

Table 5.3
Smallest eigenvalue of the preconditioned Jacobians: $\widetilde{J}_{0}$ and $\widetilde{J}_{5}$, condition number ratio and reciprocal of the relative separation $\xi_{j}$, for $j=1, \ldots, 20$. Matrix TRINO.

| $j$ | $\lambda_{\min }\left(\widetilde{J}_{0}\right)$ | $\lambda_{\min }\left(\widetilde{J}_{5}\right)$ | $\frac{\kappa\left(\widetilde{J}_{0}\right)}{\kappa\left(\widetilde{J}_{5}\right)}$ | $\xi_{j}$ | $j$ | $\lambda_{\min }\left(\widetilde{J}_{0}\right)$ | $\lambda_{\min }\left(\widetilde{J}_{5}\right)$ | $\frac{\kappa\left(\widetilde{J}_{0}\right)}{\kappa\left(\widetilde{J}_{5}\right)}$ | $\xi_{j}$ |
| ---: | :---: | :---: | ---: | ---: | ---: | :---: | :---: | ---: | ---: |
| 1 | .0211 | .0542 | 2.57 | 1.57 | 11 | .0039 | .0192 | 4.89 | 27.99 |
| 2 | .0093 | .0432 | 4.64 | 7.55 | 12 | .0058 | .0151 | 2.59 | 31.45 |
| 3 | .0154 | .0403 | 2.62 | 3.79 | 13 | .0031 | .0127 | 4.15 | 34.85 |
| 4 | .0051 | .0256 | 5.01 | 13.69 | 14 | .0045 | .0285 | 6.29 | 36.78 |
| 5 | .0168 | .0417 | 2.48 | 5.91 | 15 | .0050 | .0284 | 5.68 | 24.74 |
| 6 | .0028 | .0316 | 11.13 | 37.25 | 16 | .0085 | .0234 | 2.75 | 30.27 |
| 7 | .0024 | .0349 | 14.64 | 51.94 | 17 | .0027 | .0197 | 7.33 | 81.48 |
| 8 | .0199 | .0329 | 1.65 | 5.13 | 18 | .0017 | .0307 | 18.49 | 51.52 |
| 9 | .0075 | .0149 | 1.99 | 22.62 | 19 | .0137 | .0378 | 2.76 | 11.28 |
| 10 | .0065 | .0196 | 2.99 | 19.11 | 20 | .0074 | .0296 | 3.99 | 22.98 |

It is found that there is a constant grow of the smallest eigenvalue from $k=0$ to $k=5$. Moreover the condition number of the preconditioned matrix reduces by a factor varying from $1.65(j=8)$ to $18.49(j=18)$, the reduction of the condition number being more important when $\xi_{j}$ is large, i.e. when the initial Jacobian is ill-conditioned. Referring now to Theorem 3.7 we may observe that, being in this test case $\lambda_{\max }\left(\widetilde{J}_{k}\right) \approx 1.5$ for every eigenpair,

$$
\left\|E_{k}\right\|=\left\|I-\widetilde{J}_{k}\right\|=\max \left\{\lambda_{\max }\left(\widetilde{J}_{k}\right)-1,1-\lambda_{\min }\left(\widetilde{J}_{k}\right)\right\}=1-\lambda_{\min }\left(\widetilde{J}_{k}\right) .
$$

From Table 5.1 we then could also easily compute $\left\|E_{k}\right\|$, for $k=0,5$. For instance for $j=18$ we find $\left\|E_{0}\right\|=.9983$ and $\left\|E_{5}\right\|=.9693$ showing that even a small reduction of $\left\|E_{k}\right\|$ may lead to an important reduction in the condition number of $\widetilde{J}_{k}$.

In Figure 5.1 we plot the condition number of the preconditioned Jacobian for two selected eigenpairs $(j=7,18)$, vs outer iteration index using $k_{\max }=0$, i.e. using $P_{0}$ as the preconditioner for all the Newton systems, or $k_{\max }=10$, i.e. using the BFGS preconditioner with no restart. From the figure we notice that the condition number of $\widetilde{J}_{k}$ remains roughly constant through the nonlinear iterations with $P_{k}=P_{0}$ while it decreases significantly if the BFGS preconditioner is employed.

FIG. 5.1. Condition number of the preconditioned matrices $J_{k}^{1 / 2} P_{k} J_{k}^{1 / 2}$ vs outer iteration number, in solving the trino problem for $k_{\max }=0,10$ and two different eigenpair levels $(j=7$ and $j=18)$.

5.2. Influence of parameter $k_{\text {max }}$. We now report the results of our DACG-Newton method in the computation of the 20 leftmost eigenpairs of matrices HYB2D and MONTE-CARLO. The overall results are summarized in Tables 5.4 and 5.5 where we include CPU times and number of matrix vector products (MVP) for both the DACG initial phase and the Newton iteration. The overall outer Newton iterations (outer its) are also given. From the tables we notice that whatever the value of $k_{\max }$ there is an improvement in the total number of MVP and CPU time compared with keeping the initial preconditioner fixed throughout the nonlinear process. The improvement is also irrespective of the maximum number of PCG iterations Imax ${ }_{P C G}$. Observe that increasing $k_{\max }$ also the outer iteration number decreases, meaning that the proposed preconditioner, together with accelerating the correction equation solution, also speeds up nonlinear convergence to the desired eigenvector. The CPU time values account for the fact that the overhead introduced by the application of $P_{k+1}$ for high $k_{\max }$ values is not important. To this end it is worth emphasizing that in most cases 5 outer iterations are enough to allow convergence of the Newton method and this also explains why setting $k_{\max } \geq 5$ the results do not substantially change.

Considering for example the case $\operatorname{ImAx}_{P C G}=20$, matrix MONTE-CARLO, the number of MV products in the Newton phase reduces from an initial 5295 to a final value of 2121 obtained with $k_{\max } \geq 5$. We finally observe that the DACG-Newton algorithm is always superior to "pure" DACG method (run up to a relative residual smaller than $\tau_{D A C G}=10^{-8}$ ) in terms of MV products and CPU time as reported in the last row of both tables.

We also present two pictures (Figures 5.2 and 5.3), where the relative residual norm $\left\|\boldsymbol{r}_{k, l}\right\|$, computed by (4.2) is plotted vs Newton cumulative linear iteration index for two selected eigenvalue levels. The problem is mONTE-CARLO with $\operatorname{ImAx}_{P C G}=20$. Again we let vary $k_{\max } \in[0,10]$.

TABLE 5.4
Total number of iterations, number of MV products and CPU times for DACG-Newton algorithm with various $k_{\max }$ values and two different values of $\operatorname{Imax}_{P C G}$. Matrix HYB2D. The initial preconditioner fill-in is $\sigma=2.19$.

|  |  | DACG |  | Newton |  |  | TOT |  |
| :---: | ---: | :---: | :---: | ---: | ---: | ---: | ---: | ---: |
| IMAX $_{P C G}$ | $k_{\max }$ | its | CPU | outer its | MVP | CPU | MVP | CPU |
| 10 | 0 | 944 | 3.03 | 261 | 2730 | 7.85 | 3674 | 10.88 |
|  | 1 | 944 | 2.98 | 160 | 1647 | 4.93 | 2591 | 7.91 |
|  | 5 | 944 | 2.97 | 110 | 1134 | 3.50 | 2078 | 6.47 |
| 20 | 0 | 944 | 2.99 | 118 | 1879 | 5.15 | 2823 | 8.14 |
|  | 5 | 944 | 2.99 | 87 | 1297 | 3.77 | 2241 | 6.76 |
| DACG |  | 4033 | 11.67 |  |  |  | 4033 | 11.67 |

Table 5.5
Total number of iterations, number of MV products and CPU times for DACG-Newton algorithm with various $k_{\max }$ values and three different values of $\operatorname{Imax}_{P C G}$. Matrix MONTE-CARLO. The initial preconditioner fill-in is $\sigma=2.10$.

|  |  | DACG |  | Newton |  |  | TOT |  |
| :---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| IMAX $_{P C G}$ | $k_{\max }$ | its | CPU | outer its | MVP | CPU | MVP | CPU |
| 30 | 0 | 1921 | 15.98 | 148 | 3969 | 30.10 | 4890 | 46.08 |
|  | 1 | 1921 | 15.94 | 120 | 2799 | 22.06 | 4720 | 38.00 |
|  | 3 | 1921 | 15.81 | 102 | 2264 | 18.13 | 4185 | 33.94 |
|  | 10 | 1921 | 15.87 | 103 | 2242 | 18.22 | 4163 | 34.09 |
| 20 | 0 | 1921 | 15.85 | 267 | 5295 | 39.88 | 7216 | 55.73 |
|  | 1 | 1921 | 15.84 | 155 | 2998 | 23.88 | 4919 | 39.72 |
|  | 2 | 1921 | 16.00 | 133 | 2615 | 21.23 | 4536 | 37.23 |
|  | 3 | 1921 | 15.86 | 126 | 2337 | 19.16 | 4258 | 35.02 |
|  | 5 | 1921 | 15.78 | 114 | 2121 | 17.58 | 4042 | 33.36 |
|  | 10 | 1921 | 15.96 | 114 | 2121 | 17.67 | 4042 | 33.63 |
| 10 | 0 | 1921 | 15.85 | 1078 | 11783 | 92.04 | 13704 | 107.85 |
|  | 3 | 1921 | 15.79 | 259 | 2740 | 23.71 | 4661 | 39.50 |
|  | 5 | 1921 | 15.93 | 230 | 2434 | 21.89 | 4355 | 37.82 |
|  | 10 | 1921 | 16.01 | 193 | 2042 | 18.84 | 3963 | 34.85 |
| DACG |  | 7307 | 57.31 |  |  |  | 7307 | 57.31 |

The Figures confirm the acceleration of convergence provided by the proposed preconditioner: there is a factor $3 \div 4$ gain in the total number of iterations, when passing from $k_{\max }=0$ to $k_{\text {max }}=10$.
5.3. Role of the initial preconditioner. We report in this section results of the behavior of our preconditioner depending on the sparsity of $\widehat{P}_{0}$. We selected two different sets of parameters for the IC preconditioner than those employed in Section 5.2 , namely LFIL $=10, \tau_{I C}=0.1$ (test case $\# 1$, sparser preconditioner), and LFIL $=50, \tau_{I C}=10^{-4}$ (test case $\# 2$, preconditioner more filled-in). For test case \# 1 we obtained $\sigma=1.00$ and used $\operatorname{ImAx}_{P C G}=30$ while for test case \# 2 we obtained $\sigma=9.04$ and used $\operatorname{Imax}_{P C G}=10$. The results are summarized in Table 5.6 for the computation of the 20 smallest eigenvalues of the MONTE-CARLO matrix. We report only the results regarding the Newton phase, mentioning that in this case we chose $\tau_{D A C G}=0.1$.

The improvement in MV products/CPU time provided by the BFGS preconditioner is impressive with the sparser initial preconditioner, while in test case \# 2 the optimal number of iterations is reached with $k_{\max }=3$.

Fig. 5.2. Convergence profile of the relative residual norm vs cumulative inner iterations for eigenvalue \# 12, matrix monte-carlo.


Fig. 5.3. Convergence profile of the relative residual norm vs cumulative inner iterations for eigenvalue \# 15, matrix monte-carlo.

5.4. Eigensolution of the largest matrices. We report the results obtained in evaluating $n_{e i g}=10$ eigenpairs of EMILIA-923 which arises from the regional geomechanical model of a deep hydrocarbon reservoir. This matrix is obtained discretizing the structural problem with tetrahedral Finite Elements. Due to the complex geometry of the geological formation it was not possible to obtain a computational grid characterized by regularly shaped elements. This matrix is publicly available in the University of Florida Sparse Matrix Collection at http://www.cise.ufl.edu/ research/sparse/matrices. To obtain an efficient initial preconditioner we selected LFIL $=50$ and $\tau_{I C}=10^{-5}$ as the IC parameters which gave raise to a sparsity ratio $\sigma=2.14$. DACG was run until a very high tolerance $\tau_{D A C G}=0.2$ was reached.

In Table 5.7 we report the MVP number and CPU time together with the CPU time taken

Table 5.6
Total number of iterations, number of MV products and CPU times for DACG-Newton algorithm with various $k_{\text {max }}$. Matrix MONTE-CARLO with two different initial preconditioners.

| test case \# 1 |  |  |  | test case \# 2 |  |  |  |
| ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| $k_{\text {max }}$ | outer its | MVP | CPU | $k_{\max }$ | outer its | MVP | CPU |
| 0 | 952 | 28097 | 174.62 | 0 | 86 | 709 | 24.54 |
| 1 | 340 | 10032 | 64.09 | 1 | 82 | 614 | 20.79 |
| 3 | 241 | 7008 | 47.94 | 3 | 77 | 554 | 19.49 |
| 5 | 214 | 6097 | 42.64 | 5 | 77 | 554 | 20.69 |
| 10 | 193 | 5419 | 38.69 | 10 | 77 | 554 | 20.69 |

by the preconditioner construction, which is, in this case, a not negligible part of the overall computing time. The DACG-Newton method is shown to take great advantage from the BFGS preconditioner even for $k_{\max }=1$, displaying a halving of the MV products and CPU time with respect to reusing the same initial preconditioner. Note that in this case a very low DACG accuracy $\left(\tau_{D A C G}=0.2\right)$ is sufficient to provide a good initial vector for the subsequent Newton phase.

TABLE 5.7
Total number of iterations, number of MV products and CPU times for DACG-Newton algorithm with various $k_{\text {max }}$ values for problem Emilia-923.

|  |  | IC | DACG |  | Newton |  |  | TOT |  |
| :---: | ---: | ---: | ---: | :---: | ---: | ---: | ---: | ---: | ---: |
| ImAX $_{P C G}$ | $k_{\max }$ | CPU | its | CPU | outer its | MVP | CPU | MVP | CPU |
| 20 | 0 | 219.1 | 565 | 780.2 | 147 | 2657 | 3788.9 | 3232 | 4788.2 |
|  | 1 | 219.1 | 565 | 780.2 | 75 | 1273 | 1781.0 | 1838 | 2780.3 |
|  | 5 | 219.1 | 565 | 780.2 | 63 | 922 | 1299.0 | 1487 | 2299.5 |
| DACG |  | 219.1 | 7512 | 10313.9 |  |  |  | 7512 | 10533.0 |

Matrix DBLP represents the Laplacian of a graph describing collaboration network of computer scientists. Nodes are authors and edges are collaborations in published papers, the edge weight is the number of publications shared by the authors [21]. It is well-known that the smallest eigenvalue is zero (with multiplicity one) corresponding to an eigenvector with all unity components. We are therefore interested in the 20 smallest strictly positive eigenvalues. This matrix is also characterized by a high clustering of the eigenvalues, which makes the problem difficult to solve due to the consequent ill-conditioning of the Jacobian matrices. In our runs, we used default parameters listed in Table 5 with the exception of $\tau_{D A C G}=0.1$. The preconditioner density was in this case $\sigma=1.84$.

The results are reported in Table 5.8. DACG with $\tau_{D A C G}=10^{-8}$ could not converge to the desired eigenpairs, namely for $j=12$ it reached the maximum number of iterations (5000) which produced stagnation in the convergence to the subsequent eigenpairs. Also DACG-Newton with $k_{\max }=0$ reached the maximum number of outer iterations already at level $j=2$. Setting $k_{\max }=1$ was instead sufficient to lead DACG-Newton to convergence. Also in this case higher values of $k_{\max }$ provided faster convergence.
6. Comparison with Jacobi-Davidson. The algorithm presented and analyzed in the previous sections is here compared with the well-known Jacobi-Davidson (JD) method. For the details of this method we refer to the original paper [34], as well as to successive works [35, 20, 29] which analyze both theoretically and experimentally a number of variants of this method. In this paper, we followed the implementation suggested in the previously cited work [29], i.e. we made use of the PCG method as the inner solver, with the same initial preconditioner as that used in

Table 5.8
Total number of iterations, number of MV products and CPU times for $D A C G$-Newton algorithm with various $k_{\max }$ values for problem DBLP. Symbol $\ddagger$ stands for no convergence.

|  |  | DACG |  | Newton |  |  | TOT |  |
| :---: | ---: | :---: | :---: | ---: | ---: | ---: | ---: | ---: |
| ImAx $_{P C G}$ | $k_{\max }$ | its | CPU | outer its | MVP | CPU | MVP | CPU |
| 20 | 0 | 620 | 376.7 | $\ddagger$ | $\ddagger$ | $\ddagger$ | - | - |
|  | 1 | 620 | 376.7 | 172 | 3015 | 1696.8 | 3625 | 2073.5 |
|  | 3 | 620 | 376.7 | 153 | 2157 | 1239.7 | 2777 | 1616.4 |
|  | 5 | 620 | 376.7 | 191 | 2126 | 1189.0 | 2746 | 1565.7 |
|  | 10 | 620 | 376.7 | 156 | 1964 | 1147.7 | 2580 | 1524.4 |
| DACG |  | $\ddagger$ | $\ddagger$ |  |  |  | - | - |

the DACG-Newton method. Also the exit tests used in the two methods are identical for both the outer iteration and the inner PCG solver. In the JD implementation two parameters are crucial for its efficiency namely $m_{\min }$ and $m_{\max }$, the smallest and the largest dimension of the subspace where the Rayleigh Ritz projection takes place. After some attempts, we found that $m_{\min }=5$ and $m_{\max }=10$ were on the average the optimal values of such parameters. In all the examples and both solvers we set $\mathrm{Imax}_{P C G}=20$.

The results of the comparison are summarized in Table 6.1 where we also specify the tolerance $\tau_{D A C G}$ selected for each problem. It is found that the two methods behave very similarly, being Jacobi-Davidson slightly more performing on all the problems with the exception of matrix DBLP.

Table 6.1
Comparison between DACG-Newton and Jacobi-Davidson.

| problem | $n_{\text {eig }}$ | DACG-Newton |  |  |  | Jacobi-Davidson |  |  |
| :--- | :--- | :--- | :--- | ---: | ---: | ---: | ---: | ---: |
|  |  | $\tau_{D A C G}$ | MVP | outer its | CPU | MVP | outer its | CPU |
| HYB2D | 20 | 0.01 | 2241 | 87 | 6.76 | 1543 | 150 | 5.95 |
| MONTE-CARLO | 20 | 0.01 | 4042 | 114 | 33.36 | 2833 | 178 | 28.53 |
| DBLP | 20 | 0.1 | 2580 | 156 | 1524.40 | 2916 | 187 | 1698.00 |
| EMILIA-923 | 10 | 0.2 | 1487 | 63 | 2299.50 | 1472 | 95 | 2242.40 |

Regarding problem EMILIA-923 we provide in Figure 6.1 the plot of the relative residual norm vs cumulative linear iteration as per equation (4.2) for both DACG-Newton method (Newton phase only) and JD, corresponding to levels $j=1,2$ and 8 . We can appreciate the very similar convergence profiles of these two methods. The DACG-Newton algorithm is faster for lower $j$ values while the opposite holds for high values of $j$ where the Rayleigh-Ritz projection seems to win against the BFGS acceleration.
7. Concluding remarks. We have developed and theoretically analyzed a sequence of preconditioners aiming at accelerating the PCG method in the solution of the correction equation. This equation is to be solved at each Newton iteration to approximate a few eigenpairs of an SPD matrix. Both theoretical analysis and experimental results onto a heterogeneous set of test matrices reveal that the BFGS sequence of preconditioners greatly improves the PCG efficiency as compared to using an initially evaluated fixed preconditioner. The DACG-Newton method with the aforementioned preconditioner proves a robust and efficient algorithm for the partial eigensolution of SPD matrices and makes "pure" Newton method competitive with Jacobi-Davidson without making use of any Rayleigh-Ritz projection. On the average the latter method proves a little bit more performing than the one proposed in this work, and this is mainly due to the excessive DACG preprocessing time to devise a good initial vector for the subsequent Newton phase. However, we wonder whether the preconditioning technique studied in this work may be

Fig. 6.1. Convergence profile of the relative residual norm vs cumulative inner iterations for $D A C G$-Newton and JD methods. Matrix emilia-923. Eigenvalues $j=1$ (top figure), $j=2$ (middle figure) and $j=8$ (bottom figure).



seen as an alternative to Jacobi-Davidson or, rather, a possible improvement of it. At present we have neither theoretical nor experimental evidence in favor of this second option. We therefore let as future work the attempt to insert our preconditioner in the framework of the Jacobi-Davidson method. We will also compare the proposed algorithm with the recent implementations of Inexact Arnoldi's (Lanczos') method [23] where the inner linear system is solved with a variable accuracy depending on the closeness to the wanted eigenvector.

The sequence of linear systems (1.2), the correction equation, has in common with the normal equations to be solved at each interior point iteration the fact that the matrices involved get illconditioned as the iteration proceeds. The BFGS sequence of preconditioners developed in this paper is expected to perform well also for preconditioning the normal equations since:

1. The bounded deterioration property, proved in Theorem 3.7, is expected to mitigate the ill-conditioning of the linear systems toward the interior point solution.
2. The approach described in the previous sections allows to perform only a (either complete or inexact) factorization of the initial Jacobian, thus saving on the cost of subsequent factorizations which is know to represent the main computational burden [11] of the whole interior point method for large and sparse constrained optimization problems.

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