RATIONAL KRYLOV FOR NONLINEAR EIGENPROBLEMS, AN ITERATIVE PROJECTION METHOD

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Key words. nonlinear eigenvalue problem, rational Krylov, Arnoldi, projection method

AMS subject classification. 65F15, 65F50, 35P30

Abstract. In recent papers Ruhe [10], [12] suggested a rational Krylov method for nonlinear eigenproblems knitting together a secant method for linearizing the nonlinear problem and the Krylov method for the linearized problem. In this note we point out that the method can be understood as an iterative projection method. Similar to the Arnoldi method presented in [13], [14] the search space is expanded by the direction from residual inverse iteration. Numerical methods demonstrate that the rational Krylov method can be accelerated considerably by replacing an inner iteration by an explicit solver of projected problems.

1. Introduction.

In this note we consider the nonlinear eigenvalue problem

$$A(\lambda)x = 0 \tag{1.1}$$

where $A(\lambda) \in \mathbb{C}^{n\times n}$ is a family of matrices depending on a complex parameter $\lambda \in D \subset \mathbb{C}$. As in the linear case a parameter λ is called an eigenvalue of problem (1.1) if the equation (1.1) has a nontrivial solution $x \neq 0$ which is called an eigenvector corresponding to λ. We assume in this note that the matrix $A(\lambda)$ is large and sparse.

For sparse linear eigenproblems iterative projection methods where approximations to the wanted eigenvalues and corresponding eigenvectors are obtained from projections to subspaces which are expanded in the course of the algorithm are very efficient. Methods of this type are the Lanczos algorithm for symmetric problems, and Arnoldi's method and the Jacobi-Davidson method, e.g., for more general problems. Taking advantage of shift–and–invert techniques in Arnoldi's method one gets approximate eigenvalues closest to the shift. Ruhe [11] generalized this approach suggesting the rational Krylov method where several shifts are used in one run, thus getting good approximations to all eigenvalues in a union of regions around the shifts chosen.

In some sense, Ruhe [10] generalized the rational Krylov approach to sparse nonlinear eigenvalue problems by nesting the linearization of problem (1.1) by Lagrangean interpolation and the solution of the resulting linear eigenproblem by Arnoldi's method. Similar to the rational Krylov process he constructs a sequence V_k of subspaces of $\mathbb{C}^n$, and at the same time he updates Hessenberg matrices H_k which approximate the projection of $A(\sigma)^{-1}A(\lambda_k)$ to V_k. Here σ denotes a shift (which similarly as in the rational Krylov method for linear problems can be updated in the course of the algorithm) and λ_k an approximation to the wanted eigenvalue of (1.1). Then a Ritz vector x_k of H_k corresponding to an eigenvalue of small modulus approximates an eigenvector of the nonlinear problem from which a (hopefully) improved eigenvalue approximation of problem (1.1) is obtained.

To make the method converge Ruhe in [12] introduced an inner iteration which enforces the residual $r_k = A(\sigma)^{-1}A(\lambda_k)x_k$ to be orthogonal to the search space V_k,

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a property which is automatically satisfied for linear eigenproblems. This inner iteration is presented heuristically not noticing that it actually is nothing else but a solver of the projected nonlinear eigenproblem $V_k^H A(\sigma)^{-1}A(\lambda)V_k s = 0$. Thus, the rational Krylov method for nonlinear eigenproblems can be interpreted as an iterative projection method, where the inner iteration can be replaced by any solver of dense nonlinear eigenproblems, and numerical examples demonstrate that the method can be accelerated considerably in this way.

Although motivated in a completely different manner the search space V_k is expanded in the same way as in the Arnoldi method for nonlinear eigenproblems introduced in [13], [14]. However, differently from rational Krylov in the Arnoldi approach the original problem $A(\lambda)x = 0$ is projected to V_k. Thus, the nonlinear Arnoldi method preserves symmetry properties of problem (1.1), which can be exploited when solving the projected problems.

This note is organized as follows. Section 2 summarizes the rational Krylov method as introduced by Ruhe [10], [12]. In Section 3 we give the interpretation as an iterative projection method, and comment on modifications and improvements. Section 4 compares the original method as implemented in [4] with its modification where the inner iteration is replaced by a direct solver of the projected problem, and with the Arnoldi method for a rational eigenproblem governing the mechanical vibrations of a fluid–solid structure.

2. The rational Krylov method. In [10] Ruhe proposed the following rational Krylov method which was used by Hager and Wiberg [3] to solve a rational eigenvalue problem governing the damped vibrations of a structure using a constitutive law of a standard linear viscoelastic solid.

Linearizing the nonlinear family $A(\lambda)$ by Lagrange interpolation between two points σ and μ one gets

$$A(\lambda) = \frac{\lambda-\sigma}{\mu-\sigma}A(\mu) + \frac{\mu-\lambda}{\mu-\sigma}A(\sigma) + \text{higher order terms.} \tag{2.1}$$

Keeping σ fixed for several steps, iterating on μ and neglecting the remainder in the Lagrange interpolation one obtains

$$(A(\lambda_{j-1}) - \theta A(\sigma))x = 0, \quad \theta = \frac{\lambda_j - \lambda_{j-1}}{\lambda_j - \sigma}, \tag{2.2}$$

or equivalently the linear eigenproblem

$$(A(\sigma)^{-1}A(\lambda_{j-1}) - \theta I)x = 0, \quad \lambda_j = \lambda_{j-1} + \frac{\theta}{1-\theta}(\lambda_{j-1} - \sigma). \tag{2.3}$$

If the dimension n of problem (1.1) is small then this linear eigenproblem can be used to approximate an eigenvalue of the nonlinear problem, and choosing the smallest eigenvalue of (2.3) in modulus for every j one can expect convergence to an eigenvalue close to the initial approximation λ_1.

For large and sparse matrices Ruhe suggested to combine the linearization (2.3) with an Arnoldi process. Assume that the method has performed j steps, yielding approximations $\lambda_1, \ldots, \lambda_j$ to an eigenvalue, orthonormal vectors $v_1, \ldots, v_j$, and an upper Hessenberg matrix $H_{j,j-1} \in \mathbb{C}^{j\times(j-1)}$ such that the Arnoldi recursion

$$T(\lambda_{j-1})V_{j-1} = V_j H_{j,j-1}, \tag{2.4}$$

is fulfilled (at least approximately), where $T(\lambda) = A(\sigma)^{-1}A(\lambda)$, and $V_j = [v_1, \ldots, v_j]$.

In the linear case the Matrix $H_{j,j-1}$ would be expanded by adding one column at the right, and a zero row at the bottom, such that

$$\tilde{H}_{j+1,j} = \begin{pmatrix} H_{j,j-1} & k_j \\ 0 & \|r_\perp\| \end{pmatrix} \tag{2.5}$$

where $k_j = V_j^H r_j$, $r_j = T(\lambda_j)v_j$, and $r_\perp = r_j - V_j V_j^H v_j$. Due to the nonlinearity of $T(\cdot)$ however the next Arnoldi relation

$$T(\lambda_j)V_j = V_{j+1}\tilde{H}_{j+1,j} \tag{2.6}$$

with $v_{j+1} = r_\perp/\|r_\perp\|$ will not hold. From (2.1) it follows

$$T(\lambda_j) \approx \frac{\lambda_j - \sigma}{\lambda_{j-1} - \sigma} T(\lambda_{j-1}) - \frac{\lambda_j - \lambda_{j-1}}{\lambda_{j-1} - \sigma} I = \frac{1}{1-\theta} T(\lambda_{j-1}) - \frac{\theta}{1-\theta} I.$$

Therefore, Ruhe suggested to update H according to

$$H_{j+1,j} = \begin{pmatrix} \frac{1}{1-\theta} H_{j,j-1} - \frac{\theta}{1-\theta} I_{j,j-1} & k_j \\ 0 & \|r_\perp\| \end{pmatrix} \tag{2.7}$$

to maintain the approximate fulfillment of the Arnoldi recurrence. He arrived at a first version of the rational Krylov method in Algorithm 1. In step 5: $H_{j,j}$ denotes the submatrix of $H_{j+1,j}$ which is obtained by dropping the last row.

Algorithm 1 Rational Krylov method; preliminary version

1: Start with initial vector v_1 with $\|v_1\| = 1$, and initial λ_1 and σ
2: $r = A(\sigma)^{-1}A(\lambda_1)v_1$
3: **for** $j = 1, 2, \ldots$ until convergence **do**
4: orthogonalize $h_j = V^H r$, $r_\perp = r - Vh_j$, $h_{j+1,j} = \|r_\perp\|$
5: $\theta = \min$ eig $H_{j,j}$ with corresponding eigenvector s
6: $\lambda_{j+1} = \lambda_j + \frac{\theta}{1-\theta}(\lambda_j - \sigma)$
7: $H_{j+1,j} = \frac{1}{1-\theta} H_{j+1,j} - \frac{\theta}{1-\theta} I_{j+1,j}$
8: $v_{j+1} = r_\perp/\|r_\perp\|$
9: $r = A(\sigma)^{-1}A(\lambda_{j+1})v_{j+1}$
10: **end for**

Since the method turned out to be inefficient Ruhe [12] suggested to modify λ, H and s in an inner iteration until the residual $r = A(\sigma)^{-1}A(\lambda)V_j s$ is enforced to be orthogonal to V_j, and to expand the search space only after the inner iteration has converged.

If $H_{j,j}$ has already been updated according to step 7: then $H_{j,j}s = 0$, and with

$$k_j = V_j^H A(\sigma)^{-1}A(\lambda)V_j s = V_j^H r$$

we have approximately

$$A(\sigma)^{-1}A(\lambda)V_j \begin{bmatrix} I_{j-1} & \tilde{s} \\ 0 & s_j \end{bmatrix} = V_j[H_{j,j-1}\,,\, k_j] + re_j^T$$

where $\tilde{s}$ is the leading $j-1$ vector of s. Multiplying by the inverse of the matrix in brackets from the right and by V_j^H from the left one gets the new Hessenberg matrix

$$\hat{H}_{j,j} = [H_{j,j-1}\,,\, k_j] \begin{bmatrix} I_{j-1} & -s_j^{-1}\tilde{s} \\ 0 & s_j^{-1} \end{bmatrix} = [H_{j,j-1}\,,\, -s_j^{-1}H_{j,j-1}\tilde{s} + s_j^{-1}k_j],$$

and $H_{j,j-1}\tilde{s} + s_j h_s = 0$ finally yields that the last column of $H_{j,j}$ has to be replaced by $h_j + s_j^{-1}k_j$. Thereafter λ and H have to be updated according to steps 5: – 7: of Algorithm 1, and these steps have to be repeated until (hopefully) the residual has become orthogonal to the search space V_j.

The final version of the rational Krylov method is contained in Algorithm 2 where we neglected details about locking of converged eigenvalues, purging of unwanted directions in the search space, and updating of the pole σ.

Algorithm 2 Rational Krylov method; final version

1: start with initial vector $V = [v_1]$ with $\|v_1\| = 1$, initial λ and σ ; set $j = 1$
2: set $h_j = 0_j$; $s = e_j$; $x = v_j$;
3: compute $r = A(\sigma)^{-1}A(\lambda)x$ and $k_j = V_j^H r$
4: **while** $\|k_j\|$ >ResTol **do**
5: orthogonalize $r = r - V_j^H k_j$
6: set $h_j = h_j + k_j s_j^{-1}$
7: $\theta = \min$ eig $H_{j,j}$ with corresponding eigenvector s
8: $x = V_j s$
9: update $\lambda = \lambda + \frac{\theta}{1-\theta}(\lambda - \sigma)$
10: update $H_{j,j} = \frac{1}{1-\theta}H_{j,j} - \frac{1}{1-\theta}I$
11: compute $r = A(\sigma)^{-1}A(\lambda)x$ and $k_j = V_j^H r$
12: **end while**
13: compute $h_{j+1,j} = \|r\|$
14: **if** $|h_{j+1,j}s_j|$ >EigTol **then**
15: $v_{j+1} = r/h_{j+1,j}$; $j = j+1$; GOTO 2:
16: **end if**
17: Accept eigenvalue $\lambda_i = \lambda$ and eigenvector $x_i = x$
18: If more eigenvalues wanted, choose next θ and s, and GOTO 8:

3. Rational Krylov, an iterative projection method. Ruhe motivated the inner iteration and the requirement to make sure that the residual is orthogonal to the search space only by analogy to the linear case where it is satisfied automatically. Hager in his thesis [2] states: "The inner iteration is heuristically proposed, the condition for the inner iteration to converge and when it converges to what it actually converges are left to the domain of future research, we are looking forward to forthcoming papers of Ruhe." So, obviously both authors were not aware that the inner iteration is nothing else but a solver of the projected problem

$$V^H A(\sigma)^{-1}A(\lambda)Vs = 0. \tag{3.1}$$

We were not able to prove the local convergence of the inner iteration which can be rewritten as Algorithm 3. However the following Lemma is obvious.

LEMMA 3.1. *If the inner iteration converges, then it converges to a solution* $(\hat{\lambda}, x)$*,* $x = Vs$ *of the projected nonlinear eigenproblem (3.1).*

Algorithm 3 Inner iteration

1: Start with V such that $V^HV = I_j$, initial λ and σ and $H \approx V^HA(\sigma)^{-1}A(\lambda)V$
2: Replace last column of H by $k = V^HA(\sigma)^{-1}A(\lambda_1)v_j$
3: **for** $j = 1, 2, \ldots$ until convergence **do**
4: $\theta = \min$ eig H with corresponding eigenvector s
5: $\lambda_{j+1} = \lambda_j + \frac{\theta}{1-\theta}(\lambda_j - \sigma)$
6: $k = V^HA(\sigma)^{-1}A(\lambda_{j+1})Vs$
7: $H = \frac{1}{1-\theta}H - \frac{1}{1-\theta}I + \frac{1}{s_j}ke_j^T$
8: **end for**

Hence, the final version of rational Krylov is an iterative projection method where in every step the nonlinear eigenproblem $A(\sigma)^{-1}A(\lambda)x = 0$ is projected to a search space V, and V is expanded by (the orthogonal complement of) the the residual $r = A(\sigma)^{-1}A(\lambda)Vs$ of the Ritz pair (with respect to V), and one ends up with Algorithm 4

Algorithm 4 Rational Krylov method, an iterative projection method

1: start with initial vector $V = [v_1]$ with $\|v_1\| = 1$, initial λ and σ
2: **for** $j = 1, 2, \ldots$ until convergence **do**
3: solve projected eigenproblem $V^HA(\sigma)^{-1}A(\lambda)Vs = 0$ for (λ, s)
4: compute Ritz vector $x = Vs$ and residual $r = A(\sigma)^{-1}A(\lambda)x$
5: orthogonalize $r = r - VV^Hr$
6: expand searchspace $V = [V\ ,\ r/\|r\|]$
7: **end for**

Two observations are at hand. First, the inner iteration is a solver of a nonlinear eigenproblem (3.1) of small dimension. Hence, it can be replaced in STEP 3: of Algorithm 4 by any method for dense nonlinear eigenproblems like solvers taking advantage of the characteristic equation [5], [6], [17], inverse iteration [9], the method of successive linear problems [9] which are all quadratically convergent, or residual inverse iteration [7].

Secondly, expanding the search space it is not necessary to use the residual of the problem that is projected to the search space but every direction is fine which has a high approximation potential for the eigenvector wanted next. Following this line the second author in [13] proposed an iterative projection method for problem (1.1) expanding the search space by the orthogonal complement of $r = A(\sigma)^{-1}A(\lambda)Vs$ where (λ, Vs) is a Ritz pair of the projected problem

$$V^HA(\lambda)Vs = 0. \tag{3.2}$$

This choice was motivated by the residual inverse iteration which is known to converge linearly where the contraction constant satisfies $\mathcal{O}(|\sigma - \lambda|)$.

A further disadvantage when considering the projected problem (3.1) instead of (3.2) is the fact that symmetry properties of the underlying problem (1.1) are destroyed. If for instance $A(\cdot)$ is a family of real symmetric matrices such that the eigenvalues of problem (1.1) allow a minmax characterization then this property is inherited by the projected problems (3.2), and they can be solved efficiently by safeguarded iteration [15] which converges quadratically or even cubically. The Arnoldi method for this type of problems was proposed in [14]. Similarly symmetry properties

of the spectrum for conservative gyroscopic eigenproblems or Hamiltonian problems which can be exploited in the solution process of the projected problem are destroyed if problem (3.1) is used.

The numerical example in the next section demonstrates that the inner iteration in Algorithm 3 usually does not converge very fast, and the original rational Krylov method in Algorithm 2 is inferior to other iterative projection methods. However, there is one advantage of Ruhe's approach. The solvers for dense nonlinear eigenproblems need the explicit form of the projected problem (3.1) or (3.2) whereas Algorithm 2 only needs a procedure that yields the vector $A(\sigma)^{-1}A(\lambda)x$ for a given vector x.

4. Numerical experiments. To test the methods we consider a mathematical model which describes the problem governing free vibrations of a tube bundle immersed in a slightly compressible fluid under the following simplifying assumptions: The tubes are assumed to be rigid, assembled in parallel inside the fluid, and elastically mounted in such a way that they can vibrate transversally, but they can not move in the direction perpendicular to their sections. The fluid is assumed to be contained in a cavity which is infinitely long, and each tube is supported by an independent system of springs (which simulates the specific elasticity of each tube). Due to these assumptions, three-dimensional effects are neglected, and so the problem can be studied in any transversal section of the cavity. Considering small vibrations of the fluid (and the tubes) around the state of rest, it can also be assumed that the fluid is irrotational.

Mathematically this problem can be described in the following way (cf. [8], [1]). Let $\Omega \subset \mathbb{R}^2$ (the section of the cavity) be an open bounded set with locally Lipschitz continuous boundary Γ. We assume that there exists a family $\Omega_j \neq \emptyset$, $j = 1, \dots, K$, (the sections of the tubes) of simply connected open sets such that $\bar{\Omega}_j \subset \Omega$ for every j, $\bar{\Omega}_j \cap \bar{\Omega}_i = \emptyset$ for $j \neq i$, and each Ω_j has a locally Lipschitz continuous boundary Γ_j. With these notations we set $\Omega_0 := \Omega \setminus \bigcup_{j=1}^{K} \Omega_j$. Then the boundary of Ω_0 consists of $K+1$ connected components which are Γ and Γ_j, $j = 1, \dots, K$.

We denote by $H^1(\Omega_0) = \{u \in L^2(\Omega_0) : \nabla u \in L^2(\Omega_0)^2\}$ the standard Sobolev space equipped with the usual scalar product. Then the eigenfrequencies and the eigenmodes of the fluid-solid structure are governed by the following variational eigenvalue problem (cf. [8], [1])

Find $\lambda \in \mathbb{R}$ and $u \in H^1(\Omega_0)$ such that for every $v \in H^1(\Omega_0)$

$$c^2 \int_{\Omega_0} \nabla u \cdot \nabla v \, dx = \lambda \int_{\Omega_0} uv \, dx + \sum_{j=1}^{K} \frac{\lambda \rho_0}{k_j - \lambda m_j} \int_{\Gamma_j} un \, ds \cdot \int_{\Gamma_j} vn \, ds. \tag{4.1}$$

Here u is the potential of the velocity of the fluid, c denotes the speed of sound in the fluid, ρ_0 is the specific density of the fluid, k_j represents the stiffness constant of the spring system supporting tube j, m_j is the mass per unit length of the tube j, and n is the outward unit normal on the boundary of Ω_0.

We consider the rational eigenvalue problem (4.1) where Ω is the ellipse with center $(0,0)$ and length of semiaxes 8 and 4, and Ω_j, $j = 1, \dots, 9$ are circles with radius 0.3 and centers $(-4,-2)$, $(0,-2)$, $(4,-2)$, $(-5,0)$, $(0,0)$, $(5,0)$, $(-4,2)$, $(0,2)$ and $(4,2)$. We assume that all constants in problem (4.1) are equal to 1.

Discretizing problem (4.1) by finite elements one gets a rational matrix eigenvalue

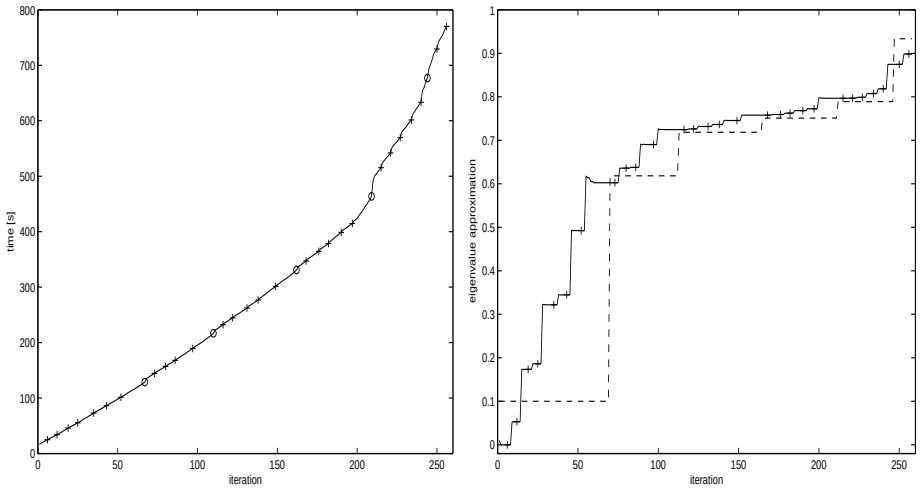

Fig. 1: Time consumption and convergence history for rational Krylov

problem

$$A(\lambda)x := -Ax + \lambda Bx + \frac{\lambda}{1-\lambda}Cx = 0 \tag{4.2}$$

where C collects the contributions of all tubes. A, B, and C are symmetric matrices, A and C are positive semidefinite, and B is positive definite. In our example the dimension is $n = 36040$.

Problem (4.2) has 28 eigenvalues $\lambda_1 \leq \cdots \leq \lambda_{28}$ in the interval $J_1 = (0, 1)$ (cf. [15]), and a large number of eigenvalues greater than 1.

We determined approximations to the eigenvalues in $[0, 1)$ by the rational Krylov method as implemented in [4], by the iterative projection method from Algorithm 4 where the projected rational eigenproblems were solved linearizing the equivalent quadratic eigenproblem $(1-\lambda)V^T A(\lambda)Vy = 0$, and by the nonlinear Arnoldi method from [14], i.e. the iterative projection method (3.2), where the projected problems were solved by safeguarded iteration. All three methods were able to find all 28 eigenvalues.

The experiments were run under MATLAB 6.5 on an Intel Centrino M processor with 1.7 GHz and 1 GB RAM. Figures 1 to 3 show the time consumption and the convergence history of the three methods where in every case the initial pole was chosen to be $\sigma = 0.1$, and the iteration was terminated if the residual was less than 10^{-6}. In all plots plus signs indicate found eigenvalues, and circles mark changes of the pole σ.

In the plots on the right the solid line indicates the total time consumption of the iteration, and in plots 2. and 3. the dashed lines mark the the time needed for solving the projected nonlinear eigenproblems, which is only a very small portion of the total CPU time. Replacing the inner iteration in Ruhe's approach by solving (3.2) directly reduces the computing time by more than 50 %, and the nonlinear Arnoldi method is even more efficient and needs only 11 % of the nonlinear rational Krylov method.

Neither the rational Krylov method in its original form nor its modification with an explicit solver of the projected problem (3.1) was able to determine eigenvalues larger than the pole of problem (4.2) in a systematic way. For different choices of initial

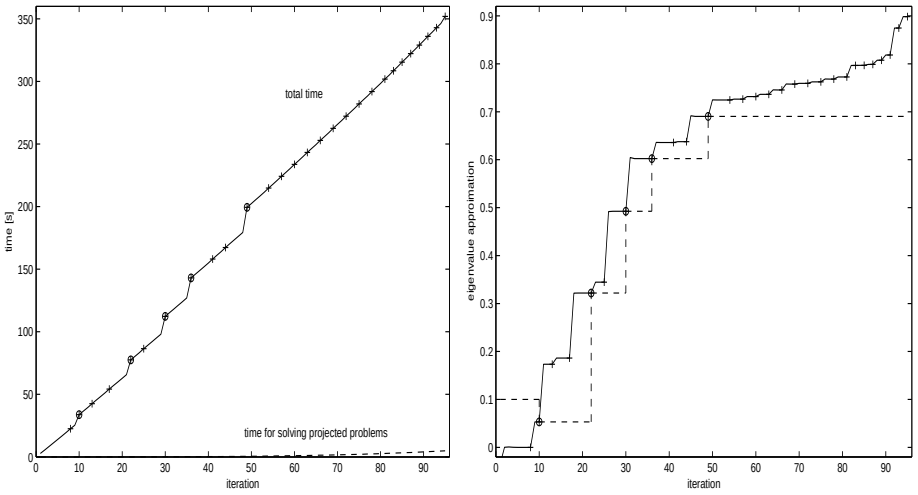

Fig. 2: Time consumption and convergence history for Algorithm 4

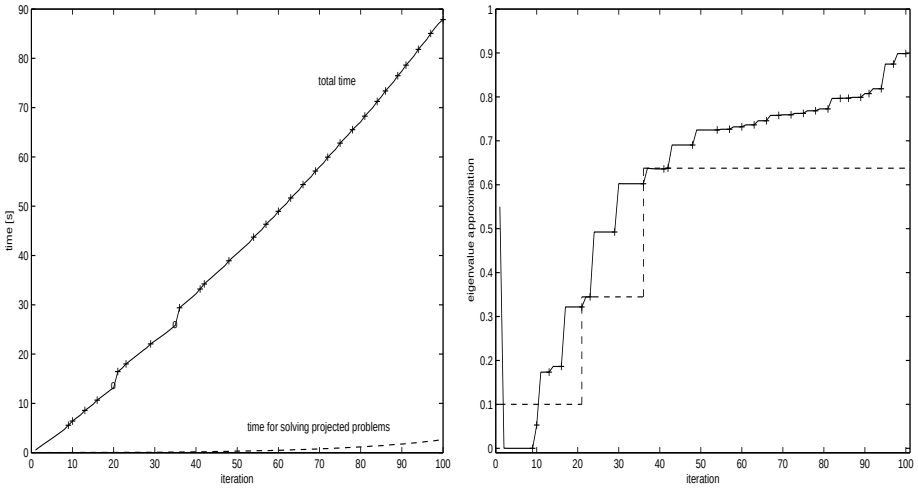

Fig. 3: Time consumption and convergence history for Arnoldi

approximations for σ and μ they both found only two or three eigenvalues before the diverged. The nonlinear Arnoldi method taking advantage of the symmetry of problem (4.2) and of the fact that its eigenvalues can be characterized as minmax values of a Rayleigh functional (cf. [16]) computed eigenvalues greater than 1 one after the other without problems. Figure 4 shows the time consumption and the convergence history of Arnoldi's method for the 15 eigenvalues in the interval $(1, 2.5)$.

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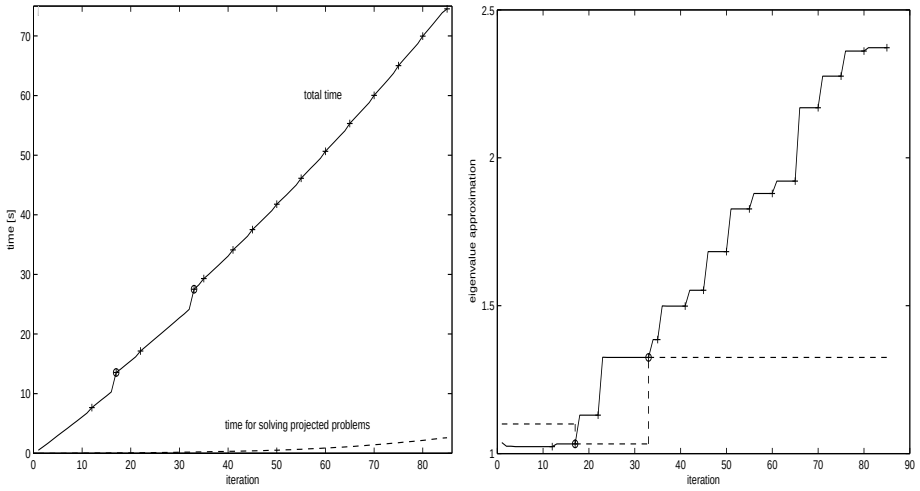

Fig. 4: Time consumption and convergence history for eigenvalues in $(1, 2.5)$

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