

# PROJECTION METHODS FOR NONLINEAR SPARSE EIGENVALUE PROBLEMS

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**Key words.** nonlinear eigenvalue problem, iterative projection method, Jacobi–Davidson method, Arnoldi method, rational Krylov method, automated multi-level substructuring

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**Abstract.** This paper surveys numerical methods for general sparse nonlinear eigenvalue problems with special emphasis on iterative projection methods like Jacobi–Davidson, Arnoldi or rational Krylov methods and the automated multi-level substructuring. We do not review the rich literature on polynomial eigenproblems which take advantage of a linearization of the problem.

**1. Introduction.** In this paper we consider the nonlinear eigenvalue problem

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

where  $T(\lambda) \in \mathbb{C}^{n \times n}$  is a family of matrices depending on a parameter  $\lambda \in D$ , and  $D \subset \mathbb{C}$  is an open set. As in the linear case,  $\lambda \in D$  is called an eigenvalue of problem (1.1) if equation (1.1) has a nontrivial solution  $x \neq 0$ . Then  $x$  is called an eigenvector corresponding to  $\lambda$ .

Nonlinear eigenvalue problems arise in a variety of applications. The most widely studied class in applications is the quadratic eigenvalue problem with

$$T(\lambda) := \lambda^2 M + \lambda C + K \tag{1.2}$$

that arises in the dynamic analysis of structures, see [30, 54, 77, 87] and the references therein. Here, typically the stiffness matrix  $K$  and the mass matrix  $M$  are real symmetric and positive (semi-)definite, and the damping matrix is general. In most applications one is interested in a small number of eigenvalues with largest real part. Another source for quadratic problems are vibrations of spinning structures yielding conservative gyroscopic systems [17, 33, 53, 113], where  $K = K^T$  and  $M = M^T$  are real positive (semi-)definite, and  $C = -C^T$  is real skew-symmetric. Then the eigenvalues are purely imaginary, and one is looking for a few eigenvalues which are closest to the origin.

There are many other applications leading to quadratic eigenvalue problems. A detailed survey has recently been given in [93].

Quadratic eigenvalue problems are special cases of polynomial eigenvalue problems

$$T(\lambda)x := \sum_{j=0}^k \lambda^j A_j x = 0 \tag{1.3}$$

with coefficients  $A_j$  in  $\mathbb{R}^{n \times n}$  or  $\mathbb{C}^{n \times n}$ . An important application of polynomial eigenvalue problems is the solution of optimal control problems which by the linear version of Pontryagin’s maximum principle lead to problem (1.3), see e.g. [67]. Other polynomial eigenvalue problems of higher degree than two arise when discretizing a linear

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eigenproblem by dynamic elements [77, 95, 96] or by least squares elements [79, 80], i.e. if one uses ansatz functions in a Rayleigh–Ritz approach which depend polynomially on the eigenparameter.

To determine the relevant energy states and corresponding wave functions of a three dimensional semiconductor quantum dot one has to determine the smallest eigenvalues and corresponding eigenfunctions of the Schrödinger equation

$$-\nabla \cdot \left( \frac{\hbar^2}{2m_j(\lambda)} \nabla u \right) + V_j u = \lambda u, \quad x \in \Omega_q \cup \Omega_m, \quad (1.4)$$

where  $\Omega_q$  and  $\Omega_m$  denote the domain occupied by the quantum dot and the surrounding matrix of a different material, respectively. For  $j \in \{m, q\}$ ,  $m_j$  is the electron effective mass and  $V_j$  the confinement potential. Assuming non-parabolicity for the electron's dispersion relation the electron effective mass  $m_j(\lambda)$  is constant on the quantum dot and the matrix for every fixed energy level  $\lambda$ , and is a rational function of  $\lambda$ . Discretizing (1.4) by finite element or finite volume methods yields a rational matrix eigenvalue problem [57, 58, 62, 106, 107].

Further rational eigenproblems

$$T(\lambda)x := -Kx + \lambda Mx + \sum_{j=1}^p \frac{\lambda}{\sigma_j - \lambda} C_j x = 0 \quad (1.5)$$

where  $K = K^T$  and  $M = M^T$  are positive definite, and  $C_j = C_j^T$  are matrices of small rank govern free vibration of plates with elastically attached masses [91, 98, 103] and vibrations of fluid solid structures [12, 13, 76, 100], and a similar problem

$$T(\lambda)x := -Kx + \lambda Mx + \lambda^2 \sum_{j=1}^p \frac{1}{\omega_j - \lambda} C_j x = 0 \quad (1.6)$$

arises when a generalized linear eigenproblem is condensed exactly [75, 94]. These problems (1.4), (1.5), and (1.6) have real eigenvalues which can be characterized as minmax values of a Rayleigh functional [98], and in all of these cases one is interested in a small number of eigenvalues at the lower end of the spectrum.

Another type of rational eigenproblem is obtained if free vibrations of a structure are modeled using a viscoelastic constitutive relation to describe the behavior of a material [36, 37]. A finite element model takes the form

$$T(\omega) := \left( \omega^2 M + K - \sum_{j=1}^k \frac{1}{1 + b_j \omega} \Delta K_j \right) x = 0 \quad (1.7)$$

where the stiffness and mass matrices  $K$  and  $M$  are positive definite,  $k$  denotes the number of regions with different relaxation parameters  $b_j$ , and  $\Delta K_j$  is an assemblage of element stiffness matrices over the region with the distinct relaxation constants.

In principle the rational problems (1.4), (1.5), (1.6), and (1.7) can be turned into polynomial eigenvalue problems by multiplying with an appropriate scalar polynomial in  $\lambda$ . Notice, however, that the degree of the polynomial can become very large and that roots of the denominators produce spurious eigenvalues (with very high multiplicity for (1.5)) which may hamper the numerical solution.

A genuine nonlinear dependence on the eigenparameter appears in dynamic element methods when using non-polynomial ansatz functions [77] or in the stability analysis of vibrating systems under state delay feedback control [18, 42, 43, 92].

Almost all these examples are finite dimensional approximations (typically finite element models) of operator eigenvalue problems and hence are large and sparse. Usually only a small number of eigenvalues in a specific region of the complex plane and associated eigenvectors are of interest. Numerical methods have to be adapted to these requirements and should exploit the sparsity of the coefficient matrices to be efficient in storage and computing time.

For linear sparse eigenproblems  $T(\lambda) = \lambda B - A$  very efficient methods are iterative projection methods (Lanczos method, Arnoldi method, Jacobi–Davidson method, e.g.), where approximations to the wanted eigenvalues and eigenvectors are obtained from projections of the eigenproblem to subspaces of small dimension which are expanded in the course of the algorithm. Essentially two types of methods are in use: methods which project the problem to a sequence of Krylov spaces like the Lanczos or the Arnoldi method [3], and methods which aim at a specific eigenpair expanding a search space by a direction which has a high approximation potential for the eigenvector under consideration like the Jacobi–Davidson method [3].

The Krylov subspace approaches take advantage of the linear structure of the underlying problem and construct an approximate incomplete Schur factorization (or incomplete spectral decomposition in the Hermitian case) from which they derive approximations to some of the extreme eigenvalues and corresponding eigenvectors, whereas the second type aims at the wanted eigenvalues one after the other using the Schur decomposition only to prevent the method from converging to eigenpairs which have been obtained already in a previous step.

For general nonlinear eigenproblems a normal form like the Schur factorization does not exist. Therefore, generalizations of iterative projection methods to general nonlinear eigenproblems always have to be of the second type. Krylov subspace methods can be applied only to nonlinear problems if they are equivalent to a linear eigenproblem. For instance, it is well known that every polynomial eigenproblem can be linearized in several ways [30, 54], one of them being the straightforward manner which results in an eigenproblem for a block Frobenius matrix. However, applying a Krylov subspace method to a linearization always increases the dimension of the problem by the factor  $k$  (the degree of the polynomial), and secondly symmetry properties which the original system may have in general are destroyed by linearization.

In this paper we review projection methods for general (i.e. not necessarily polynomial) sparse nonlinear eigenproblems. Although we have in mind sparse eigenproblems Section 2 summarizes methods for dense nonlinear eigenproblems which are needed in the projection methods in Sections 3 and 4. Iterative projection methods, which generalize the Jacobi–Davidson approach for linear problems in the sense that the search space in every step is expanded by a vector with high approximation potential for the eigenvector wanted next are presented in Section 3. Section 4 contains the generalization of the automated multi-level substructuring method to nonlinear eigenproblems. The paper closes with some numerical examples in Section 4 demonstrating the efficiency of projection methods.

**2. Methods for dense nonlinear eigenproblems.** In this section we review methods for dense nonlinear eigenproblems. The size of the problems that can be treated with these numerical methods is limited to a few thousand depending on the available storage capacities. Moreover, they require several factorizations of varying matrices to approximate one eigenvalue, and therefore, they are not appropriate for large and sparse problems. However, they are needed to solve the projected eigenproblem in most of the iterative projection methods for sparse problems. These iterative

projection methods make use of the sparse matrix structure and typically require only matrix vector multiplication with the coefficient matrices plus possibly sparse approximate factorizations of matrices, when shift-and-invert is used to get eigenvalues in the interior of the spectrum. Again here the available storage sets the limit for the system sizes that can be dealt with. Using the sparsity and the symmetry structure of the coefficient matrices, nowadays problems of size on the order of  $n = 10^7$  can be treated.

For general nonlinear eigenvalue problems, the classical approach is to formulate the eigenvalue problem as a system of nonlinear equations and to use variations of Newton's method or the inverse iteration method.

For the characteristic equation

$$\det T(\lambda) = 0. \quad (2.1)$$

it was suggested in [50, 51] to use a  $QR$ -decomposition with column pivoting  $T(\lambda)P(\lambda) = Q(\lambda)R(\lambda)$ , where  $P(\lambda)$  is a permutation matrix which is chosen such that the diagonal elements  $r_{jj}(\lambda)$  of  $R(\lambda)$  are decreasing in magnitude, i.e.  $|r_{11}(\lambda)| \geq |r_{22}(\lambda)| \geq \dots \geq |r_{nn}(\lambda)|$ . Then  $\lambda$  is an eigenvalue if and only if  $r_{nn}(\lambda) = 0$ .

Applying Newton's method to this equation, one obtains the iteration

$$\lambda_{k+1} = \lambda_k - \frac{1}{e_n^H Q(\lambda_k)^H T'(\lambda_k) P(\lambda_k) R(\lambda_k)^{-1} e_n}. \quad (2.2)$$

for approximations to an eigenvalue of problem (2.1), where  $e_n$  denotes the  $n$ -th unit vector. Approximations to left and right eigenvectors can be obtained from

$$y_k = Q(\lambda_k) e_n \quad \text{and} \quad x_k = P(\lambda_k) R(\lambda_k)^{-1} e_n.$$

An improved version of this method was suggested in [44, 45], and a similar approach was presented in [114] via a representation of Newton's method using the LU factorization of  $T(\lambda)$ . However, this relatively simple idea is not efficient, since it computes eigenvalues one at a time and needs several  $\mathcal{O}(n^3)$  factorizations per eigenvalue. It is, however, useful in the context of iterative refinement of computed eigenvalues and eigenvectors.

Another method that also solves the purpose of iterative refinement is the nonlinear version of inverse iteration. For linear eigenproblems  $Ax = \lambda x$  it is well known that inverse iteration is equivalent to Newton's method applied to the nonlinear system

$$\begin{pmatrix} Ax - \lambda x \\ v^H x - 1 \end{pmatrix} = 0$$

where  $v \in \mathbb{C}^n$  is suitably chosen. Correspondingly, for the nonlinear problem

$$F(x, \lambda) := \begin{pmatrix} T(\lambda)x \\ v^H x - 1 \end{pmatrix} = 0 \quad (2.3)$$

one step of Newton's method yields

$$\begin{pmatrix} T(\lambda_k) & T'(\lambda_k)x_k \\ v^H & 0 \end{pmatrix} \begin{pmatrix} x_{k+1} - x_k \\ \lambda_{k+1} - \lambda_k \end{pmatrix} = - \begin{pmatrix} T(\lambda_k)x_k \\ v^H x_k - 1 \end{pmatrix}. \quad (2.4)$$

The first component gives

$$x_{k+1} = -(\lambda_{k+1} - \lambda_k) T(\lambda_k)^{-1} T'(\lambda_k) x_k, \quad (2.5)$$

i.e. the direction of the new approximation to an eigenvector is  $u_{k+1} := T(\lambda_k)^{-1}T'(\lambda_k)x_k$ . Assuming that  $x_k$  is already normalized by  $v^H x_k = 1$  the second component of (2.4) reads  $v^H x_{k+1} = v^H x_k$ , and multiplying equation (2.5) by  $v^H$  yields

$$\lambda_{k+1} = \lambda_k - \frac{v^H x_k}{v^H u_{k+1}}.$$

Hence, for nonlinear eigenproblems inverse iteration obtains the form given in Algorithm 1.

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**Algorithm 1** Inverse iteration

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- 1: Start with  $\lambda_0, x_0$  such that  $v^H x_0 = 1$
  - 2: **for**  $k = 0, 1, 2, \dots$  until convergence **do**
  - 3:   solve  $T(\lambda_k)u_{k+1} = T'(\lambda_k)x_k$  for  $u_{k+1}$
  - 4:    $\lambda_{k+1} = \lambda_k - (v^H x_k)/(v^H u_{k+1})$
  - 5:   normalize  $x_{k+1} = u_{k+1}/v^H u_{k+1}$
  - 6: **end for**
- 

This algorithm (being a variant of Newton's method) converges locally and quadratically to  $(x, \lambda)$  [1, 72].

The normalization condition can be updated in each step of inverse iteration. It was suggested in [81] to use  $v_k = T(\lambda_k)^H y_k$  for the normalization, where  $y_k$  is an approximation to a left eigenvector. Then the update for  $\lambda$  becomes

$$\lambda_{k+1} = \lambda_k - \frac{y_k^H T(\lambda_k)x_k}{y_k^H T'(\lambda_k)x_k},$$

which is the Rayleigh functional for general nonlinear eigenproblems proposed in [54], and which can be interpreted as one Newton step for solving the equation  $f_k(\lambda) := y_k^H T(\lambda)x_k = 0$ . For linear Hermitian eigenproblems this gives cubic convergence if  $\lambda_k$  is updated by the Rayleigh quotient [15, 74]. The same is true [79] for symmetric nonlinear eigenproblems having a Rayleigh functional if we replace statement 4 in Algorithm 1 by  $\lambda_{k+1} = p(u_{k+1})$ , where  $p(u_{k+1})$  denotes the real root of  $u_{k+1}^H T(\lambda)u_{k+1} = 0$  closest to  $\lambda_k$ .

In [71] Newton's method is considered for the complex function  $\beta(\lambda)$  defined by

$$T(\lambda)u = \beta(\lambda)x, \quad s^H u = \kappa,$$

where  $\kappa$  is a given constant, and  $x$  and  $u$  are given vectors. This approach generalizes the method (2.2), inverse iteration, and a method proposed in [73]. It was proved that the rate of convergence is quadratic, and that cubic convergence can be obtained if not only  $\lambda$ , but also  $x$  and/or  $s$  are updated appropriately, thus unifying the results in [1, 50, 51, 54, 72, 73].

The disadvantage of inverse iteration with respect to efficiency is the large number of factorizations that are needed for each of the eigenvalues. The obvious idea then is to use a simplified version of inverse iteration, and to solve the linear system  $T(\sigma)u_{k+1} = T'(\lambda_k)u_k$  for  $u_{k+1}$  in step 3 of Algorithm 1 for some fixed shift  $\sigma$  close to the wanted eigenvalues. For linear problems  $T(\lambda) = A - \lambda I$  this method converges (although only linearly) to an eigenpair of  $Ax = \lambda x$ . In the nonlinear case it converges to an eigenpair of the linear problem  $T(\sigma)x = \gamma T'(\tilde{\lambda})x$  ( $\gamma \neq 0$  and  $\tilde{\lambda}$  depending on the

normalization condition) from which we can not recover an eigenpair of the nonlinear problem (1.1).

A remedy against this wrong convergence was proposed in [70]. Assuming that  $T(\lambda)$  is twice continuously differentiable, then Algorithm 1 gives

$$\begin{aligned} x_k - x_{k+1} &= x_k + (\lambda_{k+1} - \lambda_k)T(\lambda_k)^{-1}T'(\lambda_k)x_k \\ &= T(\lambda_k)^{-1}(T(\lambda_k) + (\lambda_{k+1} - \lambda_k)T'(\lambda_k))x_k \\ &= T(\lambda_k)^{-1}T(\lambda_{k+1})x_k + \mathcal{O}(|\lambda_{k+1} - \lambda_k|^2). \end{aligned}$$

Neglecting the second order term one gets

$$x_{k+1} = x_k - T(\lambda_k)^{-1}T(\lambda_{k+1})x_k.$$

The advantage of this approach is that replacing  $\lambda_k$  by a fixed shift  $\sigma$  does not lead to misconvergence. The method can be implemented as in Algorithm 2, see [70]

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**Algorithm 2** Residual inverse iteration

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- 1: Let  $v$  be a normalization vector and start with an approximations  $\sigma$  and  $x_1$  to an eigenvalue and corresponding eigenvector of (1.1) such that  $v^H x_1 = 1$
  - 2: **for**  $k = 1, 2, \dots$  until convergence **do**
  - 3:   solve  $v^H T(\sigma)^{-1}T(\lambda_{k+1})x_k = 0$  for  $\lambda_{k+1}$   
       or set  $\lambda_{k+1} = p(x_k)$  if  $T(\lambda)$  is Hermitian and  $\lambda_{k+1}$  is real
  - 4:   compute the residual  $r_k = T(\lambda_{k+1})x_k$
  - 5:   solve  $T(\sigma)d_k = r_k$  for  $d_k$
  - 6:   set  $z_{k+1} = x_k - d_k$
  - 7:   normalize  $x_{k+1} = z_{k+1}/v^H z_{k+1}$
  - 8: **end for**
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If  $T(\lambda)$  is twice continuously differentiable, if  $\hat{\lambda}$  is a simple zero of  $\det T(\lambda) = 0$ , and if  $\hat{x}$  is an eigenvector normalized by  $v^H \hat{x} = 1$ , then the residual inverse iteration converges for all  $\sigma$  sufficiently close to  $\hat{\lambda}$ , and one has the estimate

$$\frac{\|x_{k+1} - \hat{x}\|}{\|x_k - \hat{x}\|} = \mathcal{O}(|\sigma - \hat{\lambda}|) \quad \text{and} \quad |\lambda_{k+1} - \hat{\lambda}| = \mathcal{O}(\|x_k - \hat{x}\|^q),$$

where  $q = 2$  if  $T(\lambda)$  is Hermitian,  $\hat{\lambda}$  is real, and  $\lambda_{k+1}$  solves  $x_k^H T(\lambda_{k+1})x_k = 0$  in Step 3, and  $q = 1$  otherwise, see [70].

A variant of this approach is the method of successive linear approximations suggested in [81].

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**Algorithm 3** Method of successive linear problems

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- 1: Start with an approximation  $\lambda_1$  to an eigenvalue of (1.1)
  - 2: **for**  $k = 1, 2, \dots$  until convergence **do**
  - 3:   solve the linear eigenproblem  $T(\lambda_k)u = \theta T'(\lambda_k)u$
  - 4:   choose an eigenvalue  $\theta$  smallest in modulus
  - 5:    $\lambda_{k+1} = \lambda_k - \theta$
  - 6: **end for**
- 

If  $T$  is twice continuously differentiable, and  $\hat{\lambda}$  is an eigenvalue of problem (1.1) such that  $T'(\hat{\lambda})$  is nonsingular and 0 is an algebraically simple eigenvalue of  $T'(\hat{\lambda})^{-1}T(\hat{\lambda})$ , then the method in Algorithm 3 converges quadratically to  $\hat{\lambda}$ , see [105].

The discussed versions of inverse iteration apply to general nonlinear eigenproblems, although for Hermitian problems and real eigenvalues inverse iteration and residual inverse iteration converge faster if the eigenvalue approximations are updated using the Rayleigh functional. For Hermitian problems that allow a variational characterization of their eigenvalues [16, 34, 35, 78, 99, 101, 109], an alternative is to use the safeguarded iteration. The method was introduced in [112] for overdamped problems, and was studied in [110] for the nonoverdamped case.

Let  $J \subset \mathbb{R}$  be an open interval which may be unbounded, and assume that  $T(\lambda) \in \mathbb{C}^{n \times n}$  is a family of Hermitian matrices the elements of which are differentiable. Suppose that for every  $x \in \mathbb{C}^n \setminus \{0\}$  the real equation

$$f(\lambda, x) := x^H T(\lambda) x = 0 \quad (2.6)$$

has at most one solution  $\lambda \in J$ . Then equation (2.6) defines a functional  $p$  on some subset  $D \subset \mathbb{C}^n$  which obviously generalizes the Rayleigh quotient for linear pencils  $T(\lambda) = \lambda B - A$ , and which is called the Rayleigh functional of the nonlinear eigenvalue problem (1.1). If one assumes further that  $x^H T'(p(x)) x > 0$  for every  $x \in D$  (generalizing the definiteness requirement for linear pencils), then by the implicit function theorem  $D$  is an open set, and differentiating the identity  $x^H T(p(x)) x = 0$  one obtains, that the eigenvectors of (1.1) are stationary points of  $p$ .

Under these conditions in [109] a minmax principle for the nonlinear eigenproblem (1.1) was proved if the eigenvalues are enumerated appropriately. A value  $\lambda \in J$  is an eigenvalue of (1.1) if and only if  $\mu = 0$  is an eigenvalue of the matrix  $T(\lambda)$ , and by Poincaré's maxmin principle there exists  $m \in \mathbb{N}$  such that

$$0 = \max_{\dim V=m} \min_{x \in V, x \neq 0} \frac{x^H T(\lambda) x}{\|x\|^2}.$$

Then one assigns this  $m$  to  $\lambda$  as its number and calls  $\lambda$  an  $m$ -th eigenvalue of problem (1.1).

Under the above assumptions it was shown in [109] that for every  $m \in \{1, \dots, n\}$  problem (1.1) has at most one  $m$ -th eigenvalue in  $J$ , which can be characterized by

$$\lambda_m = \min_{\dim V=m, D \cap V \neq \emptyset} \sup_{v \in D \cap V} p(v). \quad (2.7)$$

Conversely, if

$$\lambda_m := \inf_{\dim V=m, D \cap V \neq \emptyset} \sup_{v \in D \cap V} p(v) \in J, \quad (2.8)$$

then  $\lambda_m$  is an  $m$ -th eigenvalue of (1.1), and the characterization (2.7) holds. The minimum is attained by the invariant subspace of  $T(\lambda_m)$  corresponding to its  $m$  largest eigenvalues, and the supremum is attained by any eigenvector of  $T(\lambda_m)$  corresponding to  $\mu = 0$ .

The enumeration of eigenvalues and the fact that the eigenvectors of (1.1) are the stationary vectors of the Rayleigh functional suggests the Algorithm 4 called safeguarded iteration for computing the  $m$ -th eigenvalue.

It was shown in [105, 110] that the safeguarded iteration has the following convergence properties.

- (i) If  $\lambda_1 := \inf_{x \in D} p(x) \in J$  and  $x_1 \in D$  then the safeguarded iteration converges globally to  $\lambda_1$ .

**Algorithm 4** Safeguarded iteration

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- 1: Start with an approximation  $\sigma_1$  to the  $m$ -th eigenvalue of (1.1)
  - 2: **for**  $k = 1, 2, \dots$  until convergence **do**
  - 3:   determine an eigenvector  $x_k$  corresponding to the  $m$ -largest eigenvalue of  $T(\sigma_k)$
  - 4:   solve  $x_k^H T(\sigma_{k+1}) x_k = 0$  for  $\sigma_{k+1}$
  - 5: **end for**
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- (ii) If  $\lambda_m \in J$  is a  $m$ -th eigenvalue of (1.1) which is simple, then the safeguarded iteration converges locally and quadratically to  $\lambda_m$ .
- (iii) Let  $T(\lambda)$  be twice continuously differentiable, and assume that  $T'(\lambda)$  is positive definite for  $\lambda \in J$ . If  $x_k$  in step 3 of Algorithm 4 is chosen to be an eigenvector corresponding to the  $m$  largest eigenvalue of the generalized eigenproblem  $T(\sigma_k)x = \mu T'(\sigma_k)x$ , then the convergence is even cubic.

**3. Iterative projection methods.** For sparse linear eigenvalue problems

$$Ax = \lambda x \tag{3.1}$$

iterative projection methods like the Lanczos, Arnoldi, rational Krylov or Jacobi–Davidson method are well established. The basic idea of all these methods is the construction of a search space followed by projection of problem (3.1) onto this subspace. This leads to a small dense problem that is then handled by one of the standard techniques, and the eigenvalues of the projected problem are used as approximations to the eigenvalues of the large sparse problem. The main feature of all these methods is that matrix factorizations are avoided as much as possible and the generation of the search space is usually done via an iterative procedure that is based on matrix vector products that can be cheaply obtained.

Two basic types of iterative projection methods are in use: The first type consists of methods that take advantage of the linear structure of the underlying problem and construct an approximate incomplete Schur factorization. It expands the subspaces independently of the eigenpair of the projected problem and uses Krylov subspaces of  $A$  or  $(A - \sigma I)^{-1}$  for some shift  $\sigma$ . These methods include the Arnoldi, Lanczos or rational Krylov method. The other type of methods aim at a particular eigenpair and choose the expansion such that it has a high approximation potential for a desired eigenvalue/eigenvector or invariant subspace. An example for this approach is the Jacobi–Davidson method.

The Arnoldi method together with its variants is a standard solver for sparse linear eigenproblems. A detailed discussion is contained in [3]. It is implemented in the package ARPACK [56] and the MATLAB command `eigs`. The method typically converges to the extreme eigenvalues first. If one is interested in eigenvalues in the interior of the spectrum, or eigenvalues close to a given focal point  $\sigma$ , one can apply the method in a shift-and-invert fashion, i.e. to the matrix  $(A - \sigma I)^{-1}$ . In this case one has to determine a factorization of  $A - \sigma I$  which, however, may be prohibitive for very large problems.

An obvious idea is, to use an inner–outer iteration, and to solve linear systems  $(A - \sigma I)x = r$  only approximately by an iterative method. However, methods like the Lanczos algorithm and the Arnoldi algorithm are very sensitive to perturbations in the iterations, and therefore they require highly accurate solutions of these linear systems. Therefore, the inner–outer iterations may not offer an efficient approach for these methods (see [31, 32, 52, 55, 66]).

A way out of this dilemma is the Jacobi–Davidson method. Let  $(x, \theta)$  be an approximation to an eigenpair obtained by a projection method with subspace  $V$ . We assume that  $\|x\| = 1$ ,  $\theta = x^H A x$ , and  $r := Ax - \theta x \perp x$ . Then a suitable candidate for expanding the search space is  $v := (A - \theta I)^{-1} r$  which corresponds to one step of inverse iteration with initial guess  $(x, \theta)$ . Unfortunately, for truly large problems this vector is unavailable, and one has to employ an iterative method to solve the linear system  $(A - \theta I)v = r$  approximately.

If  $x$  is already close to an eigenvector  $\hat{x}$ , and  $v$  usually even closer to  $\hat{x}$ , then the plane  $\text{span}\{x, v + e\}$  can be far away from  $\text{span}\{x, v\}$  even for a small perturbation  $e$  (i.e. the angle between these two planes can be quite large), and then the projection to the expanded space will not yield an essential progress of accuracy.

Clearly,  $\text{span}\{x, x + \alpha v\} = \text{span}\{x, v\}$  for every  $\alpha \neq 0$ , and if  $\alpha$  is chosen such that  $x$  and  $x + \alpha v$  are orthogonal, then the angle between  $\text{span}\{x, v\}$  and  $\text{span}\{x, x + \alpha v + e\}$  will be quite small for a small perturbation  $e$  of  $x + \alpha v$ . Hence, replacing  $v$  by  $x + \alpha v$  increases the robustness of the iterative projection method (cf. [108]), and if  $V$  is expanded by an inexact representation of  $x + \alpha v$  with small error  $e$ , one can still expect similar convergence properties as for inverse iteration.

If  $\alpha$  is chosen such that  $x$  and  $z = x + \alpha v$  are orthogonal, i.e.

$$z = x - \frac{x^H x}{x^H (A - \theta I)^{-1} x} (A - \theta I)^{-1} r,$$

then  $z$  solves the linear system, called correction equation

$$(I - x x^H)(A - \theta I)(I - x x^H)z = -r, \quad z \perp x. \quad (3.2)$$

The resulting iterative projection method called Jacobi–Davidson method was introduced in [90] in a completely different way, and it is well established for very large eigenproblems.

Both, the shift-and-invert Arnoldi method and the Jacobi–Davidson method have to solve a large linear system. However, while in the Arnoldi method this system in general needs to be solved very accurately to get fast convergence, numerical experiments demonstrate that in the Jacobi–Davidson method it suffices to solve this system approximately to maintain fast convergence. Typically only a small number of steps of a preconditioned Krylov subspace method are sufficient to obtain a good expansion  $z$  for the search space  $V$ .

Details of the Jacobi–Davidson method for various types of linear eigenvalue problems can be found in [3]. Implementations in FORTRAN and MATLAB can be downloaded from <http://www.math.ruu.nl/people/sleijpen>.

Many, but not all of the ideas in these projection methods can be generalized also to nonlinear eigenproblems. In the following we discuss generalizations of iterative projection methods to nonlinear eigenproblems. There are many papers on Arnoldi’s method for polynomial and in particular quadratic eigenvalue problems taking advantage of linearization, i.e. their equivalence to linear eigenproblems of higher dimension. Recently, several structure preserving methods of this type have been developed [2, 4, 9, 25, 29, 38, 39, 40, 41, 60, 59, 65, 68, 69, 93, 111]. We will not consider methods for polynomial eigenvalue problems based on linearization here, but we will only discuss iterative projection methods which are applied directly to the general nonlinear eigenproblem (1.1). We already pointed out that in this case the search spaces have to be expanded by directions that have a high approximation potential for the next wanted eigenvector.

Assume that  $V$  is an orthonormal basis of the current search space. Let  $(\theta, y)$  be a solution of the projected problem  $V^H T(\lambda) V y = 0$ , and let  $x = Vy$  be the corresponding Ritz vector. Then there are two candidates for expanding  $V$  suggested by the methods in Section 2:  $\tilde{v} = T(\theta)^{-1} T'(\theta) x$  motivated by inverse iteration, and  $\hat{v} = x - T^{-1}(\sigma) T(\theta) x$  corresponding to residual inverse iteration.

The following two subsections will take advantage of these directions. Expanding a given search space  $V$  by  $\tilde{v}$  results in the Jacobi–Davidson method considered in Subsection 3.1, and expanding it by  $\hat{v}$  yields an Arnoldi type methods treated in Subsection 3.2.

**3.1. Jacobi–Davidson method.** For the robustness reasons already discussed for linear eigenproblems in Section 3 we do not expand the current search space  $V$  by the direction of inverse iteration, i.e.  $\tilde{v} = T(\theta)^{-1} T'(\theta) x$ , but by  $z := x + \alpha \tilde{v}$  where  $\alpha$  is chosen such that  $x$  and  $z$  are orthogonal, i.e.

$$z = x + \alpha \tilde{v}, \quad \alpha = -\frac{x^H x}{x^H T(\theta)^{-1} T'(\theta) x}.$$

Then  $z$  solves the correction equation

$$\left( I - \frac{T'(\theta) x x^H}{x^H T'(\theta) y} \right) T(\theta) \left( I - \frac{x x^H}{x^H x} \right) z = T(\theta) x, \quad z \perp x. \quad (3.3)$$

As in the linear case (3.3) does not have to be solved exactly to maintain fast convergence, but usually a few steps of a Krylov subspace solver with an appropriate preconditioner suffice to obtain a good expansion direction of the search space. This natural generalization of the Jacobi–Davidson method was suggested in [88, 89] for polynomial eigenvalue problems, and was studied in [10, 104] for general nonlinear eigenproblems.

In the correction equation (3.3) the operator  $T(\theta)$  is restricted to map the subspace  $x^\perp$  into itself. Hence, if  $K \approx T(\theta)$  is a preconditioner of  $T(\theta)$  then a preconditioner for an iterative solver of (3.3) should be modified correspondingly to

$$\tilde{K} := \left( I - \frac{T'(\theta) x x^H}{x^H T'(\theta) x} \right) K \left( I - \frac{x x^H}{x^H x} \right).$$

With left-preconditioning equation (3.3) becomes

$$\tilde{K}^{-1} \tilde{T}(\theta) z = -\tilde{K}^{-1} r, \quad z \perp x. \quad (3.4)$$

where

$$\tilde{T}(\theta) := \left( I - \frac{T'(\theta) x x^H}{x^H T'(\theta) x} \right) T(\theta) \left( I - \frac{x x^H}{x^H x} \right).$$

It was already pointed out in [90] for linear eigenproblems that taking into account the projectors in the preconditioner, i.e. using  $\tilde{K}$  instead of  $K$  in a preconditioned Krylov solver, raises the cost only slightly. In every step one has to solve one linear system  $Kw = y$ , and to initialize the solver requires only one additional solve.

A template for the Jacobi–Davidson method for the nonlinear eigenvalue problem (1.1) is given in Algorithm 5. In the following we comment on some of its steps. A detailed discussion is contained in [10, 104].

**Algorithm 5** Nonlinear Jacobi–Davidson method

- 
- 1: Start with an initial basis  $V$ ,  $V^H V = I$ ;  $m = 1$
  - 2: determine preconditioner  $K \approx T(\sigma)^{-1}$ ,  $\sigma$  close to first wanted eigenvalue
  - 3: **while**  $m \leq$  number of wanted eigenvalues **do**
  - 4:   compute an approximation to the  $m$ -th wanted eigenvalue  $\lambda_m$  and corresponding eigenvector  $x_m$  of the projected problem  $V^H T(\lambda) V x = 0$
  - 5:   determine the Ritz vector  $u = V x_m$  and the residual  $r = T(\lambda_m)u$
  - 6:   **if**  $\|r\|/\|u\| < \epsilon$  **then**
  - 7:     accept approximate eigenpair  $(\lambda_m, u)$ ; increase  $m \leftarrow m + 1$ ;
  - 8:     reduce search space  $V$  if indicated
  - 9:     determine new preconditioner  $K \approx T(\lambda_m)^{-1}$  if necessary
  - 10:    choose approximation  $(\lambda_m, u)$  to next eigenpair
  - 11:    compute residual  $r = T(\lambda_m)u$ ;
  - 12:   **end if**
  - 13: Find approximate solution of correction equation
- 

$$\left(I - \frac{T'(\lambda_m)uu^H}{u^H T'(\lambda_m)u}\right)T(\sigma)\left(I - \frac{uu^H}{u^H u}\right)z = -r \quad (3.5)$$

(by preconditioned Krylov solver, e.g.)

- 14: orthogonalize  $z = z - VV^H z$ ,  $v = z/\|z\|$ , and expand subspace  $V = [V, v]$
  - 15: update projected problem
  - 16: **end while**
- 

- (i) In step 1 of Algorithm 5 any preinformation such as a small number of known approximate eigenvectors of problem (1.1) corresponding to eigenvalues close to  $\sigma$  or of eigenvectors of a contiguous problem can and should be used.

If no information on eigenvectors is at hand, and if one is interested in eigenvalues close to the parameter  $\sigma \in D$ , one can choose an initial vector at random, execute a few Arnoldi steps for the linear eigenproblem  $T(\sigma)u = \theta u$  or  $T(\sigma)u = \theta T'(\sigma)u$ , and choose the eigenvector corresponding to the smallest eigenvalue in modulus or a small number of Schur vectors as initial basis of the search space. Starting with a random vector without this preprocessing usually will yield a value  $\lambda_m$  in step 4 which is far away from  $\sigma$  and will avert convergence.

For certain rational eigenproblems governing free vibrations of fluid–solid structures, and of plates with elastically attached masses where the rational term is of small rank we discussed the choice of the initial space  $V$  for the nonlinear Arnoldi method in [64, 98]. These considerations are valid for the Jacobi–Davidson method, as well.

- (ii) Preconditioning is a key to a successful iterative solver. A comprehensive exposition of many useful preconditioning techniques can be found in [11, 86].
- (iii) As the subspaces expand in the course of the algorithm the increasing storage or the computational cost for solving the projected eigenvalue problems may make it necessary to restart the algorithm and purge some of the basis vectors. Since a restart destroys information on the eigenvectors and particularly on the one the method is just aiming at, we restart only if an eigenvector has just converged.

An obvious way to restart is to determine a Ritz pair  $(\mu, u)$  from the projection

to the current search space  $\text{span}(V)$  approximating an eigenpair wanted next, and to restart the Jacobi–Davidson method with this single vector  $u$ . However, this may discard too much valuable information contained in  $\text{span}(V)$ , and may slowdown the speed of convergence too much. Therefore, thick restarts with subspaces spanned by the Ritz vector  $u$  and a small number of eigenvector approximations obtained in previous steps which correspond to eigenvalues closest to  $\mu$  are preferable.

- (iv) A crucial point in iterative methods for general nonlinear eigenvalue problems when approximating more than one eigenvalue is to inhibit the method to converge to the same eigenvalue repeatedly. For linear eigenvalue problems this can be easily done. Krylov subspace solvers construct an orthogonal basis of the ansatz space not aiming at a particular eigenvalue, and one gets approximations to extreme eigenvalues without replication (at least if reorthogonalization is employed). If several eigenvalues are computed by the linear Jacobi–Davidson method then one determines an incomplete Schur factorization thus preventing the method from approaching an eigenvalue which was already obtained previously (cf. [27]). For nonlinear problems a similar normal form does not exist and this presents one of the most difficult tasks in achieving good convergence. See [10, 27, 61, 65, 97] for different approaches in this direction.
- (iv) If the projected problem in step 3 is solved by the method of successive linear problems, by linearization or by one of the symmetry preserving methods which solve in each iteration step a linear eigenproblem then at the same time one gets approximations to further eigenpairs of the nonlinear problem which can be exploited to get a good initial approximation to the next wanted eigenpair.
- (v) Often the family of matrices  $T(\lambda)$  has the form

$$T(\lambda) = \sum_{j=1}^p f_j(\lambda) C_j$$

with complex functions  $f_j$  and fixed matrices  $C_j \in \mathbb{C}^{n \times n}$ . Then the projected problem has the form

$$T_{V_k}(\lambda) = \sum_{j=1}^p f_j(\lambda) V_k^H C_j V_k =: \sum_{j=1}^p f_j(\lambda) C_{j,k} \quad (3.6)$$

and the matrices  $C_{j,k}$  can be updated according to

$$C_{j,k+1} = \begin{pmatrix} C_{j,k} & V_k^H C_j v \\ v^H C_j V_k & v^H C_j v \end{pmatrix}. \quad (3.7)$$

**3.2. An Arnoldi type method.** Expanding the current search space  $V$  by the direction  $\hat{v} = x - T^{-1}(\sigma)T(\theta)x$  suggested by residual inverse iteration generates similar robustness problems as for inverse iteration. If  $\hat{v}$  is close to the desired eigenvector, then an inexact evaluation of  $\hat{v}$  spoils the favorable approximation properties of residual inverse iteration.

Similarly as in the Jacobi–Davidson method one could replace  $\hat{v}$  by  $z := x + \alpha \hat{v}$  where  $\alpha$  is chosen that  $x^H z = 0$ , and one could determine an approximation to  $z$  solving a correction equation. However, since the new search direction is orthonormalized

against the previous search space  $V$  and since  $x$  is contained in  $V$  we may choose the new direction  $v = T(\sigma)^{-1}T(\theta)x$  as well. This direction satisfies the orthogonality condition  $x^H v = 0$  at least in the limit as  $\theta$  approaches a simple eigenvalue  $\hat{\lambda}$  (cf. [108]), i.e.

$$\lim_{\theta \rightarrow \hat{\lambda}} x^H T(\sigma)^{-1}T(\theta)x = 0.$$

For the linear problem  $T(\lambda) = A - \lambda B$  this is exactly the Cayley transform with pole  $\sigma$  and zero  $\theta$ . Since

$$(A - \sigma B)^{-1}(A - \theta B) = I + (\theta - \sigma)(A - \sigma B)^{-1}B$$

and Krylov spaces are shift-invariant, the resulting projection method expanding  $V$  by  $v$  is nothing else but the shift-and-invert Arnoldi method.

If the linear system  $T(\sigma)v = T(\theta)x$  is too expensive to solve for  $v$  we may choose as new direction  $v = MT(\theta)x$  with  $M \approx T(\sigma)^{-1}$ , and for the linear problem we obtain an inexact Cayley transform or a preconditioned Arnoldi method. The resulting iterative projection method which was introduced in [65] for quadratic eigenvalue problems and was studied in [97, 102] for general nonlinear eigenproblems is called nonlinear Arnoldi method in spite the fact that differently from the linear case no Krylov space is determined in the course of the algorithm and no Arnoldi recursion holds.

Since the speed of convergence depends crucially on  $|\sigma - \lambda|$  it will be advisable to change the shift or more generally the preconditioner  $M$  in the course of the algorithm if the convergence to the current eigenvalue becomes too slow. In this case one actually obtains a method which generalizes the rational Krylov method for linear problems in [84]. Thus the name nonlinear rational Krylov method would be even more appropriate. But this notation was already introduced in [84, 85] for a different method which we will also discuss below.

A template for the preconditioned nonlinear Arnoldi method with restarts and varying preconditioner is given by Algorithm 6.

Since the residual inverse iteration with fixed pole  $\sigma$  converges linearly, and the contraction rate satisfies  $\mathcal{O}(|\sigma - \lambda_m|)$ , it is reasonable to update the preconditioner if the convergence (measured by the quotient of the last two residual norms before convergence) has become too slow.

For several other recent variations and generalizations of the Arnoldi method for quadratic or general polynomial eigenvalue problems, see [4, 28, 41, 65, 93].

**3.3. Rational Krylov method.** A different approach was proposed in [82, 84, 85] generalizing the rational Krylov approach for linear eigenproblems [83] to sparse nonlinear eigenvalue problems by nesting the linearization of problem (1.1) by Regula falsi and the solution of the resulting linear eigenproblem by Arnoldi's method, where the Regula falsi iteration and the Arnoldi recursion are knit together. Similarly as in the rational Krylov process for linear eigenproblems a sequence  $V_k$  of subspaces of  $\mathbb{C}^n$  is constructed, and at the same time Hessenberg matrices  $H_k$  are updated which approximate the projection of  $T(\sigma)^{-1}T(\lambda_k)$  to  $V_k$ . Here  $\sigma$  denotes a shift and  $\lambda_k$  an approximation to the wanted eigenvalue of (1.1). Then a Ritz vector 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. Hence, in this approach the two numerical subtasks reducing the large dimension to a much smaller one and solving a nonlinear eigenproblem

**Algorithm 6** Nonlinear Arnoldi Method

---

```

1: start with an initial shift  $\sigma$  and an initial basis  $V$ ,  $V^H V = I$ ;
2: determine a preconditioner  $M \approx T(\sigma)^{-1}$ ,  $\sigma$  close to the first wanted eigenvalue
3: while  $m \leq$  number of wanted eigenvalues do
4:   compute an appropriate eigenvalue  $\theta$  and corresponding eigenvector  $y$  of the
     projected problem  $T_V(\theta)y := V^H T(\theta)V y = 0$ .
5:   determine the Ritz vector  $u = V y$  and the residual  $r = T(\theta)u$ 
6:   if  $\|r\|/\|u\| < \epsilon$  then
7:     accept  $\lambda_m = \theta$ ,  $x_m = u$ , increase  $m \leftarrow m + 1$ 
8:     determine new preconditioner  $M \approx T(\sigma)^{-1}$  if indicated
9:     restart if necessary
10:    choose approximations  $\theta$  and  $u$  to next eigenvalue and eigenvector
11:    determine residual  $r = T(\theta)u$ 
12:  end if
13:   $v = Mr$ 
14:   $v = v - V V^H v$ ,  $\tilde{v} = v/\|v\|$ ,  $V = [V, \tilde{v}]$ 
15:  reorthogonalize if necessary
16:  update projected problem  $T_V(\theta) = V^H T(\theta)V$ 
17: end while

```

---

which are solved separately in the Jacobi–Davidson and the Arnoldi methods in Sections 3.1 and 3.2 are attacked simultaneously. This method was applied in [36, 37] to the rational eigenvalue problem (1.7) governing damped vibrations of a structure.

Linearizing the nonlinear family  $T(\lambda)$  by Lagrange interpolation between two points  $\mu$  and  $\sigma$  one gets

$$T(\lambda) = \frac{\lambda - \mu}{\sigma - \mu} T(\sigma) + \frac{\lambda - \sigma}{\mu - \sigma} T(\mu) + \text{higher order terms.} \quad (3.8)$$

Keeping  $\sigma$  fixed for several steps, iterating on  $\mu$ , neglecting the remainder in the Lagrange interpolation, and multiplying by  $T(\sigma)^{-1}$  from the right one obtains

$$T(\sigma)^{-1} T(\lambda_{j-1}) w = \theta w \quad \text{with } \theta = \frac{\lambda_j - \lambda_{j-1}}{\lambda_j - \sigma} \quad (3.9)$$

predicting a singularity at

$$\lambda_j = \lambda_{j-1} + \frac{\theta}{1 - \theta} (\lambda_{j-1} - \sigma). \quad (3.10)$$

For large and sparse matrices the linearization (3.9) is combined with a linear Arnoldi process. Assume that the method has performed  $j$  steps, yielding approximations  $\lambda_1, \dots, \lambda_j$  to an eigenvalue, orthonormal vectors  $v_1, \dots, v_j$ , and an upper Hessenberg matrix  $H_{j,j-1} \in \mathbb{C}^{j \times (j-1)}$  such that the Arnoldi recursion

$$T(\sigma)^{-1} T(\lambda_{j-1}) V_{j-1} = V_j H_{j,j-1}, \quad (3.11)$$

is fulfilled (at least approximately), where  $V_j = [v_1, \dots, v_j]$ .

Updating the matrix  $H_{j,j-1}$  according to the linear theory yields

$$\tilde{H}_{j+1,j} = \begin{pmatrix} H_{j,j-1} & k_j \\ 0 & \|r_\perp\| \end{pmatrix} \quad (3.12)$$

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

$$T(\sigma)^{-1}T(\lambda_j)V_j = V_{j+1}\tilde{H}_{j+1,j}, \quad v_{j+1} = v_\perp / \|v_\perp\|.$$

To satisfy it at least approximately one takes advantage of Lagrangian interpolation

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

where  $A(\lambda) := T(\sigma)^{-1}T(\lambda)$ , and updates  $H$  according to

$$H_{j+1,j} = \begin{pmatrix} \frac{1}{1-\theta} H_{j,j-1} - \frac{\theta}{1-\theta} I_{j,j-1} & k_j \\ 0 & \|r_\perp\| \end{pmatrix}. \quad (3.13)$$

This yields a first version of the rational Krylov method, which unfortunately is not very efficient.

In [84] it was suggested to modify  $\lambda$  and  $H$  in an inner iteration until the residual  $r = T(\sigma)^{-1}T(\lambda)V_j s$  is enforced to be orthogonal to  $V_j$ , and to expand the search space only after the inner iteration has converged which gives Algorithm 7.

---

**Algorithm 7** Rational Krylov method

---

- 1: start with initial vector  $V = [v_1]$  with  $\|v_1\| = 1$ , initial  $\lambda$  and  $\sigma$ ; set  $j = 1$
  - 2: set  $h_j = 0$ ;  $s = e_j$ ;  $x = v_j$ ;
  - 3: compute  $r = T(\sigma)^{-1}T(\lambda)x$  and  $k_j = V_j^H r$
  - 4: **while**  $\|k_j\| > \text{ResTol}$  **do**
  - 5:   orthogonalize  $r = r - V_j^H k_j$
  - 6:   set  $h_j = h_j + k_j s_j^{-1}$
  - 7:    $\theta = \min \text{ eig } H_{j,j}$  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  $r = T(\sigma)^{-1}T(\lambda)x$  and  $k_j = V_j^H r$
  - 12: **end while**
  - 13: compute  $h_{j+1,j} = \|r\|$
  - 14: **if**  $|h_{j+1,j} s_j| > \text{EigTol}$  **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  $\theta$  and  $s$ , and GOTO 8:
- 

The inner iteration is nothing else but a solver of the projected problem

$$V_j^H T(\sigma)^{-1}T(\lambda)V_j s = 0. \quad (3.14)$$

Hence, although motivated originally in a completely different way, the rational Krylov method is an iterative projection method, where the nonlinear eigenproblem  $T(\sigma)^{-1}T(\lambda)x = 0$  is projected to a search space  $V$ , and  $V$  is expanded by the orthogonal complement (with respect to  $V$ ) of the residual  $r = T(\sigma)^{-1}T(\lambda)V s$  of the Ritz pair, and one ends up with Algorithm 8.

**Algorithm 8** Rational Krylov method, an iterative projection method

- 
- 1: start with initial vector  $V = [v_1]$  with  $\|v_1\| = 1$ , initial  $\lambda$  and  $\sigma$
  - 2: **for**  $j = 1, 2, \dots$  until convergence **do**
  - 3:   solve projected eigenproblem  $V^H T(\sigma)^{-1} T(\lambda) V s = 0$  for  $(\lambda, s)$   
by inner iteration
  - 4:   compute Ritz vector  $x = V s$  and residual  $r = T(\sigma)^{-1} T(\lambda) x$
  - 5:   orthogonalize  $r = r - V V^H r$
  - 6:   expand search space  $V = [V, r/\|r\|]$
  - 7: **end for**
- 

The inner iteration in step 3 of Algorithm 8 can be replaced by any dense solver of Section 2, and numerical examples in [46] demonstrate that the method can be accelerated considerably this way.

It is a disadvantage of the rational Krylov method that symmetry properties which the original problem may have are destroyed if the projected problem (3.14) is considered instead of  $V_j^H T(\lambda) V_j s = 0$  in the Arnoldi method or the Jacobi–Davidson algorithm. But on the other hand, the solvers in Section 2 need the explicit form of the projected problem whereas the inner iteration in Algorithm 7 only needs a procedure that yields the vector  $T(\sigma)^{-1} T(\lambda) x$  for a given  $x$ .

**4. Automated Multi-Level Substructuring.** Over the last few years, a new method for performing frequency response and eigenvalue analysis of complex finite element (FE) structures known as Automated Multi-Level Substructuring (AMLS for short) has been developed [5, 6, 7, 8, 47].

In AMLS the large finite element model is recursively divided into many substructures on several levels based on the sparsity structure of the system matrices. Assuming that the interior degrees of freedom of substructures depend quasistatically on the interface degrees of freedom, and modeling the deviation from quasistatic dependence in terms of a small number of selected substructure eigenmodes, the size of the finite element model is reduced substantially yet yielding satisfactory accuracy over a wide frequency range of interest. Recent studies ([47, 49], e.g.) in vibro-acoustic analysis of passenger car bodies where very large FE models with more than one million degrees of freedom appear and several hundreds of eigenfrequencies and eigenmodes are needed have shown that AMLS is considerably faster than Lanczos type approaches.

From a mathematical point of view AMLS is a projection method where the ansatz space is constructed by exploiting Schur complements of submatrices and truncation of spectral representations of subproblems. Differently from the methods in Section 3 it is a one-shot method, i.e. the search spaces are not expanded in the course of the algorithm, but depending on certain parameters the ansatz space is constructed, and if the solution of the projected method at the end turns to be not accurate enough, one has to repeat the reduction process with improved parameters.

We are concerned with the linear eigenvalue problem

$$Kx = \lambda Mx \tag{4.1}$$

where  $K \in \mathbb{R}^{n \times n}$  and  $M \in \mathbb{R}^{n \times n}$  are symmetric and positive definite matrices.

We first consider the component mode synthesis method (CMS method) which is the essential building block of the AMLS method. Assume that the graph of the

matrix  $|K| + |M|$  is partitioned into  $r$  substructures such that the rows and columns of  $K$  can be reordered in the following way:

$$K = \begin{pmatrix} K_{\ell\ell 1} & \dots & O & K_{\ell i 1} \\ \vdots & \ddots & \vdots & \vdots \\ O & \dots & K_{\ell\ell r} & K_{\ell i r} \\ K_{i\ell 1} & \dots & K_{i\ell r} & K_{ii} \end{pmatrix},$$

and  $M$  after reordering has the same block form. Here  $K_{\ell\ell j}$ ,  $j = 1, \dots, r$  is the local stiffness matrix corresponding to the  $j$ -th substructure,  $i$  denotes the set of interface vertices, and  $K_{\ell i j}$  describes the interaction of the interface degrees of freedom and the  $j$ -th substructure.

We distinguish only between local and interface degrees of freedom. Then  $K$  and  $M$  have the following form:

$$K = \begin{pmatrix} K_{\ell\ell} & K_{\ell i} \\ K_{i\ell} & K_{ii} \end{pmatrix} \quad \text{and} \quad M = \begin{pmatrix} M_{\ell\ell} & M_{\ell i} \\ M_{i\ell} & M_{ii} \end{pmatrix}. \quad (4.2)$$

We transform the matrix  $K$  to block diagonal form using block Gaussian elimination, i.e. we apply the congruence transformation

$$P = \begin{pmatrix} I & -K_{\ell\ell}^{-1}K_{\ell i} \\ 0 & I \end{pmatrix}$$

to the pencil  $(K, M)$  to obtain the equivalent pencil

$$(P^T K P, P^T M P) = \left( \begin{pmatrix} K_{\ell\ell} & 0 \\ 0 & \tilde{K}_{ii} \end{pmatrix}, \begin{pmatrix} M_{\ell\ell} & \tilde{M}_{\ell i} \\ \tilde{M}_{i\ell} & \tilde{M}_{ii} \end{pmatrix} \right). \quad (4.3)$$

Here  $K_{\ell\ell}$  and  $M_{\ell\ell}$  stay unchanged, and

$$\begin{aligned} \tilde{K}_{ii} &= K_{ii} - K_{\ell i}^T K_{\ell\ell}^{-1} K_{\ell i} \quad \text{is the Schur complement of } K_{\ell\ell} \\ \tilde{M}_{\ell i} &= M_{\ell i} - M_{\ell\ell} K_{\ell\ell}^{-1} K_{\ell i} = \tilde{M}_{i\ell}^T \\ \tilde{M}_{ii} &= M_{ii} - M_{i\ell} K_{\ell\ell}^{-1} K_{\ell i} - K_{i\ell} K_{\ell\ell}^{-1} M_{\ell i} + K_{i\ell} K_{\ell\ell}^{-1} M_{\ell\ell} K_{\ell\ell}^{-1} K_{\ell i}. \end{aligned}$$

We further transform the pencil (4.3) taking advantage of a modal basis for the local degrees of freedom. To this end we consider the eigenvalue problem

$$K_{\ell\ell} \Phi = M_{\ell\ell} \Phi \Omega, \quad \Phi^T M_{\ell\ell} \Phi = I, \quad (4.4)$$

where  $\Omega$  is a diagonal matrix containing the eigenvalues. Then applying the congruence transformation  $\text{diag}\{\Phi, I\}$  to (4.2) yields the equivalent pencil

$$\left( \begin{pmatrix} \Omega & 0 \\ 0 & \tilde{K}_{ii} \end{pmatrix}, \begin{pmatrix} I & \Phi^T \tilde{M}_{\ell i} \\ \tilde{M}_{i\ell} \Phi & \tilde{M}_{ii} \end{pmatrix} \right). \quad (4.5)$$

In structural dynamics (4.5) is called Craig-Bampton form of the eigenvalue problem (4.1) corresponding to the partitioning (4.2). In terms of linear algebra it results from block Gaussian elimination to reduce  $K$  to block diagonal form, and diagonalization of the block  $K_{\ell\ell}$  using a spectral basis.

Selecting some eigenmodes of problem (4.4), usually the ones associated with eigenvalues below a cut off threshold, and dropping the rows and columns in (4.5) corresponding to the other modes one arrives at the component mode synthesis method

(CMS) [14]. Hence, if the diagonal matrix  $\Omega_1$  and the matrix  $\Phi_1$  contain the eigenvalues and eigenvectors to keep, respectively, then the eigenproblem (4.5) is reduced to

$$\begin{pmatrix} \Omega_1 & 0 \\ 0 & \tilde{K}_{ii} \end{pmatrix} y = \lambda \begin{pmatrix} I & \tilde{M}_{\ell i} \\ \tilde{M}_{i\ell} & \tilde{M}_{ii} \end{pmatrix} y \quad (4.6)$$

with

$$\tilde{M}_{\ell i} = \Phi_1^T (M_{\ell i} - M_{\ell\ell} K_{\ell\ell}^{-1} K_{\ell i}) = \tilde{M}_{i\ell}^T.$$

AMLS generalizes CMS in the following way. Again the graph of  $|K| + |M|$  is partitioned into a small number of subgraphs, but more generally than in CMS these subgraphs in turn are substructured on a number  $p$  of levels yielding a tree topology for the substructures. This induces the following partitioning of the index set  $I = \{1, \dots, n\}$  of degrees of freedom. Let  $I_1$  be the set of indices corresponding to interface degrees of freedom on the coarsest level, and for  $j = 2, \dots, p$  define  $I_j$  to be the set of indices of interface degrees of freedom on the  $j$ -th level which are not contained in  $I_{j-1}$ . Finally, let  $I_{p+1}$  be the set of interior degrees of freedom on the finest level.

With these notations AMLS works as follows. Its first step is the CMS method with cut-off frequency  $\tau_1$  applied to the finest substructuring, i.e.  $I_{p+1}$  is the set of local degrees of freedom, and  $\tilde{I}_{p+1} := \cup_{j=1}^p I_j$  is the set of interface degrees of freedom. After  $j$  steps,  $1 \leq j \leq p-1$ , one derives a reduced pencil

$$\left( \begin{pmatrix} \Omega_f & O & O \\ O & K_{\ell\ell}^{(j)} & K_{\ell i}^{(j)} \\ O & K_{i\ell}^{(j)} & K_{ii}^{(j)} \end{pmatrix}, \begin{pmatrix} M_{ff}^{(j)} & M_{f\ell}^{(j)} & M_{fi}^{(j)} \\ M_{\ell f}^{(j)} & M_{\ell\ell}^{(j)} & M_{\ell i}^{(j)} \\ M_{if}^{(j)} & M_{i\ell}^{(j)} & M_{ii}^{(j)} \end{pmatrix} \right). \quad (4.7)$$

where  $f$  denotes the degrees of freedom obtained in the spectral reduction in the previous steps,  $\ell$  collects the indices in  $I_{p+1-j}$ , and  $i$  corresponds to the index set  $\cup_{k=1}^{p-j} I_k$  of interface degrees of freedom on levels which are not yet treated. Applying the CMS method to the south-east  $2 \times 2$  blocks of the matrices, i.e. annihilating the off-diagonal block  $K_{\ell i}^{(j)}$  by block Gaussian elimination, and reducing the set of  $\ell$ -indices by spectral truncation with cut-off frequency  $\tau_{j+1}$  one arrives at the next level.

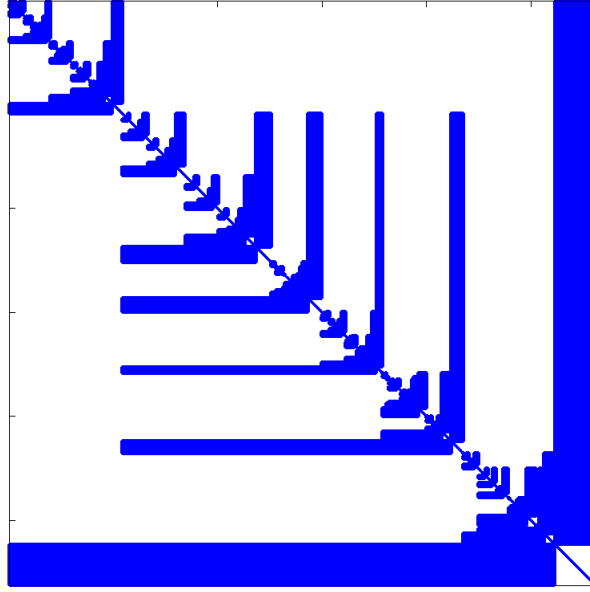
After  $p$  CMS steps one obtains the reduced problem

$$\left( \begin{pmatrix} \Omega_p & O \\ O & K_{\ell\ell}^{(p)} \end{pmatrix}, \begin{pmatrix} M_{ff}^{(p)} & M_{f\ell}^{(p)} \\ K_{\ell f}^{(p)} & M_{\ell\ell}^{(p)} \end{pmatrix} \right), \quad (4.8)$$

and a final spectral truncation of the lower-right blocks with cut-off frequency  $\tau_{p+1}$  yields the reduction of problem (4.1) by AMLS, which is a projected problem

$$\mathcal{K}y = \lambda \mathcal{M}y. \quad (4.9)$$

Here the stiffness matrix  $\mathcal{K}$  has become diagonal, and the mass matrix is projected to a matrix  $\mathcal{M}$  the diagonal of which is the identity, and the only off-diagonal blocks containing non-zero elements are the ones describing the coupling of the substructures and its interfaces. Fig. 4.1 shows the structure of the resulting mass matrix.

FIG. 4.1. *Transformed mass matrix*


This short description of AMLS neglects the algorithmically important fact that all matrices  $K_{\ell\ell}^{(j)}$  and  $M_{\ell\ell}^{(j)}$  are block diagonal. Hence, the annihilation of the off-diagonal blocks  $K_{\ell i}^{(j)}$  and the spectral reduction on each level is quite inexpensive. Implementation details can be found in [19, 47].

The original eigenproblem (4.1) is equivalent to a rational eigenvalue problem of the same dimension as the projected problem in AMLS, which can be interpreted as exact condensation of the original eigenproblem with respect to an appropriate basis. Its eigenvalues at the lower end of the spectrum can be characterized as minmax values of a Rayleigh functional of this rational eigenproblem. Comparing the Rayleigh quotient of the projected problem and the Rayleigh functional of the rational problem the following a priori bound for the error of the AMLS method was proved in [20].

**THEOREM 4.1.** *Let  $K, M \in \mathbb{R}^{n \times n}$  be symmetric and positive definite, and let  $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$  be the eigenvalues of problem (4.1), which we assume to be ordered by magnitude. Let the graph of  $|K| + |M|$  be substructured with  $p$  levels, and denote by  $\tilde{\lambda}_1^{(\nu)} \leq \tilde{\lambda}_2^{(\nu)} \leq \dots$  the eigenvalues obtained by AMLS with cut-off threshold  $\omega_\nu$  on level  $\nu$ .*

*If  $m \in \mathbb{N}$  such that*

$$\lambda_m < \min_{\nu=0, \dots, p} \omega_\nu \leq \lambda_{m+1}$$

*then it holds*

$$\frac{\tilde{\lambda}_j^{(p)} - \lambda_j}{\lambda_j} \leq \prod_{\nu=0}^p \left( 1 + \frac{\lambda_j^{(\nu)}}{\omega_\nu - \lambda_j^{(\nu)}} \right) - 1, \quad j = 1, \dots, m. \quad (4.10)$$

Since the final problem is a projection of each of the intermediate eigenproblems in the AMLS reduction, it follows from the minmax characterization that  $\lambda_j^{(\nu)} \leq \tilde{\lambda}_j^{(p)}$  for

$\nu = 0, \dots, p$ . Therefore the a priori bound (4.10) can be replaced by the computable bound

$$\frac{\tilde{\lambda}_j^{(p)} - \lambda_j}{\lambda_j} \leq \prod_{\nu=0}^p \left( 1 + \frac{\tilde{\lambda}_j^{(p)}}{\omega_\nu - \tilde{\lambda}_j^{(p)}} \right) - 1, \quad j = 1, \dots, m. \quad (4.11)$$

Numerical examples demonstrate that the error bound in (4.10) overestimates the true relative error of AMLS by one or two orders of magnitude. However, an example in [20] demonstrates that the bound can not be improved without further assumptions.

**4.1. AMLS for nonlinear eigenproblems.** To generalize the AMLS method to nonlinear eigenproblems

$$T(\lambda)x = 0 \quad (4.12)$$

we identify an essential linear part of  $T(\cdot)$ , i.e. we rewrite problem (4.12) as

$$Kx - \lambda Mx - R(\lambda)x = 0, \quad (4.13)$$

where  $K \in \mathbb{C}^{n \times n}$  and  $M \in \mathbb{C}^{n \times n}$  are Hermitian and positive definite matrices, and

$$R(\lambda) = K - \lambda M - T(\lambda) \quad (4.14)$$

is a perturbation of the linear eigenproblem  $Kx = \lambda Mx$ , which is not necessarily small but has a small influence on the eigenparameters and eigenvectors of interest.

Once the multi-level substructuring transformation of the linear pencil  $(K, M)$  has been accomplished with a given cut-off frequency we obtain a matrix  $\Phi_{\text{AMLS}}$  of substructure modes on all levels, and a projected eigenproblem

$$\mathcal{K}y = \lambda \mathcal{M}y \quad (4.15)$$

of much smaller dimension, where  $\mathcal{K} = \Phi_{\text{AMLS}}^H K \Phi_{\text{AMLS}}$  and  $\mathcal{M} = \Phi_{\text{AMLS}}^H M \Phi_{\text{AMLS}}$ .

This information can be used in two ways to solve the nonlinear eigenvalue problem approximately: First, we may project the nonlinear eigenproblem (4.12) to the subspace of  $\mathbb{C}^n$  spanned by substructure modes which were kept in the AMLS reduction, i.e.

$$\Phi_{\text{AMLS}}^H T(\lambda) \Phi_{\text{AMLS}} y = \mathcal{K}y - \lambda \mathcal{M}y - \Phi_{\text{AMLS}}^H R(\lambda) \Phi_{\text{AMLS}} y = 0. \quad (4.16)$$

In particular this projection can be performed easily, if the remainder  $R(\lambda)$  has the form

$$R(\lambda) = \sum_{j=1}^p f_j(\lambda) C_j$$

where  $f_j(\lambda)$  are given complex functions and  $C_j \in \mathbb{C}^{n \times n}$  are given matrices, which quite often have the same sparsity structure as the pencil  $(K, M)$  or some other simple structure. In this case the projection  $\Phi_{\text{AMLS}}^H R(\lambda) \Phi_{\text{AMLS}}$  could be determined simultaneously with the matrices  $\mathcal{K}$  and  $\mathcal{M}$  in the course of the AMLS reduction.

Secondly, we may determine Ritz pairs  $(\lambda_j, \Phi_{\text{AMLS}} y_j)$ ,  $j = 1, \dots, m$  of the linear problem  $Kx = \lambda Mx$  corresponding to eigenvalues in the wanted region from the

projected problem (4.15), and project the nonlinear problem to the subspace spanned by these Ritz vectors. Thus we get

$$X^H T(\lambda) X z = \Lambda z - \lambda z - X^H R(\lambda) X z = 0 \quad (4.17)$$

where  $\Lambda = \text{diag}\{\lambda_1, \dots, \lambda_m\}$  and  $X = (x_1, \dots, x_m)$ .

Problem (4.17) is equivalent to the projection of problem (4.16) to the space spanned by the eigenvectors  $y_1, \dots, y_m$  of (4.15) corresponding to  $\lambda_1, \dots, \lambda_m$ . Hence, we can expect, that the first approach will yield better approximations. Examples, however, demonstrate that the loss of accuracy is often negligible.

In either case we arrive at a projected nonlinear eigenvalue problem of much smaller dimension which can be solved by an appropriate method, i.e. a dense solver if the projected problem is small, or by linearization if the underlying problem is a polynomial eigenproblem, or by an iterative projection method of Arnoldi or Jacobi–Davidson type.

This approach was applied successfully to gyroscopic eigenproblems [21, 23] and to rational eigenproblems governing vibrations of fluid–solid structures and damped vibrations of structures [22, 24].

**5. Numerical examples.** To test the projection methods we consider two types of problems, a rational eigenproblem governing damped vibrations of a structure which has non–real eigenvalues, and a finite element model of free vibrations of a fluid–solid structure, which is symmetric and has a Rayleigh functional such that the projected problems can be solved by safeguarded iteration. The discretized problems were generated using FEMLAB [26], and the nonlinear eigenproblems were solved under MATLAB 7.1 [63] on an Intel Pentium D processor with 4 GByte RAM and 3.2 GHz.

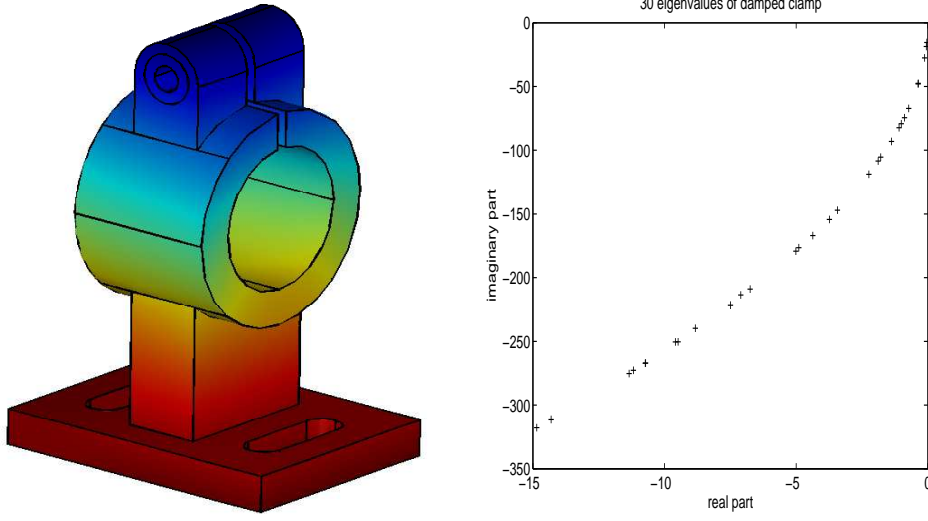
**5.1. Damped vibrations of a structure.** We consider a finite element model of a vibrating structure with nonproportional damping. Using a viscoelastic constitutive relation to describe the behavior of a material in the equations of motions yields a rational eigenvalue problem for the case of free vibrations [37]. A finite element model obtains the form

$$T(\omega)x := \left( \omega^2 M + K - \sum_{j=1}^J \frac{1}{1 + b_j \omega} \Delta K_j \right) x = 0 \quad (5.1)$$

where  $M$  is the consistent mass matrix,  $K$  is the stiffness matrix with the instantaneous elastic material parameters used in Hooke’s law,  $J$  denotes the number of regions with different relaxation parameters  $b_j$ , and  $\Delta K_j$  is an assemblage of element stiffness matrices over the regions with distinct relaxation constants. The real part of an eigenvalue is the exponential rate with which the motion described by the corresponding eigenvector  $x$  decays. The imaginary part is the (damped) angular frequency with which the motion described by  $x$  oscillates.

We consider the feeder clamp in Fig. 5.1 from the model library of FEMLAB [26] which is clamped at its bottom. The instantaneous Young’s modulus is set to  $E = 2.06 \times 10^{11}$  Pa, the instantaneous Poisson’s rate is  $\nu = 0.3$ , and the density is set to  $\rho = 7800$  kg/m<sup>3</sup>. For the nonproportional damping we use in addition the following parameters,  $\Delta\nu = 0.28$ , and  $\Delta E = 6 \times 10^{10}$  Pa, and the relaxation constant is set to  $b = 1 \times 10^{-3}$ .

Discretizing this problem by linear Lagrangian elements we obtained the rational eigenproblem (5.1) of dimension 193617. For symmetry reasons we determined only

FIG. 5.1. *feeder clamp* / *eigenvalues*TABLE 5.1  
*Iterative projection methods: Feeder clamp problem*

Preconditioner		Arnoldi		Jacobi–Davidson		rational Krylov	
threshold	CPU	# iter.	CPU	# iter.	CPU	# iter.	CPU
$10^{-2}$	41	601	4137	166	1736	412	9033
$10^{-3}$	127	226	2004	129	1144	163	3053
$10^{-4}$	348	109	847	105	1203	78	2268

eigenvalues with negative imaginary part, and we computed 30 of them one after another with decreasing imaginary part. We solved this problem by the Jacobi–Davidson, the nonlinear Arnoldi, and the rational Krylov method, where we preconditioned by an incomplete LU decomposition with different drop tolerances. The projected eigenproblems were solved by inverse iteration, and we accepted an eigenpair if the residual norm was less than  $10^{-4}$ .

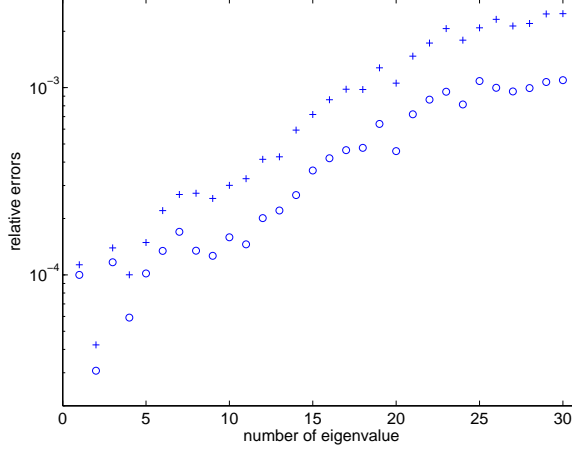
Table 5.1 contains the CPU time for determining the eigenpairs (excluding the time needed to determine the preconditioner which is displayed separately in column 2) and the number of iterations for three different preconditioners. If the preconditioner is very accurate, then the Arnoldi method is faster than the Jacobi–Davidson method, but if only a coarse preconditioner is available than Jacobi–Davidson outperforms the Arnoldi method. This was also observed for many other examples of different kinds. In any case the rational Krylov iteration is inferior to the other two methods.

Applying the AMLS method to the linear eigenvalue problem

$$Kx = \lambda Mx \quad (5.2)$$

with cut-off frequency  $\lambda_c = 1.2e7$  and  $\lambda_c = 2.4e7$ , respectively, and applying the transformations and projections to the matrix  $\Delta K$  simultaneously, we obtained an

FIG. 5.2. Feeder clamp: relative errors of 30 eigenvalues



eigenvalue problem

$$\left(\omega^2 \mathcal{M} + \mathcal{K} - \frac{1}{1+b\omega} \Delta \mathcal{K}\right) y = 0 \quad (5.3)$$

of dimensions  $d_1 = 1252$  and  $d_2 = 2723$ , which required 364 and 374 seconds, respectively.

Multiplying (5.3) by  $1 + b\omega$  one gets a polynomial eigenvalue problem of degree 3 which is equivalent to the linearized eigenvalue problem

$$\begin{pmatrix} O & I & O \\ O & O & I \\ \Delta \mathcal{K} - \mathcal{K} & -b\mathcal{K} & -\mathcal{M} \end{pmatrix} \begin{pmatrix} y \\ \omega y \\ \omega^2 y \end{pmatrix} = \omega \begin{pmatrix} I & O & O \\ O & I & O \\ O & O & b\mathcal{M} \end{pmatrix} \begin{pmatrix} y \\ \omega y \\ \omega^2 y \end{pmatrix} \quad (5.4)$$

of dimension  $3d_j$ ,  $j \in \{1, 2\}$ . Approximations to the desired 30 eigenvalues of (5.1) can be obtained from problem (5.4) by the MATLAB function `eigs` (i.e. by ARPACK) requiring 16 and 76 seconds, respectively. The maximum relative error is  $2.5e - 3$  for the projected problem of dimension 1252, and  $1.09e - 3$  for the problem of dimension 2723. Fig. 5.2 shows the relative errors of the AMLS method for the rational eigenproblem (5.1) where circles correspond to dimension 2723 and plus signs to 1252.

The solution time for the projected problem can be further reduced to 3.1 seconds, if problem (5.3) is projected to the 72 dimensional subspace spanned by the eigenvectors of the linear eigenproblem  $\mathcal{K}y = \lambda \mathcal{M}y$  corresponding to eigenvalues not exceeding  $\tilde{\lambda} = 5 \times 10^5$ . This approach obviously is equivalent to determining Ritz vectors of the linear problem  $Kx = \lambda Mx$  corresponding to eigenvalues not exceeding  $\tilde{\lambda}$  and projecting problem (5.1) to the space spanned by these Ritz vectors. For the projected problem of dimension 2723 the maximum relative error is raised only slightly to  $1.11e - 3$ .

**5.2. Vibrations of a fluid–solid structure.** 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. [12, 13, 76]). Let  $\Omega \subset \mathbb{R}^2$  (the section of the cavity) be an open bounded set with Lipschitz boundary  $\Gamma$ . We assume that there exists a family  $\Omega_j \neq \emptyset$ ,  $j = 1, \dots, p$ , (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  $\Omega_j$  has a Lipschitz boundary  $\Gamma_j$ . With these notations we set  $\Omega_0 := \Omega \setminus \bigcup_{j=1}^p \Omega_j$ .

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. [12, 13])

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

$$c^2 \int_{\Omega_0} \nabla u \cdot \nabla v \, dx = \lambda \int_{\Omega_0} uv \, dx + \sum_{j=1}^p \frac{\lambda \rho_0}{k_j - \lambda m_j} \int_{\Gamma_j} un \, ds \cdot \int_{\Gamma_j} vn \, ds. \quad (5.5)$$

Here  $u$  is the potential of the velocity of the fluid,  $c$  denotes the speed of sound in the fluid,  $\rho_0$  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  $\Omega_0$ .

The eigenvalue problem is non-standard in two respects: The eigenparameter  $\lambda$  appears in a rational way in the boundary conditions, and the boundary conditions are nonlocal. Let  $\sigma_j := k_j/m_j$  denote the poles of problem (5.5) ordered by magnitude, and let  $\sigma_0 = 0$  and  $\sigma_{p+1} = \infty$ . Then the eigenvalues of (5.5) in each of the intervals  $(\sigma_j, \sigma_{j+1})$ ,  $j = 0, \dots, p$  can be characterized as minmax values of a Rayleigh functional, and therefore (5.5) has a countable set of eigenvalues each of finite multiplicity [100].

In particular we consider the rational eigenvalue problem (5.5) where  $\Omega$  is the ellipse with center  $(0,0)$  and length of semiaxes 8 and 4, and  $\Omega_j$ ,  $j = 1, \dots, 9$  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  $c = 1$ ,  $\rho_0 = 1$  and  $m_j = 1$  for all  $j$ . For the stiffness constants  $k_j$  we assume  $k_1 = k_2 = k_3 = 1$ ,  $k_4 = k_5 = k_6 = 2$ , and  $k_7 = k_8 = k_9 = 3$ .

Discretizing problem (5.5) by linear Lagrangian elements one gets a rational matrix eigenvalue problem

$$T(\lambda)x := -Kx + \lambda Mx + \frac{\lambda}{1-\lambda} C_1 C_1^T x + \frac{\lambda}{2-\lambda} C_2 C_2^T x + \frac{\lambda}{3-\lambda} C_3 C_3^T x = 0 \quad (5.6)$$

where  $K$  and  $M$  are symmetric and positive (semi-)definite, and  $C_j \in \mathbb{R}^{n \times 6}$ ,  $j = 1, 2, 3$ , collects the contributions of the three groups of tubes in the nonlocal boundary conditions. In our example the dimension is  $n = 143064$ .

Problem (5.6) has 18, 15, and 14 eigenvalues in the interval  $J_1 = (0, 1)$ ,  $J_2 = (1, 2)$ , and  $J_3 = (2, 3)$ , respectively, and a large number of eigenvalues in  $(3, \infty)$ , 18 of which

TABLE 5.2  
*Iterative projection methods: Fluid–solid structure*

method	$J_1$	$J_2$	$J_3$	$J_4$	$\Sigma$
Arnoldi	69	94	103	154	420
Jacobi–Davidson	200	251	235	347	1033

are contained in  $J_4 := (3, 5)$  (cf. [64]). In each of the intervals  $J_j$  the eigenvalues can be characterized as minmax values of a Rayleigh functional [100]. This property is preserved by the orthogonal projection methods of Arnoldi and Jacobi–Davidson type, and therefore the eigenvalues can be determined one after the other solving the projected problems by safeguarded iteration [97]. The rational Krylov method destroys the symmetry, and we were not able to determine the eigenvalues by the rational Krylov method in a systematic way.

Preconditioning by the (complete) LU factorization of  $T(\sigma)$  for fixed  $\sigma \in J_j$  and starting with initial search spaces according to [64, 98] the Arnoldi and the Jacobi–Davidson method needed the computing times given in Tab. 5.2. Notice, that the Arnoldi method outperforms the Jacobi–Davidson method due to the accurate preconditioner.

The reduction of problem (5.6) by AMLS with the base problem  $Kx = \lambda Mx$  and a cut-off frequency of 100 generated a rational eigenvalue problem

$$-\mathcal{K}y + \lambda \mathcal{M}y + \frac{\lambda}{1-\lambda} \mathcal{C}_1 \mathcal{C}_1^T y + \frac{\lambda}{2-\lambda} \mathcal{C}_2 \mathcal{C}_2^T y + \frac{\lambda}{3-\lambda} \mathcal{C}_3 \mathcal{C}_3^T y = 0 \quad (5.7)$$

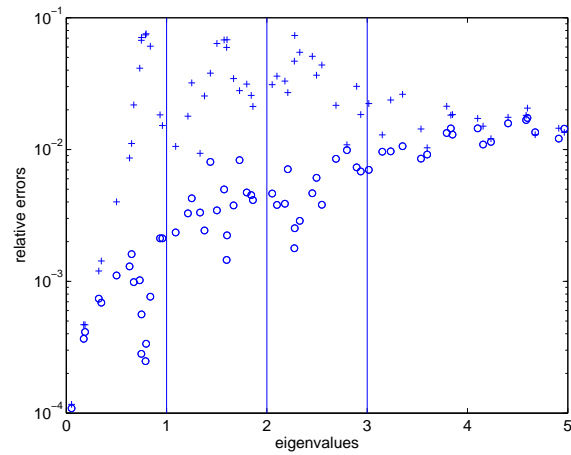
of dimension 915. In principle this problem could be multiplied by  $(1-\lambda)(2-\lambda)(3-\lambda)$  yielding a polynomial eigenvalue problem of degree 4. Linearization would result in a linear eigenvalue problem of dimension 3660 which could be solved by a sparse solver like ARPACK. However, since  $\text{rank}(\mathcal{C}_j) = 6$ ,  $j = 1, 2, 3$ , the polynomial eigenproblem and its linearization have eigenvalues  $\lambda_j = j$ ,  $j = 1, 2, 3$  each of multiplicity 909, which would impede the computation of the eigenvalues in the interval  $[0, 5]$ .

Since the projected problem (5.7) inherits the symmetry properties of problem (5.6) we solved it by the nonlinear Arnoldi method, which required 231 seconds for reducing the base problem  $Kx = \lambda Mx$  by AMLS and transforming the matrices  $\mathcal{C}_1$ ,  $\mathcal{C}_2$ , and  $\mathcal{C}_3$  simultaneously, and 35 seconds for solving the projected problem (5.7). Hence, the total CPU time was 266 seconds.

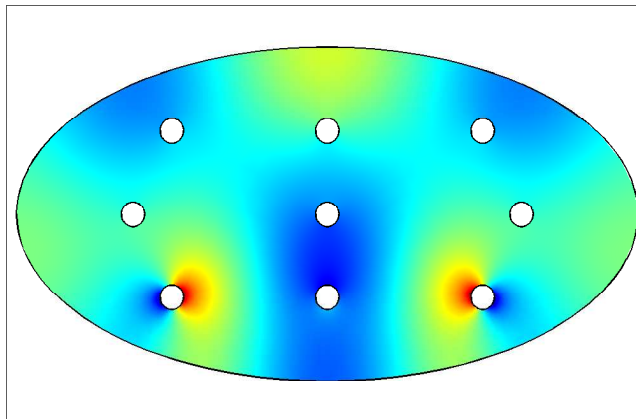
The relative errors are displayed as plus signs in Fig. 5.3. The maximum error is 0.076 which is quite large for a cut-off frequency being 20 times larger than the largest desired eigenvalue. This difficulty is caused by the fact that the rational eigenproblem (5.6) is not just a small perturbation of the base problem  $Kx = \lambda Mx$  used in the AMLS reduction (for instance, (5.6) has 18 eigenvalues in the interval  $[0, 1)$  whereas the linear problem  $Kx = \lambda Mx$  has only 12). There are eigenvectors of problem (5.6) which have large amplitudes close to some of the tubes which can not be approximated well by the AMLS basis consisting of eigenmodes of interfaces and substructures. Fig. 5.4 shows one of these eigenfunctions.

It is interesting to note that these eigenfunctions do not correspond to eigenvalues which are close to a pole. Fig. 5.5 shows the eigenfunction corresponding to an eigenvalue  $\lambda_{18}$  close to the pole  $\sigma_1 = 1$  which can be easily approximated by the base vectors.

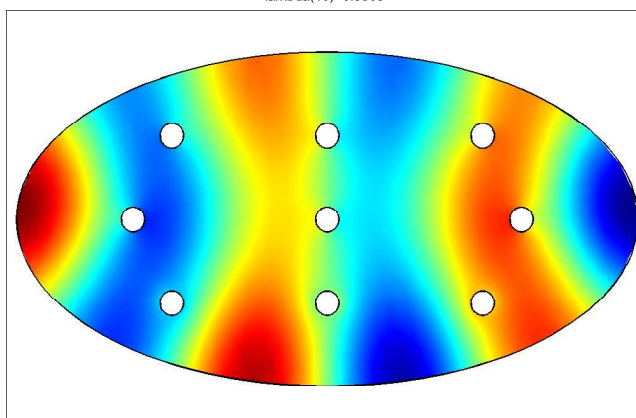
To improve the approximation properties of AMLS we complemented the 503

FIG. 5.3. *Relative errors for fluid–solid structure*FIG. 5.4. *Eigenvector corresponding to  $\lambda_{13} = 0.7506$* 

lambda(13)=0.7506

FIG. 5.5. *Eigenvector corresponding to  $\lambda_{18} = 0.9585$* 

lambda(18)=0.9585



interface degrees of freedom on the coarsest level which were generated by the automatic graph partitioner METIS [48] for the base problem  $Kx = \lambda Mx$  by the 1728 unknowns corresponding to nonzero row entries of the matrix  $[C_1, C_2, C_3]$ . Applying AMLS with the cut-off frequency 100 we obtained a reduced problem of the type (5.7) of dimension 924 which we solved by the nonlinear Arnoldi method. The maximum relative error was reduced to 0.017. The relative errors are displayed in Fig. 5.3 as circles. The total CPU time was 376 seconds, 342 seconds for the AMLS reduction, and 34 seconds for the solution of the reduced problem.

The gain in computing time by the AMLS method for this 2 dimensional problem is not as pronounced as in our previous example since the matrices are less populated, and the preconditioner in the nonlinear Arnoldi method requires much less storage and arithmetic operations.

The alternative way of solving the nonlinear eigenproblem by projecting it to a subspace spanned by a moderate number of Ritz vectors obtained from the AMLS method for the linear base problem leads to bad approximations in this problem. For instance, if problem (5.6) is projected to the space (of dimension 88) spanned by the Ritz vectors corresponding to the Ritz values not exceeding 10 (twice the maximal wanted eigenvalue), the maximum relative error for the eigenvalues in the interval  $[0, 1)$  is 0.15.

**6. Conclusions.** We have discussed projection methods for large scale nonlinear eigenvalue problems. Iterative projection methods of Jacobi–Davidson and of Arnoldi type are efficient, where the Arnoldi method usually is faster if an accurate preconditioner is available, whereas the Jacobi–Davidson method is more robust for only coarse preconditioners. For truly large eigenproblems the automated multi-level substructuring method outperforms iterative projection methods if an essential linear part can be identified such that the remainder has only a small influence on the eigenpairs of interest.

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