

# ITERATIVE PROJECTION METHODS FOR LARGE-SCALE NONLINEAR EIGENVALUE PROBLEMS \*

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## Abstract

In this presentation we review iterative projection methods for sparse nonlinear eigenvalue problems which have proven to be very efficient. Here the eigenvalue problem is projected to a subspace  $\mathcal{V}$  of small dimension which yields approximate eigenpairs. If an error tolerance is not met then the search space  $\mathcal{V}$  is expanded in an iterative way with the aim that some of the eigenvalues of the reduced matrix become good approximations to some of the wanted eigenvalues of the given large matrix. Methods of this type are the nonlinear Arnoldi method, the Jacobi–Davidson method, and the rational Krylov method.

**Keywords:** eigenvalue, eigenvector, iterative projection method, robust expansion, Jacobi–Davidson method, nonlinear Arnoldi method, structure preservation.

## 1 Introduction

The term nonlinear eigenvalue problem is not used in a unique way in the literature. Searching Google scholar for 'nonlinear eigenvalue problem' most of the 386.000 hits consider parameter dependent operator equations

$$T(\lambda, u) = 0$$

which are nonlinear with respect to the state variable  $u$ , and they discuss the structure of the solution set including its dependence on the parameter, bifurcation and Hopf bifurcation of solutions, the existence of quasi-periodic solutions and chaotic behaviour

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of solutions, positivity of solutions, multiplicity of solution, and the (change of) stability of solutions, e.g..

In this paper we consider the following straightforward generalisation of linear eigenvalue problems which is also called nonlinear eigenvalue problem: Let  $T(\lambda)$  be a family of operators depending on a complex parameter  $\lambda$ . Find  $\lambda$  such that the homogeneous problem

$$T(\lambda)x = 0 \tag{1}$$

has a nontrivial solution  $x \neq 0$ . As in the linear case,  $\lambda$  with this property is called an eigenvalue of problem (1), and  $x$  is called a corresponding eigenvector. Since we are interested in numerical methods for these nonlinear eigenvalue problems we restrict ourselves to the case that  $T(\lambda) \in \mathbb{C}^{n \times n}$  is a family of matrices defined on an open set  $D \subset \mathbb{C}$ .

A wide abundance of applications requires the solution of a nonlinear eigenvalue problem the most studied class of which is the quadratic eigenvalue problem

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

that arises in the dynamic analysis of structures, see [31, 64, 95, 106] 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 [25, 28, 36, 63, 139], 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 like vibrations of fluid-solid structures [17], lateral buckling analysis [94], corner singularities of anisotropic material [2, 104], vibro-acoustics [10, 92], stability analysis in fluid mechanics [15], constrained least squares problems [32], and regularisation of total least squares problems [62, 108, 109], to name just a few. [117] surveys quadratic eigenvalue problems, its many applications, its mathematical properties, and some numerical solution techniques.

Polynomial eigenvalues

$$T(\lambda)x = \sum_{j=0}^k \lambda^j A_j x = 0 \tag{3}$$

of higher degree than two arise when discretising a linear eigenproblem by dynamic elements [95, 119, 120] or by least squares elements [97, 98] (i.e. if one uses ansatz functions in a Rayleigh–Ritz approach which depend polynomially on the eigenparameter). Further important applications of polynomial eigenvalue problems are the solution of optimal control problems which by the linear version of Pontryagin’s maximum principle lead to problem (3) [81], singularities in linear elasticity [55–58], nonlinear integrated optics [14], and the electronic behaviour of quantum dots [48, 49].

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

$$-\nabla \cdot \left( \frac{\hbar^2}{2m_j(\lambda)} \nabla u \right) + V_j u = \lambda u, \quad x \in \Omega_q \cup \Omega_m, \quad (4)$$

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  $\lambda$ . Discretising (4) by finite element or finite volume methods yields a rational matrix eigenvalue problem [11, 68, 69, 73, 77, 130, 131].

Further rational eigenproblems

$$T(\lambda)x := -Kx + \lambda Mx + \sum_{j=1}^p \frac{\lambda}{\sigma_j - \lambda} C_j x = 0 \quad (5)$$

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 [113, 115, 126] and vibrations of fluid solid structures [18, 19, 93, 124], and a similar problem

$$T(\lambda)x := -Kx + \lambda Mx + \lambda^2 \sum_{j=1}^p \frac{1}{\omega_j - \lambda} C_j x = 0 \quad (6)$$

arises when a generalised linear eigenproblem is condensed exactly [91, 118]. These problems (4), (5), and (6) have real eigenvalues which can be characterised as minmax values of a Rayleigh functional [134, 135], 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 a rational eigenproblem is obtained for free vibrations of a structure if one uses a viscoelastic constitutive relation to describe the behaviour of a material [39, 40]. A finite element model then obtains the form

$$T(\omega) := \left( \omega^2 M + K - \sum_{j=1}^k \frac{1}{1 + b_j \omega} \Delta K_j \right) x = 0 \quad (7)$$

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. Similar problems describe viscoelastically damped vibrations of sandwich structures [21, 26, 114]

In principle the rational problems (4) – (7) can be turned into polynomial eigenvalue problems by multiplying with an appropriate scalar polynomial in  $\lambda$ . Notice, however,

that important structural properties like symmetry and variational characterisations of eigenvalues can get lost. Moreover, the degree of the polynomial can become very large and roots of the denominators produce spurious eigenvalues (with very high multiplicity for problem (5)) which may hamper the numerical solution.

A general nonlinear dependence on the eigenparameter was already considered by Przemieniecki [95] when studying dynamic element methods with non-polynomial ansatz functions. In the past few years general nonlinear eigenproblems appear more often as the modelling of physical objects becomes more involved and numerical methods even for large scale problem are available. A typical example describing the resonance frequencies of an accelerator cavity is [50, 70, 71]

$$T(\lambda) = K - \lambda M + i \sum_{j=1}^p \sqrt{\lambda - \sigma_j} W_j \quad (8)$$

where  $K$  and  $M$  are symmetric and positive definite, and  $W_j$  are symmetric matrices of small rank modelling the coupling of the accelerator to its surrounding. Further examples appear in vibrations of poroelastic structures [22, 23], vibro-acoustic behaviour of piezoelectric/poroelastic structures [7, 8], stability of acoustic pressure levels in combustion chambers [65], and in the stability analysis of vibrating systems under state delay feedback control [27, 46, 47, 53, 116].

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. They should take advantage of structure properties like symmetry 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 desired eigenvalues and eigenvectors are obtained from projections of the underlying 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 [4], 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 Davidson and the Jacobi–Davidson method [4].

The Krylov subspace approaches take advantage of the linear structure of the underlying problem and construct an approximate incomplete Schur factorisation (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 factorisation does not exist. Therefore, generalisations of Krylov subspace methods can be applied only to nonlinear problems if they are equivalent to a linear eigenproblem.

A standard approach to treating the polynomial eigenvalue problem (1) both theoretically and numerically is linearisation, i.e. to transform (3) into an equivalent linear eigenvalue problem  $L(\lambda)X = \lambda GX - HX = 0$  where  $G, H \in \mathbb{C}^{n\ell \times n\ell}$  and  $X \in \mathbb{C}^{n\ell}$  which then can be solved by a standard eigenvalue solver. Most widely used in practice are companion forms [31, 64] one of which is

$$L(\lambda) = \lambda \begin{pmatrix} A_k & 0 & \dots & 0 \\ 0 & I_n & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & I_n \end{pmatrix} + \begin{pmatrix} A_{k-1} & A_{k-2} & \dots & A_0 \\ -I_n & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & -I_n & 0 \end{pmatrix}. \quad (9)$$

They are easily constructed, but their disadvantage is that the dimension of the problem increases by the factor  $k$  (the degree of the polynomial), and secondly structural properties such as symmetry which the original system may have in general are destroyed by a linearisation.

In many applications the polynomial eigenproblem has some structure that should be reflected in its linearisation, and should be exploited in its numerical solution for efficiency, stability and accuracy reasons. In [9] a two-sided Lanczos process (introduced in [13] for quadratic eigenproblems) is applied to a symmetric/skew-symmetric linearisation of a gyroscopic system thus preserving the property that the eigenvalues appear as purely imaginary pairs and avoiding complex arithmetic. More generally, in [2, 3, 84] polynomial eigenproblems are considered the spectrum of which have Hamiltonian structure, i.e. its eigenvalues appear in quadruples  $\{\lambda, \bar{\lambda}, -\lambda, -\bar{\lambda}\}$  or in real or purely imaginary pairs  $\{\lambda, -\lambda\}$ . A linearisation was studied that transforms the problem into a Hamiltonian/skew-Hamiltonian pencil for which a structure preserving skew-Hamiltonian, isotropic, implicitly restarted shift-and-invert Arnoldi algorithm called SHIRA [83] was designed. More generally, [75] introduced an approach to constructing linearisations of polynomial eigenvalue problems which generalises the companion forms, and which gave rise to linearisations preserving symmetry [41], definiteness [35, 42, 86], and respecting palindromic and odd-even structures [74].

There are also Krylov type methods for quadratic eigenvalue problems which do not take advantage of linearisations. [67] proposed a generalisation of the Arnoldi method to the monic quadratic matrix polynomial  $\lambda^2 I - \lambda A - B$ . Reducing the matrices  $A$  and  $B$  simultaneously to generalised Hessenberg matrices  $H_k = Q_k^H A Q_k$  and  $K_k = Q_k^H B Q_k$  by a sequence of orthogonal matrices  $Q_k$  a quadratic pencil  $\theta^2 I - \theta H_k - K_k$  of much smaller dimension is derived the Ritz pairs of which approximate eigenpairs of the original pencil. In [43, 44] this approach is generalized to polynomial eigenproblems. In [5, 6, 72, 137] second order Krylov subspaces for monic quadratic pencils are introduced which are spanned by mixed powers of the matrices  $A$  and  $B$  and corresponding projection methods.

For general nonlinear eigenproblems the rational Krylov approach for linear eigenproblems [100] is generalised in [101, 102] by nesting the linearisation of problem (1) by Lagrangian interpolation and the solution of the resulting linear eigenproblem by Arnoldi's method, where the Regula falsi iteration and the Arnoldi recursion are knit together. The name is a little misleading since no Krylov space is constructed but the method can be interpreted as a projection method where the search spaces are expanded by directions with high approximation potential for the eigenvector wanted next, namely by the vector obtained by some residual inverse iteration [54].

This method has the drawback, that potential symmetry properties of the underlying problem are destroyed which is not the case for the Arnoldi method in [121, 125] which expands the search space by a different residual inverse iteration (again no Krylov space appears; the name is chosen because the method reduces to the shift-and-invert Arnoldi method if applied to a linear eigenproblem). Expanding the search space by an approximate inverse iteration one arrives at a Jacobi–Davidson method introduced in [111] for polynomial eigenvalue problems and in [12] and [127] for general nonlinear eigenproblems.

In this paper we review the iterative projection methods for general (i.e. not necessarily polynomial) sparse nonlinear eigenproblems which generalise 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. We do not review the quickly growing literature on projection methods for polynomial and rational eigenvalue problems which take advantage of linearisation in particular exploiting structure properties of the underlying problem. Although we have in mind sparse eigenproblems Section 2 summarises methods for dense nonlinear eigenproblems which are needed in the iterative projection methods of Jacobi–Davidson, Arnoldi and rational Krylov type presented in Section 3. The paper closes with a numerical example in Section 4 demonstrating the efficiency of the methods.

## 2 Methods for dense nonlinear eigenproblems

In this section we shortly outline methods for dense nonlinear eigenproblems (more detailed presentation are given in [82, 128, 129]). Typically, these methods require several factorisations of varying matrices to approximate one eigenvalue, and therefore, they are not appropriate for large and sparse problems but are limited to a few thousands unknowns depending on the available storage capacity. However, they are needed within projection methods for sparse problems to solve the nonlinear projected problems of small dimension.

## 2.1 Methods based on the characteristic equation

Obviously  $\lambda$  is an eigenvalue of the nonlinear problem (1), if and only if it is a root of the characteristic equation

$$\det T(\lambda) = 0. \quad (10)$$

In [59,60] it was suggested to use a QR-factorisation 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. Then  $\lambda$  is an eigenvalue if and only if  $r_{nn}(\lambda) = 0$ .

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

$$\lambda_{k+1} = \lambda_k - \frac{1}{e_n^H Q(\lambda_k)^H T'(\lambda_k) P(\lambda_k) R(\lambda_k)^{-1} e_n}, \quad (11)$$

for approximations to an eigenvalue of problem (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 [51, 52] and also quadratic convergence was shown. A similar approach was presented in [140], via a representation of Newton's method using the  $LU$ -factorisation of  $T(\lambda)$ . Other variations of this method can be found in [141, 142]. However, this relatively simple idea is not efficient, since it computes eigenvalues one at a time and needs several  $\mathcal{O}(n^3)$  factorisations per eigenvalue. It is, however, useful in the context of iterative refinement of computed eigenvalues and eigenvectors.

## 2.2 Inverse iteration

For linear eigenproblems one obtains inverse iteration by applying Newton's method to  $Ax - \lambda x = 0$  augmented by a scaling condition  $v^H x = 1$  with a suitably chosen vector  $v$ . Accordingly, Newton's method for the nonlinear system

$$F(x, \lambda) := \begin{pmatrix} T(\lambda)x \\ v^H x - 1 \end{pmatrix} = 0 \quad (12)$$

reads

$$\begin{pmatrix} T(\lambda_k) & T'(\lambda_k)x_k \\ v^H & 0 \end{pmatrix} \begin{pmatrix} x_{k+1} - x_k \\ \lambda_{k+1} - \lambda_k \end{pmatrix} = - \begin{pmatrix} T(\lambda_k)x_k \\ v^H x_k - 1 \end{pmatrix}. \quad (13)$$

The first component gives the direction of the new approximation to an eigenvector  $u_{k+1} := T(\lambda_k)^{-1} T'(\lambda_k)x_k$ . Assuming that  $x_k$  is already normalised by  $v^H x_k = 1$  the second component of (13) reads  $v^H x_{k+1} = v^H x_k$ , and multiplying the first component by  $v^H$  yields

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

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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:   normalise  $x_{k+1} = u_{k+1}/v^H u_{k+1}$
  - 6: **end for**
- 

Hence, for nonlinear eigenproblems inverse iteration obtains the form given in Algorithm 1. Being a variant of Newton's method this algorithm converges locally and quadratically to  $(x, \lambda)$  [1, 88].

As in the linear case the normalisation condition can be modified in each step of inverse iteration. It was suggested in [99] to use  $v_k = T(\lambda_k)^H y_k$  for the normalisation, 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 [64], 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 [20, 90]. The same is true [97] 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  $\lambda_k$ . Similarly, the two-sided Rayleigh quotient iteration for linear eigenvalue problems [90] was generalised to nonlinear eigenvalue problems and was shown to be locally and cubically convergent [105, 107].

In [87] 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 generalises the method (11), inverse iteration, and a method proposed in [89]. 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, 59, 60, 64, 88, 89].

### 2.3 Residual inverse iteration

For linear eigenproblems inverse iteration can be replaced by a simplified version  $x_{k+1} = (A - \sigma I)^{-1}x_k$  with fixed  $\sigma$  converging to an eigenvector corresponding to the eigenvalue of  $A$  next to  $\sigma$ . The convergence is only linear but the method has the advantage that only one factorisation of the matrix  $A - \sigma I$  is necessary.

In contrast to the linear case replacing step 3 in Algorithm 1 by  $T(\sigma)x_{k+1} = T'(\lambda_k)x_k$  with a fixed shift  $\sigma$  results in misconvergence. It is easily seen that this



iteration 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 normalisation condition) from which we can not recover an eigenpair of the nonlinear problem (1).

A remedy against this wrong convergence was proposed in [85]. 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 [85]

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**Algorithm 2** Residual inverse iteration

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- 1: Let  $v$  be a normalisation vector and start with an approximations  $\sigma$  and  $x_1$  to an eigenvalue and corresponding eigenvector of (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  $\lambda_{k+1} = p(x_k)$  is  $T(\lambda)$  is Hermitian
  - 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: normalise  $x_{k+1} = z_{k+1}/v^H z_{k+1}$
  - 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 normalised 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 [85].

## 2.4 Successive linear approximations

A first order approximation of problem (1) is

$$T(\lambda)x \approx (T(\tilde{\mu}) - \theta T'(\tilde{\mu}))x = 0, \quad \theta = \tilde{\mu} - \lambda. \quad (14)$$

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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)
  - 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**
- 

This suggests the method of successive linear problems in Algorithm 3 introduced in [99].

If  $T$  is twice continuously differentiable, and  $\hat{\lambda}$  is an eigenvalue of problem (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  $\lambda$ , see [128].

## 2.5 Safeguarded iteration

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 characterisation of their eigenvalues [24, 37, 38, 96, 123, 134, 135], an alternative is to use the safeguarded iteration. The method was introduced in [138] for overdamped problems, and was studied in [86, 136] 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 continuous. Suppose that for every  $x \in \mathbb{C}^n \setminus \{0\}$  the real equation

$$f(\lambda, x) := x^H T(\lambda)x = 0 \tag{15}$$

has at most one solution  $\lambda \in J$ . Then equation (15) defines a functional  $p$  on some subset  $D \subset \mathbb{C}^n$  which obviously generalises the Rayleigh quotient for linear pencils  $T(\lambda) = \lambda B - A$ , and which is called the Rayleigh functional of the nonlinear eigenvalue problem (1).

Assume that

$$(\lambda - p(x))x^H T(\lambda)x > 0 \quad \text{for every } \lambda \in J, \lambda \neq p(x)$$

(generalising the definiteness requirement for linear pencils), and enumerate the eigenvalues of (1) in  $J$  in the following way: A value  $\lambda \in J$  is an eigenvalue of (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).

Under the above assumptions it was shown in [134,135] that for every  $m \in \{1, \dots, n\}$  problem (1) has at most one  $m$ -th eigenvalue in  $J$ , which can be characterised by

$$\lambda_m = \min_{\dim V=m, D \cap V \neq \emptyset} \sup_{v \in D \cap V} p(v). \quad (16)$$

Conversely, if

$$\lambda_m := \inf_{\dim V=m, D \cap V \neq \emptyset} \sup_{v \in D \cap V} p(v) \in J, \quad (17)$$

then  $\lambda_m$  is an  $m$ -th eigenvalue of (1), and the characterisation (16) 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 suggests Algorithm 4 called safeguarded iteration for computing the  $m$ -th eigenvalue.

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**Algorithm 4** Safeguarded iteration

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- 1: Start with an approximation  $\sigma_1$  to the  $m$ -th eigenvalue of (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**
- 

It was shown in [86, 136] 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  $\lambda_1$ .
- (ii) If  $\lambda_m \in J$  is a  $m$ -th eigenvalue of (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 generalised 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

$$Ax = \lambda x \quad (18)$$

iterative projection methods like the Lanczos, Arnoldi, rational Krylov or Jacobi–Davidson method are very efficient. Here the dimension of the eigenproblem is reduced by projecting it to a subspace of much smaller dimension, and the reduced problem is solved by a fast technique for dense problems. The subspaces are expanded in the course of the algorithm in an iterative way with the aim that some of the eigenvalues of the reduced matrix become good approximations of some of the wanted eigenvalues of the given large matrix.

Two types of iterative projection methods are in use: methods which expand the subspaces independently of the eigenpair of the projected problem and which use Krylov subspaces of  $A$  or  $(A - \sigma I)^{-1}$  for some shift  $\sigma$  like the Arnoldi method or Lanczos method or rational Krylov method, and methods which aim at a particular eigenpair and choose the expansion  $q$  such that it has a high approximation potential for a wanted eigenvector like the Jacobi–Davidson method.

Today the Lanczos method together with its variants is a standard solver for sparse linear eigenproblems. A detailed discussion is contained in [4]. 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 applies 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 factorisation 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 [33, 34, 61, 66, 80]).

A way out of this dilemma is the Jacobi–Davidson method which is more robust to inexact expansions of search spaces. Let  $(x, \theta)$  be an approximation to an eigenpair obtained by a projection method with subspace  $\mathcal{V}$ . We assume that  $\|x\| = 1$ ,  $\theta = x^H Ax$ , 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 Rayleigh quotient 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.

Actually, we are not interested in the direction  $v$  but in an expansion of  $\mathcal{V}$  which contains  $v$ , and for every  $\alpha \neq 0$  the vector  $u = x + \alpha v$  is as qualified as  $v$ . It was shown in [133] that the most robust expansion of this type is obtained if  $x$  and  $x + \alpha v$  are orthogonal, and it is easily seen that this  $u$  solves the so called correction equation

$$(I - xx^H)(A - \theta I)(I - xx^H)u = -r, \quad u \perp x. \quad (19)$$

The resulting iterative projection method called Jacobi–Davidson method was introduced in [112] in a completely different way, and it is well established for very large eigenproblems.

### 3.1 Jacobi–Davidson method

The same considerations hold true also for the nonlinear eigenproblems (1). Assume that we are given a search space  $\mathcal{V}$  and a matrix  $V$  with orthonormal columns containing a basis of  $\mathcal{V}$ . Let  $(y, \theta)$  be an eigenpair of the projected problem

$$V^H T(\lambda) V y = 0 \quad (20)$$

and  $x = V y$  be the corresponding Ritz vector. A direction with high approximation potential is given by inverse iteration  $\tilde{v} = T(\theta)^{-1} T'(\theta) x$ . For robustness reasons discussed for the linear case we expand  $\mathcal{V}$  by  $v = x + \alpha \tilde{v}$  where  $\alpha$  is chosen such that  $x^H(x + \alpha \tilde{v}) = 0$ , i.e.

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

Then  $v$  solves the correction equation

$$\left( I - \frac{T'(\theta) x x^H}{x^H T'(\theta) x} \right) T(\theta) \left( I - \frac{x x^H}{x^H x} \right) z = T(\theta) x, \quad v \perp x. \quad (21)$$

As in the linear case (21) 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 generalisation of the Jacobi–Davidson method was suggested in [110, 111] for polynomial eigenvalue problems, and was studied in [12, 127, 132] for general nonlinear eigenproblems.

In the correction equation (21) 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 (21) should be modified correspondingly to

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

It was already pointed out in [112] 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 iteration step of the Krylov solver for (21) one has to solve one linear system  $\tilde{K} w = y$ , and to initialise requires only one additional solve.

A template for the Jacobi–Davidson method for the nonlinear eigenvalue problem (1) is given in Algorithm 5. In the following we comment on some of its steps. A detailed discussion is contained in [12, 127, 132].

- (i) In step 1 of Algorithm 5 preinformation such as known approximate eigenvectors of problem (1) or eigenvectors of contiguous problems can be introduced into the algorithm.

---

**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

$$\left(I - \frac{T'(\lambda_m) u u^H}{u^H T'(\lambda_m) u}\right) T(\sigma) \left(I - \frac{u u^H}{u^H u}\right) z = -r \quad (22)$$

(by preconditioned Krylov solver, e.g.)

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

If no information on eigenvectors is at hand, and we are interested in eigenvalues close to the parameter  $\sigma \in D$ , one can choose an initial vector at random, execute a few Lanczos or Arnoldi steps for the linear eigenproblem  $T(\sigma)u = \theta u$  or  $T(\sigma)u = \theta T'(\sigma)u$ , and choose  $V$  by orthogonalising eigenvectors corresponding to small eigenvalues in modulus. 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.

Rational eigenvalue problems governing free vibrations of fluid-solid structures require a particular initial space the choice of which is discussed in [122]

- (ii) Preconditioning is a key to a successful iterative solver. A comprehensive exposition of many useful preconditioning techniques can be found in [16, 103].
- (iii) Since the dimension of the projected problems are usually small they can be solved by any method for dense nonlinear eigenvalue problems discussed in Section 2.

A crucial point in iterative projection methods for general nonlinear eigenvalue problems when approximating more than one eigenvalue is to inhibit the method to converge to the same eigenvalue repeatedly. In the linear case this is no problem. 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 reorthogonalisation is employed). If several eigenvalues are computed by the Jacobi–Davidson method then one determines an incomplete Schur factorisation thus preventing the method from approaching an eigenvalue which was already obtained previously (cf. [29]). For nonlinear problems a similar normal form does not exist.

If  $T(\lambda)$  is a family of real symmetric or Hermitian matrices and  $D$  is a real interval such that the eigenvalues are maxmin values of a Rayleigh functional then the projected problems inherit this property. The eigenvalues can be determined one after the other by safeguarded iteration, and approximating the  $m$ -th eigenvalue usually enough information about the next eigenvector is gathered to compute the  $(m + 1)$ -th eigenvalue safely. This approach which was discussed in [12] has the advantage that it is most unlikely that the method converges to an eigenvalue that has already been found previously.

Similarly, in the general case one can order the eigenvalues by their distance to a fixed parameter  $\sigma_0$ , and approximate them one after the other by the method of successive linear problems. If already  $m - 1$  eigenvalues of (1) closest to  $\sigma_0$  have been determined, and  $\mu_0$  is an approximation to the eigenvalue wanted next, we iteratively perform the following three steps until convergence: we solve the linear eigenproblem  $V^H T(\mu_\ell) V y = \theta v^H T'(\mu_\ell) V y$ , choose the eigenvalue  $\hat{\theta}$  such that  $|\sigma_0 - (\mu_\ell - \hat{\theta})|$  is  $m$ -smallest among the eigenvalues  $\theta$ , and set  $\mu_{\ell+1} = \mu_\ell - \hat{\theta}$ .

A disadvantage of this method is the fact that consecutive eigenvalues  $\lambda_{m-1}$  and  $\lambda_m$  usually will not be close to each other, and therefore, a preconditioner which was adequate for one eigenvalue can yield slow convergence of the iterative solver for the next eigenvalue [132]. Hence, this method should be used only if a small number of eigenvalues close to a parameter is wanted.

Quite often the nonlinear eigenvalue problem under consideration is a (small) perturbation of a linear eigenvalue problem. In (7) we considered a rational eigenproblem governing the free vibrations of a structure using a viscoelastic constitutive relation to describe the behaviour of the material. It is well known that often the eigenmodes of the damped and the undamped problem do not differ very much although the eigenvalues do. Therefore, it is reasonable to determine an eigenvector  $y$  of the undamped and projected problem  $(\omega^2 V^H M V - V^H K V) y = 0$  corresponding to the  $m$ -smallest eigenvalue  $\omega_m^2$ , determine an approximate eigenvalue  $\tilde{\omega}$  of the nonlinear projected problem from the complex equation  $y^H V^H T(\omega) V y = 0$  or  $e^H V^H T(\sigma)^{-1} T(\omega) V y = 0$ , and correct it by one of the methods in Section 2.

- (iv) 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.

Since some of the solvers of the nonlinear projected eigenproblems take advantage of some enumeration of the eigenvalues it is natural to keep the eigenvectors that have been converged in the course of the algorithm. Otherwise this enumeration would be perturbed. We therefore continue with an orthonormal basis of  $X_m := \text{span}\{x_1, \dots, x_m\}$ . If an approximation to an eigenvector wanted next is obtained cheaply we add it to  $X_m$ . A local restart procedure which is particularly suitable if a very large number of eigenvalues is desired or eigenvalue in the interior of the spectrum is discussed in [76].

- (v) Some of the eigensolvers discussed in Section 2 can be used to get approximations to the eigenvector and eigenvalue wanted next. In this case we continue with these approximations. If no information on the next eigenvalue and eigenvector can be gained cheaply we continue with the current approximations.
- (vi)  $v$  is orthogonalised with respect to the current search space  $V$  by classical Gram–Schmidt. It may be replaced by modified Gram–Schmidt for stability reasons. Notice, however, that the classical Gram–Schmidt procedure is able to use BLAS3, and thus can be faster than classical Gram–Schmidt by a better use of cache.

### 3.2 Nonlinear Arnoldi 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 favourable 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 orthonormalised 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. [130]), 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 [78, 79] for quadratic eigenvalue problems and was studied in [121, 125] 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.

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

---

**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  $T_V(\theta)y := V^H T(\theta)Vy = 0$ .
  - 5:   determine the Ritz vector  $u = Vy$  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:     $v = v - VV^H v$ ,  $\tilde{v} = v/\|v\|$ ,  $V = [V, \tilde{v}]$
  - 15:    reorthogonalise if necessary
  - 16:    update projected problem  $T_V(\theta) = V^H T(\theta)V$
  - 17: **end while**
- 

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 generalisations of the Arnoldi method for quadratic or general polynomial eigenvalue problems, see [5, 6, 30, 45, 70, 71, 78, 79, 117].

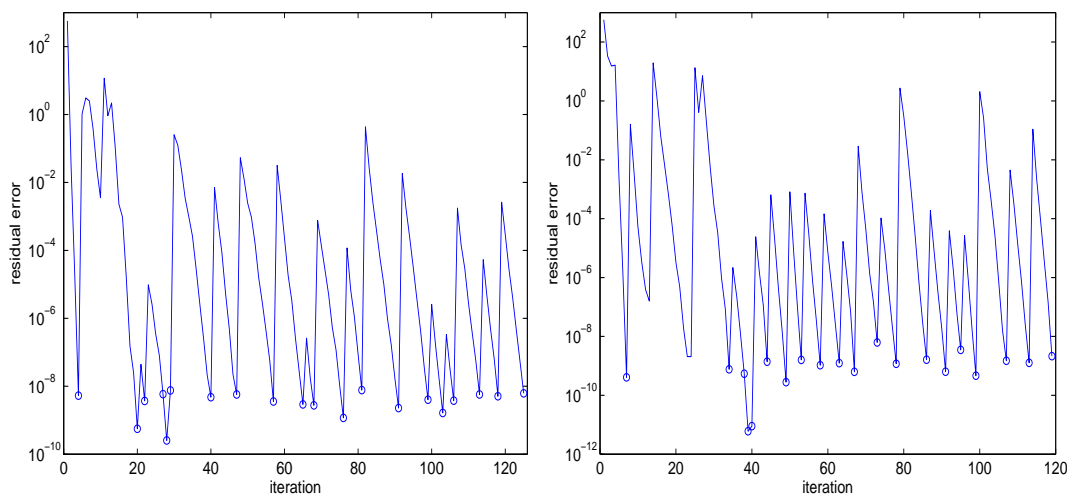


Figure 1: Convergence history of nonlinear Arnoldi and Jacobi-Davidson method

## 4 Numerical example

To demonstrate the numerical behaviour of the iterative projection method we consider the delay differential equation

$$u_t(x, t) = \Delta u(x, t) + a(x)u(x, t) + b(x)u(x, t - \tau t), \quad t > 0, x \in [0, \pi] \times [0, t]. \quad (23)$$

Semi-discretising with finite differences with respect to  $x$  and the ansatz  $u(x, t) = e^{\lambda t}u(x)$  yields the nonlinear eigenvalue problem

$$T(\lambda)x = \lambda x + Ax + e^{-\lambda\tau}Bx = 0. \quad (24)$$

We tested both iterative projection methods for a problem of this type of dimension  $n = 39601$ . Since  $T(\lambda)$  is symmetric and the conditions of the minmax characterisation are satisfied the projected problems can be solved by the safeguarded iteration, and the eigenvalues can be determined safely one after the other. Further numerical experiments (including some with nonreal eigenvalues) are reported in [82, 125, 128, 129, 131, 132].

The experiments were run under MATLAB2007a on an Intel Core Duo CPU with 2.13 Hz and 2.96 GB RAM. We computed the 20 smallest eigenvalues. Figure 1 shows the convergence history for both methods, the nonlinear Arnoldi method on the left and the Jacobi–Davidson method on the right, where the preconditioner was chosen to be the LU factorisation of  $T(\sigma)$  for some  $\sigma$  close to the smallest eigenvalue and was kept during the whole computation. For both methods an average of approximately 6 iterations are needed to find an eigenvalue. Notice however, that for the nonlinear Arnoldi only one solve with the preconditioner is needed to expand the search space, whereas the Jacobi–Davidson method requires the approximate solution of a correction equation. It is noteworthy that there are eigenvalues which are quite close to each other,  $\lambda_7 = 16.97703$  and  $\lambda_8 = 16.98516$ , e.g., which does not hamper the convergence.

Preconditioner	Arnoldi		Jacobi–Davidson	
	# iter.	CPU	# iter.	CPU
LU	125	14.9	119	38.4
inc. LU, $10^{-3}$	241	34.2	143	44.7
inc. LU, $10^{-2}$	1001	245.0	177	58.2

Table 1: Nonlinear Arnoldi and Jacobi–Davidson method

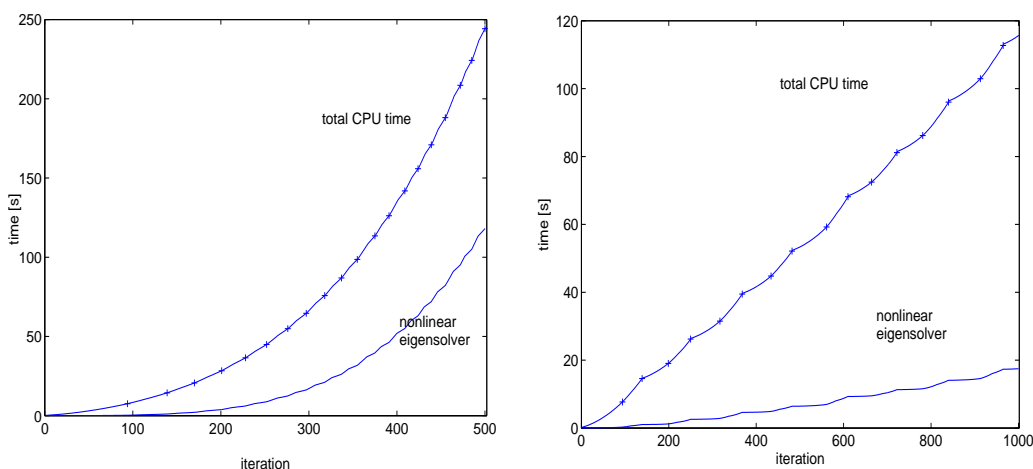


Figure 2: Time consumption of nonlinear Arnoldi method without and with restarts

Table 1 contains the CPU time for both methods where we employed the LU factorisation as well as incomplete LU factorisations for two cut off levels,  $10^{-3}$  and  $10^{-2}$  and did not reduce the search space during the iterations. It is observed that for an accurate preconditioner the nonlinear Arnoldi method is much faster than the Jacobi–Davidson method, whereas for a coarse preconditioner the Jacobi–Davidson method is the clear winner. The same observation was made for many other examples, the Jacobi–Davidson method is more robust with respect to coarse preconditioners than the nonlinear Arnoldi method.

The CPU times in Table 1 correspond to the projection methods without restart. Figure 2 shows on the left the time consumption of the nonlinear Arnoldi method with incomplete LU preconditioner with threshold  $10^{-2}$  as well as the share which is required for solving the projected eigenvalue problems. It demonstrates the necessity of restarts since the superlinear time consumption is mainly caused by the eigensolvers. On the right Figure 2 shows the behaviour of the nonlinear Arnoldi method if the method is restarted whenever the dimension of the search space exceeds 100 after the computation of an eigenvalue had been completed.

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