BROYDEN’S METHOD FOR NONLINEAR EIGENPROBLEMS

ELIAS JARLEBRING

Abstract. Broyden’s method is a general method commonly used for nonlinear systems of equations, when very little information is available about the problem. We develop an approach based on Broyden’s method for nonlinear eigenvalue problems. Our approach is designed for problems where the evaluation of a matrix vector product is computationally expensive, essentially as expensive as solving the corresponding linear system of equations. We show how the structure of the Jacobian matrix can be incorporated into the algorithm to improve convergence. The algorithm exhibits local superlinear convergence for simple eigenvalues, and we characterize the convergence. We show how deflation can be integrated and combined such that the method can be used to compute several eigenvalues. A specific problem in machine tool milling, coupled with a PDE is used to illustrate the approach. The simulations are done in the julia programming language, and are provided as publicly available module for reproducability.

1. Introduction. We here consider the nonlinear eigenvalue problem (NEP) defined by

\begin{equation}
M(\lambda)v = 0
\end{equation}

where $M : \mathbb{C} \rightarrow \mathbb{C}^{n \times n}$ is an analytic function of $\lambda$. This problem can equivalently be written as a system of nonlinear equations

\begin{equation}
F\left(\begin{bmatrix} v \\ \lambda \end{bmatrix}\right) = 0
\end{equation}

where

\begin{equation}
F\left(\begin{bmatrix} v \\ \lambda \end{bmatrix}\right) := \begin{bmatrix} M(\lambda)v \\ c^Hv - 1 \end{bmatrix}
\end{equation}

under the assumption that $c$ is not orthogonal to the eigenvector. The normalization condition $c^Hc = 1$ is selected such that $F$ is analytic and therefore complex differentiable, which would not be the case if we were to select $\|v\|_2 = v^Hv = 1$ instead.

This class of NEPs has been studied for decades, as can be seen in summary references [36, 32, 46] and the benchmark collection [2]. Several standard approaches for NEPs of the type (1.1) are based on Newton’s method. The Newton approach for NEPs was proposed already in 1950 [43], and later developed further in [34, 36]. The residual inverse iteration [33] is an implicit Newton method [24] and forms the basis of the nonlinear Arnoldi method [45]. More recently, block variants of Newton’s method has been developed [27]. There is a summary of many methods [18] of which many are Newton methods or can be interpreted as flavors of Newton’s method. The QR-approach for banded matrices in [14] is based on Kublanovskaya’s approach [28] which is also a Newton method applied to the $(n, n)$-element of the R-matrix in the QR-factorization of $M(\lambda)$. Two-sided Newton approaches and Jacobi-Davidson approaches have been studied in [27]. Considerable convergence theory and specialization of the Newton type approaches can be found in the literature, e.g., convergence theory [40, 41, 42] as well as inexact solves and preconditioning [39].

These Newton-approaches depend on explicit access to the matrix $M(\lambda)$, in ways which are not available. Most methods depend on direct access of $M(\lambda)$ and/or that the NEP can be expressed in an affine form

\begin{equation}
M(\lambda) = M_1f_1(\lambda) + \cdots + M_mf_m(\lambda)
\end{equation}
where \( f_1, \ldots, f_m \) are analytic functions and \( m \ll n \). The availability of an affine form typically means that when \( m \) is small, the projected problem \( V^T M(\lambda) Wz = 0 \) can normally be solved in a computationally cheap way. The matrix \( M(\lambda) \) and an affine form are not always available in applications. We illustrate this further in Section 7 with a problem stemming from the analysis of time-periodic delay-differential equations.

The approach presented here is based on Broyden’s method for nonlinear systems of equations; see \([7]\) and more recent summaries in \([10, 14]\). Broyden’s method is also based on Newton’s method, but the Jacobian approximation is updated (typically with a rank-one matrix) in order to avoid the computation of the Jacobian matrix. An attractive feature of Broyden’s method is that only one function evaluation per iteration is required. In the context of NEPs this implies that we do not need an affine form and nor a direct accurate access to the Jacobian matrix.

In common for many structured iterative methods, application of a general purpose approach to a specific problem leads to structures which can be exploited in the algorithm. We derive in Section 3 a structure of Broyden method iterates when applied to (1.2), which allows us to improve the approach. We show how this can be integrated with a deflation technique (in Section 4). In this context we also show how restarting can be carried out in a natural way. A local convergence is also characterized (in Section 5). We show how the convergence is related to Jordan structure in the sense of \([10, 19]\). More precisely, we show how the convergence is given by the existence of solutions to the equation

\[
\sum_{i=0}^{a} \frac{M^{(i)}(\lambda)}{i!} v_{a-i} = 0
\]

where \( v_0 \) is a singular vector of \( M(\lambda) \).

We present numerical results of simulations for several problems in Section 6 and Section 7 in order to illustrate the properties of the method and its competitiveness for the time-periodic time-delay system.

2. Background and basic algorithm. We briefly summarize the specific version of Broyden’s method which will be the basis of our algorithm on. We use a damped version of Broyden’s method, as described e.g., in \([1, Section 7]\). The derivation follows from the Newton-like update equation

\[
J_k \Delta x_k = -F(x_k)
\]

where the next approximation is computed with a damped update equation

\[
x_{k+1} = x_k + \gamma_k \Delta x_k
\]

The choice of the damping parameter \( \gamma_k \) will be tuned to our setting, essentially to avoid taking too large steps (as we shall further describe in Remark \([3,3]\)). The next matrix \( J_{k+1} \) will satisfy (what is commonly called) the secant condition

\[
J_{k+1}(x_{k+1} - x_k) = F(x_{k+1}) - F(x_k)
\]

where \( J_{k+1} \) is a rank-one modification of \( J_k \). We will focus on updates of the form,

\[
J_{k+1} = J_k + \frac{1}{\Vert \Delta x_k \Vert^2} z_{k+1} \Delta x_k^H.
\]
By combining (2.1), (2.3) and (2.4), it is clear that $z_{k+1}$ can be directly computed from

\begin{equation}
(2.5) \quad z_{k+1} = \frac{1}{\gamma_k} (F(x_{k+1}) - (1 - \gamma_k)F(x_k)).
\end{equation}

In the literature on Broyden’s method (without damping), e.g., the original work [7], the relation (2.4) with choice (2.5) is typically viewed as the minimization of the update matrix $J_{k+1} - J_k$ with respect to the Frobenius norm and maintaining the secant condition (2.3).

The equations (2.1), (2.2), (2.5) and (2.4) form an explicit algorithm where the state consists of a vector $x_k$ and a matrix $J_k$, taking the role of a Jacobian matrix. This algorithm is called Broyden’s good method. (Our algorithm can be modified to carry out bad Broyden’s method. We focus on the good Broyden method, for simplicity.)

An unfavorable aspect from a computational perspective is that the linear system in (2.6) needs to be solved in every step. There are several ways to avoid this. Instead of storing with the inverse of $J_k$ we can store its inverse $H_k = J_k^{-1}$. and state the algorithm in terms of $H_k$ instead of $J_k$. We see immediately that (2.1) becomes

\begin{equation}
(2.6) \quad \Delta x_k = -H_k F(x_k)
\end{equation}

Similarly, the update equation (2.4) can be reformulated in terms of $H_k$. More precisely, by applying the Sherman-Morrison-Woodbury formula [17, Section 2.1.4], we obtain

\begin{align*}
(2.7a) & \quad H_{k+1} = J_{k+1}^{-1} = \left( J_k + \frac{1}{\|\Delta x_k\|^2} z_{k+1} \Delta x_k^H \right)^{-1} \\
(2.7b) & \quad = J_k^{-1} - \frac{J_k^{-1} z_{k+1} \Delta x_k^H J_k^{-1}}{\|\Delta x_k\|^2 + \Delta x_k^H J_k^{-1} z_{k+1}} \\
(2.7c) & \quad = H_k - \frac{H_k z_{k+1} \Delta x_k^H H_k}{\|\Delta x_k\|^2 + \Delta x_k^H H_k z_{k+1}}.
\end{align*}

By using (2.5) and (2.8) we see that $H_k z_{k+1} = \frac{1}{\gamma}(H_k F(x_{k+1}) + (1 - \gamma)\Delta x_k)$ and the following equivalent alternative relation for $H_{k+1}$

\begin{equation}
(2.8) \quad H_{k+1} = H_k - \frac{(H_k F(x_{k+1}) + (1 - \gamma)\Delta x_k) \Delta x_k H_k}{\Delta x_k^H (H_k F(x_{k+1}) + \Delta x_k)}
\end{equation}

**Example 2.1.** In order to illustrate the differences between the two versions of Broyden’s method in terms of round-off error we carry out simulations on a small example (for reproducability). We consider the quadratic eigenvalue problem

$M(\lambda) = A_0 + A_1 \lambda + A_2 \lambda^2$

where $A_0$, $A_1$ and $A_2$ were randomly generated. We carried out the simulation for both $H$-version and $J$-version in single precision, as well as a simulation in sufficiently high precision such that the result iteration can be treated as exact. The residual norm
history is given in Figure 2.1. We see that the H-version follows the exact error history (computed with high precision arithmetic) worse than the J-version. The algorithm presented in the next section follows the trajectory even better (T-variant). Although the differences between the methods are small in this example, it illustrates what can be seen in longer simulations (in Section 6).

![Iteration history and zoomed iteration history](image)

**Figure 2.1. Round-off error illustration.**

3. Structure exploiting Broyden method.

3.1. Structure of the iterates. We now consider nonlinear systems of equations with a particular structure:

\[
F(\lambda, \begin{bmatrix} v \\ u \end{bmatrix}) = \begin{bmatrix} M(\lambda) & U(\lambda) \\ C^H & 0 \end{bmatrix} \begin{bmatrix} v \\ u \end{bmatrix} - b \in \mathbb{C}^{n+p+1}
\]

where $C^H \in \mathbb{C}^{(p+1) \times n}$, $U(\lambda) \in \mathbb{C}^{n \times p}$, $v \in \mathbb{C}^n$ and $u \in \mathbb{C}^p$. We will also consistently partition $b$ as $b^T = [b^T_1 \ b^T_2]$.

This structure includes the nonlinear equation formulation in (1.3) as the special case $p = 0$ and $b = e_{n+1}$. We take this more general approach in order to incorporate deflation in a natural way, as we will describe in Section 4. The Jacobian of this problem can be derived explicitly:

\[
J(\lambda, \begin{bmatrix} v \\ u \end{bmatrix}) = \begin{bmatrix} M(\lambda) & U(\lambda) \\ C^H & 0 \end{bmatrix} \begin{bmatrix} v \\ u \end{bmatrix} + \begin{bmatrix} M'(\lambda)v + U'(\lambda)u \\ 0 \\ 0 \end{bmatrix} \in \mathbb{C}^{(n+p+1) \times (n+p+1)}
\]

We first note that the structure of the Jacobian and the iterates are preserved in Broyden’s method, when we denote

\[
x_k = \begin{bmatrix} v_k \\ u_k \\ \lambda_k \end{bmatrix}
\]
More precisely, if we initialize the Jacobian in Broyden’s method with the structure, and label the blocks as

\[
J_1 = \begin{bmatrix} M_1 & W_1 \\ C^H & 0 \end{bmatrix} \in \mathbb{C}^{(n+p+1) \times (n+p+1)}.
\]

where \( W_1 = [U_1 \ f_1] \), then this structure is preserved in the sense of the following theorem.

**Theorem 3.1 (Structured iterates of Broyden’s method).** Let \((v_1, u_1, \lambda_1)\) be such that,

\[
C \begin{bmatrix} v_{k+1} \\ U \end{bmatrix} = b_2
\]

and \( J_1 \) be set to \((3.4)\). Suppose Broyden’s method initiated with \((v_1, u_1, \lambda_1)\) and \( J_1 \) applied to \((3.1)\) does not break down, and let \((v_k, u_k, \lambda_k)\) and \( J_k, k = 2, \ldots \) be the iterates. Then, the structures \((3.5)\) and \((3.4)\) are preserved for all \( k \), i.e., for \( k = 2, \ldots \), we have

\[
J_k = \begin{bmatrix} M_k & W_k \\ C^H & 0 \end{bmatrix}
\]

and

\[
C \begin{bmatrix} v_{k+1} \\ U \end{bmatrix} = b_2.
\]

**Proof.** The proof is by induction. We suppose \((3.6)\) and \((3.7)\) for a specific \( k \) and prove these two equations for \( k + 1 \). It is clear from \((2.1)\) that \( \Delta x_k \) satisfies

\[
\begin{bmatrix} M_k & W_k \\ C^H & 0 \end{bmatrix} \Delta x_k = \begin{bmatrix} M(\lambda_k)v_k + U(\lambda_k)u_k - b_1 \\ C^H v_k - b_2 \end{bmatrix} = \begin{bmatrix} M(\lambda_k)v_k + U(\lambda_k)u_k - b_1 \\ 0 \end{bmatrix}
\]

such that \( C^H \Delta v_k = 0 \). Since \( v_{k+1} = v_k + \gamma \Delta v_k \), we have

\[
C^H v_{k+1} = C^H (v_k + \gamma \Delta v_k) = C^H v_k = b_2.
\]

which shows \((3.7)\) for \( k + 1 \). Therefore, the vector \( z_{k+1} \) has the structure

\[
z_{k+1} = \frac{1}{\gamma} \left( \begin{bmatrix} M(\lambda_{k+1})v_{k+1} + U(\lambda_{k+1}) - b_1 \\ C^H v_{k+1} - b_2 \end{bmatrix} - (1 - \gamma_k) \begin{bmatrix} M(\lambda_k)v_k + U(\lambda_k) - b_1 \\ C^H v_k - b_2 \end{bmatrix} \right) = \frac{1}{\gamma} \begin{bmatrix} M(\lambda_{k+1})v_{k+1} + U(\lambda_{k+1}) - b_1 - (1 - \gamma_k)(M(\lambda_k)v_k + U(\lambda_k) - b_1) \\ 0 \end{bmatrix}
\]

The matrix \( J_k \) is updated according to \((2.4)\). The last block row of the update in \((2.4)\) is zero, since the last block row of is \( z_{k+1} = 0 \). Therefore, we can define some \( J_{k+1} \) and \( W_{k+1} \) such that \((3.6)\) is satisfied for \( k + 1 \).

**3.2. Structured Broyden.** With the objective to improve Broyden’s method for nonlinear systems of equations of the form \((3.1)\), we now show how the structure proven in Theorem 3.1 can be implicitly preserved. The \( J \)-version is straightforward to modify to incorporate the structure, by consideration of the blocks of \((2.1)\) in \( J_k \Delta x = -F(x_k) \) as follows. We multiply the first block row of equation \((2.1)\) from the left with \( C^H M_k^{-1} \), i.e.,

\[
C^H M_k^{-1} \begin{bmatrix} M_k \Delta v_k + W_k \Delta \lambda_k \\ X \end{bmatrix} = -C^H M_k^{-1} \Delta r_k,
\]

\[
(3.8)
\]
where the residual $r_k$ is defined as

$$\label{eq:r_k} r_k = M(\lambda_k)v_k + U(\lambda_k)u_k - b_1.$$  

By using that $C^H\Delta v_k = C^H(v_{k+1} - v_k)/\gamma_k = (b_1 - b_1)/\gamma_k = 0$ due Theorem 3.1, we conclude from (3.8) that the following linear system for $\Delta u_k$ and $\Delta \lambda_k$ is satisfied

$$\label{eq:linear_system_1} - C^H M_k^{-1} r_k = (C^H M_k^{-1} W_k) \begin{bmatrix} \Delta u_k \\ \Delta \lambda_k \end{bmatrix}.$$  

Subsequently, $\Delta v_k$ is found from the first block row of (2.1), i.e.,

$$\label{eq:linear_system_2} \Delta v_k = -M_k^{-1} \left( W_k \begin{bmatrix} \Delta u_k \\ \Delta \lambda_k \end{bmatrix} + r_k \right).$$  

Hence, the solution of the linear system in (2.1) can be replaced by first solving (3.10) and then computing (3.11). This procedure can be implemented with $p + 2$ linear solves.

At first sight, nothing is gained since we need even more linear solves than the $J$-version. However, similar to the $H$-version, we can now formulate the algorithm by representing an inverse. More precisely, instead of storing $M_k$ we store,

$$T_k = M_k^{-1}.$$  

The reasoning with exploitation of the Jacobian in the $J$-version can be translated as follows. Equation (3.10) can be replaced by computing

$$\label{eq:Z_k} Z_k = T_k W_k$$  

which allows us to compute the corresponding linear system in $p + 1$ unknowns:

$$\begin{bmatrix} \Delta u_k \\ \Delta \lambda_k \end{bmatrix} = -(C^H Z_k)^{-1}(C^H T_k r_k),$$  

from which we can form

$$\Delta v_k = -Z_k \begin{bmatrix} \Delta u_k \\ \Delta \lambda_k \end{bmatrix} - T_k r_k.$$  

For notational convenience we now set $I^H := [I \ 0] \in \mathbb{R}^{n \times (n+p+1)}$. After updating the iterates

\begin{align*}
  &v_{k+1} = v_k + \gamma \Delta v_k \\
  &u_{k+1} = u_k + \gamma \Delta u_k \\
  &\lambda_{k+1} = \lambda_k + \gamma \Delta \lambda_k
\end{align*}  

we compute a new residual corresponding to $r_{k+1}$ using (3.9) and define $\tilde{z}_{k+1}$ as

$$\tilde{z}_{k+1} = I^T z_{k+1} = \frac{1}{\gamma_k} (r_{k+1} - (1 - \gamma_k) r_k).$$  

By again applying the Sherman-Morrison-Woodbury formula, we see that we can directly update $T_k$

$$T_{k+1} = T_k - \frac{1}{\| \Delta x_k \|^2 + \Delta x_k^H I T_k I^T z_{k+1}} T_k I^T z_{k+1} \Delta x_k^H T_k.$$
which can be further simplified to not contain $x$-dependence,

\begin{equation}
T_{k+1} = T_k + T_k \hat{z}_{k+1} a_{k+1}^H
\end{equation}

where $a_{k+1}^H := -\Delta v^H_k T_k / (\|\Delta v_k\|^2 + \|\Delta u_k\|^2 + |\Delta \lambda_k|^2 + \Delta v^H_k T_k \hat{z}_{k+1})$. We can subsequently update $W_k$ with

\begin{equation}
W_{k+1} = W_k + \hat{z}_{k+1} b_{k+1}^H
\end{equation}

where $b_{k+1}^H = [\Delta u_k^H \ (\Delta \lambda_k)^H] / (\|\Delta v\|^2 + \|\Delta u\|^2 + |\Delta \lambda|^2)$. Finally, as a consequence of the fact that $T_k$ and $W_k$ are updated with rank-one matrices, we can also compute $Z_{k+1}$ by a rank one update of $Z_k$ rather than using the definition (3.12). By combining (3.18) and (3.19) we find that

\begin{equation}
Z_{k+1} = T_{k+1} W_{k+1} = Z_k + T_k \hat{z}_k (a_{k+1}^H W_k + (1 + a_{k+1}^H \hat{z}_{k+1}) b_{k+1}^H).
\end{equation}

We now note that the above equations form an algorithm, which does not contain explicitly $J_k$, nor $x_k$, and implicitly preserves the preserves the Jacobian structure in Theorem 3.1. The algorithm is summarized in Algorithm 1. For implementation details, such as how to update $T_k$, $W_k$ and $Z_k$ by using only two vector operations, we refer to the publicly available software, further described in Section 6. As a consequence of the derivation, we have the following equivalence.

**Theorem 3.2 (Equivalence Broyden methods).** The $J$-version of Broyden’s method applied to (3.1), i.e., the iteration defined by (2.1), (2.2) and (2.3) is equivalent to the structured Broyden’s method, i.e., the iteration defined by (3.13), (3.14), (3.15), (3.18), (3.19) and (3.20). Moreover, the states of the algorithms are related by

\begin{equation}
J_k = \begin{bmatrix} T_k^{-1} & W_k \\ C^H & 0 \end{bmatrix}.
\end{equation}

**Remark 3.3 (Selection of damping).** The damping parameter is used to prevent the algorithm from taking too big steps in a pre-asymptotic phase, which can otherwise lead divergence or convergence to an (undesired) solution far away. In practice, we observed that the $\lambda$-approximation in the beginning of the iteration often generated new approximations far away from the true solution. Therefore, we capped the step by selection

\begin{equation}
\gamma_k = \min(1, t/|\Delta x_k|)
\end{equation}

where $\tau$ is a threshold parameter.

This implies $||x_{k+1} - x_k|| < t$ and in particular that $|\lambda_{k+1} - \lambda_k| \leq t$. This choice was determined based on numerical simulations. Another option would be the Armijo-steplength, as used, e.g., in the context of Newton’s method for NEPs in [27]. In contrast to (3.22), the standard implementation of Armijo step-steplength involves function evaluations, and is not competitive in our situation. We note that there is very little general conclusive theoretical analysis concerning how the damping parameter is best chosen in a Broyden setting, as e.g., pointed out in [1].

4. Deflation.
Algorithm 1 Structured Broyden’s method

Input: Starting values:
- Vectors: \( v_1 \in \mathbb{C}^n, u_1 \in \mathbb{C}^p, \lambda_1 \in \mathbb{C} \) approximating solution to (3.1)
- Matrices: \( C^H \in \mathbb{C}^{(p+1) \times n}, T_1 \in \mathbb{C}^{n \times n} \) and \( W_1 \in \mathbb{C}^{n \times (p+1)} \) approximating (3.2)

Input must satisfy \( C^H v_1 = b_2 \).

Output: \( v_m, u_m, \lambda_m, T_m, W_m \)

1: Compute \( r_1 \) according to (3.9)
2: Compute \( Z_1 \) according to (3.12)
3: while \( k = 1, 2, \ldots \) until convergence do
4: Compute \( \Delta u_k, \Delta \lambda_k \) by solving the linear system (3.13) in \( p+1 \) variables
5: Compute \( \Delta v_k \) with (3.14)
6: Select the damping parameter \( \gamma_k \), e.g., as in Remark 3.3
7: Update the iterates by computing \( v_{k+1}, u_{k+1} \) and \( \lambda_{k+1} \) with (3.15)
8: Compute \( r_{k+1} \) according to (3.9)
9: Compute \( \tilde{z}_{k+1} \) using \( r_k \) and \( r_{k+1} \) and (3.16)
10: Compute \( Z_{k+1} \) with (3.20)
11: Compute \( W_{k+1} \) with (3.19)
12: Compute \( T_{k+1} \) with (3.18)
13: end while

4.1. A deflated NEP. Structured Broyden’s method can be directly applied to (1.3) to compute an eigenpair of (1.1), as was illustrated in Example 2.1. In order to provide the possibility to compute several eigenvalues in a robust way, we here develop a deflation technique, which can be integrated with the structured Broyden’s method. Our reasoning is inspired by the work on invariant pairs for NEPs in [27] and deflation [11]. These works, in turn, are inspired by ideas for quadratic eigenvalue problems [30, 31, 3].

The essential conclusion of our reasoning provided below is that we can define an augmented NEP as

\[
G(\lambda) = \begin{bmatrix} M(\lambda) & U(\lambda) \\ X^H & 0 \end{bmatrix}
\]

whose eigenvalues are essentially the same as the original NEP except for some eigenvalues which are removed. (We postpone the definition of \( X \) and the function \( U(\lambda) \) until after the discussion of invariant pairs below.) Note that if we add an orthogonalization constraint to \( G(\lambda)w = 0 \) as in (1.2) with a particular vector \( e^H = [c_1^H \ 0] \), we obtain a nonlinear system of with the structure of the previous section, i.e., (3.1). Our construction is based on applying Algorithm 1 to this problem.

For the derivation of this approach we need the concepts of invariant pairs, orthogonalization conditions and augmented invariant pairs, which we briefly summarize. See [27, 11] and [12] for a detailed characterization. Without loss of generality, let \( M \) in (1.1) be decomposed as a sum of products of matrices and functions as in (1.4). This decomposition always exists, although in computation it does not always lead to efficient algorithms if \( m \) is large. We will only use this decomposition for theoretical purposes and not in the final algorithm. An invariant pair of (1.1) is defined as a pair \( (X, S) \in \mathbb{C}^{n \times p} \times \mathbb{C}^{p \times p} \) which satisfies

\[
0 = M_1Xf_1(S) + \cdots + M_mXf_m(S),
\]
where \( f_i(S) \in \mathbb{C}^{m \times m} \) are matrix functions of \( f_i, i = 1, \ldots, m \). By computing a Schur decomposition of \( S \), it is possible to show that the eigenvalues of \( S \) are eigenvalues of (1.1). For standard eigenvalue problems, we usually require that the columns of \( X \) (which form a basis of an invariant subspace) are linearly independent. This is done in order to prevent the same eigenspace to appear several times in the invariant pair. In practice (still linear eigenvalue problems) this is usually achieved by imposing that the columns of \( X \) are orthonormal. The concept of minimality formalizes this reasoning. The minimality concept is slightly different in the nonlinear case, due to the fact that several eigenvalues can have the same eigenvector (or correspondingly for invariant subspaces). The generalization is not expressed terms of the column span \( X \), but instead of the column span of

\[
\begin{bmatrix}
X \\
\vdots \\
XS^{\ell-1}
\end{bmatrix}
\]

If there exists \( \ell \in \mathbb{N} \) such that (4.2) has full column rank, then the pair is called minimal, and the smallest \( \ell \) such that (4.2) has full column rank, is called the minimality index of the pair \((X, S)\). As pointed out in [12], for minimal invariant pairs \( \ell = 1 \) is generic.

The concept of invariant pairs was used in a natural way to construct a deflation technique for (simplified) Newton method and a Jacobi-Davidson method in [12] and [11]. The main idea is to compute invariant pairs one column at a time. Given an invariant pair \((X, S)\), vectors \( v, u \) and \( \lambda \) are computed such that the extended pair

\[
(\hat{X}, \hat{S}) = \left( \begin{bmatrix} X & v \end{bmatrix}, \begin{bmatrix} S & u \\ \lambda \end{bmatrix} \right)
\]

is also an invariant pair. In [11, Lemma 6.1.3] the minimality is guaranteed by imposing orthogonality to the columns of (4.2),

\[
\begin{bmatrix}
X \\
\vdots \\
XS^{\ell-1}
\end{bmatrix}^H \begin{bmatrix}
\hat{X} \\
\vdots \\
\hat{X}S^{\ell-1}
\end{bmatrix} = 0
\]

In this way, we avoid reconvergence, i.e., if an eigenvalue is contained in \( S \), the algorithm will not find this eigenvalue again, unless it has multiplicity greater than one.

The condition that the extended pair (4.3) is invariant, is equivalent to a more explicit condition, shown in the following lemma.

**Lemma 4.1 (Lemma 6.1.1 of [11]).** Let \((X, S)\) be an invariant pair of the nonlinear eigenvalue problem (1.1). Then, the extended pair (4.3) is an invariant pair if and only if

\[
M(\lambda)v + U(\lambda)u = 0
\]

where

\[
U(\lambda) = \frac{1}{2\pi i} \oint_\Gamma M(\xi)(\xi I - \Lambda)^{-1}(\xi - \lambda)^{-1} d\xi.
\]

\[
M(\lambda)v + U(\lambda)u = 0
\]
If \( \lambda \not\in \lambda(S) \) we have additionally (as formalized in [11, Lemma 6.2.2])

\[
U(\lambda) = M(\lambda)X(\lambda I - S)^{-1}.
\]

In this work we will in practice extensively use (4.7) rather than the slightly more general definition (4.6).

We now focus on the case \( \ell = 1 \); see Remark 4.3 for discussion of general case.

By combining equations (4.5) and (4.4) we reach the nonlinear eigenvalue problem corresponding to (4.1) where

\[
\begin{bmatrix}
M(\lambda)U(\lambda)X
\end{bmatrix}^{T}
\]

is an eigenvector of the NEP \( G(\lambda) \), given by (4.1).

This reasoning is formalized in the following theorem, which can be interpreted as a complement to [12, Theorem 3.6] where we also stress that imposing orthogonality is not restricting the set of minimal invariant pairs. We state the theorem in terms of similarity transformations. The pair \((X, S)\) is a minimal invariant pair, if and only if \((XZ, Z^{-1}SZ)\) is a minimal invariant where \(Z \in \mathbb{C}^{p \times p}\) is invertible [11, Lemma 3.2.3]. We say that \((X, S)\) and \((XZ, Z^{-1}SZ)\) are equivalent by similarity transformation.

**Theorem 4.2 (Index one extensions).** Suppose \((X, S)\) is a minimal invariant pair with index one. Then, all minimal invariant pairs with index one of the form (4.3) are equivalent by similarity transformation to the minimal invariant pairs with index one of the form (4.3) where \(v, u, \lambda\) are solutions to

\[
\begin{bmatrix}
M(\lambda) & U(\lambda)
\end{bmatrix}^{T} = 0,
\]

and \(\|v\| + \|u\| \neq 0\).

**Proof.** Let \(Z = R^{-1}P\) be the similarity transformation, defined by the QR-factorization of \(X = QR\) (where \(Q \in \mathbb{C}^{n \times p}\) and \(R \in \mathbb{C}^{p \times p}\) is invertible since the columns of \(X\) are linearly independent) and the Schur factorization \(RSR^{-1} = PRP^{H}\).

From this transformation we see that \((X, S)\) is equivalent by similarity transformation to \((XZ, Z^{-1}SZ)\) where \(XZ\) is orthogonal and \(Z^{-1}SZ\) upper triangular. By a change of variable, the condition (4.8) is unmodified by the transformation. Hence, without loss of generality we can assume that \(X\) is orthogonal and \(S\) upper triangular.

Suppose \((\hat{X}, \hat{S})\) is an augmented minimal invariant pair (with extensions that do not necessarily satisfy (4.8)). With the similarity transformation

\[
Z = \begin{bmatrix}
I & -X^{H}v \\
0 & 1
\end{bmatrix} \in \mathbb{C}^{(p+1) \times (p+1)}
\]

we can, by using Lemma 4.1, verify that (4.8) is satisfied by selecting vectors corresponding \((v, u, \lambda)\) as \((\hat{X}Ze_{p+1}, [I_{p} 0]Z^{-1}SZe_{p+1}, \lambda)\). The converse holds due to the fact that a solution satisfying (4.8) forms a vector \(v\) which is orthogonal to \(X\), and non-zero since the extension would otherwise be non-minimal.

**Remark 4.3 (Minimality index greater than one).** The generalization of the above reasoning to a higher minimality index can be seen as follows. The orthogonality condition (4.4) with \(\ell = 2\) implies that \(v, u, \lambda\) must satisfy

\[
(X^{H} + \lambda S^{H}X^{H})v + S^{H}X^{H}Xu = 0.
\]

Unlike the case \(\ell = 1\), this expression depends on both \(u\) and \(\lambda\). As pointed out in a more general form in [12], the analogous NEP to (4.8) becomes

\[
\begin{bmatrix}
M(\lambda) & U(\lambda) \\
X^{H} + \lambda S^{H}X^{H} & S^{H}X^{H}X
\end{bmatrix}^{T} = 0.
\]
Unfortunately, when we include a normalization condition as in \( (1.2) \), this problem does not lead to a nonlinear equation of the form \( (3.1) \) which we need for structured Broyden method. It includes more blocks and more \( \lambda \)-dependence,

\[
0 = \begin{bmatrix} M(\lambda) & U(\lambda) \\ C_1^H(\lambda) & C_2^H \\ e_1^H & 0 \end{bmatrix} \begin{bmatrix} v \\ u \end{bmatrix} - b \in \mathbb{C}^{1+1},
\]

where \( C_1^H(\lambda) = X^H + \lambda S^H X^H \) and \( C_2^H = S^H X^H X \). This prevents us from using structured Broyden in the same way. We can however apply Broyden’s method (without exploiting the same amount of structure), which we illustrate in the simulations in Section 3. In this sense, our algorithm presented in the next section can in principle be constructed with a higher minimality index, but we cannot use the same amount of structure. In this paper we develop an efficient algorithm for \( \ell = 1 \), and propose to use the slower variant without structure exploitation for problems where eigenpairs share eigenvectors. For most problems stemming from PDEs, \( \ell = 1 \) is generic.

4.2. Structured Broyden with deflation. The previous section showed that given an index one invariant pair, we can compute an extension of that invariant pair by solving the NEP \( (4.1) \). All extensions are represented by this extended NEP according to Theorem 4.2. Since \( (4.1) \) combined with the normalization condition with \( e^H = [e_1^H 0] \) leads to a nonlinear system of equation of the structure \( (3.1) \) and we can use Algorithm 1 to solve it.

This structured extension of the invariant pair can be combined with Algorithm 1. Algorithm 2 shows this combination, including handling of invariant pairs and starting values. We now provide further details and justification of the algorithm, and show how restarting can be incorporated.

Recall that our method is mainly intended for problems where the matrix vector product \( M(\lambda)z \) is computationally expensive. At step 8 of Algorithm 1 we need to compute the residual \( (3.9) \) which in our setting contains terms \( M(\lambda)v \) and \( U(\lambda)w \); each of these involving one matrix vector product with \( M(\lambda) \). When we use Algorithm 1 we can combine \( M \) with the formula for \( U \) in \( (1.7) \) and compute the residual \( (3.9) \) directly by using only matrix vector product.

\[
r_{k+1} = M(\lambda_{k+1})v_{k+1} + U(\lambda_{k+1})u_{k+1} = M(\lambda_{k+1})(v_{k+1} + X(\lambda_{k+1}I - S)^{-1}u_{k+1}).
\]

Our algorithm requires starting values for each extension of the invariant pair. Although starting values are usually tuned to the applications, and this can also be done in our case, we here propose a quite general application-independent procedure to select starting values. We base the starting values on previously computed information, which can be viewed as a restarting procedure. Starting values are required for \( M_1 = T_1^{-1}, W_1, v_1, u_1 \) and \( \lambda_1 \). If we are interested in eigenvalues close to a target \( \sigma \), we propose (Step 1) to use \( M_1 \approx M(\sigma) \) (or \( M_1 = M(\sigma) \) if it can be computed cheaply) and set \( \lambda_1 = \sigma \).

The eigenvector approximation \( (v_1 \in \mathbb{C}^n \text{ and } u_1 \in \mathbb{C}^p) \) are computed following an approximation of one step of the method called safeguarded iteration \( (3.2) \) Algorithm 4) in Step 6. Eigenvector approximations in safeguarded iteration are extracted by selecting the eigenvector corresponding to a small eigenvalue of the matrix \( M(\lambda) \). We select \( v_1 \) and \( u_1 \) in this way but applied to the extended deflated NEP \( (1.11) \), by replacing the blocks of the matrix with approximations, \( M(\lambda_1) \approx M_1 \) and \( U(\lambda_1) \approx U_0 \), where \( U_0 \) is computed directly from \( (1.7) \) by using \( p \) matrix vector products.
We see by comparing (3.21) and (3.2) that $W_0$ should be an approximation of $[U(\lambda_0) \ M'(\lambda_0)v_0 + U'(\lambda_0)u_0]$. The approximation of $U(\lambda_0)$ is chosen as the already computed $U_0$. The formula for $U(\lambda)$ in (4.7) gives us directly that

$$U'(\lambda) = -M(\lambda)X(\lambda I - S)^{-2} + M'(\lambda)X(\lambda I - S)^{-1}.$$

In order to compute a starting value of the last column of $W_0$ we use that the chain-rule for differentiation applied to $U(\lambda)$ implies

$$M'(\lambda_1)v_1 + U'(\lambda_1)u_1 = M'(\lambda_1)(v_1 + X(\lambda_1 I - S)^{-1}u_1) - M(\lambda_1)X(\lambda_1 I - S)^{-2}u_1 =$$

$$M'(\lambda_1)(v_1 + X(\lambda_1 I - S)^{-1}u_1) - U(\lambda_1)(\lambda_1 I - S)^{-1}u_1.$$

Unless the matrix vector action of the derivative $M$ is explicitly available, the first term can be approximated by central finite difference, and the second term by using the already computed $U_1$, i.e., $U(\lambda_1)(\lambda_1 I - S)^{-1}u_1 \approx U_1(\lambda_1 I - S)^{-1}u_1$. This is done in step 8.

In Step 11 we expand the invariant pair again if the problem exhibits symmetry. It is straightforward to show that if $\overline{M(\lambda)} = M(\lambda)$ for all $\lambda$, then an eigenpair $(v, \lambda)$ implies that $(\overline{\lambda}, \overline{X})$ is an eigenpair which can be included in the invariant pair if $\lambda \notin \mathbb{R}$. The new complex conjugate pair $(\overline{\lambda}, \overline{X})$ is included by carrying out a Gram-Schmidt orthogonalization against $X$, and storing the Gram-Schmidt coefficients in the new column of $S$.

**Algorithm 2** Deflated Broyden’s method

**Input:** Target $\sigma$ and normalization vector $c \in \mathbb{C}^n \setminus \{0\}$

**Output:** A standard minimal invariant pair $(X, S) \in \mathbb{C}^{n \times p} \times \mathbb{C}^{p \times p}$ of (1.1)

1. Compute $M_1 \approx M(\sigma)$ and $T_1 \approx M(\sigma)^{-1}$
2. Set $X = \text{empty matrix}$ and $S = \text{empty matrix}$
3. Set $k = 1$
4. while $k < p$ do
5. Compute $U_1 \approx U(\sigma) \in \mathbb{C}^{n \times (k-1)}$ where $U$ is given by (4.7)
6. Compute the smallest (in modulus) eigenvalue of the matrix

$$\begin{bmatrix} M_1 & U_1 \\ X^H & 0 \end{bmatrix} \in \mathbb{C}^{(n+k-1) \times (n+k-1)}$$

and let $[v_1^T \ u_1^T]^T$ be the corresponding eigenvector normalized such that $v_1^H v_1 = 1$.
7. Impose orthogonalization (3.1) on $v_1$ by updating $v_1$ and $u_1$.
8. Compute $f_1 \approx M'(\sigma)v_1 - U_1(\sigma I - S)^{-1}u_1$, e.g., with finite difference for $M'(\sigma)v_1$.
9. Run structured Broyden for NEPs (Algorithm 1) with $C = [X \ c]$ starting value $(\sigma, v_1, u_1)$ and Jacobian approximation $(T_1, W_1) = (T_1, [U_1 \ f_1])$. Save output in $(\lambda, v, u)$ and $(T_N, [U_N \ f_N])$
10. Expand invariant pair according to (4.3).
11. $k = k + 1$
12. If NEP has conjugate pair symmetry, expand also with conjugate eigenpair.
13. end while
5. Convergence theory. Due to its equivalence with Broyden’s method, the convergence of our approach can be characterized with more general results. In particular, Broyden’s method has asymptotic local superlinear convergence in general \[15, 6\]. However, the theory for superlinear convergence only holds under the assumption that the Jacobian at the solution is invertible. If this is not satisfied you can invoke theory for Broyden’s method of singular Jacobians \[9\], which implies (in general) linear convergence with a convergence factor equal to the reciprocal golden ratio. We characterize the singularity of the Jacobian of our particular problem.

The singularity of the Jacobian of many iterative methods for NEPs are directly given from the multiplicity (or Jordan chain structure) of the solution to the NEP, cf. \[41, 26, 23, 42\]. Our construction is equivalent to applying Broyden’s method to the augmented NEP \((4.1)\). Therefore, the Jacobian singularity of the augmented system \((3.1)\) can be characterized with the multiplicity of the augmented NEP \((4.1)\). Since the augmented problem is an artificially constructed NEP, we find it more insightful to characterize the Jacobian singularity in terms of the eigenvalue multiplicity of the original NEP \((1.1)\).

We note that the Jacobian of \((3.1)\) is given by

\[
J_* = \begin{bmatrix}
M(\lambda) & U(\lambda) & M'(\lambda)v + U'(\lambda)u
X^H & M'(\lambda)v + U'(\lambda)u
\end{bmatrix}
\]

and provide two convergence results. It turns out that the condition that the vector \(c\) should not be orthogonal to the eigenvector generalizes to the condition that matrix

\[
\begin{bmatrix}
X^H
\end{bmatrix}
\begin{bmatrix}
X
v_1
\end{bmatrix}
\]

needs to be non-singular, which is needed in the following theorem which gives a precise condition for the Jacobian to be singular.

**Theorem 5.1 (Jacobian singularity).** Suppose \((X, S)\) is a minimal index one invariant pair of \((1.1)\), where \(X\) is orthogonal and \(S\) upper triangular. Suppose \(\lambda_1, v_1\) is an eigenpair of \((1.1)\) such that \((5.2)\) is non-singular, and suppose \(M'(\lambda_1)v_1\) has null space of dimension one. Moreover, assume \(\lambda_1 \notin \lambda(S)\) and \(v_1 \notin \text{Range}(X)\). Then

\[
\begin{bmatrix}
v
u
\lambda
\end{bmatrix} = \begin{bmatrix}
(I - X^HX)v_1 \\
(\lambda_1 I - S)X^HV_1 \\
\lambda_1
\end{bmatrix}
\]

is a solution to \((4.8)\). Moreover, the Jacobian \((5.1)\) corresponding to this solution is singular if and only if there exists a Jordan chain of length two, i.e., there exists a vector \(v_2\) such that

\[
M(\lambda_1)v_2 + M'(\lambda_1)v_1 = 0.
\]

**Proof.** We verify \((5.3)\) directly by inserting into \((4.8)\) and using the formula for \(U\) in \((4.7)\) and that \(M(\lambda_1)v_1 = 0\). In order to establish when the Jacobian is singular we give necessary and sufficient conditions for the existence of non-trivial \(z_1, z_2, z_3\) such that

\[
\begin{bmatrix}
M(\lambda) & U(\lambda) & M'(\lambda)v + U'(\lambda)u
X^H & M'(\lambda)v + U'(\lambda)u
\end{bmatrix}
\begin{bmatrix}
z_1
z_2
z_3
\end{bmatrix} = 0.
\]

13
By using the formula for $U'(\lambda_1)$ in (4.9) and the formula for the solution vector (5.3), the first block equation becomes

$$\lambda_1 dz_1 + X(\lambda I - S)^{-1} z_2 + X(\lambda I - S)^{-1} X^H v_1 z_3 + M'(\lambda_1) v_1 z_3 = 0$$

We separate the rest of the proof into two cases.

- Suppose $z_3 = 0$, such that (5.6) reduces to $M(\lambda)(z_1 + X(\lambda I - S)^{-1} z_2) = 0$. Since $M(\lambda_1)$ has a one-dimensional null space, we must have $z_1 + X(\lambda I - S)^{-1} z_2 = \beta v_1$. By multiplication from left with $[X \ c]^T$, combining this with the last rows in (5.5) and using the assumption (5.2) we see that $\beta = 0$ and $z_2 = 0$. Consequently, $z_1 = 0$, such that $z_1, z_2, z_3$ are identically zero and do not form a non-trivial singular vector. Hence, any non-trivial singular vector must satisfy $z_3 \neq 0$.

- If we assume that $z_3 \neq 0$, we can without loss of generality assume that $z_3 = 1$. Clearly (5.6) can only be zero if there exists a vector $v_2$ such that (5.4) is satisfied. Moreover, $z_1$ and $z_2$ must satisfy for some value $\beta$,

$$z_1 + X(\lambda I - S)^{-1} z_2 + X(\lambda I - S)^{-1} X^H v_1 = v_2 + \beta v_1$$

We obtain that

$$\begin{bmatrix} X^H \\ c^H \end{bmatrix} \begin{bmatrix} \lambda I - S)^{-1} z_2 \\ -\beta \end{bmatrix} = \begin{bmatrix} X^H \\ c^H \end{bmatrix} \begin{bmatrix} -X(\lambda I - S)^{-1} X^H v_1 + v_2 \end{bmatrix}$$

This linear system has a solution since (5.2) is invertible by assumption, and directly gives us a singular vector from a vector $v_2$ satisfying (5.3). It is non-trivial since $z_3 = 1$.

\section{Example 5.2 (Double eigenvalue).} The convergence properties for a singular Jacobian matrix can be observed in practice, and we illustrate this with the NEP presented in [23] (and also [23, 26]). The problem is a delay eigenvalue problem $M(\lambda) = -\lambda I + A_0 + A_1 e^{-\tau \lambda}$ constructed such that it has a double non-semisimple eigenvalue at $\lambda_* = 3\pi i$. The error history of Algorithm 2 with $\sigma = 0$ and $M_0 = M(\sigma)$ is given in Figure 5.1. We clearly see that we have linear convergence the first time the iteration converges to $\lambda_*$. The second time the iteration converges to $\lambda_*$ we have superlinear convergence, consistent with the fact that the eigenvalue has multiplicity two (and not three). Once one of the double eigenvalues has been deflated, the Jacobian is singular, i.e., the convergence behaves as the convergence for simple eigenvalue.

We also observe (consistent with theory [4]) that the linear convergence has convergence factor equal to the reciprocal golden ratio, i.e., approximately 0.618.

\section{6. Simulations for quadratic time-delay system.} We provide results of simulations for various NEPs. Our implementation is in the Julia programming language [4, version 0.6.2 using a quad-core, 16 GB RAM, Intel i7-4600U CPU with 2.10GH [4]).

In order to show the properties of our approach we apply now apply the algorithm to the following problem

$$M(\lambda) = -\lambda^2 I + A_0 + A_1 e^{-\lambda}$$

where the matrices are the same as those in [13]. The simulations of this section are intended to illustrate method properties, and we do not claim that this method is the best method for this type of problem.

\footnote{The simulations are publicly available online: \url{http://www.math.kth.se/~eliasj/src/broyden}}
Figure 5.1. Convergence for the problem with a double eigenvalue at $\lambda_\ast = 3\pi i$. We clearly observe linear convergence the first time the iteration converges to $\lambda_\ast$, and fast superlinear convergence the second time it converges to $\lambda_\ast$.

We first illustrate the structure exploitation. In Figure 6.1 we see the convergence of the discussed versions of Broyden’s method. Figure 6.1a and Figure 6.1b show the same simulation but with different $x$-axis. The structure exploiting Broyden method (Algorithm 1) converges (slightly) faster in terms of iterations, although they are equivalent in exact arithmetic. The structure exploiting Broyden method is considerably faster than the other variants in terms of computation time.

The relevance of the damping is illustrated in Figure 6.3. No damping (or a very large $t$) typically leads to faster convergence, but robustness is lost as the solution can start diverging. The parameter $t$ can be viewed as a trade-off parameter, between robustness and convergence speed.

In order to illustrate the value of superlinear convergence, we compare the algorithm residual inverse iteration as described in [33], which is a very well established method. Residual inverse iteration is an implicit quasi-Newton method [24] and exhibits linear convergence. We see in Figure 6.4 that our proposed method is faster in terms of iterations. In the residual inverse iteration we have pre-computed an LU-factorization, in order speed up the computation of the linear solves.

In order to illustrate that a higher minimality index can allow you to compute more than $n$ eigenvalues, we adapted to idea described in Remark 4.3. A comparison with $\ell = 2$ can be seen in Figure 6.2 with $n = 5$. Minimality index $\ell = 2$ provides the possibility to compute $2n = 10$ eigenvalues.

7. Simulations for time-periodic delay-differential equation. The following problem is called time-periodic delay-differential equation. We consider a linear (time-varying) delay-differential equation

$$\dot{y}(t) = A(t)y(t) + B(t)y(t - \tau)$$

where $A(t), B(t) \in \mathbb{C}^{n \times n}$ are periodic functions with period $\tau$. We briefly summarize a stability characterization which leads to a NEP. See description of certain applications [29] and references therein and a number of numerical methods [38] [21] [22] [20] [5] for details. The observation that (7.1) can be characterized with a NEP was also used in [35]. We consider the ODE (without delay) associated with (7.1)

$$\dot{p}(t) = C(t, \lambda)p(t),$$
where
\[ C(t, \lambda) := A(t) + B(t)e^{-\lambda \tau} - \lambda I. \]
We define a NEP \( M(\lambda) \) by the action on a vector as
\[ M(\lambda)v = p(\tau) - v \]
where \( p(\tau) \) is the solution \( p(t) \) of (7.2) at \( t = \tau \) with initial condition \( p(0) = v. \)

The solutions of the NEP defined by (7.3), correspond to \((\lambda, v)\) such that \( p(\tau) = v = p(0) \), i.e., the starting value and final vector of \( p \) are the same and \( p \) can be viewed as a periodic function. From Floquet theory one can show that the stability of (7.1) is determined from the right-most solution \( \lambda \). The value \( \mu = e^{\tau \lambda} \) is called the characteristic multiplier, which is greater than one for right-half plane solutions to the NEP.

Note that the NEP given by (7.3), has an action defined by a solution to an ODE, i.e., the action is computationally expensive and it is of the type we consider in this work.
7.1. Benchmark problem. Time-periodic time-delay systems has been considerably used in models and studied in for specific applications in the literature. Certain vibrations in machine tool milling can be modeled with time-periodic time-delay systems, where dominant modes correspond to the undesirable machine tool chatter. The delay in this case stems from the fact that the cut of the previous lap has an influence on the current lap. The periodicity stems from the periodicity in the force, and modeling of the cutting tooth which is periodic in time due to the rotation. We consider a specific setup used as a benchmark in several papers. See [21] [22] [20] and references therein. The equations of motion are second order but can be reformulated into a first order time-periodic time-delay system

\[
\dot{y} = \begin{bmatrix}
0 & \frac{1}{m} \\
-\omega_0^2 & -2\zeta\omega_0
\end{bmatrix} y(t) + \begin{bmatrix}
0 \\
\frac{a_p w(t)}{m}
\end{bmatrix} y(t - \tau)
\]

By consideration of the projection of the application of the force (as described in [35]), the time-periodic coefficient becomes

\[w(t) = H(t - \tau/2)(\sin^2(\phi(t)))K_R + \cos(\phi(t)) \sin(\phi(t))K_T\]

where \(H(t)\) is the heaviside function and \(\phi(t) = 2\pi t/\tau\). We see that if the force modeling is not considered, \(w(t)\) is constant the problem reduces to the (easier) standard
time-delay system.

We carried out simulations with parameters \( a_p = m = \tau = \omega_0 = \zeta = 1 \), and solved the time-dependent ODE with Runge-Kutta 4 with \( N \) discretization points. The convergence as a function of iteration is given in Figure 7.1b.

One of the most successful numerical approaches for this problem correspond to discretizations of operator formulations, e.g., a spectral discretization of the monodromy operator in [8] and [5]. In practice, this involves the solution of a large (linear) eigenvalue problem. A comparison with the approach in [8] is shown in Figure 7.1a. We clearly see that the discretization in [8] and our approach lead to algebraic convergence, of similar order. That is, although a spectral discretization is used in [8], the observed convergence with respect to ODE-discretization is not exponential, but only algebraic. This is expected since the \( A(t) \) has a discontinuous derivative, and one cannot in general expect exponential convergence for PDEs which have discontinuous derivatives.

7.2. Benchmark problem with PDE coupling. In order to also take into account vibrations in the workpiece in the milling, a model which couples a PDE was presented in [35]. A discretization of the PDE leads to the following problem. Let \( D_{xx} = \frac{1}{h^2} \text{tridiag}(1, -2, 1) \in \mathbb{R}^{N \times N} \) where \( h = 1/N \). The identity operator in the finite-element basis is denoted \( P^{-1} \) and \( p_n = Pe_n \). The time-periodic time-delay
We carried out simulations for a discretization with \(N = 5000\), i.e., \(n = 10002\) on a computer with 64 GB of RAM. The results are presented in Figure 7.2. The action of the ODE was discretized with \(N = 15\), whereas the approximation of \(M(\sigma)\) was computed with \(N = 7\). The problem is stiff, and we therefore used an implicit time-stepping scheme. The inverse of the identity was treated in a way that avoids computing a full matrix. This problem is of such size that our implementation of the approach of [8] was not applicable due to the high demand of memory resources.

8. Conclusions and outlook. Broyden’s method, a standard approach for non-linear systems of equations, has here been developed to and turned into a useful algorithm for certain types of NEPs. Broyden’s method has been developed and studied considerable in the literature. Several techniques seem to carry over directly, such as limited memory versions [10, 44], or variations, such as the (so-called) bad Broyden’s method [7] can be specialized completely analogous to our approach. In order to maintain generality we have intentionally not pursued a detailed study of the ODE-solver used in the specific application in Section 7.2. A more specialized result using the structure of the matrices would probably lead to even further efficiency, but would be beyond the scope of this paper about methods for NEPs rather than the
specific problem Section 7.2.

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