An integral method for solving nonlinear eigenvalue problems

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Abstract

We propose a numerical method for computing all eigenvalues (and
the corresponding eigenvectors) of a nonlinear holomorphic eigenvalue
problem that lie within a given contour in the complex plane. The
method uses complex integrals of the resolvent operator, applied to
at least \( k \) column vectors, where \( k \) is the number of eigenvalues inside
the contour. The theorem of Keldysh is employed to show that the
original nonlinear eigenvalue problem reduces to a linear eigenvalue
problem of dimension \( k \). No initial approximations of eigenvalues and
eigenvectors are needed. The method is particularly suitable for mod-
erate large eigenvalue problems where \( k \) is much smaller than the
matrix dimension. We also give an extension of the method to the
case where \( k \) is larger than the matrix dimension. The quadrature
errors caused by the trapezoid sum are discussed for the case of an-
alytic closed contours. Using well known techniques it is shown that
the error decays exponentially with an exponent given by the product
of the number of quadrature points and the minimal distance of the
eigenvalues to the contour.

1 Introduction

We consider nonlinear eigenvalue problems of the form

\[
T(z)v = 0, \quad v \in \mathbb{C}^m, v \neq 0, z \in \Omega,
\]

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where $T : \Omega \to \mathbb{C}^{m,m}$ is assumed to be holomorphic in some domain $\Omega \subset \mathbb{C}$. The computation of all eigenvalues and eigenvectors inside $\Omega$ usually requires to solve two problems (see [13],[1] for recent reviews):

1. Approximate localization and separation of eigenvalues in suitable domains resp. intervals,

2. accurate computation of eigenvalues and associated eigenvectors by an iterative method.

The global problem of localization can be substantially simplified if minimum-maximum characterizations similar to the linear case hold [23],[20]. Voss and co-workers have combined these principles with locally convergent methods of Arnoldi or Jacobi-Davidson type (see [21],[2],[22]), and in this way provided an effective means for computing all eigenvalues.

Another case where both problems can be solved, is for polynomials

$$T(z) = \sum_{j=0}^{p} T_j (z - z_0)^j, \quad T_j \in \mathbb{C}^{m,m}.$$ 

This eigenvalue problem can be reduced to a linear eigenvalue problem of dimension $pm$, and this is the path taken by the MATLAB routine polyeig. Quite a few papers in the literature either analyze this linearization approach or generalize methods from linear eigenvalues to the polynomial case.

In the general holomorphic case we just have a power series near each $z_0 \in \Omega$

$$T(z) = \sum_{j=0}^{\infty} T_j (z - z_0)^j, \quad |z - z_0| \text{ small}, \quad T_j \in \mathbb{C}^{m,m}.$$ 

One may then use polynomial truncation and the polynomial solver for getting good initial estimates of the eigenvalues. However, the success of this method strongly depends on the radius of convergence and on the decay of the coefficient matrices. Also, it may be necessary to compute power series at many different points in $\Omega$.

Finally, we refer to the recent approach of Kressner [11], who uses the fact that any holomorphic matrix function can be written as

$$T(z) = \sum_{j=1}^{p} f_j(z) T_j, \quad T_j \in \mathbb{C}^{m,m}$$

with holomorphic functions $f_j : \Omega \mapsto \mathbb{C}$ (such a representation always exists for some $p \leq m^2$). Then a Newton-type iteration is devised in [11] that allows
to compute a group of eigenvalues and an associated subspace. Though the convergence of this method is surprisingly robust to the choice of initial values, it remains a method for solving the local problem.

In this paper we tackle the global problem by using contour integrals, which seem to be the only available tool in the general holomorphic case. The idea is to use the theorem of Keldysh [9], [10], which provides an expansion of $T(z)^{-1}$ in a neighborhood $U \subset \Omega$ of an eigenvalue $\lambda \in \Omega$ as follows:

$$T(z)^{-1} = \sum_{j=-\kappa}^{\infty} S_j (z - \lambda)^j, \quad z \in U \setminus \{\lambda\}, \quad S_j \in \mathbb{C}^{m,m}, \quad S_{-\kappa} \neq 0.$$  \hspace{1cm} (2)

More specifically, Keldysh’ theorem gives a representation of the singular part in (2) in terms of generalized eigenvectors of $T(z)$ and its adjoint $T^H(z)$. A good reference for the underlying theory is [15] which we briefly review in Section 2.

Numerical methods based on contour integrals seem not to have attracted much attention in the past. A notable exception are exponential integrators and, more recently, approaches to compute analytic functions of matrices via suitably transformed contour integrals, see [7], [8, 13.3.2]. In particular, the exponential convergence of the trapezoid sum is proved in [7].

Our goal is to compute all eigenvalues and the associated eigenvectors that lie within a given closed contour $\Gamma$ in $\Omega$. The main algorithm is described in Section 3. Suppose that $k \leq m$ eigenvalues of (1) lie inside $\Gamma$. Then our method reduces the nonlinear eigenvalue problem to a linear one of dimension $k$ by evaluating the contour integrals

$$A_p = \frac{1}{2\pi i} \int_{\Gamma} z^p T(z)^{-1} \hat{V} dz, \quad p = 0, 1.$$ \hspace{1cm} (3)

Here $\hat{V} \in \mathbb{C}^{m,k}$ is generally taken as a random matrix. The contour integrals in (3) are calculated approximately by the trapezoid sum. If $N$ quadrature points are used, this requires to solve $Nk$ linear systems, which is the main numerical effort. As a consequence, our method is limited to moderately large nonlinear eigenvalue problems for which a fast (sparse) direct solver is available.

In Section 4 we apply the algorithm to several examples, showing that a moderate number of quadrature nodes ($N \approx 25$) is usually sufficient to get good estimates of eigenvalues and eigenvectors. Based on [4], we prove in Section 4 that the quadrature error decays exponentially with an exponent that depends on the product of the number of quadrature nodes and the smallest distance of the eigenvalues to the contour.
In the final Section 5 we deal with two problems that are typical for non-linear eigenvalue problems and that do not occur in the linear case: First, there can be much more eigenvalues than the matrix dimension (e.g. characteristic functions for delay equations) and, second, eigenvectors belonging to different eigenvalues can be linearly dependent, even if the number of eigenvalues is less than the matrix dimension. In Section 5 we extend our integral method such that it applies to the case \( k > m \) and that it can also handle rank defects of eigenspaces. For the extended integral method it is necessary to evaluate \( A_p \) from (3) for indices \( 0 \leq p \leq 2 \lceil \frac{k}{m} \rceil - 1 \). Numerical examples show that this extension is suitable for solving both aforementioned problems.

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2 Nonlinear eigenvalues and Keldysh’ Theorem

The material in this section is largely based on the monograph \[15\]. It contains a general study of meromorphic operator functions that have values in spaces of Fredholm operators of index 0. For our purposes it is sufficient to consider matrix valued mappings

\[ T : \Omega \subset \mathbb{C} \to \mathbb{C}^{m,m}, \]

that are holomorphic in some open domain \( \Omega \). We write this as \( T \in H(\Omega, \mathbb{C}^{m,m}) \).

For a matrix \( A \) we denote by \( R(A) \) and \( N(A) \) its range and nullspace, respectively.

**Definition 2.1.** A number \( \lambda \in \Omega \) is called an **eigenvalue** of \( T(\cdot) \) if \( T(\lambda)v = 0 \) for some \( v \in \mathbb{C}^m, v \neq 0 \). The vector \( v \) is then called a (right) **eigenvector**. By \( \sigma(T) \) we denote the set of all eigenvalues and by \( \rho(T) = \Omega \setminus \sigma(T) \) we denote the **resolvent set**.

The eigenvalue \( \lambda \) is called **simple** if

\[ N(T(\lambda)) = \text{span}\{v\}, v \neq 0 \quad T'(\lambda)v \notin R(T(\lambda)). \]

**Theorem 2.2.** Every eigenvalue \( \lambda \in \sigma(T) \) of \( T \in H(\Omega, \mathbb{C}^{m,m}) \) is isolated, i.e. \( U \setminus \{\lambda\} \subset \rho(T) \) for some neighborhood \( U \) of \( \lambda \).

Moreover, \( T(z) \) is meromorphic at \( \lambda \), i.e. there exist \( \kappa \in \mathbb{N} \) and \( S_j \in \mathbb{C}^{m,m} \) for \( j \geq -\kappa \) such that \( S_{-\kappa} \neq 0 \) and

\[ T(z)^{-1} = \sum_{j=-\kappa}^{\infty} S_j (z - \lambda)^j, \quad z \in U \setminus \{\lambda\}. \]
Remark 2.3. The number $\kappa$ is uniquely determined and called the order of the pole at $\lambda$.

The Theorem of Keldysh (see Theorem 2.6 below) gives a representation of the singular part
\[
-\frac{1}{\kappa} \sum_{j=-\kappa}^{\infty} S_j(z - \lambda)^j
\]
in terms of (generalized) eigenvectors of $T$ and $T^H$. It goes back to Keldysh [9] with a proof given in [10]. Generalizations of Keldysh’ theorem were derived by Trofimov [19], who introduced the concept of root polynomials, and by Marcus and Sigal [12] and Gohberg and Sigal [5] who used factorizations of operator functions. A simple direct proof was found by Mennicken and Möller [14] who later gave a concise approach to the whole theory in [15].

For the motivation of the algorithm in the next section it is instructive to first state Keldysh’ theorem for simple eigenvalues. In this case Definition 2.1 implies for the adjoint $T^H(z)$
\[
N(T^H(\lambda)) = \text{span}\{w\} \quad \text{for some} \quad w \in \mathbb{C}^m, w \neq 0,
\]
\[
w^H T'(\lambda) v \neq 0.
\]
Without loss of generality we can normalize $v$ and $w$ such that
\[
w^H T'(\lambda) v = 1.
\]
(5)

Then we are still free to further normalize either $|w| = 1$ or $|v| = 1$.

Theorem 2.4. Assume $\lambda \in \Omega$ is a simple eigenvalue of $T \in H(\Omega, \mathbb{C}^{m,m})$ with eigenvectors normalized as in (5). Then there is a neighborhood $\mathcal{U} \subset \Omega$ of $\lambda$ and a holomorphic function $R \in H(\mathcal{U}, \mathbb{C}^{m,m})$ such that
\[
T(z)^{-1} = \frac{1}{z - \lambda}vw^H + R(z), \quad z \in \mathcal{U} \setminus \{\lambda\}.
\]
(6)

Moreover, let $C \subset \Omega$ be a compact subset that contains only simple eigenvalues $\lambda_n$, $n = 1, \ldots, k$ with eigenvectors $v_n, w_n$ satisfying
\[
T(\lambda_n)v_n = 0, \quad w_n^HT(\lambda_n) = 0, \quad w_n^HT'(\lambda_n)v_n = 1.
\]
(7)

Then there is a neighborhood $\mathcal{U}$ of $C$ in $\Omega$ and a holomorphic function $R \in H(\mathcal{U}, \mathbb{C}^{m,m})$ such that
\[
T(z)^{-1} = \sum_{n=1}^{k} \frac{1}{z - \lambda_n}v_nw_n^H + R(z), \quad z \in \mathcal{U} \setminus \{\lambda_1, \ldots, \lambda_k\}.
\]
(8)
Proof. The first part is a special case of Theorem 2.6 below. For the second part, note that eigenvalues are isolated and hence we can choose a neighborhood $C \subset U \subset \Omega$ such that $\sigma(T) \cap U = \{\lambda_1, \ldots, \lambda_k\}$. Then the function

$$R(z) = T(z)^{-1} - \sum_{n=1}^{k} \frac{1}{z - \lambda_n} v_n w_n^H$$

is holomorphic in $U \cap \rho(T)$ and by the first part it is also holomorphic in suitable neighborhoods of $\lambda_n, n = 1, \ldots, k$.

**Definition 2.5.** Let $T \in H(\Omega, \mathbb{C}^{m,m})$ and $\lambda \in \Omega$.

(i) A function $v \in H(\Omega, \mathbb{C}^m)$ is called a root function of $T$ at $\lambda$ if

$$v(\lambda) \neq 0, \quad T(\lambda)v(\lambda) = 0.$$ 

The order of the zero $z = \lambda$ of $T(z)v(z)$ is called the multiplicity of $v$ at $\lambda$ and denoted by $s(v)$.

(ii) A tuple $(v_0, \ldots, v_{n-1}) \in (\mathbb{C}^m)^n, n \geq 1$ is called a chain of generalized eigenvectors (CGE) of $T$ at $\lambda$ if $v(z) = \sum_{j=0}^{n-1} (z-\lambda)^j v_j$ is a root function of $T$ at $\lambda$ of multiplicity $s(v) \geq n$.

(iii) For a given $v_0 \in N(T(\lambda)), v_0 \neq 0$ the number

$$r(v_0) = \max\{s(v) : v \text{ is a root function of } T \text{ at } \lambda \text{ with } v(\lambda) = v_0\}$$

is finite and called the rank of $v_0$.

(iv) A system of vectors in $\mathbb{C}^m$

$$V = \{v_j^\ell, 0 \leq j \leq m_\ell - 1, 1 \leq \ell \leq L\}$$

is called a canonical system of generalized eigenvectors (CSGE) of $T$ at $\lambda$ if the following conditions hold:

(a) The vectors $v_0^1, \ldots, v_L^1$ form a basis of $N(T(\lambda))$,

(b) The tuple $(v_0^\ell, \ldots, v_0^{m_\ell - 1})$ is a CGE of $T$ at $\lambda$ for $\ell = 1, \ldots, L$,

(c) $m_\ell = \max\{r(v_0) : v_0 \in N(T(\lambda)) \setminus \text{span}\{v_0^\nu : 0 \leq \nu < \ell\}\}$

for $\ell = 1, \ldots, L$.

One can show that a CSGE always exists and that the numbers $m_\ell$ are ordered according to

$$m_1 \geq m_2 \geq \ldots \geq m_L.$$ 

They are called the partial multiplicities of $T$ at $\lambda$. With these notions we can state the following general theorem, see [15, Theorem 1.6.5].
Theorem 2.6 (Keldysh). Let $T \in H(\Omega, \mathbb{C}^{m,m})$ be given with $\rho(T) \neq \emptyset$. For $\lambda \in \sigma(T)$ let

$$V = (v_j^\ell, 0 \leq j \leq m_\ell - 1, 1 \leq \ell \leq L)$$

be a CSGE of $T$ at $\lambda$. Then there exists a CSGE

$$W = (w_j^\ell, 0 \leq j \leq m_\ell - 1, 1 \leq \ell \leq L)$$

of $T^H$ at $\lambda$, a neighborhood $U$ of $\lambda$ and a function $R \in H(U, \mathbb{C}^{m,m})$ such that

$$T(z)^{-1} = \sum_{\ell=1}^{L} \sum_{j=1}^{m_\ell} (z - \lambda)^{-j} \sum_{\nu=0}^{m_\ell-j} v_{\nu j}^\ell w_{m_\ell-j-\nu}^{\ell H} + R(z), \quad z \in U \setminus \{\lambda\}.$$  (9)

The system $W$, for which (9) holds, is the unique CSGE of $T^H$ at $\lambda$ that satisfies the following conditions

$$r(w_j^\ell) = m_\ell$$

$$\sum_{\alpha=0}^{j} \sum_{\beta=1}^{m_\nu} u_{j-\alpha}^{\ell H} T_{\alpha+\beta}^{\nu} v_{m_\nu-\beta}^\nu = \delta_{\nu j} \delta_0, 0 \leq j \leq m_\ell - 1, 1 \leq \ell, \nu \leq L, \quad (10)$$

where

$$T_j = \frac{1}{j!} T^{(j)}(\lambda), \quad j \geq 0.$$  (11)

Remark 2.7. Rather than using generalized eigenvectors one can also write $T(z)^{-1}$ in terms of left and right root functions, see [15, Th.1.5.4].

The representation (9) shows that the order $\kappa$ of the pole in (4) is given by

$$\kappa = \max\{m_\ell : \ell = 1, \ldots, L\}.$$ 

Further, the number $L = \dim(N(T(\lambda)))$ is the geometric multiplicity while $\sum_{\ell=1}^{L} m_\ell$ is the algebraic multiplicity of $\lambda$. In the semi-simple case $m_\ell = 1, \ell = 1, \ldots, L$, equations (9) and (11) simplify to

$$T(z)^{-1} = (z - \lambda)^{-1} \sum_{\ell=1}^{L} v_0^\ell w_0^{\ell H} + R(z),$$

$$w_0^\ell T'(\lambda) v_0^\nu = \delta_{\ell \nu}, \quad 1 \leq \ell, \nu \leq L, \quad (6)$$

which in case $L = 1$ further simplify to (6) and (5).

Consider now all eigenvalues inside a compact set $C \subset \Omega$. In the same way as (5) followed from (6), we obtain from Theorem 2.6 the following corollary.
Corollary 2.8. Let \( C \subset \Omega \) be compact and \( T \in H(\Omega, \mathbb{C}^{m,m}) \). Then \( C \) contains at most finitely many eigenvalues \( \lambda_n, n = 1, \ldots, n(C) \) with corresponding CSGEs

\[
V_n = \left( v_j^{\ell,n}, 0 \leq j \leq m_{\ell,n} - 1, 1 \leq \ell \leq L_n \right), \quad n = 1, \ldots, n(C).
\]

Let

\[
W_n = \left( w_j^{\ell,n}, 0 \leq j \leq m_{\ell,n} - 1, 1 \leq \ell \leq L_n \right), \quad n = 1, \ldots, n(C)
\]

be the corresponding CSGEs of \( T^H \) such that

\[
r(w_0^{\ell,n}) = m_{\ell,n}
\]

and with 

\[
T_{j,n} = \frac{1}{j!} T^{(j)}(\lambda_n)
\]

\[
\sum_{\alpha=0}^{j} \sum_{\beta=1}^{m_{\nu,n}} w_{j-\alpha}^{\ell,n} T_{\alpha+\beta,n} v_{m_{\nu,n}-\beta}^{\nu,n} = \delta_{\nu \ell} \delta_{0j}, \quad 0 \leq j \leq m_{\ell,n} - 1, 1 \leq \ell, \nu \leq L_n.
\]

Then there exists a neighborhood \( C \subset U \subset \Omega \) and a function \( R \in H(U, \mathbb{C}^{m,m}) \) such that for all \( z \in U \setminus \{\lambda_1, \ldots, \lambda_n(C)\} \)

\[
T(z)^{-1} = \sum_{n=1}^{n(C)} \sum_{\ell=1}^{L_n} \sum_{j=1}^{m_{\ell,n}} (z - \lambda_j)^{-j} \sum_{\nu=0}^{m_{\ell,n} - j} v_{\nu,n} w_{m_{\ell,n} - j - \nu}^{\ell,n} + R(z).
\]

As a consequence of the corollary it follows that the order of the pole in (4) is given by

\[
\kappa = \max\{m_{\ell,n} : 0 \leq \ell \leq L_n, 1 \leq n \leq n(C)\}.
\]

Consider now a contour \( \Gamma \subset \Omega \), i.e. a simple closed curve that has its interior \( \text{int}(\Gamma) \subset \Omega \). An easy consequence of the residue theorem is the following result.

Theorem 2.9. Let \( T \in H(\Omega, \mathbb{C}^{m,m}) \) have no eigenvalues on the contour \( \Gamma \subset \Omega \) and denote by \( \lambda_n, n = 1, \ldots, n(\Gamma) \) the eigenvalues in the interior \( \text{int}(\Gamma) \subset \Omega \). Then with the CSGEs from Corollary 2.8 we have for any \( f \in H(\Omega, \mathbb{C}) \)

\[
\frac{1}{2\pi i} \int_{\Gamma} f(z) T(z)^{-1} dz = \sum_{n=1}^{n(\Gamma)} \sum_{\ell=1}^{L_n} \sum_{j=1}^{m_{\ell,n}} \frac{f^{(j-1)}(\lambda_n)}{(j-1)!} \sum_{\nu=0}^{m_{\ell,n} - j} v_{\nu,n} w_{m_{\ell,n} - \nu-j}^{\ell,n}.
\]
If all eigenvalues are simple the formula reads

\[ \frac{1}{2\pi i} \int_{\Gamma} f(z)T(z)^{-1}dz = \sum_{n=1}^{n(\Gamma)} f(\lambda_n)v_nw_n^H, \]  

(13)

where \(v_n, w_n\) are left and right eigenvectors corresponding to \(\lambda_n\) and normalized according to

\[ w_n^HT(\lambda_n)v_n = 1, \quad n = 1, \ldots, n(\Gamma). \]  

(14)

**Proof.** Corollary 2.8 applies to \(C = \text{int}(\Gamma) \cup \Gamma\), where the function \(f(z)T(z)^{-1}\) has residues at \(\lambda_j\) given by the right-hand side of (12). The special case \(L_n = 1, m_{0n} = 1, n = 1, \ldots, n(\Gamma)\) yields equation (13). \(\square\)

### 3 The algorithm for a few eigenvalues

In the following we set up an algorithm for computing all eigenvalues of \(T \in H(\Omega, \mathbb{C}^{m,m})\) inside a given contour \(\Gamma\) in \(\Omega\). We assume that the sum of all algebraic multiplicities

\[ k = \sum_{n=1}^{n(\Gamma)} L_n \sum_{\ell=1}^{m_{\ell,n}} \]  

(15)

is less than or equal to the system dimension \(m\). For the opposite case we refer to Section 5. In high-dimensional problems we actually expect to have \(k \ll m\).

#### 3.1 Simple eigenvalues inside the contour

As in the second part of Theorem 2.9 let us assume that all eigenvalues \(\lambda_1, \ldots, \lambda_{n(\Gamma)}\) in \(\text{int}(\Gamma)\) are simple so that \(k = n(\Gamma)\). We introduce the matrices

\[ V = (v_1 \ldots v_k), \quad W = (w_1 \ldots w_k) \in \mathbb{C}^{m,k}. \]

We assume that we have chosen a matrix

\[ \hat{V} \in \mathbb{C}^{m,l}, \quad k \leq l \leq m, \]

such that

\[ W^H\hat{V} \in \mathbb{C}^{k,l} \text{ has rank } k. \]  

(16)

In particular, this implies \(\text{rank}(W) = k\). In the applications we choose \(\hat{V}\) at random (see Section 4), so that (16) can be expected to hold in a generic sense.
if \( \text{rank}(W) = k \). We note that (in contrast to linear eigenvalue problems) it is easy to construct nonlinear eigenvalue problems for which \( W \) is rank deficient. However, this seems to be a nongeneric situation for typical applications. In addition to (16) we assume

\[
\text{rank}(V) = k, \tag{17}
\]

which again is expected to hold in generic cases.

Next we compute the two integrals

\[
A_0 = \frac{1}{2\pi i} \int_{\Gamma} T(z)^{-1}\hat{V}dz \in \mathbb{C}^{m,l} \tag{18}
\]

\[
A_1 = \frac{1}{2\pi i} \int_{\Gamma} zT(z)^{-1}\hat{V}dz \in \mathbb{C}^{m,l}. \tag{19}
\]

The evaluation of these integrals by quadrature rules is by far the most expensive part of the algorithm and will be discussed below. Note also, that in the linear case \( T(z) = zI - A \) the matrix \( A_0 \) is obtained by applying to \( \hat{V} \) the Riesz projector onto the invariant subspace associated with all eigenvalues inside \( \Gamma \).

By (13) we obtain

\[
A_0 = \sum_{n=1}^{k} v_n w_n^H \hat{V} = VW^H \hat{V}. \tag{20}
\]

Similarly,

\[
A_1 = \sum_{n=1}^{k} \lambda_n v_n w_n^T \hat{V} = V \Lambda W^H \hat{V}, \quad \Lambda = \text{diag}(\lambda_n, n = 1, \ldots, k). \tag{21}
\]

In the next step we compute the singular value decomposition (SVD) of \( A_0 \) in reduced form

\[
VW^H \hat{V} = A_0 = V_0 \Sigma_0 W_0^H \tag{22}
\]

where \( V_0 \in \mathbb{C}^{m,k}, \Sigma_0 = \text{diag}(\sigma_1, \ldots, \sigma_k), W_0 \in \mathbb{C}^{l,k}, V_0^H V_0 = I_k, W_0^H W_0 = I_k. \)

Note that the rank conditions (16), (17) show that \( \text{rank}(A_0) = k \), hence \( A_0 \) has singular values

\[
\sigma_1 \geq \ldots \sigma_k > 0 = \sigma_{k+1} = \ldots = \sigma_l.
\]

By the rank condition (17) we have

\[
R(A_0) = R(V) = R(V_0). \tag{23}
\]
Since both, $V_0$ and $V$ are $m \times k$ matrices and $V_0$ has orthonormal columns, we obtain

$$V = V_0 S, \quad S = V_0^H V \in \mathbb{C}^{k,k} \text{ nonsingular.} \quad (23)$$

With (20), (23) we find $V_0 SW^H \hat{V} = V_0 \Sigma_0 W_0^H$ and thus

$$W^H \hat{V} = S^{-1} \Sigma_0 W_0^H.$$  

This relation is used to eliminate $W^H \hat{V}$ from $A_1 = V_0 S \Lambda W^H \hat{V}$. We obtain

$$V_0^H A_1 = S \Lambda W^H \hat{V} = S \Lambda S^{-1} \Sigma_0 W_0^H,$$

which upon multiplication by $W_0 \Sigma_0^{-1}$ from the right finally gives

$$S \Lambda S^{-1} = V_0^H A_1 W_0 \Sigma_0^{-1}. \quad (24)$$

Note that the right-hand side is a computable matrix which is diagonalizable and has as eigenvalues exactly the eigenvalues of $T$ inside the contour. We summarize the result in a theorem.

**Theorem 3.1.** Suppose that $T \in H(\Omega, \mathbb{C}^{m,m})$ has only simple eigenvalues $\lambda_1, \ldots, \lambda_k$ inside the contour $\Gamma$ in $\Omega$ with left and right eigenvectors normalized as in (14). Moreover, let a matrix $\hat{V} \in \mathbb{C}^{m,l}$ be given such that $k \leq l \leq m$ and the rank conditions (16), (17) are satisfied. Then the matrix

$$B = V_0^H A_1 W_0 \Sigma_0^{-1} \in \mathbb{C}^{k,k}, \quad (25)$$

given by (18), (19) and the SVD (22), is diagonalizable with eigenvalues $\lambda_1, \ldots, \lambda_k$. From the eigenvectors $s_1, \ldots, s_k \in \mathbb{C}^k$ of $B$ one obtains the eigenvectors of $T$ through

$$v_n = V_0 s_n, \quad n = 1, \ldots, k.$$

**Remarks 3.2.** (a) For reasons of numerical stability we may replace $A_1$ by

$$\tilde{A}_1 = \frac{1}{2\pi i} \int_{\Gamma} (z - z_0) T(z)^{-1} \hat{V} dz = A_1 - z_0 A_0.$$

For example, in case of a circle $\Gamma$, one can take $z_0$ as its center. Then (21) holds with $\Lambda - z_0$ instead of $\Lambda$ and the matrix $\tilde{B} = V_0^H \tilde{A}_1 W_0 \Sigma_0^{-1}$ has eigenvalues $\lambda_n - z_0$. Therefore, the eigenvalues of $T$ are found by adding $z_0$ to the eigenvalues of $\tilde{B}$.

(b) The rank conditions in the theorem are crucial. Assume, for example, that $A_0 = WV^H \hat{V}$ has rank $k_0 < k$. Then the SVD (22) holds with matrices $W_0 \in \mathbb{C}^{l,k_0}, V_0 \in \mathbb{C}^{m,k_0}$ and $\Sigma_0 = \text{diag}(\sigma_1, \ldots, \sigma_{k_0})$. Moreover, we have
In (23), \( S \in \mathbb{C}^{k_0,k} \), \( B \in \mathbb{C}^{k_0,k_0} \) in (25). Finally we find \( B = S \Lambda \tilde{S} \) where \( \tilde{S} = W^H \hat{W} S_0^{-1} \) satisfies \( S \tilde{S} = I_{k_0} \). Except for the case, when \( S \) has some zero columns this does not lead to a useful relation between the eigenvalues of \( B \) and \( \Lambda \). For numerical computations we therefore recommend to test the residuals \( ||T(\lambda_n)v_n|| \), see Section 3.3. A general cure of this rank deficient case is provided by the generalized algorithm in Section 5 which, however, is computationally more expensive.

### 3.2 Multiple eigenvalues inside the contour

Let us consider the general case where \( T \in H(\Omega, \mathbb{C}^{m,m}) \) has no eigenvalues on the contour \( \Gamma \) but may have multiple eigenvalues inside. We apply Corollary 2.8 to the compact set \( \mathcal{C} = \Gamma \cup \text{int}(\Gamma) \) and assume that the matrix composed of all CSGEs that belong to eigenvalues inside \( \Gamma \),

\[
V = \begin{pmatrix} v_{\ell,n}^j, & 0 \leq j \leq m_{\ell,n} - 1, & 1 \leq \ell \leq L_n, & 1 \leq n \leq n(\Gamma) \end{pmatrix},
\]

has rank \( k \), cf. (15). Then, using Theorem 2.9 with \( f(z) = 1 \) shows that \( A_0 \), as defined in (18), satisfies

\[
A_0 = \sum_{n=1}^{n(\Gamma)} \sum_{\ell=1}^{L_n} \sum_{\nu=0}^{m_{\ell,n} - 1} v_{\nu}^{,\ell,n} w_{m_{\ell,n} - 1 - \nu}^{,\ell,nH} \hat{V}.
\]

Further, we assume that the matrix

\[
W^H \hat{V} \in \mathbb{C}^{k,l}
\]

has maximum rank \( k \), where

\[
W = \begin{pmatrix} w_{\ell,n}^{,\ell,n}, & 0 \leq \nu \leq m_{\ell,n} - 1, & 1 \leq \ell \leq L_n, & 1 \leq n \leq n(\Gamma) \end{pmatrix} \in \mathbb{C}^{m,k},
\]

is normalized as in Theorem 2.6. With Theorem 2.9 we then find

\[
A_1 = \sum_{n=1}^{n(\Gamma)} \sum_{\ell=1}^{L_n} \left[ \lambda_n \sum_{\nu=0}^{m_{\ell,n} - 1} v_{\nu}^{,\ell,n} w_{m_{\ell,n} - 1 - \nu}^{,\ell,nH} + \sum_{\nu=0}^{m_{\ell,n} - 2} v_{\nu}^{,\ell,n} w_{m_{\ell,n} - 2 - \nu}^{,\ell,nH} \right] \hat{V} = V \Lambda W^H \hat{V},
\]

where \( \Lambda \) has Jordan normal form

\[
\Lambda = \begin{pmatrix} J_1 & \cdots & J_{n(\Gamma)} \end{pmatrix}, \quad J_n = \begin{pmatrix} J_{n,1} & \cdots & J_{n,L_n} \end{pmatrix}, \quad J_{n,\ell} = \begin{pmatrix} \lambda_n & 1 & \cdots \end{pmatrix}.
\]

(29)
As in Section 3.1 the next steps are the SVD (22) for $A_0$ and the computation of $B = V_0^H A_1 W_0 \Sigma_0^{-1} \in \mathbb{C}^{k,k}$. Then $B$ has eigenvalues $\lambda_1, \ldots, \lambda_{n(\Gamma)}$ and its Jordan normal form has the same partial multiplicities as $T(z)$.

**Theorem 3.3.** Suppose that $T \in H(\Omega, \mathbb{C}^{m,m})$ has no eigenvalues on the contour $\Gamma$ in $\Omega$ and pairwise distinct eigenvalues $\lambda_n, n = 1, \ldots, n(\Gamma)$ inside $\Gamma$ with partial multiplicities $m_1, n \geq \ldots \geq m_{L_n,n}, n = 1, \ldots, n(\Gamma)$. Moreover, assume that the matrix of generalized eigenvectors from (26) and the matrix $W_0 \Sigma_0^{-1}$ from (27) have rank $k$ with $k$ given by (15). Then the matrix $B \in \mathbb{C}^{k,k}$ from (25) has Jordan normal form (29) with the same eigenvalues $\lambda_n$ and partial multiplicities $m_{\ell,n}$ ($\ell = 1, \ldots, L_n, n = 1, \ldots, n(\Gamma)$). Suitable CSGEs for $T$ can be obtained from corresponding CSGEs $s_{\ell,n}^j$ for $B$ via

$$v_{\ell,n}^j = V_0 s_{\ell,n}^j, \quad 0 \leq j \leq m_{\ell,n} - 1, 1 \leq \ell \leq L_n, 1 \leq n \leq n(\Gamma).$$

**Remark 3.4.** Essentially, the theorem reduces the nonlinear problem for eigenvalues inside a contour to a linear eigenvalue problem for a $k \times k$-matrix. The linear eigenvalue problem inherits the multiplicity structure of the nonlinear problem. As usual, computing the Jordan normal form is not a stable process and other forms, such as the Schur form, are recommended. A closer look at the derivation of the algorithm (22), (24) shows that it is sufficient to have a rank revealing QR-decomposition. One would then replace $W_0 \Sigma_0^{-1}$ in (24) by the inverse of the maximum rank upper triangular submatrix.

### 3.3 Quadrature and numerical realization

The major step in the algorithm consists in evaluating the integrals (18) and (19) by numerical quadrature and by solving the linear systems involved in the evaluation of the integrand. We assume that $\Gamma$ has a $2\pi$-periodic smooth parameterization

$$\varphi \in C^1(\mathbb{R}, \mathbb{C}), \quad \varphi(t + 2\pi) = \varphi(t) \quad \forall t \in \mathbb{R}.$$ 

Of particular interest is the real analytic case $\varphi \in C^{\infty}(\mathbb{R}, \mathbb{C})$. Taking equidistant nodes $t_j = \frac{2\pi j}{N}, j = 0, \ldots, N$ and using the trapezoid sum, we find the following approximations

$$A_0 = \frac{1}{2\pi i} \int_0^{2\pi} T(\varphi(t))^{-1} \hat{V} \varphi'(t) dt \approx$$

$$A_{0,N} = \frac{1}{iN} \sum_{j=0}^{N-1} T(\varphi(t_j))^{-1} \hat{V} \varphi'(t_j), \quad (30)$$
where we used $\varphi(t_0) = \varphi(t_N)$. Similarly,

$$A_1 \approx A_{1,N} = \frac{1}{iN} \sum_{j=0}^{N-1} T(\varphi(t_j))^{-1} \hat{V} \varphi(t_j) \varphi'(t_j). \tag{31}$$

In order to compute $A_{0,N}$ we need to solve $Nl$ linear systems with $N$ different matrices $T(\varphi(t_j)), j = 0, \ldots, N-1$ and with $l$ different right-hand sides each. Note that we can use the solutions of these linear systems to compute $A_{1,N}$ at almost no extra cost. For the special case of a circle $\varphi(t) = \mu + Re^{it}$ we obtain the formulas

$$A_{0,N} = \frac{R}{N} \sum_{j=0}^{N-1} T(\varphi(t_j))^{-1} \hat{V} \exp\left(\frac{2\pi i j}{N}\right),$$

$$A_{1,N} = \mu A_{0,N} + \frac{R^2}{N} \sum_{j=0}^{N-1} T(\varphi(t_j))^{-1} \hat{V} \exp\left(\frac{4\pi i j}{N}\right).$$

The algorithm can be summarized as follows:

**Integral algorithm 1**

**Step 1:** Choose an index $l \leq m$ and a matrix $\hat{V} \in \mathbb{C}^{m,l}$ at random.

**Step 2:** Compute $A_{0,N}, A_{1,N}$ from (30,31).

**Step 3:** Compute the SVD $A_{0,N} = V \Sigma W^H$, where $V \in \mathbb{C}^{m,l}$, $W \in \mathbb{C}^{l,l}$, $V^H V = W^H W = I_l$, $\Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_l)$.

**Step 4:** Perform a rank test for $\Sigma$, i.e. find $0 < k \leq l$ such that $\sigma_1 \geq \ldots \geq \sigma_k > \text{tol}_{\text{rank}} \approx \ldots \approx \sigma_l \approx 0$.

If $k = l$ then increase $l$ and go to Step 1.

Else let $V_0 = V(1 : m, 1 : k), W_0 = W(1 : l, 1 : k)$ and $\Sigma_0 = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_k)$.

**Step 5:** Compute $B = V_0^H A_{1,N} W_0 \Sigma_0^{-1} \in \mathbb{C}^{k,k}$.

**Step 6:** Solve the eigenvalue problem for $B$

$$BS = SA, S = (s_1 \ldots s_k), A = \text{diag}(\lambda_1, \ldots, \lambda_k).$$

If $\|T(\lambda_j)v_j\| \leq \text{tol}_{\text{res}}$ and $\lambda_j \in \text{int}(\Gamma)$ accept $v_j = V_0 s_j$ as eigenvector and $\lambda_j$ as eigenvalue.

**Remarks 3.5.** (a) If we find $k = l$ positive singular values in Step 4 then we take this as an indication that there may be more than $l$ eigenvalues (including multiplicities) inside $\Gamma$. We then increase $l$ until a rank drop is detected in Step 4.

(b) In general, it is more efficient to compute $A_{1,N}$ in Step 5, when the index $k$ has been determined. Then one has to store the solutions of the linear
systems solved during the evaluation of $A_{0,N}$.

(c) As noted in Remark 3.2(b) the algorithm may fail due to linear dependency of (generalized) eigenvectors. Therefore, we include a test of the residual. Moreover, as the experiments in Section 4 show, eigenvalues close to the contour, either inside or outside $\Gamma$, may lead to difficulties in the rank test. Therefore, the trivial test $\lambda_j \in \text{int}(\Gamma)$ is included in Step 6 as well.

(d) In Step 6 we assumed that eigenvalues are simple. If multiplicities occur or $B$ is only brought into upper triangular form, then the eigenvalues can still be read off from the diagonal, and the structure of eigenvectors can be retrieved from $V_0S$.

4 Error analysis and numerical examples

4.1 Error analysis

Standard results on the trapezoid sum for holomorphic periodic integrands imply exponential convergence at a rate that depends on the number of nodes times the width of the horizontal strip of holomorphy, see [3], [4, 4.6.5]. Applications of these results to the computation of matrix functions via contour integrals appear in [7].

Theorem 4.1. Let $f \in H(S(d_-, d_+), \mathbb{C})$ be $2\pi$-periodic on the strip

$$S(d_-, d_+) = \{ z \in \mathbb{C} : -d_- < \text{Im } z < d_+ \}, \quad d_+ > 0.$$ 

Then the error of the trapezoid sum

$$E_N(f) = \frac{1}{2\pi} \int_0^{2\pi} f(x)dx - \frac{1}{N} \sum_{j=0}^{N-1} f\left(\frac{2\pi j}{N}\right)$$

satisfies for all $0 < r_- < d_-, 0 < r_+ < d_+$

$$|E_N(f)| \leq \max_{\text{Im}(z)=r_+} |f(z)| G(e^{-Nr_+}) + \max_{\text{Im}(z)=r_-} |f(z)| G(e^{-Nr_-}),$$

where $G(x) = \frac{x}{1-x}, x \neq 1$.

Remark 4.2. Note that Theorem 4.1 is a slight variation of [4, 4.6.5] since $f$ is not assumed to be real on $[0, 2\pi]$ and the strip $S(d_-, d_+)$ can be unsymmetric, in general.

In the following we state and prove the corresponding result for integrals over circles which will be used in the sequel.
Theorem 4.3. Let $f \in H(A(a_-, a_+), \mathbb{C})$ be holomorphic on the annulus

$$A(a_-, a_+) = \{ z \in \mathbb{C} : \frac{1}{a_-} < \frac{|z|}{R} < a_+ \}, \quad a_\pm > 1,$$

for some $R > 0$. Then the error of the trapezoid sum

$$E_N(f) = \frac{1}{2\pi i} \int_{|z|=R} f(z) dz - \frac{R}{N} \sum_{j=0}^{N-1} f(R \omega_N^j) \omega_N^j, \quad \omega_N = \exp\left(\frac{2\pi i}{N}\right),$$

satisfies for all $1 < \rho_- < a_-, 1 < \rho_+ < a_+$

$$|E_N(f)| \leq \max_{|z| = \rho_+} |f(z)| G(\rho_+^{-N}) + \max_{\rho_-|z| = R} |f(z)| G(\rho_-^N).$$

Proof. We use the Laurent expansion of $f$ (see e.g. [6])

$$f(z) = \sum_{k=-\infty}^{\infty} f_k z^k, \quad f_k = \frac{1}{2\pi i} \int_{|z|=R} f(z) z^{k-1} dz,$$

which converges uniformly on compact subdomains of the annulus. By a simple computation,

$$E_N(z^k) = \begin{cases} -R_{\ell N} \rho_+^\ell, & k + 1 = \ell N, \ell \in \mathbb{Z} \setminus \{0\}, \\ 0, & \text{otherwise.} \end{cases}$$

Applying $E_N$ to (34) leads to

$$E_N(f) = -\sum_{\ell=1}^\infty (f_{\ell N} R_{\ell N} + f_{-\ell N} R^{-\ell N}).$$

From Cauchy’s Theorem and a standard estimate we obtain

$$|f_{\ell N} R_{\ell N}| = \left| \frac{R_{\ell N}}{2\pi i} \int_{|z|=R} f(z) z^{\ell N-1} dz \right| \leq \frac{R_{\ell N}}{2\pi} \max_{|z|=\rho_+^N} |f(z)| (\rho_+^N)^{-\ell N-1} \rho_+^{-\ell N}.$$

In a similar way,

$$|f_{-\ell N} R^{-\ell N}| \leq \max_{\rho_-|z|=R} |f(z)| \rho_-^{-\ell N}.$$

Using these estimates in (35) completes the proof. \qed
The proof shows that the $\rho_-\text{-term}$ can be discarded in (33) if the principal term in the Laurent expansion vanishes (i.e. $f_k = 0$ for $k \leq -1$). Likewise, the $\rho_+\text{-term}$ disappears when $f_k = 0$ for $k \geq 0$. For the function

$$f(z) = (z - \lambda)^{-j}, \quad j \geq 1,$$

the principal term vanishes for $|\lambda| > R$ while the secondary term vanishes for $|\lambda| < R$. Example (36) is crucial for the application to the meromorphic functions from Section 3. Therefore, we note the following explicit formula.

**Lemma 4.4.** The error of the trapezoid sum (32) for the function (36) in case $N \geq j$ is given as follows,

$$E_N((z - \lambda)^{-j}) = \frac{(-1)^{j-1} \lambda^{-j}}{(j-1)!} \left\{ \frac{g^{j-1}}{dx^j}(x^j G(x^{-N}))|_{x = \frac{R}{\lambda}}, \quad |\lambda| < R, \right. \quad |\lambda| > R.$$

In particular,

$$E_N((z - \lambda)^{-j}) = \begin{cases} O(\lambda^{-j} \left( \frac{|\lambda|}{R} \right)^{N-j+1}), & |\lambda| < R, \\ O(\lambda^{-j} \left( \frac{R}{|\lambda|} \right)^{N-j+1}), & |\lambda| > R. \end{cases}$$

**Remark 4.5.** If $f \in H(A(a_-, a_+), \mathbb{C})$ is meromorphic on an open neighborhood of the closed annulus $A(a_-, a_+)^c$, then the estimate (33) can be sharpened as follows

$$E_N(f) = O(a_+^{-N} + a_-^{-N}).$$

In order to see this, first consider the singular part that belongs to poles on the boundary of $A(a_-, a_+)$, and use Lemma 4.4. Then apply Theorem 4.3 to the remaining part on a slightly larger annulus.

Consider a general contour $\Gamma$ in $\Omega$ with $2\pi$-periodic parametrization $\varphi(t), t \in [0, 2\pi]$. Moreover, assume that $\varphi$ has a $2\pi$-periodic holomorphic extension to a strip

$$\varphi \in H(S(d_-, d_+), \Omega), \quad \varphi(z + 2\pi) = \varphi(z).$$

For definiteness, we also assume that

$$\varphi(z) \begin{cases} \in \text{int}(\Gamma), & 0 < \text{Im}(z) < d_+, \\ \notin \text{int}(\Gamma), & -d_- < \text{Im}(z) < 0. \end{cases}$$

Common examples are circles $\varphi(z) = z_0 + Re^{iz}$ with $z \in \mathbb{C}$ and ellipses $\varphi(z) = a \cos(z) + b \sin(z)$ with $|\text{Im}(z)| < \text{artanh}(\min(\frac{a}{b}, \frac{b}{a})).$
Let \( g \in H(\Omega, \mathbb{C}) \), then the error of the trapezoid sum for \( f(z) = g(\varphi(z))\varphi'(z) \), \( z \in S(d_-, d_+) \) is

\[
E_N(g) = \frac{1}{2\pi i} \int_\Gamma g(z)dz - \frac{1}{iN} \sum_{j=0}^{N-1} g(\varphi\left(\frac{2\pi j}{N}\right))\varphi'\left(\frac{2\pi j}{N}\right). \tag{41}
\]

From Theorem 4.1 we obtain an estimate

\[
|E_N(g)| \leq \Phi(r_+)G(e^{-Nr_+}) + \Phi(r_-)G(e^{-Nr_-}), \tag{42}
\]

where \( 0 < r_- < d_- \), \( 0 < r_+ < d_+ \) and \( \Phi(r) = \max_{\text{Im}(z)=r} |\varphi'(z)||g(\varphi(z))| \).

The following lemma gives a rough estimate of the right-hand sides for the pole function \( g(z) = (z-\lambda)^{-j}, \lambda \in \Omega \).

**Lemma 4.6.** Let \( \Omega \) be bounded and let \( \varphi \) satisfy conditions (39), (40). Then there exist constants \( C_1, C_2, C_3 > 0 \) (depending on \( \varphi, j \) but not on \( N \) or \( \lambda \in \Omega \)) such that for \( \text{dist}(\lambda, \Gamma) \leq C_3 \),

\[
|E_N((\cdot - \lambda)^{-j})| \leq C_1 \text{dist}(\lambda, \Gamma)^{-j} \exp\left(-C_2 N \text{dist}(\lambda, \Gamma)\right). \tag{43}
\]

**Proof.** For a fixed \( 0 < q < 1 \) there are bounds \( |\varphi'(z)| \leq M_+ \) for \( 0 \leq \text{Im}(z) \leq qd_+ \) and \( |\varphi'(z)| \leq M_- \) for \( 0 \leq -\text{Im}(z) \leq qd_- \). Let \( C_3 = \max(M_+d_+, M_-d_-) \) and define \( r_+ = \frac{q \text{dist}(\lambda, \Gamma)}{M_+} \). Then there exists some \( z_+ = s_+ + ir_+, 0 \leq s_+ < 2\pi \) such that

\[
\min_{\text{Im}(z)=r_+} |\lambda - \varphi(z)| = |\lambda - \varphi(z_+)| \geq |\lambda - \varphi(s_+)| - |\varphi(s_+) - \varphi(z_+)| \geq \text{dist}(\lambda, \Gamma) - M_+r_+ = (1-q)\text{dist}(\lambda, \Gamma).
\]

The first term in (42) can be estimated as follows

\[
|\Phi(r_+)G(e^{-Nr_+})| \leq M_+ \max_{\text{Im} z = r_+} |(\varphi(z) - \lambda)^{-j}|G(e^{-Nr_+}) \leq C(1-q)^{-j}M_+\text{dist}(\lambda, \Gamma)^{-j} \exp\left(-N\text{dist}(\lambda, \Gamma)\frac{q}{M_+}\right).
\]

The second term is treated analogously.

As a consequence of Lemmas 4.4 and 4.6 we obtain an exponential estimate for the errors in (30) and (31).

**Theorem 4.7.** Let \( T \in H(\Omega, \mathbb{C}) \) have maximum order \( \kappa \) of poles for the inverse in \( \Omega \), cf. Theorem 2.2. Further, let \( \Gamma \) be a simple closed contour in \( \Omega \) with \( \sigma(T) \cap \Gamma = \emptyset \) and such that the parametrization \( \varphi \) satisfies (39) and
Then there exist constants $C_1, C_2 > 0$ (depending on $T$ and $\hat{V}$ but not on $N$) such that the matrices from (30), (31) satisfy
\[
\|A_p - A_{p,N}\| \leq C_1 d(T)^{-\kappa} e^{-C_2Nd(T)}, \quad p = 0, 1,
\]
where $d(T) = \min_{\lambda \in \sigma(T)} \text{dist}(\lambda, \Gamma)$ and $d(T) = 1$ if $\sigma(T) = \emptyset$. If $\Gamma$ is a circle with parametrization $\varphi(t) = z_0 + Re^{it}$, then the following estimate holds
\[
\|A_p - A_{p,N}\| \leq C_1 \left[ \rho_-^{N-\kappa+1} + \rho_+^{N+\kappa-1} \right], \quad p = 0, 1,
\]
where
\[
\rho_- = \max_{\lambda \in \sigma(T), |\lambda - z_0| < R} \frac{|\lambda - z_0|}{R}, \quad \rho_+ = \max_{\lambda \in \sigma(T), |\lambda - z_0| > R} \frac{R}{|\lambda - z_0|}.
\]

Combining these estimates with the well-known perturbation theory for singular value decompositions [18] we find that the integral algorithm detects the correct rank $k$ of $A_{0,N}$ if $N$ is sufficiently large. Further, the perturbation theory for simple eigenvalues [18] leads to the following corollary.

**Corollary 4.8.** Let the assumptions of Theorem 3.1 and of Theorem 4.7 be satisfied. Let $\lambda_1, \ldots, \lambda_k$ be the eigenvalues of $T$ inside $\Gamma$ and let $\lambda_{1,N}, \ldots, \lambda_{k,N}$ be the eigenvalues from step 6 of the integral algorithm. With the notation from Theorem 4.7 we then have the error estimates
\[
\max_{j=1,\ldots,n(\Gamma)} |\lambda_j - \lambda_{j,N}| \leq C_1 d(T)^{-\kappa} e^{-C_2Nd(T)},
\]
in case of a general curve satisfying (39), (40), and
\[
\max_{j=1,\ldots,n(\Gamma)} |\lambda_j - \lambda_{j,N}| \leq C \left[ \rho_-^{N-\kappa+1} + \rho_+^{N+\kappa-1} \right]
\]
in case of a circle with radius $R$ and center $z_0$.

### 4.2 Numerical examples

**Example 4.9.** For the first test we choose a real quadratic polynomial
\[
T(z) = T_0 + zT_1 + z^2T_2, \quad T_j \in \mathbb{R}_{60}^{60}, j = 0, 1, 2,
\]
where $T_0, T_1, T_2$ are taken at random (rand from MATLAB). In this case we can compare with the spectrum $\sigma_{\text{polyeig}}$ resulting from MATLAB’s polyeig.

Figure 1(left) shows the result from polyeig (open circles) and the eigenvalues from Integral algorithm 1 (filled boxes) for the data
\[
\varphi(t) = Re^{it}, \quad t \in [0, 2\pi], \quad R = 0.33, \quad \text{tol}_{\text{rank}} = 10^{-4}, \quad \text{tol}_{\text{res}} = 10^{-1}.
\]
The eight eigenvalues inside the circle are detected and well approximated by the integral algorithm. Figure 1 (right) shows the errors

$$e(\lambda_j) = \min \{ |\lambda_j - \mu| : \mu \in \sigma_{\text{polyeig}} \}$$

for two characteristic eigenvalues inside the circle. Both show exponential decay with respect to $N$ at approximately the same rate.

Figure 1: Example 4.9. Eigenvalues of a quadratic eigenvalue problem from polyeig (open circles) and Integral algorithm 1 (filled squares) with $N = 150$ (left). Difference $e(\lambda_j)$ of eigenvalues $\lambda_1 \approx 0.30578$ (filled circles) and $\lambda_2 \approx 0.0961 - 0.1315i$ (open circles) between polyeig and the integral algorithm versus the number of nodes $N$ (right).

Figure 2: Example 4.9. Singular values versus $N$ for a fixed number of $l = 11$ columns in the integral algorithm (left), reduction of the number of singular values by the rank test of the adaptive algorithm versus $N$ (right).

While Figure 1 (left) results from the integral algorithm with an adaptive number $l$ of columns (which yields $l = 8$ at $N = 150$), the computations in
Figure 1(right) are done with a fixed number of \( l = 11 \) columns. For this case we show the behavior of the 11 largest singular values of \( A_{0,N} \) in Figure 2 (left). Sufficient separation of singular values already occurs at values \( N \approx 25 \), much smaller than 150. Figure 2 (right) shows how the adaptive algorithm reduces the number of singular values from \( l = 23 \) at \( N = 20 \) to \( l = 8 \) for \( N \geq 95 \).

**Example 4.10.** For the next experiment we take random complex entries in (44), a fixed number \( l = 10 \) of columns, and the same circle as in (45). Again, the 6 eigenvalues inside the circle from *polyeig* are well approximated by the integral algorithm, see Figure 3 (left).

![Figure 3: Example 4.10. Eigenvalues from polyeig (open circles) and eigenvalues from the integral algorithm for a random quadratic complex matrix polynomial (left), singular values of integral algorithm with \( l = 10 \) columns versus the number \( N \) of quadrature nodes for the same example (right).](image)

But this time the singular values do not separate as well as in Figure 2 (left). Two of them decay rather slowly, while two others, due to eigenvalues very close but outside the contour, remain of order one. However, this behavior does not result in spurious eigenvalues. On the contrary, if we keep \( l = 10 \) for the eigenvalue computation, then this yields the 6 eigenvalues inside and in addition the four eigenvalues lying closest to the contour, but outside. Such a behavior is also suggested by our error analysis in Section 4.1 according to which the principle error term depends on the distance of eigenvalues to the contour, both for eigenvalues inside and outside. Computational experience shows that only very small singular values (\( \approx 10^{-10} \)) lead to spurious eigenvalues and these can be easily avoided by the residual test in Step 6.
Example 4.11. This example, taken from [17] and [11], is a finite element discretization of a nonlinear boundary eigenvalue problem

\[-u''(x) = \lambda u(x), 0 \leq x \leq 1, u(0) = 0 = u'(1) + \frac{\lambda}{\lambda - 1}u(1).\]

The matrix function is

\[T(z) = T_1 + \frac{1}{1-z}e_me^T - zT_3,\]

where

\[T_1 = m \begin{pmatrix} 2 & -1 & \cdot & \cdot & \cdot & \cdot \\ -1 & 2 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 2 & -1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & -1 & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & 1 \end{pmatrix}, \quad T_3 = \frac{1}{6m} \begin{pmatrix} 4 & 1 & \cdot & \cdot & \cdot \\ 1 & 4 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 4 & 1 & \cdot \\ \cdot & \cdot & \cdot & 1 & 2 \end{pmatrix}.\]

We use \(m = 400\) and compute five eigenvalues in the interval \([2, 298]\). Again Figure 4 (left) shows the real eigenvalues in the circle which agree with those from [11]. Note that we avoided the singularity of \(T\) at \(z = 1\). The residuals of the computed eigenvectors and eigenvalues decay exponentially as expected, see Figure 4 but not as smooth as in the previous examples.

![Figure 4: Example 4.11](image)

Figure 4: Example 4.11. Eigenvalues from the integral algorithm for the finite element discretization of a nonlinear boundary eigenvalue problem (left), decay of residuals \(\text{res}(\lambda_j) = ||T(\lambda_j)(v_j)||\) for \(\lambda_1 \approx 24\) (open circles), \(\lambda_2 \approx 123\) (filled circles) versus the number \(N\) of quadrature nodes for the same example (right).
Example 4.12. Consider the quadratic polynomial

\[ T(z) = T_0 + (z - a)(b - z)T_1, \quad a < b \in \mathbb{R}, \quad T_0, T_1 \in \mathbb{R}^{15,15}, \]  

(46)

where \( T_0 \) has zeroes in the first column. All other entries of \( T_0, T_1 \) are chosen at random. Then \( T(z) \) has different eigenvalues \( a \) and \( b \) with the same eigenvector \( e^1 \in \mathbb{R}^m \). This is a critical case since the rank condition (17) is violated. In Figure 5 (left) we show the results of polyeig and of the integral algorithm (with \( l = 5 \) and the data from (45)). There are three eigenvalues inside the circle. Both eigenvalues \( a = -0.2 \) and \( b = 0.1 \) are missed by the integral method, while the third one is found, though at lower accuracy than in the previous examples. Figure 5 shows that only one singular value stays of order one when \( N \) is increased. This example will be reconsidered in Section 5.

![Figure 5: Example 4.11. Eigenvalues from polyeig (open circles) and eigenvalues from the integral algorithm for a quadratic matrix polynomial with rank defect (left), singular values of integral algorithm with \( l = 5 \) columns versus the number \( N \) of quadrature nodes for the same example (right).](image)

5 The algorithm for many eigenvalues

In this section we show how the method from Section 3 can be extended to nonlinear eigenvalue problems with more eigenvalues than the dimension of the system, i.e. \( m < k \), and to the rank deficient cases, see Remark 3.2 and Example 4.12.
5.1 Construction of algorithm

In case \( m < k \) condition (17) is always violated and there is no matrix \( \hat{V} \) satisfying (16). Therefore, we compute more integrals of type (18), (19), namely

\[
A_p = \frac{1}{2\pi i} \int_{\Gamma} z^p T(z)^{-1} \hat{V} dz \in \mathbb{C}^{m,l}, \quad p \in \mathbb{N}.
\]

Here we assume that \( \hat{V} \in \mathbb{C}^{m,l} \) with \( l \leq m \). In fact, in case \( k > m \) we set \( \hat{V} = I_m \) instead of making a random choice.

From Theorem 2.9 we obtain

\[
A_p = V \Lambda_p W^H \hat{V}, \quad p \in \mathbb{N},
\]

(47)

where \( V, W \in \mathbb{C}^{m,k} \) are given by (26) and (28) and \( \Lambda \) has the normal form (29).

Now we choose \( K \in \mathbb{N}, K \geq 1 \) and form the \( Km \times Kl \) matrices

\[
B_0 = \begin{pmatrix}
A_0 & \cdots & A_{K-1} \\
\vdots & \ddots & \vdots \\
A_{K-1} & \cdots & A_{2K-2}
\end{pmatrix}, \quad B_1 = \begin{pmatrix}
A_1 & \cdots & A_K \\
\vdots & \ddots & \vdots \\
A_K & \cdots & A_{2K-1}
\end{pmatrix}.
\]

(48)

From (47) we find the representations

\[
B_0 = \begin{pmatrix}
V \\
\vdots \\
V \Lambda^{K-1}
\end{pmatrix} (W^H \hat{V} \cdots \Lambda^{K-1} W^H \hat{V}),
\]

(49)

and

\[
B_1 = \begin{pmatrix}
V \\
\vdots \\
V \Lambda^{K-1}
\end{pmatrix} \Lambda (W^H \hat{V} \cdots \Lambda^{K-1} W^H \hat{V}).
\]

(50)

We assume that \( K \) has been chosen such that the following rank condition holds

\[
\text{rank} \begin{pmatrix}
V \\
\vdots \\
V \Lambda^{K-1}
\end{pmatrix} = k.
\]

(51)

The smallest index having this property is called the minimality index in [11]. In case \( k > m \) this can be expected to hold if we choose

\[(K - 1)m < k \leq Km.\]
In case $k \leq m$ with $\text{rank}(V) < k$ (see Remark 3.2(b)) the following lemma shows that (51) holds for $K$ larger than the sum of the maximal ranks at all eigenvalues.

**Lemma 5.1.** Let the assumptions of Corollary 2.8 be satisfied. Then the rank condition (51) holds with $k$ as defined in (15) for $K \geq n(C)$

$$
\sum_{n=1}^{n(C)} \max_{1 \leq \ell \leq L_n} m_{\ell,n}.
$$

**Proof.** Let $M_n = \max_{1 \leq \ell \leq L_n} m_{\ell,n}$ and $M = \sum_{n=1}^{n(C)} M_n$. Assume that $VA^j x = 0, j = 0, \ldots, M - 1$ for some $x \in \mathbb{C}^m$. For any $n \in \{1, \ldots, n(C)\}$ and $0 \leq \beta \leq M_n - 1$ consider the polynomial

$$
P_{n,\beta}(z) = (z - \lambda_n)^\beta \prod_{r=1, r \neq n}^{n(C)} (z - \lambda_r)^{M_r}.
$$

By our assumption $0 = VP_{n,\beta}(A)x$. We partition according to (29)

$$
V = (V_1 \cdots V_{n(C)}), V_n = (V_{n,1} \cdots V_{n,L_n}), V_{n,\ell} = (v_{0,\ell}^{\ell,n} \cdots v_{m_{\ell,n}-1}^{\ell,n}),
$$

$$
x = (x_1 \cdots x_{n(C)}), x_n = (x_{1,n} \cdots x_{L_n,n}), x_{\ell,n} = (x_{0,\ell}^{\ell,n} \cdots x_{m_{\ell,n}-1}^{\ell,n}).
$$

Using $(J_n - \lambda_n)^{M_n} = 0$ for $\hat{n} \neq n$ we obtain

$$
0 = \sum_{\ell=1}^{L_n} \prod_{\hat{n} \neq n, m_{\ell,n} \geq 1}^{n(C)} (J_{n,\ell} - \lambda_{\hat{n}})^{M_{\hat{n}}}(J_{n,\ell} - \lambda_n)^\beta x_{\ell,n}.
$$

From this we conclude by induction on $\beta = M_n - 1, \ldots, 0$ that

$$
x_{\nu,\ell}^{\nu,n} = 0, \quad \text{if } \beta \leq \nu \leq m_{\ell,n} - 1.
$$

For $\beta = M_n - 1$, equation (52) reads

$$
0 = \prod_{\hat{n} \neq n}^{n(C)} (\lambda_n - \lambda_{\hat{n}})^{M_{\hat{n}}} \sum_{\ell=1, m_{\ell,n} = M_n}^{L_n} v_{0,\ell}^{\ell,n} x_{\ell,n}^{\ell,n},
$$

and thus (53) holds for $\beta = M_n$ by the linear independence of the vectors $v_{0,\ell}^{\ell,n}$ (cf. Definition 2.5 (iv)). For the induction step we use (52) with $\beta - 1$ instead of $\beta$. Together with (53) we find

$$
0 = \prod_{\hat{n} \neq n}^{n(C)} (\lambda_n - \lambda_{\hat{n}})^{M_{\hat{n}}} \sum_{\ell=1, m_{\ell,n} \geq \beta}^{L_n} v_{0,\ell}^{\ell,n} x_{\ell,n}^{\ell,n},
$$

$$
25
$$
which shows that (53) holds for $\beta - 1$. Thus we have shown $x = 0$ and this finishes the proof.

The computational procedure is now a straightforward generalization of Section 3.1. First compute $B_0, B_1 \in \mathbb{C}^{K_m,K_l}$ from (48). In addition to (51), assume

$$\text{rank} \left( W^H \hat{V} \cdots \Lambda^{K-1}W^H \hat{V} \right) = k. \tag{54}$$

Let us abbreviate

$$V_{[K]} = \begin{pmatrix} V \\ V \Lambda^{K-1} \end{pmatrix} \in \mathbb{C}^{K_m,k}, \quad W_{[K]}^H = \begin{pmatrix} W^H \hat{V} & \cdots & \Lambda^{K-1}W^H \hat{V} \end{pmatrix} \in \mathbb{C}^{k,K_l}.$$ 

Compute the SVD

$$V_{[K]}W_{[K]}^H = B_0 = V_0 \Sigma_0 W_0^H,$$

where $V_0 \in \mathbb{C}^{K_m,k}, V_0^H V_0 = I_k, \Sigma_0 = \text{diag}(\sigma_1, \ldots, \sigma_k) \in \mathbb{C}^{k,k}$, and $W_0 \in \mathbb{C}^{K_l,k}$, $W_0^H W_0 = I_k$. From the rank conditions (51), (54),

$$\sigma_1 \geq \ldots \sigma_k > 0 = \sigma_{k+1} = \ldots = \sigma_{K_l}.$$

The rank condition (51) also implies

$$R(B_0) = R(V_{[K]}) = R(V_0).$$

Thus the matrix $S = V_0^H V_{[K]} \in \mathbb{C}^{k,k}$ is nonsingular and satisfies

$$V_{[K]} = V_0 S. \tag{55}$$

With (49), (55) we find

$$W_{[K]}^H = S^{-1} \Sigma_0 W_0^H,$$

and then from (50)

$$B_1 = V_{[K]} \Lambda W_{[K]}^H = V_0 S \Lambda S^{-1} \Sigma_0 W_0^H.$$ 

Finally, this leads to

$$D := V_0^H B_1 W_0 \Sigma_0^{-1} = S \Lambda S^{-1}. \tag{56}$$

Therefore, the analog of Theorem 3.3 is
Theorem 5.2. Suppose that $T \in H(\Omega, \mathbb{C}^{m,m})$ has no eigenvalues on the contour $\Gamma$ in $\Omega$ and pairwise distinct eigenvalues $\lambda_n, n = 1, \ldots, n(\Gamma)$ inside $\Gamma$ with partial multiplicities $m_{1,n} \geq \ldots \geq m_{L_n,n}, n = 1, \ldots, n(\Gamma)$. Assume that the rank conditions (51), (54) are satisfied with $k$ given by (15). Then the matrix $D \in \mathbb{C}^{k,k}$ from (56) has Jordan normal form (29) with the same eigenvalues $\lambda_n$ and partial multiplicities $m_{\ell,n}(\ell = 1, \ldots, L_n, n = 1, \ldots, n(\Gamma))$. Suitable CSGEs for $T$ can be obtained from corresponding CSGEs $s_j^{\ell,n}$ for $D$ via

$$v_j^{\ell,n} = V_0^{[1]} s_j^{\ell,n}, \quad 0 \leq j \leq m_{\ell,n} - 1, 1 \leq \ell \leq L_n, 1 \leq n \leq n(\Gamma),$$

where $V_0^{[1]}$ is the upper $m \times k$ block in

$$V_0 = \begin{pmatrix} V_0^{[1]} \\ \vdots \\ V_0^{[K]} \end{pmatrix}.$$  

(57)

Remark 5.3. In a sense this generalization is similar to linearizing a polynomial eigenvalue problem by increasing the dimension. Note, however, that this only becomes necessary if there are too many eigenvalues inside the contour, or if rank defects occur that are not present in linear eigenvalue problems.

The generalization of the algorithm from Section 3.3 is the following.

Integral algorithm 2

Step 1: Choose numbers $l \leq m$, $K \geq 1$ and a matrix $\hat{V} \in \mathbb{C}^{m,l}$ at random. If more than $m$ eigenvalues are expected inside $\Gamma$, let $l = m, \hat{V} = I_m$.

Step 2: Compute

$$A_{p,N} = \frac{1}{iN} \sum_{j=0}^{N-1} T(\varphi(t_j))^{-1} \hat{V} \varphi(t_j)^p \varphi'(t_j), \quad p = 0, \ldots, 2K - 1,$$

and form $B_{0,N}, B_{1,N}$ as in (48).

Step 3: Compute the SVD $B_{0,N} = V \Sigma W^H$, where $V \in \mathbb{C}^{Km,Kl}, W \in \mathbb{C}^{Kl,Kl}, V^H V = W^H W = I_{Kl}, \Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_{Kl})$.

Step 4: Perform a rank test for $\Sigma$, i.e. find $0 < k \leq Kl$ such that $\sigma_1 \geq \ldots \geq \sigma_k > \sigma_{k+1} \approx \ldots \approx \sigma_{Kl} \approx 0$. If $k = Kl$ then increase $l$ or $K$ and go to Step 1. Else let $V_0 = V(1:Km,1:k), W_0 = W(1:Kl,1:k)$ and $\Sigma_0 = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_k)$.

Step 5: Compute $D = V_0^H B_{1,N} W_0 \Sigma_0^{-1} \in \mathbb{C}^{k,k}$.
Step 6: Solve the eigenvalue problem for $D$
$$DS = SA, \ S = (s_1 \ldots s_k), \ \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_k).$$
If $\|T(\lambda_j)v_j\|$ is small and $\lambda_j \in \text{int}(\Gamma)$ accept $v_j = V_0^{[1]}s_j$ (with $V_0^{[1]}$ from (57)) as eigenvector and $\lambda_j$ as eigenvalue.

5.2 Numerical Examples

Example 5.4. We apply the integral algorithm 2 to the rank deficient example (46), where $K = 2, l = 3$ and the contour is the circle from (15). Now the eigenvalues $a = -0.2$ and $b = 1$ are reproduced correctly (see Figure 6 (left)), and three singular values survive as expected (Figure 6 (right)).

Example 5.5. Consider the characteristic equation of a delay system $\dot{x} = T_0x(t) + T_1x(t-\tau)$ from [16, Sec.2.4.2], [11], given by

$$T(z) = zI - T_0 - T_1 e^{-z\tau}, \quad T_0 = \begin{pmatrix} -5 & 1 \\ 2 & -6 \end{pmatrix}, \quad T_1 = \begin{pmatrix} -2 & 1 \\ 4 & -1 \end{pmatrix}. \quad (58)$$

In case $\tau = 1$ there are more than two eigenvalues inside the circle $\varphi(t) = z_0 + Re^{it}, \mu = -1, R = 6$. We set $l = 2, \hat{V} = I_2$ and $K = 3$ for the integral algorithm 2 and obtain with $N = 150$ five eigenvalues inside the circle, (see Figure 7 (left)), which coincide with the computed ones in [11]. Much smaller values than $N = 150$ give sufficient accuracy, since there is a good separation of singular values and a fast decay of residuals, see Figure 7 (right).
Figure 7: Example 5.5. Eigenvalues of the characteristic equation (58) inside a circle of radius 6 and with center $-1$, computed with the integral algorithm 2 with $K = 3, l = 2$. (left), residuals $||T(\lambda_j)v_j||$ for $\lambda_1 \approx -0.6 + 2.71i$, $\lambda_2 \approx -2.27 + 5.07i$ versus the number $N$ of quadrature nodes for the same example (right).

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