Connections between contour integration and rational Krylov methods for eigenvalue problems

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Abstract

Contour integration methods and rational Krylov methods are two important classes of numerical methods for computing eigenvalues in a given region of the complex plane. Using rational filtering based on a quadrature rule, we present connections between two variants of these methods. We prove for linear eigenvalue problems that with a particular choice of the starting basis matrix and the rational filter, these methods construct the same subspace and hence compute the same Ritz pairs. Consequently, this equivalence allow us to combine good properties of both worlds. Firstly, the connections of rational Krylov methods with contour integration methods provide better stopping criteria for the former based on the rank test in the latter. Secondly, this connection allows for an efficient implementation of contour integration via rational Krylov which can significantly reduce the computational cost. We also introduce the contour filtered compact rational Krylov method for nonlinear eigenvalue problems, since for these problems the connection of contour integration methods with rational filtering is lost. Finally, we illustrate the connections for both linear and nonlinear eigenvalue problems.

Keywords : rational Krylov, contour integration, rational filter, nonlinear eigenvalue problem
MSC : 65F15, 47J10.

CONNECTIONS BETWEEN CONTOUR INTEGRATION AND RATIONAL KRYLOV METHODS FOR EIGENVALUE PROBLEMS*

ROEL VAN BEEUMEN†, KARL MEERBERGEN‡, AND WIM MICHIELS‡

Abstract. Contour integration methods and rational Krylov methods are two important classes of numerical methods for computing eigenvalues in a given region of the complex plane. Using rational filtering based on a quadrature rule, we present connections between two variants of these methods. We prove for linear eigenvalue problems that with a particular choice of the starting basis matrix and the rational filter, these methods construct the same subspace and hence compute the same Ritz pairs. Consequently, this equivalence allow us to combine good properties of both worlds. Firstly, the connections of rational Krylov methods with contour integration methods provide better stopping criteria for the former based on the rank test in the latter. Secondly, this connection allows for an efficient implementation of contour integration via rational Krylov which can significantly reduce the computational cost. We also introduce the contour filtered compact rational Krylov method for nonlinear eigenvalue problems, since for these problems the connection of contour integration methods with rational filtering is lost. Finally, we illustrate the connections for both linear and nonlinear eigenvalue problems.

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AMS subject classifications. 65F15,47J10

1. Introduction.

We consider the problem of finding all eigenvalues λ located inside a compact *target set* $\Sigma \subset \Omega \subseteq \mathbb{C}$, and corresponding eigenvectors $x \in \mathbb{C}^n \setminus \{0\}$ of the nonlinear eigenvalue problem (NLEP)

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

where the matrix-valued function $A : \Omega \to \mathbb{C}^{n\times n}$ is analytic on Ω. Note that (1.1) reduces to the standard eigenvalue problem in case $A(z) := zI - A$ and to the polynomial (or rational) eigenvalue problem when $A(z)$ is a (rational) matrix polynomial.

The first class of numerical methods we consider in this paper for solving the NLEP (1.1) comprises the contour integration methods. The use of contour integrals for solving eigenvalue problems is a relatively recent development [32] compared to the history of applying such methods for finding the zeros of a scalar analytic function [16]. The first contour integral based eigensolver for computing all the eigenvalues of a matrix A inside a given contour Γ was proposed by Sakurai and Sugiura in [24]. This method reduces the eigenvalue problem to a generalized eigenvalue problem involving two Hankel matrices built up from the scalar moments

$$\mu_p := \frac{1}{2\pi i}\int_\Gamma (z-\gamma)^p\, u^*(zI-A)^{-1}v\, dz, \qquad p = 0, 1, \ldots,$$

where $\gamma \in \mathbb{C}$ belongs to the interior of the closed contour $\Gamma \subset \Omega$ and $u, v \in \mathbb{C}^n$ are chosen randomly. Note that these contour integrals μ_p are based on the resolvent

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operator $(zI-A)^{-1}$. However, the Hankel matrices become ill-conditioned when there are eigenvalues lying close to the contour. To overcome this disadvantage, a Rayleigh–Ritz type contour integration method was proposed in [25] and a connection with rational filter functions is given in [14]. Furthermore, Polizzi's FEAST algorithm [21, 30] also uses contour integrals based on the resolvent function for computing eigenvalues inside a given contour of a Hermitian pencil $Bz - A$ with B positive definite.

Generalizations of contour integration methods towards NLEPs are proposed by Sakurai and co-authors in [3, 37] and by Beyn in [9]. For a connection with rational filter functions, see [32, 31]. All these methods use (approximate) contour integrals of the resolvent operator $A(z)^{-1}$ applied to a basis matrix $V \in \mathbb{C}^{n\times k}$, with $k \leq n$,

$$\mathcal{S} := \frac{1}{2\pi i}\int_{\Gamma} f(z)A(z)^{-1}V dz, \tag{1.2}$$

where $f : \Omega \to \mathbb{C}$ is analytic on Ω and $\Gamma \subset \Omega$ is a given closed contour.

The second class of numerical methods under consideration for solving the NLEP (1.1) are the Krylov type methods. For linear eigenvalue problems, we have the shift-and-invert Arnoldi method [2] and the rational Krylov method [22, 23]. Both the implicitly restarted Arnoldi method as well as the rational Krylov method implicitly apply, respectively, a polynomial and rational filter to the Krylov vectors [10]. In case of polynomial or rational eigenvalue problems, we use linearization, i.e., the transformation of the (rational) matrix polynomial into a linear pencil with the same eigenvalues. Consequently, the eigenvalues of the constructed linearization pencil are computed by a standard algorithm of choice [19, 1, 35]. For general nonlinear eigenvalue problems, we first construct an accurate polynomial or rational approximation of the nonlinear matrix-valued function $A(\lambda)$ in (1.1) on the target set Σ. Next, we use again a linearization to convert the NLEP into a generalized linear eigenvalue problem. See, e.g., [12, 34, 13, 33].

In the literature we also find several (quasi) Newton-type methods, which we will not consider in this paper. Examples, among others, are the residual inverse iteration method [20], the block Newton method [17], and Jacobi–Davidson projection methods [8, 36, 11]. For a connection between the rational Krylov method and the Jacobi–Davidson algorithm we refer to [23] and for a connection between Newton's method and the Newton rational Krylov method to [34].

In this paper, we present several connections between variants of the rational Krylov method and the contour integration method for solving both linear and nonlinear eigenvalue problems. The connecting feature in the linear case is rational filtering, i.e., contour integration methods have an interpretation of applying a rational function to a subspace, whereas the rational Krylov method can be used for implicitly applying a rational filter to a Krylov subspace. We will prove that with a particular choice of the starting basis matrix in the contour integration methods in combination with well chosen shifts in the rational Krylov method, both methods construct the same subspace and compute the same Ritz values for linear eigenvalue problems. The mathematical connections between these two important classes of eigensolvers allows us to combine interesting properties of both classes. In the nonlinear case on the other hand, the situation is somewhat different because contour integration methods for solving NLEPs have lost their connection with rational filtering. However, we will show that for NLEPs a rational (contour) filtering process is still possible in the compact rational Krylov framework [35].

The paper is organized as follows. In the first part, sections 2 to 4, we focus on the

linear eigenvalue problem, $Ax = \lambda x$, in order to keep notation simple. Sections 2 and 3 briefly review the basic contour integration algorithm and the rational Krylov method, respectively. We also discuss their important properties needed in the remainder of the paper. Section 4 introduces the contour filtered rational Krylov method and contains the central proof of this paper about the mathematical equivalence between this two classes of eigensolvers for the linear eigenvalue problem. We also discuss the differences in implementation details here. Next, in section 5 we discuss some connections for NLEPs and introduce the contour filtered CORK method. In section 6 we illustrate the connections for both linear and nonlinear eigenvalue problems. Finally, the main conclusions are summarized in section 7.

2. Contour integration methods. For computing all eigenvalues of a matrix A inside a given closed curve Γ, we consider the projection methods which derive their projections from complex contour integrals. In these contour integration methods, discretizing the contour integrals of the resolvent operator applied to a basis matrix (1.2), in particular the moment matrices of order p

$$\mathcal{M}_p := \frac{1}{2\pi i}\int_\Gamma z^p (zI - A)^{-1} V dz, \qquad p = 0, 1, \ldots, \tag{2.1}$$

plays a central role. By using a quadrature rule to approximate the contour integral in (2.1), we obtain the discretized moment matrices

$$M_p := \sum_{j=0}^{N-1} \omega_j z_j^p (z_j I - A)^{-1} V, \qquad p = 0, 1, \ldots, \tag{2.2}$$

where z_j are the quadrature nodes and ω_j the corresponding weights.

2.1. Spectral projections and rational filter functions. To illustrate the connections between moment matrices and rational filter functions [5], we first focus on the 0th moment matrix $\mathcal{M}_0$. Let

$$\mathcal{P} := \frac{1}{2\pi i}\int_\Gamma (zI - A)^{-1} dz \tag{2.3}$$

be the spectral projector associated with the eigenspace corresponding to the eigenvalues of A contained within Γ [15]. Then, we have $\mathcal{M}_0 = \mathcal{P}V$, i.e., the contour integral $\mathcal{M}_0$ computes a projection of V onto the eigenspace of interest.

By using a quadrature rule, with nodes $z_0, z_1, \ldots, z_{N-1}$ and corresponding weights $\omega_0, \omega_1, \ldots, \omega_{N-1}$, to discretize the spectral projector $\mathcal{P}$ (2.3), we obtain the following approximate projector

$$P := \sum_{j=0}^{N-1} \omega_j (z_j I - A)^{-1}. \tag{2.4}$$

Note that, by making use of matrix functions, we have $P = b_0(A)$, where

$$b_0(z) := \sum_{j=0}^{N-1} \frac{\omega_j}{z_j - z}, \tag{2.5}$$

is the rational function with poles z_j and residues ω_j. When P acts on a matrix V and λ is an eigenvalue of A for which $|b_0(\lambda)|$ is small, then the components of V in the directions of eigenvectors of A corresponding to λ will be reduced.

We now illustrate that the discretized moment matrices M_p (2.2) can also be interpreted as rational filters of the matrix A applied to the basis matrix V. Therefore, let the p-th order rational filter function b_p be defined as follows

$$b_p(z) := \sum_{j=0}^{N-1} \frac{\omega_j z_j^p}{z_j - z}, \qquad p = 0, 1, \ldots, \tag{2.6}$$

where z_j and ω_j are equal to the quadrature nodes and weights in (2.2), respectively. Consequently, we have

$$M_p = b_p(A)V, \qquad p = 0, 1, \ldots, \tag{2.7}$$

which is the central connection between contour integration and rational filtering.

Furthermore, the rational filter functions as well as the dicretized moment matrices satisfy a recurrence relation under the following assumption on the quadrature nodes and weights.

ASSUMPTION 2.1. *Let the quadrature nodes and weights (z_j, ω_j) satisfy*

$$\sum_{j=0}^{N-1} \omega_j z_j^p = 0, \tag{2.8}$$

for $p = 0, 1, \ldots, p_{max}$.

Note that Assumption 2.1 corresponds to exactly integrating $\int_\Gamma z^p dz = 0$, which is, for example, the case for the trapezoidal rule with $p_{\max} = 1$ and for Gauss–Legendre quadrature with $p_{\max} = 2N - 1$.

LEMMA 2.2. *Let b_p be defined in* (2.6) *and suppose that Assumption* 2.1 *holds. Then the rational filter functions have the following recurrence relations*

$$b_{p+1}(z) = z b_p(z) = z^{p+1} b_0(z),$$

for $p = 0, 1, \ldots, p_{max}$.

Proof. By definition of b_p and (2.8), we have

$$b_{p+1}(z) - z b_p(z) = \sum_{j=0}^{N-1} \frac{\omega_j z_j^{p+1}}{z_j - z} - z \sum_{j=0}^{N-1} \frac{\omega_j z_j^p}{z_j - z} = \sum_{j=0}^{N-1} \omega_j z_j^p \frac{z_j - z}{z_j - z} = \sum_{j=0}^{N-1} \omega_j z_j^p = 0.$$

Using induction completes the proof. ∎

The interpretation of the discretized moment matrices as rational filter functions of A applied to the basis matrix V, together with the recurrence relation between these filter functions, results in the following theorem.

THEOREM 2.3. *Let M_p and b_p be defined in* (2.2) *and* (2.6)*, respectively, and suppose that Assumption* 2.1 *holds. Then the discretized moment matrices have the following recurrence relations*

$$M_{p+1} = A M_p = A^{p+1} M_0.$$

for $p = 0, 1, \ldots, p_{max}$.

Proof. The proof immediately follows from (2.7) and Lemma 2.2. ∎

2.2. Basic algorithm. Contour integration methods appear in the literature in all kinds of flavors. They mainly differ in the way the contour integrals are discretized, i.e., the chosen quadrature rule, the order of the rational filter, and whether the contour filter is recursively repeated or not. A basic version of the contour integration method for a matrix A is outlined in Algorithm 1.

Algorithm 1: Contour integration method

Input: Basis matrix $V \in \mathbb{C}^{n\times k}$.

for $j = 1, 2, \ldots$ **do**

1 Compute the discretized moment matrix M_0 (2.2).
2 QR factorization $M_0 =: UR$.
3 Solve $(U^*AU)X = X\Lambda$.
4 Update $V = UX$.

end

Note that Algorithm 1 both includes, among others, the CIRR method [25, 14], Beyn's method [9], and FEAST [21, 30]. The first two correspond to only one iteration of Algorithm 1 and use the trapezoidal rule in step 1 to discretize the contour integral M_0, whereas the latter is fundamentally a subspace iteration method using Gauss–Legendre quadrature in step 1 of Algorithm 1.

All these methods have in common that they reduce in step 3 the original eigenvalue problem to the following small eigenvalue problem, or a variant of,

$$(U^*AU)\, t = \lambda t, \tag{2.9}$$

where U is an orthogonal basis matrix for the discretized moment matrix M_0. In [9] both the 0th and 1st discretized moment matrices are computed and the eigenvalues are obtained from the $U^*M_1R^{-1}$. However, by using Theorem 2.3, i.e., $M_1 = AM_0$, we obtain the same eigenvalues as in (2.9).

Moreover, Algorithm 1 has a rational filter interpretation since by definition (2.7) step 1 acts as a rational filter of the matrix A applied to the basis matrix V. This can be summarized as follows.

PROPOSITION 2.4. *Let the rational filter $b_0(z)$ be defined as in* (2.5)*. Then the effect of performing one iteration of Algorithm* 1 *onto the basis matrix V corresponds to applying the contour filter φ_c of the matrix A to it, i.e.,*

$$\operatorname{range}(M_0) = \operatorname{range}(\varphi_c(A)V),$$

where $\varphi_c(z) := b_0(z)$.

2.3. Rank test. A contour integral method for computing all eigenvalues inside a given contour Γ can also provide an estimate for the number of eigenvalues lying inside Γ. Therefore, the so called *rank test* is used, i.e., an economy-size singular value decomposition of the discretized moment matrix M_0, see e.g., [9].

Suppose first that the number of columns, k, of the starting matrix V is larger than the actual number of eigenvalues, ℓ, lying inside Γ: $\ell < k$. Then, for a sufficiently high number of quadrature nodes, a rank drop can be detected in M_0 from its singular values, i.e.,

$$\sigma_1 \geq \cdots \geq \sigma_\ell > \mathrm{tol}_{\mathrm{rank}} > \sigma_{\ell+1} \approx \cdots \approx \sigma_k \approx 0,$$

where tol_{rank} is a given tolerance. However, in case we find $\ell = k$, it can be an indication that there may be more than ℓ eigenvalues (including multiplicities) inside Γ. Consequently, k can be increased until a rank drop is detected.

3. Rational Krylov method. The rational Krylov method [22, 23] is a generalization of the shift-and-invert Arnoldi method for solving generalized linear eigenvalue problems. There are two main differences between the two methods. Firstly, instead of a fixed shift for the Arnoldi method, the rational Krylov method allows to change the shift (or pole) at every iteration. Secondly, the rational Krylov method collects the information about the eigenvalues in a pair of Hessenberg matrices.

3.1. Algorithm. The rational Krylov (sequence) algorithm for a matrix $A \in \mathbb{C}^{n\times n}$ and a starting vector $v_1 \in \mathbb{C}^n$ constructs an orthonormal basis V_m for the subspace $\mathcal{Q}_m$ spanned by

$$\mathcal{Q}_m := \text{span}\left\{v_1, v_2, \cdots, v_m\right\},$$

where

$$v_{j+1} := (A - \sigma_j I)^{-1} v_j, \qquad j = 1, \ldots, m-1,$$

with $\sigma_j \in \mathbb{C}$ are the shifts. Algorithm 2 gives an outline, including also shifts at ∞.

Algorithm 2: Rational Krylov method

Input: Starting vector v_1, with $\|v_1\| = 1$, and shifts $\sigma_1, \ldots, \sigma_{m-1} \in \mathbb{C} \cup \infty$.

for $j = 1, \ldots, m-1$ **do**

1 Compute: $w := \begin{cases} (A - \sigma_j I)^{-1} v_j, & \sigma_j \neq \infty \\ A v_j, & \sigma_j = \infty \end{cases}$.

2 Orthogonalize: $w := w - V_j h_j$, where $h_j = V_j^* w$.

3 Get new vector: $v_{j+1} = w / h_{j+1,j}$, where $h_{j+1,j} = \|w\|$.

end

4 Compute Ritz pairs: (λ_i, x_i).

By elimination of w in the jth iteration of Algorithm 2 and combining all iterations, we obtain the recurrence relation of the rational Krylov method

$$A V_m \underline{K}_{m-1} = V_m \underline{L}_{m-1}, \tag{3.1}$$

where the jth columns of the two $m \times (m-1)$ upper Hessenberg matrices $\underline{K}_{m-1}$ and $\underline{L}_{m-1}$ are, respectively,

$$\begin{aligned} \underline{k}_j &:= \underline{h}_j, & \underline{l}_j &:= \sigma_j \underline{h}_j + \underline{e}_j, & &\text{for } \sigma_j \neq \infty, \\ \underline{k}_j &:= \underline{e}_j, & \underline{l}_j &:= \underline{h}_j, & &\text{for } \sigma_j = \infty, \end{aligned}$$

with $\underline{h}_j$ the coefficients of the Gram–Schmidt orthogonalization process and $\underline{e}_j$ the jth column of the identity matrix I_m extended with a zero at the bottom. Note that by this definition, we have

$$\sigma_j = \frac{l_{j+1,j}}{k_{j+1,j}}, \qquad j = 1, \ldots, m-1,$$

and in each iteration step j, we assume that $|k_{j+1,j}| + |l_{j+1,j}| \neq 0$. Then, we call the pair $(\underline{K}_j, \underline{L}_j)$ *unreduced* [6].

Approximations for the eigenvalues and corresponding eigenvectors of A can be obtained from the top left upper parts of the Hessenberg matrices $\underline{K}_{m-1}$ and $\underline{L}_{m-1}$.

DEFINITION 3.1 (Ritz pair). *Let (λ_i, s_i) satisfy*

$$L_{m-1}s_i = \lambda_i K_{m-1}s_i, \qquad s_i \neq 0.$$

Then we call $(\lambda_i, x_i := V_m \underline{K}_{m-1} s_i)$ a Ritz pair of A.

Every iteration of Algorithm 2 is characterised by the matrices V, $\underline{K}$, and $\underline{L}$. Therefore, in order to ease notation in the remainder, we introduce the term *RKS triple* [10] to refer to the rational Krylov process (3.1).

DEFINITION 3.2 (RKS triple of order $j-1$). *The triple $\left(V_j, \underline{K}_{j-1}, \underline{L}_{j-1}\right)$ with $V_j \in \mathbb{C}^{n\times j}$ and $\underline{K}_{j-1}, \underline{L}_{j-1} \in \mathbb{C}^{j\times(j-1)}$ is called an RKS triple of order $j-1$ for A, if*

1. *it satisfies the rational Krylov recurrence relation* (3.1)*,*
2. *$\underline{K}_{j-1}$ and $\underline{L}_{j-1}$ are upper Hessenberg matrices with $(\underline{K}_{j-1}, \underline{L}_{j-1})$ unreduced, and*
3. *none of the $\sigma_i = l_{i+1,i}/k_{i+1,i}$, $i = 1, \ldots, j-1$ is an eigenvalue of A.*

3.2. Implicit rational filtering. The rational Krylov algorithm can also be used for the application of a rational filter on its subspace V [10]. This implicit rational filtering process with the matrix A consists of an expansion phase followed by a restarting phase. We now review the main results of implicit rational filtering in the rational Krylov method.

Suppose that after $k-1$ iterations of Algorithm 2, we have an RKS triple of order $k-1$ and let the rational filter be defined as follows

$$\varphi_{rks}(z) := \prod_{j=0}^{N-1} \frac{\alpha_j z - \beta_j}{z - z_j}, \tag{3.2}$$

where the poles $z_j \in \mathbb{C}$ and the shift pairs (α_j, β_j) are chosen such that $\alpha_i z_j \neq \beta_i$ and $\alpha_i \sigma_\ell \neq \beta_i$ for all $i, j = 0, 1, \ldots, N-1$ and $\ell = 1, \ldots, k-1$. Then, for applying the rational filter $\varphi_{rks}(A)$ to V_k, we first perform N additional RKS iterations with shifts

$$\sigma_k := z_0,\ \sigma_{k+1} := z_1,\ \ldots,\ \sigma_{k+N-1} := z_{N-1}. \tag{3.3}$$

Hence, we obtain an RKS triple of order $m-1$ with $m := k+N$. Secondly, this RKS triple is again reduced to one of order $k-1$ via the restarting procedure described in the following theorem.

THEOREM 3.3. *Let $\left(V_m, \underline{K}_{m-1}, \underline{L}_{m-1}\right)$ be an RKS triple of order $m-1$ for the matrix A satisfying* (3.3) *and define, for given $Q \in \mathbb{C}^{m\times k}$ and $Z \in \mathbb{C}^{(m-1)\times(k-1)}$ with $Q^*Q = I_k$ and $Z^*Z = I_{k-1}$,*

$$V_k^+ := V_m Q, \qquad \underline{K}_{k-1}^+ := Q^* \underline{K}_{k-1} Z, \qquad \underline{L}_{k-1}^+ := Q^* \underline{L}_{k-1} Z.$$

Then there are such Q and Z so that $\left(V_k^+, \underline{K}_{k-1}^+, \underline{L}_{k-1}^+\right)$ is an RKS triple with

$$\operatorname{range}\left(V_k^+\right) = \operatorname{range}\left(\varphi_{rks}(A) V_k\right),$$

where $\varphi_{rks}(z)$ is the rational filter given by (3.2).

Proof. See De Samblanx *et al.* [10, Theorems 4.2–4.3]. ∎

For the construction of V_k^+ from the poles z_j and the shift pairs (α_j, β_j), we refer to [10]. It can be efficiently implemented and only involves operations on the Hessenberg matrices $\underline{K}_{m-1}$ and $\underline{L}_{k-1}$ in order to compute Q and Z.

Remark that this implicit rational filtering process in the rational Krylov method can also be repeated in order to apply $\varphi_{rks}(A)$ multiple times. Furthermore, note that in case we choose the shift pairs $(\alpha_j, \beta_j) = (1, \lambda_j)$, with λ_j the unwanted Ritz values, we perform implicit restarting with *exact shifts*, i.e., the exact shifts results in purging the unwanted Ritz values and leaves the other ones untouched [29, 10].

4. Connections for linear eigenvalue problems. In this section, we propose the contour filtered rational Krylov method and prove its mathematical equivalence to contour integration methods for the linear eigenvalue problem. The key ingredients are the rational filter interpretation of the discretized moment matrices (2.7) and the implicit rational filtering performed by the rational Krylov method.

4.1. Contour filtered rational Krylov method. The application of a rational filter in the rational Krylov method allows for any rational filter of the form (3.2). In case we choose this filter $\varphi_{rks}(z)$ equal to the contour filter $\varphi_c(z) := b_0(z)$, i.e.,

$$\varphi_{rks}(z) := \prod_{j=0}^{N-1} \frac{\alpha_j z - \beta_j}{z - z_j} = \sum_{j=0}^{N-1} \frac{\omega_j}{z - z_j} =: \varphi_c(z), \tag{4.1}$$

we obtain the contour filtered rational Krylov method, outlined in Algorithm 3.

Algorithm 3: Contour filtered rational Krylov method

Input: RKS triple of order $k-1$: $\left(V_k, \underline{K}_{k-1}, \underline{L}_{k-1}\right)$.

for $j = 1, 2, \ldots$ **do**

1 EXPAND by performing N RKS iterations with shifts $z_0, z_1, \ldots, z_{N-1}$:

$$\left(V_{k+N}, \underline{K}_{k+N-1}, \underline{L}_{k+N-1}\right).$$

2 REDUCE by using Theorem 3.3 with $\varphi_{rks} = \varphi_c$ (4.1):

$$\left(V_k, \underline{K}_{k-1}, \underline{L}_{k-1}\right) := \left(V_k^+, \underline{K}_{k-1}^+, \underline{L}_{k-1}^+\right).$$

end

3 Perform 1 RKS iteration with shift $\sigma = \infty$:

$$\left(V_{k+1}, \underline{K}_k, \underline{L}_k\right).$$

4 Compute Ritz pairs from Hessenberg pair (L_k, K_k).

Algorithm 3 takes an RKS triple of order $k-1$ as input, i.e., $k-1$ iterations of Algorithm 2, and performs in every iteration j the implicit rational filtering procedure described in section 3.2 (steps 1–2). Next in step 3, an additional rational Krylov iteration with a shift at ∞ is performed, yielding the following recurrence relation

$$AV_k K_k = V_{k+1} \underline{L}_k. \tag{4.2}$$

Finally, k Ritz values are obtained from solving the small eigenvalue problem (L_k, K_k) in step 4.

Remark that, by (4.1) and Theorem 3.3, Algorithm 3 has a rational (contour) filter interpretation. This can be summarized as follows.

PROPOSITION 4.1. *Let the rational filter $b_0(z)$ be defined as in* (2.5)*. Then the effect of performing one iteration of Algorithm* 3 *onto the basis matrix V_k corresponds to applying the contour filter φ_c of the matrix A to it, i.e.,*

$$\text{range}\left(V_k^+\right) = \text{range}\left(\varphi_c(A)V_k\right),$$

where $\varphi_c(z) := b_0(z)$ and V_k^+ the Krylov basis after step 2 in iteration j.

4.2. Mathematical equivalence based on rational filtering. We now prove the equivalence between contour integration methods (Algorithm 1) and the contour filtered rational Krylov method (Algorithm 3). Remark that the former obtains the Ritz values from computing the eigenvalues of the projected matrix U^*AU, whereas the latter obtains them directly from computing the eigenvalues of the Hessenberg pair (L, K). For the remainder of this section, we make the following assumptions.

ASSUMPTION 4.2. *Let*

(i) *the starting basis matrix $V \in \mathbb{C}^{n\times k}$ for Algorithm* 1 *be equal to V_k of the RKS triple to start Algorithm* 3 *with;*
(ii) *the rational filter function φ_{rks} in Algorithm* 3 *be equal to the rational filter function φ_c corresponding to Algorithm* 1*.*

The first assumption is motivated by the fact that a Krylov subspace, e.g., built from shifts inside or on the contour, is richer in the direction of the wanted eigenspace than a randomly chosen subspace. The second assumption states that part of the rational Krylov shifts are no free parameters any more but implicitly chosen by the contour filter.

Then, by combining Propositions 2.4 and 4.1, we obtain

$$\text{range}\left(M_0\right) = \text{range}\left(V_k^+\right), \tag{4.3}$$

where M_0 is the result of step 1 in Algorithm 1 and V_k^+ the Krylov basis after step 2 in Algorithm 3, respectively. The mathematical equivalence between Algorithms 1 and 3 extends to the obtained Ritz values and is summarized in the following theorem.

THEOREM 4.3. *Suppose that Assumption* 4.2 *holds. Then the contour filtered rational Krylov method, outlined in Algorithm* 3*, and the contour integration method, outlined in Algorithm* 1*, are mathematically equivalent, i.e., the computed Ritz values are the same.*

Proof. To prove this theorem, we only consider one iteration of the outer loops in Algorithms 1 and 3. Without loss of generality, let U in step 3 of Algorithm 1 be equal to V_k, obtained after step 2 of Algorithm 3. Then substitution in (2.9) yields

$$\left(V_k^* A V_k\right) t = \lambda t. \tag{4.4}$$

Next, multiplication of (4.2) from the left by V_k^*, yields

$$V_k^* A V_k K_k = L_k. \tag{4.5}$$

Finally, by substitution of (4.5) in (4.4) we obtain the small eigenvalue problem of Algorithm 3

$$L_k s = \lambda K_k s,$$

with $s = K_k^{-1}t$. Hence, the Ritz values computed via the contour integration method solving (2.9) and the contour filtered rational Krylov method are the same. This completes the proof. ∎

The equivalence proven in Theorem 4.3 will now be used to propose a rank test in the rational Krylov method (section 4.3). Next, the differences in implementation details of both classes of methods will be discussed (section 4.4).

4.3. Rank test in rational Krylov method. One of the advantages of using a contour integral method for computing all eigenvalues inside a given contour Γ is that, via the rank test, it also provides an estimate for the number of eigenvalues inside Γ. Based on the mathematical equivalence between contour integration methods and the contour filtered rational Krylov method, we now introduce how to perform the rank test also in Algorithm 3.

The discretized moment matrix M_0 is not readily available in the contour filtered rational Krylov method since, by (4.3), this method only builds an orthogonal basis for M_0. Therefore, the following lemma provides a relatively cheap and easy way to also compute M_0 in Algorithm 3.

THEOREM 4.4. *Suppose that Assumption* 4.2 *holds. Then the discretized moment matrix* M_0 (2.2) *can be computed as follows*

$$M_0 = \sum_{j=0}^{N-1} \omega_j V_{k+j+1} \underline{H}_{k+j} (z_j H_{k+j} - K_{k+j})^{-1} \begin{bmatrix} I_k \\ 0 \end{bmatrix},$$

where $\left(V_{k+N}, \underline{K}_{k+N-1}, \underline{L}_{k+N-1}\right)$ *is the RKS triple after step 1 of Algorithm* 3.

Proof. We start with the fact that step 1 of Algorithm 3 performs N RKS iterations, for which we have the following recurrence relation after each iteration j

$$AV_{k+j+1}\underline{H}_{k+j} = V_{k+j+1}\underline{K}_{k+j}, \tag{4.6}$$

for $j = 0, 1, \ldots, N-1$. Remark that, by definition, the last row of $z_j\underline{H}_{k+j} - \underline{K}_{k+j}$ is zero. Consequently, negation of (4.6) and adding $z_j V_{k+j+1}\underline{H}_{k+j}$ to both sides, yields

$$(z_j I - A)V_{k+j+1}\underline{H}_{k+j} = V_{k+j}(z_j H_{k+j} - K_{k+j}). \tag{4.7}$$

Next, by multiplication of (4.7) from the left by $(z_j I - A)^{-1}$ and from the right by $(z_j H_{k+j} - K_{k+j})^{-1}$ we obtain

$$(z_j I - A)^{-1} V_{k+j} = V_{k+j+1}\underline{H}_{k+j}(z_j H_{k+j} - K_{k+j})^{-1}.$$

Finally, noting that the first k columns of V_{k+j+1} are equal to V and summing up all N terms, with corresponding weights ω_j, completes the proof. ∎

For performing the rank test in Algorithm 3, we use Theorem 4.4 to compute the discretized moment matrix M_0. Consequently, the rank test is performed in exactly the same way as in contour integration methods, i.e., via an economy-size singular value decomposition of M_0.

Remark 4.5. A rank test in the contour filtered rational Krylov method is relatively cheap since it only requires linear combinations of the rational Krylov vectors and no additional linear systems solves. On the other hand, a rank test can also be performed in, for example, Arnoldi's method. But this comes with a certain cost because it will require N additional linear system solves, which is for most large-scale eigenvalue problems the dominant cost.

4.4. Differences in implementation details. The mathematical equivalence between Algorithms 1 and 3 allows now for a fair comparison between the contour integration method, which is based on computing the discretized moment matrices M_p, and the contour filtered rational Krylov method, which only uses a subspace of the discretized moment matrices.

4.4.1. Starting subspace. Contour integration methods mostly use a randomly chosen starting subspace. However, when contour integration is used as a rational filter, a good starting basis may reduce the number of outer iterations. On the other hand, the contour filtered rational Krylov method uses a (rational) Krylov subspace to start with. Constructing a Krylov subspace V is of course more expensive than starting with a random one, but the former will also be richer in the wanted eigenspace. This Krylov subspace can, for example, be easily generated by an Arnoldi process. In case the standard Arnoldi process is used, it will only involve matrix multiplications with A and vector orthogonalizations. In case the shift-and-invert Arnoldi process is used it will require an additional LU factorization, which can be reused in every iteration. When the shift is chosen appropriately, the shift-and-invert Krylov subspace usually provides a better starting subspace than a standard Krylov subspace.

4.4.2. Linear system solves. By discretization of the contour integrals with a quadrature rule with N nodes, both types of methods require N linear system solves in the core of their algorithm. But the major difference between them comprises the right hand side. While the contour integration methods have a matrix with k columns as right hand side, the contour filtered rational Krylov method solves in every iteration only a linear system with a vector as right hand side. Therefore, the use of Algorithm 3 can result in a significant reduction of the computation cost.

Remark that the contour integration method (Algorithm 1) is in fact a subspace iteration method. Therefore, this type of methods is more suitable for iterative linear system solves with low accuracy, since in this case simple implicit restarting is no longer possible in Krylov methods. Note also that Algorithm 1 computes the Ritz pairs from an explicit projection of A on the subspace. On the other hand, the rational Krylov method requires accurate linear system solves for computing the Ritz values from the Hessenberg matrices.

4.4.3. Projection and orthogonalization. The contour integration methods first construct the moment matrices and next an orthogonal basis is computed. This basis is consequently used in an explicit projection in order to obtain the small eigenvalue problem (2.9). On the other hand, the contour filtered rational Krylov method does not use an explicit projection since it solves the Hessenberg eigenvalue problem (K_k, H_k). Furthermore, the orthogonalization is distributed over all RKS iterations.

4.4.4. Memory cost. For large-scale eigenvalue problems, the dominant memory cost of contour integration methods is the storage of the starting subspace and the moment matrices. More precisely, for constructing the small eigenvalue problem (2.9) a contour integration algorithm requires two matrices of size $n \times k$. For the contour filtered rational Krylov method on the other hand, the dominant memory cost is the storage of the rational Krylov subspace. Algorithm 3 requires only one matrix but of size $n \times (k + N)$. However, this algorithm can also be implemented in such a way that the algorithm only involves a matrix of size $n \times (k+1)$ by replacing steps 1–2 by N times one RKS iteration directly followed by a restart with a rational filter with only one pole [10]. Therefore, the contour filtered rational Krylov method reduces the memory cost by almost a factor 2 compared to contour integration methods.

4.4.5. Parallel implementation. The computation of the discretized moment matrix in the contour integration method requires N independent linear system solves with the same subspace V. This is an obvious advantage for parallelism. For a parallel implementation of the rational Krylov algorithm, we refer to [26, 27, 28].

4.4.6. Generalized eigenvalue problems. So far we only considered linear eigenvalue problems in this section. However, an extension of the algorithms to generalized eigenvalue problems $Ax = \lambda Bx$ is straightforward. For contour integration methods this corresponds to replacing the identity matrix in the discretized moment matrices (2.2) by the matrix B. On the other hand for the contour filtered rational Krylov method this corresponds to replacing the shift-and-invert step in Algorithm 2 by $w = (A - \sigma_j B)^{-1} B v_j$.

5. Connections for nonlinear eigenvalue problems. In comparison to linear eigenvalue problems, the situation for the nonlinear case is somewhat different.

Firstly, the number of eigenvalues of a NLEP (inside a contour Γ) can be larger than the problem dimension n. Therefore, contour integration methods for NLEPs [3, 9, 37] also use higher order discretized moment matrices

$$\widetilde{M}_p := \sum_{j=0}^{N-1} \omega_j z_j^p A(z_j)^{-1} V, \qquad p = 0, 1, \ldots, \tag{5.1}$$

where again z_j are the quadrature nodes and ω_j the corresponding weights.

Secondly, note that in the nonlinear case the resolvent operator $(zI - A)^{-1}$ in (2.1) and (2.2) is replaced by $A(z)^{-1}$, where $A(z)$ is defined in (1.1). This implies that, in general, the connection to rational filtering is lost.

Thirdly, the rational Krylov method is not directly applicable to a NLEP of the form (1.1). Therefore, we will adopt a three phase approach [33]. First, in the *approximation* phase, the nonlinear matrix-valued function $A(\lambda)$ is approximated by an interpolating (rational) matrix polynomial on the given contour Γ. This step results in a corresponding polynomial or rational eigenvalue problem. Next, in the *linearization* phase, the polynomial or rational eigenvalue problem is converted into a larger generalized linear eigenvalue problem with the same eigenvalues, called linearization. Finally, in the *rational Krylov* phase, we solve the obtained linear eigenvalue problem by the contour filtered rational Krylov method and fully exploit the structure of the linearization pencil.

5.1. CORK framework. The compact rational Krylov (CORK) framework [35] uses a simple and generic representation of structured linearization pencils and maximally exploits its structure in the rational Krylov method.

Let $P(\lambda) \in \mathbb{C}^{n \times n}$ be a matrix polynomial of grade d which accurately approximates the nonlinear matrix-valued function $A(\lambda)$ inside and on the contour Γ. Then, we define the $dn \times dn$ structured linear pencil $\mathbf{L}(\lambda)$ as follows

$$\mathbf{L}(\lambda) = \mathbf{A} - \lambda \mathbf{B}, \tag{5.2}$$

where

$$\mathbf{A} = \left[\begin{array}{ccccc} A_0 & A_1 & \cdots & A_{d-1} \\ \hline \multicolumn{4}{c}{M \otimes I_n} \end{array}\right], \qquad \mathbf{B} = \left[\begin{array}{ccccc} B_0 & B_1 & \cdots & B_{d-1} \\ \hline \multicolumn{4}{c}{N \otimes I_n} \end{array}\right], \tag{5.3}$$

with $A_i, B_i \in \mathbb{C}^{n \times n}$ and $M, N \in \mathbb{C}^{(d-1) \times d}$. The matrices in the first block row of $\mathbf{L}(\lambda)$ are related to the coefficients of $P(\lambda)$, and the Kronecker structure below this

first block row corresponds to the linear relations between the basis functions of $P(\lambda)$. Note that the structured linearization pencil (5.3) covers many of the linearizations used in the literature. For an overview of different polynomial and rational bases, we refer to [35].

The CORK method, proposed in [35], is the result of fully exploiting the Kronecker structure of $\mathbf{L}(\lambda)$ in the rational Krylov method by decomposing V_j as follows

$$V_j = (I_d \otimes Q_j)\, U_j, \tag{5.4}$$

where $V_j \in \mathbb{C}^{dn \times j}$, $Q_j \in \mathbb{C}^{n \times r}$, and $U_j \in \mathbb{C}^{dr \times j}$, with $r < d + j$. Note that, since V_j and Q_j have orthonormal columns by definition, U_j also has orthonormal columns. Although $\mathbf{L}(\lambda)$ is of dimension dn, the CORK algorithm only involves linear system solves with $P(\sigma)$, and matrix-vector and vector-vector operations of dimension n. Hence, both the memory and computation cost is significantly reduced, compared to directly applying Algorithm 2 to $\mathbf{L}$, yielding an algorithm for large-scale NLEPs which has the same orders of magnitude as solving a linear eigenvalue problem of the same dimension n.

5.2. Contour filtered CORK method. After approximating the nonlinear matrix-valued function $A(\lambda)$ in (1.1) by an interpolating (rational) matrix polynomial $P(\lambda)$ and transforming it to the structure linearization pencil $\mathbf{L}(\lambda)$, we obtain a linear generalized eigenvalue problem. Hence, the theory and results of section 4 apply again and the connection with rational filtering is back.

We now propose the contour filtered CORK method, abbreviated by CF–CORK, as a special variant of the contour filtered rational Krylov method, outlined in Algorithm 3, applied to the pencil $\mathbf{L}(\lambda)$. In the CF–CORK method we fully exploit the Kronecker structure of the linearization matrices $\mathbf{A}$ and $\mathbf{B}$, and use the compact representation of the subspace as given in (5.4).

Using the results of section 4, the CF–CORK method is mathematically equivalent to applying contour integration onto the linearization pencil $\mathbf{L}(\lambda) = \mathbf{A} - \lambda\mathbf{B}$. But an easy equivalence directly to nonlinear contour integration is not possible because of the reasons spelled out in the beginning of this section. However, under the following assumptions, the CF–CORK method and the nonlinear contour integration methods solve linear systems with exactly the same matrices. Therefore, let the shifts $z_0, z_1, \ldots, z_{N-1}$ in Algorithm 3 be equal to the quadrature nodes used in (5.1) and a subset of the interpolation nodes for the nonlinear matrix-valued function $A(\lambda)$. Consequently, the CF–CORK method only requires linear system solves with $A(z_j)$, i.e., the same as used to construct the discretized moment matrices (5.1).

Moreover, in contrast to the nonlinear contour integration methods, the CF–CORK method allows for repeatedly applying the contour filter, as we will illustrate in section 6.2. Furthermore, there is also no need for using higher discretized moment matrices in the CF–CORK method since we can always choose the grade d such that $k \leq dn$.

6. Numerical examples. In the first example, we consider a linear eigenvalue problem and illustrate that the contour filtered rational Krylov method (Algorithm 3) produces the same results as the ones obtained via the contour integral method (Algorithm 1). In the second example, we consider the "`gun`" problem of the NLEVP collection [7] and compare the CF–CORK method to the standard CORK method using implicit restarting with exact shifts.

All numerical experiments are performed in MATLAB version 8.3.0 (R2014a) on

a Dell Latitude notebook running an Intel(R) Core(TM) i5-2540M CPU @ 2.60GHz quad core processor with 8 GB RAM.

6.1. Linear eigenvalue problem. We consider a randomly generated matrix $A \in \mathbb{R}^{100\times 100}$ with condition number $\kappa(A) \approx 3.10^4$. The eigenvalues of A are shown in Figure 1. The aim is to compute all the eigenvalues inside the unit disk Γ.

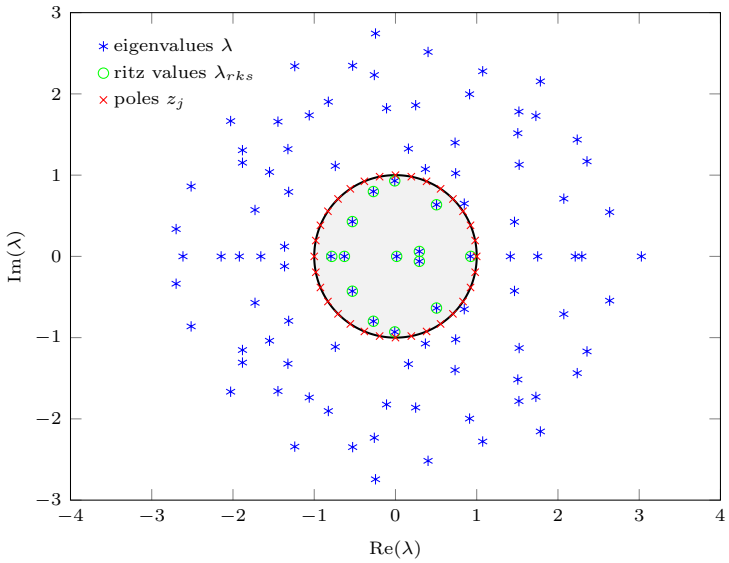


FIG. 1. *Results for the matrix A.*

In order to compute the eigenvalues in Γ, we use the unit disk filter function

$$\varphi_{rks}(z) := \prod_{j=0}^{N-1} \frac{z_j}{z - z_j} = \frac{1}{1 - z^N}, \tag{6.1}$$

where the poles are the roots of unity, $z_j = \exp(2\pi i \frac{j}{N})$, with $N = 32$. Note that (6.1) approximates the contour filter, i.e., approximately 1 inside the unit disk and 0 elsewhere [4]. As starting basis matrix V, we took a Krylov subspace V_k generated with A^{-1} and a random starting vector. Since the number of eigenvalues inside Γ is 14, we chose $k = 14$.

We will now compare the Ritz values obtained by one outer iteration of the contour integration method (Algorithm 1) to the ones obtained by one outer iteration of the contour filtered rational Krylov method (Algorithm 3). For measuring the convergence of an approximate eigenpair (λ, x), we use the relative residual norm

$$e = \frac{\|(A - \lambda I)x\|_2}{(\|A\|_1 + |\lambda|)\|x\|_2}.$$

The results are presented in Table 1. The first two columns contain the Ritz values after the first outer iteration of Algorithms 1 and 3, respectively. The mathematical equivalence between these two classes of methods is illustrated by the differences between the Ritz values $|\lambda_c - \lambda_{rks}|$, shown in column 3. Note also that their corresponding relative residual norms e_c and e_{rks}, respectively given in columns 4 and 5, are the same.

TABLE 1
Ritz values for the matrix A after the first outer iteration of Algorithms 1 and 3.

λ_c	λ_{rks}	$\lvert\lambda_c - \lambda_{rks}\rvert$	e_c	e_{rks}	$\lvert e_c - e_{rks}\rvert$
$0.0148 - 0.0000i$	$0.0148 - 0.0000i$	4.12e-14	5.31e-17	9.39e-16	8.86e-16
$0.2939 + 0.0608i$	$0.2939 + 0.0608i$	2.20e-12	1.64e-08	1.64e-08	1.29e-14
$0.2939 - 0.0608i$	$0.2939 - 0.0608i$	3.45e-12	1.64e-08	1.64e-08	5.22e-15
$-0.6284 - 0.0000i$	$-0.6284 - 0.0000i$	3.65e-12	8.93e-06	8.93e-06	1.81e-15
$-0.5306 + 0.4285i$	$-0.5306 + 0.4285i$	1.11e-12	4.04e-05	4.04e-05	4.82e-14
$-0.5306 - 0.4285i$	$-0.5306 - 0.4285i$	9.02e-13	4.04e-05	4.04e-05	3.93e-14
$-0.7842 + 0.0000i$	$-0.7842 - 0.0000i$	4.28e-12	1.25e-03	1.25e-03	5.19e-14
$0.5047 + 0.6355i$	$0.5047 + 0.6355i$	2.88e-12	2.56e-05	2.56e-05	3.10e-15
$0.5047 - 0.6355i$	$0.5047 - 0.6355i$	3.90e-12	2.56e-05	2.56e-05	4.55e-15
$-0.2718 + 0.7983i$	$-0.2718 + 0.7983i$	6.36e-12	3.76e-05	3.76e-05	3.04e-13
$-0.2718 - 0.7983i$	$-0.2718 - 0.7983i$	4.51e-12	3.76e-05	3.76e-05	2.15e-13
$0.9265 + 0.0000i$	$0.9265 + 0.0000i$	3.02e-12	4.54e-05	4.54e-05	2.80e-14
$-0.0087 + 0.9295i$	$-0.0087 + 0.9295i$	2.20e-12	3.35e-05	3.35e-05	6.27e-14
$-0.0087 - 0.9295i$	$-0.0087 - 0.9295i$	2.79e-12	3.35e-05	3.35e-05	6.71e-14

6.2. Nonlinear eigenvalue problem. We consider the "gun" problem of the NLEVP collection [7]. This is a large-scale problem that models a radio-frequency gun cavity and is of the form [18]

$$A(\lambda)x = \Big(K - \lambda M + i\sqrt{\lambda - \sigma_1^2}\, W_1 + i\sqrt{\lambda - \sigma_2^2}\, W_2\Big)x = 0, \tag{6.2}$$

where M, K, W_1 and W_2 are real symmetric matrices of size 9956×9956, K is positive semidefinite, M is positive definite, and $\operatorname{rank}(W_1) + \operatorname{rank}(W_2) = 84$. The complex square root $\sqrt{\cdot}$ corresponds to the principal branch and as in [7], we take $\sigma_1 = 0$ and $\sigma_2 = 108.8774$. For measuring the convergence of an approximate eigenpair (λ, x), we use the relative residual norm $E(\lambda, x)$ defined in [18].

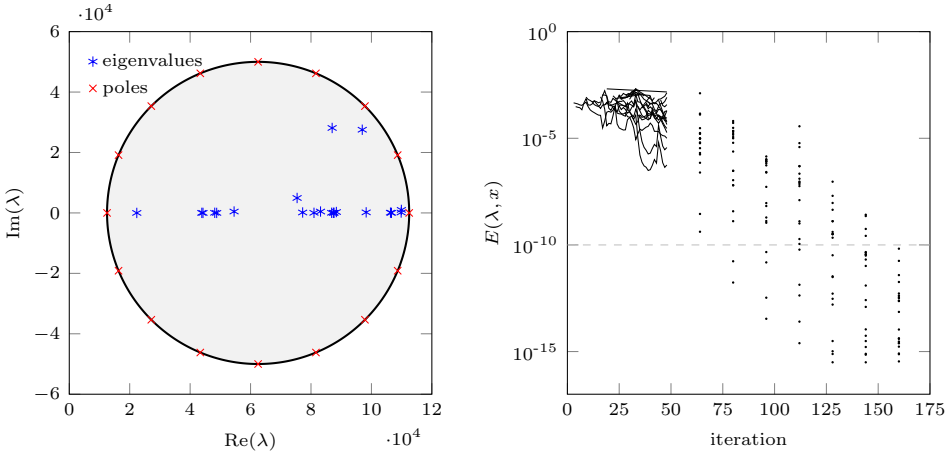
The goal is to compute all the eigenvalues inside the contour Γ, which is the circle with center $c_\Gamma = 250^2$ and radius $300^2 - 200^2$. We first approximate $A(\lambda)$ in (6.2) by an interpolating rational Newton polynomial on Γ. This results in a fixed linearization of degree $d = 40$. For more information on how to construct this linearization pencil, we refer to [13].

In a first experiment, we compute all eigenvalues inside Γ via the contour filtered CORK method (CF–CORK). Therefore, we use the following rational filter function

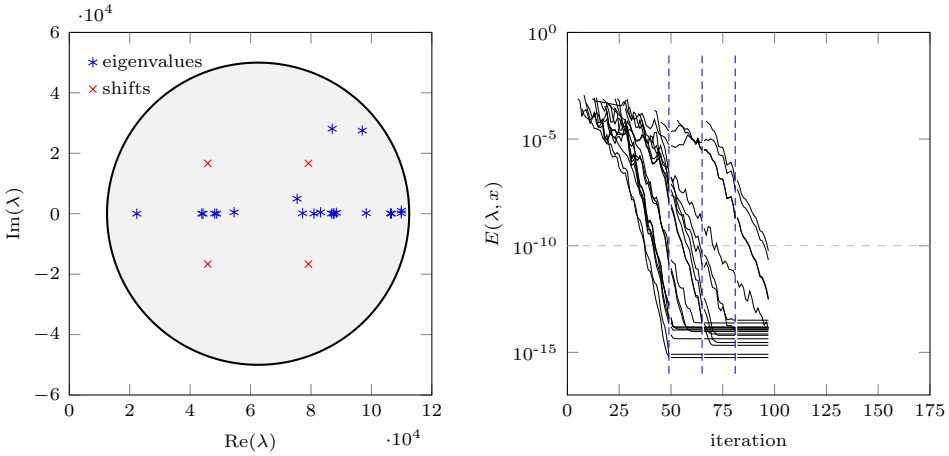
$$\varphi_{cork}(z) := \prod_{j=0}^{N-1} \frac{\beta_j}{z - z_j}, \tag{6.3}$$

where z_j are the poles, indicated by "$\times$" in Figure 2a, $\beta_j := z_j - c_\Gamma$, and $N = 16$. Note that (6.3) approximates the contour filter, i.e., approximately 1 inside Γ and 0 elsewhere. Furthermore, we started the CF–CORK method with a Krylov subspace V_k of dimension $k = 49$, generated by three times cyclically repeating the poles z_j as shifts in the rational Krylov process. The (little) convergence of the eigenpairs during the generation of V is shown in the first 48 iteration of the right graph in Figure 2a. Next, we applied 7 times the rational (contour) filter function φ_{cork} to V_k in order to obtain all 21 eigenvalues up to a relative residual norm smaller than the given tolerance of 10^{-10}. As illustrated in the right graph of Figure 2a, this sums up to a total of 160 CORK iterations.

In a second experiment, we now use the standard CORK method to compute the eigenvalues inside Γ. The differences between these two methods lies in the choice of



(a) CF–CORK method



(b) CORK method

FIG. 2. *Results for the "gun" problem: eigenvalues (left) and convergence history (right).*

the rational Krylov shifts and the restarting process: the former uses a contour filter in the restarting process, whereas the latter uses implicit restarting with exact shifts. In order to make a fair comparison, we set the maximal dimension of the Krylov subspace in the CORK method equal to 50, which was also the maximal dimension in the previous experiment. Next, we chose four shifts inside Γ, indicated by "$\times$" in Figure 2b, which we cyclicaly repeated and in every restart we selected 33 Ritz values. As stopping criteria we used the heuristic that all Ritz values inside Γ should have converged. The convergence history is shown in the right graph of Figure 2b and illustrates that all eigenvalues up to the given tolerance are obtained after only 3 restarts and in less than 100 CORK iterations.

Finally, we compare in terms of computation and memory costs the CF–CORK method to the standard CORK method. Since we chose equal maximal dimension of the Krylov subspace in both methods, both the memory cost related to storing the subspace as well as the orthogonalization cost are almost exactly the same. However,

the main difference lies in the computation cost for solving the linear systems. Note that the CF–CORK method required N LU decompositions for solving all linear systems in the first experiment, while in the second experiment the standard CORK method only required 4. Moreover, the CF–CORK requires much more iterations to converge due to the fact that the rational Krylov shifts, i.e., the poles of the contour filter (6.3), lie much further away from the wanted eigenvalues inside Γ compared to the chosen shifts inside Γ for the standard CORK method. As already noted in Remark 4.5, contour integration has a *reputation* of being more reliable for computing all eigenvalues inside a given contour, this example illustrates that it can have a much higher cost. However, the stopping criteria used in the second experiment work very well in practice.

7. Conclusions. In this paper, we have proven for linear eigenvalue problems that, under some conditions, contour integration methods and the rational Krylov method are mathematically equivalent. Next, we used this equivalence to combine the good properties of both world and introduced the contour filtered rational Krylov method. We also provided a detailed comparison, in terms of implementation details, of these two classes of methods for computing all eigenvalues inside a given closed contour. Furthermore, in order to overcome the loss of connection with rational filtering in contour integration methods for nonlinear eigenvalue problems, we have introduced the contour filtered CORK method.

The connections between these two different classes of eigensolvers have been shown by numerical examples. The experiments also show that contour integration methods, compared to rational Krylov methods using implicit restarting with exact shifts, come with a much higher cost due to a relatively high number of LU decompositions and a slower convergence requiring much more iterations.

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