ANALYSIS OF THE RATIONAL KRYLOV SUBSPACE PROJECTION METHOD FOR LARGE-SCALE ALGEBRAIC RICCATI EQUATIONS *

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Abstract. In the numerical solution of the algebraic Riccati equation $A^*X + XA - XBB^*X + C^*C = 0$, where A is large, sparse and stable, and B, C have low rank, projection methods have recently emerged as a possible alternative to the more established Newton-Kleinman iteration. In spite of convincing numerical experiments, a systematic matrix analysis of this class of methods is still lacking. We derive new relations for the approximate solution, the residual and the error matrices, giving new insights into the role of the matrix $A - BB^*X$ and of its approximations in the numerical procedure. The new results provide theoretical ground for recently proposed modifications of projection methods onto rational Krylov subspaces.

Key words. Riccati equation, rational Krylov, reduced order modelling

AMS subject classifications. 47J20, 65F30, 49M99, 49N35, 93B52

1. Introduction. We consider the numerical solution of the algebraic Riccati equation

$$A^*X + XA - XBB^*X + C^*C = 0, \tag{1.1}$$

where $A \in \mathbb{R}^{n\times n}$ is large and sparse, and $B \in \mathbb{R}^{n\times q}$, $C \in \mathbb{R}^{p\times n}$ with $q, p \ll n$; here and in the following A^* denotes the complex conjugate of A. For A stable[1], the solution matrix X of interest is the one that is symmetric positive semidefinite and such that $A - BB^*X$ remains stable. Equation (1.1) arises in many scientific and engineering applications that require controlling a dynamical system, and it has been deeply studied by applied algebraists and numerical mathematicians; we refer the reader to [29] for a thorough description of the problem and its many mathematical relations. In the recent book [11], the numerical treatment of this and related problems has been discussed, both in the small and large scale cases. In the large scale setting, with $n \gg 10^3$, a serious bottleneck is given by the fact that the possibly dense $n \times n$ matrix X cannot be stored. Most numerical methods thus approximate X by means of factored low-rank matrices, e.g., $X \approx ZZ^*$, so that only Z needs to be stored. Different approaches have been explored to solve (1.1) under this constraint, and for quite some time a variant of the Newton method, the Newton-Kleinman iteration, has been the most popular approach [28],[16],[10],[8]. Low-rank subspace iteration strategies have also been considered in the past few years, see, e.g., [1],[7],[31]. Other forms of data-sparse approximations include multilevel [19] and hierarchical [20] methods, which rely on available structure in the data.

Projection-type methods also yield low rank approximations, however they had not been used for the Riccati equation until very recently. In fact, projection methods are extensively employed in the solution of algebraic linear systems and eigenvalue problems. In the past decade, specific choices of approximation spaces have shown that projection methods are particularly effective also for *linear* matrix equations such as the Lyapunov and Sylvester equations [38]. Lately, the projection idea has been applied to the algebraic (quadratic) Riccati equation [26],[25], with surprisingly good

*Version of January 31, 2016.

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[1]An $n \times n$ matrix is stable if all its eigenvalues are in the open left half complex plane.

results, to the point that better performance is often observed than with Newton-based procedures [40]. Moreover, ad-hoc parameter selections have been proposed to further enhance particularly effective approximation spaces [31]. This strong numerical evidence however is lacking of any theoretical justification: the procedure is mainly based on its linear counterpart and therefore it seems to completely disregard the quadratic term $-XBB^*X$. Nonetheless, fast convergence to the sought after solution is usually observed.

The aim of this paper is to start an analysis that will lead to a better understanding of this class of methods. By looking at the computed quantities from different perspectives, we are able to give new insights into the role of the approximate solution X_k in the various contexts where the Riccati equation is extensively studied. We start in section 3 with model order reduction of linear dynamical systems, where approximation by projection is a recognized important tool, and show that X_k carries information on the optimal function value in the reduced control problem. In section 5 we deepen our knowledge of X_k and the associated residual, which allows us to derive new expressions for the residual matrix and justify recently proposed enhancements of a popular space in model order reduction, that is the rational Krylov subspace. A key role in our discussion will be played by the residual matrix,

$$R_k := A^*X_k + X_kA - X_kBB^*X_k + C^*C. \tag{1.2}$$

By simple algebra, it is customary to rewrite R_k as

$$R_k = (A^* - X_kBB^*)X_k + X_k(A - BB^*X_k) + C^*C + X_kBB^*X_k, \tag{1.3}$$

which highlights the occurrence of the matrix $A^* - X_kBB^*$. This matrix and its projected version will be ubiquitous in the paper, and are the true players in the approximation process. Finally, the connection between the approximation of the matrix equation and the invariant subspace setting is highlighted in section 6. While our interest was motivated by the good performance of rational Krylov methods, which are the main focus of section 5, many of the results in fact hold for more general projection methods. We believe that our analysis helps provide good ground to characterize projection methods as a natural and effective strategy for solving the Riccati equation.

The following notation and definitions will be used. For $X \in \mathbb{R}^{n\times n}$, $X \geq 0$ means that X is symmetric and positive semidefinite, while $X > 0$ means that is symmetric and positive definite. A stable matrix is a square matrix with all its eigenvalues in the open left-half complex plane. An $n \times n$ matrix A is passive if its field of values, $\{z \in \mathbb{C} : z = (x^*Ax)/(x^*x), 0 \neq x \in \mathbb{C}^n\}$, is all in the open left-half complex plane. I_n denotes the identity matrix of size n, and the subscript will be avoided whenever clear from the context. A pair (A, B) is controllable if the matrix $[B, AB, \ldots, A^{n-1}B]$ is full row rank, and (C, A) is observable if (A^*, C^*) is controllable. A pair (A, B) is stabilizable if there exists a matrix X such that $A - BB^*X$ is stable. The Euclidean norm $\|\cdot\|$ for vectors and its induced norm for matrices will be used, together with the Frobenius norm for matrices, defined as $\|A\|_F^2 = \sum_{i,j} |a_{i,j}|^2$, where $A = (a_{i,j})$.

2. Background on projection methods. Projection methods usually generate a sequence of nested approximation spaces, $\mathcal{K}_k \subseteq \mathcal{K}_{k+1}$, $k \geq 1$, where an approximate solution is determined. Let the columns of $V_k \in \mathbb{R}^{n\times d_k}$ span the space $\mathcal{K}_k$, where d_k is the space dimension, with $d_k \leq d_{k+1}$. An approximation to X in (1.1) is sought as $X_k = V_kY_kV_k^* \approx X$, where Y_k is determined by imposing some additional condition.

A Galerkin method is characterized by an orthogonality condition of the residual to the given space, namely $R_k \perp \mathcal{K}_k$, where R_k is as defined in (1.2); the orthogonality is with respect to the standard matrix inner product, so that the Galerkin condition reads

$$V_k^* R_k V_k = 0. \tag{2.1}$$

As the subspace grows, the residual is forced to belong to a smaller and smaller space. When $d_k = n$ then clearly it must be $R_k = 0$ and a solution to (1.1) is determined, in exact arithmetic. The main goal is to determine a sufficiently good approximate solution X_k for $d_k \ll n$. To obtain Y_k we substitute X_k into the expression for the residual matrix in (2.1):

$$\begin{aligned} V_k^*(A^* V_k Y_k V_k^* + V_k Y_k V_k^* A - V_k Y_k V_k^* B B^* V_k Y_k V_k^* + C^* C) V_k = 0 \\ V_k^* A^* V_k Y_k + Y_k V_k^* A V_k - Y_k V_k^* B B^* V_k Y_k + V_k^* C^* C V_k = 0, \end{aligned}$$

where we used that $V_k^* V_k = I_{d_k}$. Setting $T_k = V_k^* A V_k$, $B_k = V_k^* B$ and $C_k^* = V_k^* C^*$ we see that Y_k can be obtained by solving the reduced Riccati equation

$$T_k^* Y_k + Y_k T_k - Y_k B_k B_k^* Y_k + C_k^* C_k = 0. \tag{2.2}$$

Under the assumption that A is passive, T_k is stable, therefore (2.2) admits a unique stabilizing positive semidefinite solution Y_k, which is then used for constructing X_k.

The effectiveness of the whole procedure depends on the choice of $\mathcal{K}_k$. The approximation spaces explored in the (quite recent) literature are all based on block Krylov subspaces generated with A or with rational functions of A and starting term C^* [26],[25],[40]. In section 5 we will analyze the case of the block rational Krylov subspace, while the results of the next two sections hold for any approximation space.

3. Order reduction of dynamical systems by projection. The Riccati equation is tightly connected with the time-invariant linear system

$$\begin{cases} \dot{x}(t) = Ax(t) + Bu(t), & x(0) = x_0 \\ y(t) = Cx(t), \end{cases} \tag{3.1}$$

where $u(t)$ and $x(t)$ are the control (or input) and state vectors, while $y(t)$ is the output vector; x_0 is the initial state. We note that $x(t)$ also depends on both x_0 and $u(t)$, but this will not be explicitly reported in the notation. Let us introduce the following quadratic cost functional[2]

$$\mathcal{J}(u, x_0) = \int_0^\infty (x(t)^* C^* C x(t) + u(t)^* u(t)) dt.$$

The Riccati equation matrix X is used in the solution of the following linear-quadratic regulator problem:

$$\inf_u \mathcal{J}(u, x_0),$$

which consists in finding an *optimal control* function $u_*(t)$ associated with the system (3.1), at which the function $\mathcal{J}$ attains its infimum. The following well known result

[2]Here we consider a simplified version to make an immediate connection with the Riccati equation stated in (1.1).

connects the optimal cost problem with the solution of the algebraic Riccati equation (1.1); see, e.g., the relevant part of [29, Theorem 16.3.3] in our notation.

THEOREM 3.1. *Let the pair (A, B) be stabilizable and (C, A) observable. Then there is a unique solution $X \geq 0$ of (1.1). Moreover,*

i) For each x_0 there is a unique optimal control, and it is given by $u_*(t) = -B^*X \exp((A - BB^*X)t)x_0$ for $t \geq 0$;

ii) $J(u_*, x_0) = x_0^* X x_0$ for all $x_0 \in \mathbb{C}^n$.

The optimal control function $u_*(t)$ in the theorem above is in fact determined as $u_*(t) = -B^*Xx(t)$, giving rise to the closed-loop dynamical system

$$\dot{x}(t) = (A - BB^*X)x(t), \qquad x(0) = x_0,$$

whose solution is $x(t) = \exp((A - BB^*X)t)x_0$ for $t \geq 0$ [24].

A reduced order model aims at representing the given large dynamical system by means of a significantly smaller one. This can be done by projecting data onto a significantly smaller space. A popular strategy in this class is to use the Rational Krylov subspace to reduce the coefficient matrices by projecting them onto an appropriate vector space [3]. The solutions of the reduced system can effectively approximate the original state and control in case the space trajectories do not occupy the whole state space. In practice, this means that the original model can be well represented by far fewer degrees of freedom [2].

A quantity of interest to the control community that is used to monitor the quality of the reduced system is the transfer function, for which a large literature is available; see, e.g., [3],[9],[18],[37] and their references. Here we focus on the reduction process, and show that the subspace projection allows one to determine the optimal control of the reduced dynamical system. Let the $d_k \ll n$ orthonormal columns of $V_k \in \mathbb{R}^{n \times d_k}$ span the computed subspace, and, as in the previous section, let $T_k = V_k^* A V_k$, $B_k = V_k^* B$, $C_k^* = V_k^* C^*$. Then we can define the reduced order system

$$\begin{cases} \dot{\widehat{x}}(t) = T_k \widehat{x}(t) + B_k \widehat{u}(t), & \widehat{x}(0) = V_k^* x_0. \\ \widehat{y}(t) = C_k \widehat{x}(t), \end{cases} \tag{3.2}$$

Clearly, as $d_k \to n$ the reduced system approaches the original one. For smaller d_k, the quantity $x_k(t) = V_k \widehat{x}(t)$ is an approximate state of the original system.

COROLLARY 3.2. *The solution matrix Y_k of (2.2) is the unique non-negative solution that gives the feedback optimal control $\widehat{u}_*(t)$, $t \geq 0$, for the system (3.2).*

Proof. Let

$$\widehat{\mathcal{J}}_k(\widehat{u}, \widehat{x}_0) = \int_0^\infty (\widehat{x}(t)^* C_k^* C_k \widehat{x}(t) + \widehat{u}(t)^* \widehat{u}(t)) dt.$$

be the cost functional associated with (3.2). By applying Theorem 3.1, an optimal control for the reduced system is $\widehat{u}_*(t) = -B_k^* Y_k \exp((T_k - B_k B_k^* Y_k)t)\widehat{x}_0$, where Y_k solves the reduced Riccati equation

$$T_k^* Y + Y T_k - Y B_k B_k^* Y + C_k^* C_k = 0, \tag{3.3}$$

with the reduced state $\widehat{x}(t) = \exp((T_k - B_k B_k^* Y_k)t)\widehat{x}_0$. Equation (3.3) is precisely the Riccati equation obtained by Galerkin projection of the original large scale matrix equation (1.1) onto the given subspace. ∎

Theorem 3.1(ii) implies

$$\widehat{\mathcal{J}}_k(\widehat{u}_*, \widehat{x}_0) = \widehat{x}_0^* Y_k \widehat{x}_0 = x_0^* V_k Y_k V_k^* x_0 = x_0^* X_k x_0.$$

Therefore, if $X_k \to X$ as $d_k \to \infty$, the optimal value of the reduced functional yields an estimate to the minimum functional cost via the approximate solution $X_k = V_k Y_k V_k^*$ to the large Riccati equation.

An approximate control function $u_k(t)$ for the unreduced functional $\mathcal{J}(u_k, x_0)$ is obtained directly using the approximation X_k, bypassing the reduced functional $\widehat{\mathcal{J}}$. Indeed, if we assume that the approximate Riccati solution X_k is stabilizing, we can write

$$u_k(t) = -B^* X_k x_k(t), \qquad \text{with} \quad x_k(t) = \exp((A - BB^* X_k)t)x_0. \tag{3.4}$$

Substituting $X_k = V_k Y_k V_k^*$ we get $u_k(t) = -(B^* V_k) Y_k V_k^* \exp((A - B(B^* V_k) Y_k V_k^*)t)x_0$. The question then arises as of whether u_k and $\widehat{u}_*$ are related. Comparing this expression with that of $\widehat{u}_*(t)$, we see that they are close to each other as soon as

$$\exp((V_k^*(A - BBX_k)V_k t)V_k^* \approx V_k^* \exp((A - BB^* X_k)t).$$

Using the expansion of $\exp(z)$ in terms of power series and taking transpose conjugations, this approximation can be written as

$$(A^* - X_k BB^*)^\ell V_k \approx V_k \left(V_k^*(A^* - X_k BB^*)V_k\right)^\ell, \qquad \text{for any } \ell \in \mathbb{N}.$$

This approximation becomes an equality as soon as range(V_k) is an invariant subspace of $A^* - X_k BB^*$. In general, however, the columns of V_k do not span an invariant subspace, therefore this connection is not sufficient to connect the two control functions. The following proposition does provide a relation between the optimal reduced cost functional value with the value of the original functional at u_k.

PROPOSITION 3.3. *Assume that $A - BB^* X_k$ is stable and that u_k is defined as in (3.4). With the previous notation it holds*

$$|\mathcal{J}(u_k, x_0) - \widehat{\mathcal{J}}_k(\widehat{u}_*, \widehat{x}_0)| \le \frac{\|R_k\|}{2\alpha} x_0^* x_0,$$

where $\alpha > 0$ is such that $\|e^{(A-BB^*X_k)^* t}\| \le e^{-\alpha t}$ for all $t \ge 0$.

Proof. Using (1.3), let us write the Riccati residual equation as

$$(A - BBX_k^*)^* X_k + X_k(A - BBX_k) + X_k BB^* X_k + C^* C - R_k = 0.$$

Then

$$\begin{aligned}
\mathcal{J}(u_k, x_0) &= \int_0^\infty (u_k^* u_k + x_k^* C^* C x_k) dt \\
&= \int_0^\infty x_0^* e^{(A-BB^*X_k)^* t} (X_k BB^* X_k + C^* C) e^{(A-BB^*X_k)t} x_0 dt \\
&= x_0^* X_k x_0 + \int_0^\infty x_0^* e^{(A-BB^*X_k)^* t} R_k e^{(A-BB^*X_k)t} x_0 dt.
\end{aligned}$$

From $x_0^* X_k x_0 = \widehat{J}_k(\widehat{u}_*, \widehat{x}_0)$ and $|\int_0^\infty x_0^* e^{(A-BB^*X_k)^* t} R_k e^{(A-BB^*X_k)t} x_0 dt| \le \frac{\|R_k\|}{2\alpha} x_0^* x_0$ the result follows. ∎

This theorem establishes a linear relation between the matrix equation residual norm and the distance between the optimal value of the reduced functional and the value of the approximate unreduced functional. As the residual norm goes to zero, the two functional values coalesce, and this may occur for $d_k \ll n$, that is with a projection space of much smaller dimension than the original one.

We conclude with a remark about the type of approximation space used. In model order reduction, usually different projection spaces are used from the left and from the right, so as to expand both in terms of C^* and B. The connection between this approach and the reduction of the (symmetric) Riccati equation deserves future analysis.

4. Control stability properties of the subspace projection approximation. By using the residual equation, norm estimates for the error $X - X_k$ can be derived by using classical perturbations results. In this section we recall these classical estimates, which can have a different flavor in our setting, where the *perturbations* are not very small in general. Nonetheless, these results enable us to state that for d_k large enough the approximate solution X_k is rigorously equipped with all the nice stabilizability properties of the exact solution. Moreover, they can be used to track the progress in the approximation as the approximation space grows.

Unlike the linear equation case, a small residual norm does not necessarily imply a small error, since the Riccati equation has more than one solution. Therefore, in general an assumption is needed about the closeness of the approximate solution to the sought after one, to be able to derive information on the error norm from the residual norm.

Let X be an exact stabilizing solution, $E_k = X - X_k$ the error and $R_k = A^*X_k + X_kA - X_kBB^*X_k + C^*C$ the residual. Subtract this residual equation from (1.1). Then by adding and subtracting XBB^*X_k and $E_kBB^*X_k$ in sequence, we obtain

$$(A^* - XBB^*)E_k + E_k(A - BB^*X) + E_kBB^*E_k + R_k = 0.$$

We observe in passing that the second order term in E_k becomes negligeable for $\|E_k\| \ll 1$. From this Riccati equation for the error, under certain conditions a bound on the error can be obtained. To this end we recall the definition of the *closed-loop Lyapunov operator*

$$\Omega_X(Z) := (A - BB^*X)^*Z + Z(A - BB^*X),$$

and observe that if H is the matrix solving $(A-BB^*X)^*H+H(A-BB^*X) = -I$, then $\|H\| = \|\Omega_X^{-1}\| = \max_{Z\neq 0}(\|\Omega_X^{-1}(Z)\|/\|Z\|)$; see [27, Lemma 2]. Note that $\|\Omega_X^{-1}\|$ is the reciprocal of the sep operator for the given matrix [41]. An interesting interpretation of $\|\Omega_X^{-1}\|$ in terms of the *damping* of the closed-loop dynamical system is also given in [27].

THEOREM 4.1. [27] *Let X be a symmetric and positive semidefinite solution to (1.1) such that $A - BB^*X$ is stable. Assume that $\|X - X_k\| < 1/(3\|B\|^2\|\Omega_X^{-1}\|)$. If the residual matrix R_k satisfies $4\|B\|^2\|\Omega_X^{-1}\|^2\|R_k\| < 1$ then*

$$\|X - X_k\| \le 2\|\Omega_X^{-1}\|\,\|R_k\|.$$

We refer the reader to [17] for more refined estimates. This bound is a generalization to the nonlinear case of the well known bound for the (vector) norm of the error when approximately solving a linear system $Ax = b$. We note that the "norm of the inverse"

is replaced here with the norm of the closed-loop operator inverse, which takes into account both the linear and the quadratic coefficient matrices.

We next recall a theorem on the sensitivity of the Lyapunov equation solution.

THEOREM 4.2. [24, Theorem 2.2] *Let A be stable and let H satisfy $A^*H + HA = -I$. Let ΔA satisfy $\|\Delta A\| < 1/(2\|H\|)$. Then $A + \Delta A$ is stable.*

This result enables us to state that if the error $X - X_k$ is small enough, then X_k is stabilizable; a similar result can also be found in [27, Lemma 1].

COROLLARY 4.3. *Let $A - BB^*X$ be stable and let X_k be an approximate solution to (1.1) and $E_k = X - X_k$. If $\|BB^*E_k\| < 1/(2\|\Omega_X^{-1}\|)$, then $A - BB^*X_k$ is stable.*

Proof. We write $A - BB^*X_k = (A - BB^*X) + BB^*E_k =: \widetilde{A} + \Delta\widetilde{A}$. We thus apply Theorem 4.2 to $\widetilde{A}$, $\Delta\widetilde{A}$: $\widetilde{A}$ is stable by hypothesis; moreover, if $\|BB^*E_k\| = \|\Delta\widetilde{A}\| < 1/(2\|\Omega_X^{-1}\|)$ then $\widetilde{A} + \Delta\widetilde{A}$ is stable. □

Finally, we turn our attention to the special form of the approximate solution, that is $X_k = V_k Y_k V_k^*$. The following result shows that after k iterations of a projection method, the reduced solution matrix Y_k is stabilizing.

PROPOSITION 4.4. *Let T_k be stable and $(T_k - B_k B_k^* Y_k, C_k^*)$ controllable. Let Y_k be the approximation obtained after k iterations of the chosen projection method. Then $T_k - B_k B_k^* Y_k$ is a stable matrix.*

Proof. The symmetric matrix Y_k solves the reduced matrix equation $T_k^*Y + YT_k - YB_kB_k^*Y + C_k^*C_k = 0$. Rewriting the equation, Y_k satisfies

$$(T_k^* - Y_k B_k B_k^*)Y_k + Y_k(T_k - B_k B_k^* Y_k) + Y_k B_k^* B_k Y_k + C_k^* C_k = 0,$$

that is, Y_k formally solves a Lyapunov equation. Since $Y_k B_k^* B_k Y_k + C_k^* C_k \geq C_k^* C_k$, Theorem 5.3.2(b) in [29] ensures that the eigenvalues of $T_k - B_k B_k^* Y_k$ all lie in the open left half-plane, that is the matrix is stable. □

Next result tracks the modification in the approximate solution matrix X_k as the subspace grows. It is important to realize that in general, the matrices Y_k in the sequence are computed by solving a new and expanding Riccati equation, therefore the entries of Y_k and Y_{k+1} are not related by a simple explicit recurrence.

PROPOSITION 4.5. *Let X_j be the approximate solution onto $\mathcal{K}_j$ for $j = k, k+1$. Then for k large enough,*

$$\|X_{k+1} - X_k\| \leq 2\|\Omega_{Y_{k+1}}^{-1}\|\|R_k\|.$$

Proof. We write $X_{k+1} = V_{k+1}Y_{k+1}V_{k+1}^*$ and $X_k = V_kY_kV_k^* = V_{k+1}\check{Y}_{k+1}V_{k+1}^*$, where $\check{Y}_{k+1}$ is Y_k padded with extra rows and columns to match the dimension of Y_{k+1}, and we recall that $V_{k+1} = [V_k, \star]$. Moreover, we set $T_{k+1} = [T_k, t_{k+1}^{(1)}; (t_{k+1}^{(1)})^*, \star]$. Y_{k+1} solves the reduced equation $T_{k+1}^*Y + YT_{k+1} - YB_{k+1}B_{k+1}^*Y + C_{k+1}^*C_{k+1} = 0$. Substituting instead the matrix $\check{Y}_{k+1}$ we obtain that the residual satisfies

$$\begin{aligned}\rho_k &:= T_{k+1}^*\check{Y}_{k+1} + \check{Y}_{k+1}T_{k+1} - \check{Y}_{k+1}B_{k+1}B_{k+1}^*\check{Y}_{k+1} + C_k^*C_k\\ &= V_{k+1}^*(A^*V_{k+1}\check{Y}_{k+1}V_{k+1}^* + V_{k+1}\check{Y}_{k+1}V_{k+1}^*A - V_{k+1}\check{Y}_{k+1}V_{k+1}^*BB^*V_{k+1}\check{Y}_{k+1}V_{k+1}^* + C^*C)V_{k+1}\\ &= V_{k+1}^*(A^*X_k + X_kA - X_kBB^*X_k + C^*C)V_{k+1}.\end{aligned}$$

Therefore, $\|\rho_k\| \leq \|R_k\|$. Using Theorem 4.1, if $\|Y_{k+1} - \check{Y}_{k+1}\| < 1/(3\|B_{k+1}\|^2\|\Omega_{Y_{k+1}}^{-1}\|)$ and $\|\rho_k\| \leq 1/(4\|B_{k+1}\|^2\|\Omega_{Y_{k+1}}^{-1}\|^2)$ then

$$\|Y_{k+1} - \check{Y}_{k+1}\| \leq 2\|\Omega_{Y_{k+1}}^{-1}\|\|\rho_k\|.$$

Noticing that $\|Y_{k+1} - \check{Y}_{k+1}\| = \|X_{k+1} - X_k\|$ the result follows. □

5. Rational Krylov subspace approximation. The approximation quality of projection methods depends on the choice of the approximation space $\mathcal{K}_k$. In the case of the Lyapunov and Sylvester equations, a classical choice is the Krylov subspace $\mathcal{K}_k = \text{range}([C^*, A^*C^*, \ldots, (A^*)^{k-1}C^*])$, first introduced for this problem by Saad in [36]. Note that in general, $C^* \in \mathbb{R}^{n\times p}$ satisfies $p \geq 1$, therefore the space is in fact a "block" space, whose dimension is not greater than $d_k = pk$. More recently and motivated by the reduction of dynamical systems, rational Krylov subspaces have shown to be very attractive. For $\mathbf{s} = [s_1, s_2, \ldots]$, with $s_j \in \mathbb{C}^+$, they are given by

$$\mathcal{K}_k(A, C^*, \mathbf{s}) := \text{range}([C^*, (A - s_2 I)^{-1}C^*, \ldots, \prod_{j=1}^{k-1}(A - s_{j+1}I)^{-1}C^*]).$$

If the problem data are real, the shifts are included in conjugate pairs. Moreover, $\Re(s_j) > 0$ therefore all inverses exist for A stable. We remark that the first block of columns generating $\mathcal{K}_k$ is simply the matrix C^*; this corresponds to using an infinite parameter $s_1 = \infty$ as first shift, and this will be an assumption throughout. Including C^* into the space is crucial for convergence, since the whole constant matrix term is exactly represented in the approximation space. The effectiveness of the space now depends on the choice of the parameters s_j, $j = 2, 3, \ldots$. A lot of work has been devoted to the analysis of ideal shifts, due to the relevance of rational Krylov subspaces in eigenproblems [35],[33], matrix function evaluations [22],[14],[23], and Model Order Reduction [21],[34],[15]; we refer the readers to [38] and to the references cited above. We mention that for linear matrix equations, the choice of $s_j \in \{0, \infty\}$ seems to be particularly effective in many cases, since the computational cost of solving with the coefficient matrix at each iteration can be somewhat mitigated, without dramatically sacrificing the asymptotic convergence rate. Numerical experiments reported in [40] show that for the algebraic Riccati equation this is no longer the case: the general rational Krylov subspace appears to be superior in all considered examples, in terms of subspace dimension, if the shifts are properly selected. This comparison deserves further study [39]. For the sake of simplicity of exposition or unless it is explicitly stated, in the rest of this section and its subsections we assume that C has a single row, that is $p = 1$. There is no relevant difference for $p > 1$, except that the same shift is applied to a block of p vectors, and that the involved matrices have dimensions depending on pk.

For $k \geq 1$, the rational Krylov subspace with shifts $s_1, s_2, \ldots, s_k$ satisfies the following Arnoldi relation[3] (see, e.g., [12], [30]):

$$A^*V_k = V_k T_k^* + \hat{v}_{k+1} g_k^*, \qquad V_k^* V_k = I, \tag{5.1}$$

where $\mathcal{K}_k = \text{range}(V_k)$, and $\hat{v}_{k+1}\beta = v_{k+1}s_k - (I - V_k V_k^*)A^* v_{k+1}$ is the QR decomposition of the right-hand side matrix, and with $g_k^* = \beta h_{k+1,k} E_k^* H_k^{-1}$. The matrix

$$\begin{bmatrix} H_k \\ h_{k+1,k} E_k^* \end{bmatrix}$$

contains the orthogonalization coefficients that generate the orthonormal columns of V_{k+1} (see, e.g., [15]). We set $V_1\beta_0 = C^*$, the reduced QR factorization of C^*. By

[3] The conjugate-transposition in T_k^* is used for consistency in the notation employed for the reduced Riccati equation.

construction, the matrix $[V_k, \hat{v}_{k+1}]$ has orthonormal columns as well.

PROPOSITION 5.1. *The matrix X_k satisfies the following algebraic Riccati equation*

$$(A^* - \hat{v}_{k+1} f_k^*)X + X(A - f_k \hat{v}_{k+1}^*) - XBB^*X + C^*C = 0,$$

where $f_k = V_k g_k$ and g_k is as in (5.1).

Proof. The residual satisfies

$$\begin{aligned} R_k &= [V_k, \hat{v}_{k+1}] \begin{bmatrix} 0 & Y_k g_k \\ g_k^* Y_k & 0 \end{bmatrix} \begin{bmatrix} V_k^* \\ \hat{v}_{k+1}^* \end{bmatrix} \\ &= \hat{v}_{k+1} g_k^* Y_k V_k^* + V_k Y_k g_k \hat{v}_{k+1}^* = \hat{v}_{k+1} g_k^* V_k^* X_k + X_k V_k g_k \hat{v}_{k+1}^*. \end{aligned} \tag{5.2}$$

Substituting into equation (1.2) and collecting terms the result follows. □

Since $\|f_k^* X_k\| = \|R_k\|/\sqrt{2}$, the modified equation of Proposition 5.1 tends to the original Riccati equation as convergence takes place. However, we cannot infer that X_k is close to X in the backward error sense, since $\hat{v}_{k+1} f_k^*$ is not small in general.

5.1. The adaptive rational Krylov subspace. Several different selection strategies have been proposed for the shifts s_j. In the linear equation case, Penzl ([34]) suggested a pre-processing for the computation of a fixed number of shifts, which are then applied cyclically. More recently, a greedy adaptive strategy was proposed in [15] for the same class of problems, which determines the next shift during the computation, so that the process can automatically learn from the convergence behavior of the method. The shifts are selected by minimizing a particular rational function on an approximate and adaptively adjusted spectral region of A. In [31] it was observed that for the Riccati equation the inclusion of information on BB^* during the shift computation – in the form of eigenvalues of $V_k^*(A^* - X_k BB^*)V_k$ – may be beneficial in certain cases. In the following we aim to justify this choice. To this end, we need to set a rational function framework that parallels some of the matrix relations obtained in the previous sections.

A relation corresponding to (5.1) can be obtained by using orthogonal rational functions with respect to some inner product; see, e.g., [12]. We note that each v_j can be written as $v_j = \varphi_j(A)c/\|c\|$, for some orthogonal rational function $\varphi_j = p_j/q_{j-1}$, where p_j, q_{j-1} are polynomials of degree at most j and $j-1$, respectively. For $j = 0$ we define $\varphi_0 = 1$. Let $\Phi_{k-1}(\lambda) = [\varphi_0(\lambda), \varphi_1(\lambda), \ldots, \varphi_{k-1}(\lambda)]$. Then,

$$\lambda \Phi_{k-1}(\lambda) = \Phi_{k-1}(\lambda) T_k^* + \hat{\varphi}_k(\lambda) g_k^*; \tag{5.3}$$

from (5.3) it follows that θ is a zero of $\hat{\varphi}_k$ if and only θ is an eigenvalue of T_k. We refer to [5, section 2.2] for a similar relation, where a different Arnoldi-type relation is used.

A first attempt to justify the use of information from $A - BB^*X_k$ can be obtained by generalizing the argument in [15], working as if the problem were linear. For the sake of notational simplicity, for the rest of this section we let $\mathcal{A}_k = A - BB^*X_k$ and $\mathcal{T}_k = V_k^* \mathcal{A}_k V_k = T_k - B_k B_k^* Y_k$. Using (1.2) we can write the residual as

$$\begin{aligned} R_k &= (A^* - X_k BB^*)X_k + X_k(A - BB^*X_k) + C^*C + X_k BB^* X_k \\ &= \mathcal{A}_k^* X_k + X_k \mathcal{A}_k + \mathcal{D}_k \mathcal{D}_k^*, \end{aligned} \tag{5.4}$$

where $\mathcal{D}_k = [C^*, X_k B]$. We observe that all columns of $\mathcal{D}_k$ belong to $K_k(A^*, C^*, \mathbf{s})$, since $\mathcal{D}_k = V_k[E_1\beta_0, Y_k B_k]$.

REMARK 5.2. *The rational Krylov subspace $K_k(A^*, C^*, \mathbf{s})$ satisfies an Arnoldi-type property for the matrix $\mathcal{A}_k$. Indeed,*

$$\begin{aligned}\mathcal{A}_k^* V_k &= A^* V_k - X_k B B^* V_k \\ &= V_k T_k^* + \hat{v}_{k+1} g_k^* - V_k Y_k B_k B_k^* \\ &= V_k (T_k^* - Y_k B_k B_k^*) + \hat{v}_{k+1} g_k^* = V_k \mathcal{T}_k^* + \hat{v}_{k+1} g_k^*.\end{aligned}$$

By using the expression of the residual (5.4) as if it were the residual matrix of a Lyapunov equation, we can follow the same reasoning as in [15] for the selection of the next shift. However, as opposed to the linear case, all involved matrices now depend on the iteration k. To simplify the presentation, in the following argument we assume that $C^* = c \in \mathbb{R}^n$. Consider the shifted system $(\mathcal{A}_k^* - sI)x = c$, and an approximate solution $x_k \in K_k(\mathcal{A}_k^*, c, \mathbf{s})$. Then the residual can be written as

$$c - (\mathcal{A}_k^* - sI)V_k(\mathcal{T}_k^* - sI)^{-1} e_1 \beta_0 = \frac{\psi_k(\mathcal{A}_k)c}{\psi_k(s)}, \qquad \psi_k(z) = \prod_{j=1}^{k} \frac{z - \lambda_j}{z - s_j}, \tag{5.5}$$

where λ_j are the eigenvalues of $\mathcal{T}_k$. The next shift s_{k+1} is then determined so that

$$s_{k+1} = \arg\left(\max_{s \in \partial\mathbb{S}_k} \left| \frac{1}{\psi_k(s)} \right| \right),$$

where $\mathbb{S}_k \subset \mathbb{C}^+$ approximates the mirrored spectral region of $\mathcal{A}_k$, and $\partial\mathbb{S}_k$ is its border. Note that ψ_k is a multiple of $\hat{\varphi}_k$ in (5.3). A major practical difference from the adaptive procedure in the Lyapunov equation case is that $\mathbb{S}_k$ will change at each iteration in agreement with the modifications in the spectrum of $\mathcal{A}_k$. In fact, thanks to the Arnoldi relation of Remark 5.2, the unknown spectral region of $\mathcal{A}_k$ is replaced with the spectral region of $\mathcal{T}_k$, which is computable after the approximate solution Y_k is determined. This approach is precisely the one explored in [31] for the Riccati equation. As opposed to an adaptive shift selection based on A (see, e.g., [40]), this approach includes information on the second order coefficient matrix, which may be crucial when the term $-BB^*X$ in $A - BB^*X$ significantly modifies the spectral properties of A (see Example 5.5). In the next section we give a rigorous formalization of this argument.

5.2. A new expression for the residual and the choice of shifts. In [4] a new expression for the residual of the Sylvester equation was proposed. We extend this expression to the case of the Riccati residual matrix. The new expression allows an interpretation of the two-term sum in (5.2) by means of rational functions. Note that the result also holds for $B = 0$, therefore its proof provides a more elementary proof for the Lyapunov equation than in [4].

PROPOSITION 5.3. *Assume that the columns of C^* belong to Range(V_k), and let $\mathcal{T}_k = V_k^* \mathcal{A}_k V_k = T_k - B_k B_k^* Y_k$. Then the residual R_k satisfies*

$$R_k = \widehat{R}_k V_k^* + V_k \widehat{R}_k^*, \qquad \text{with} \quad \widehat{R}_k = A^* V_k Y_k + V_k Y_k \mathcal{T}_k + C^*(CV_k),$$

so that $\|R_k\|_F = \sqrt{2}\|\widehat{R}_k\|_F$.

Proof. By substituting $\widehat{R}_k$ in the expression for R_k we obtain,

$$\begin{aligned}\widehat{R}_k V_k^* + V_k \widehat{R}_k^* &= A^* X_k + V_k Y_k T_k V_k^* - V_k Y_k B_k B_k^* Y_k V_k^* + C^* C \\ &\quad + X_k A + V_k T_k^* Y_k V_k^* - V_k Y_k B_k B_k^* Y_k V_k^* + C^* C \\ &= R_k + 0,\end{aligned}$$

where the reduced equation (2.2) and $C^* C V V^* = C^* C$ were used; this proves the first relation. The norm relation follows from $V_k^* \widehat{R}_k = 0$, which can be readily verified. ∎

We shall call $\widehat{R}_k$ the "semi"-residual matrix. The proposition above shows that the residual norm of the Galerkin method for the Riccati equation is the same as that of an associated Sylvester equation times the constant $\sqrt{2}$. As a consequence, we can at least formally state that $V_k Y_k V_k^*$ is a solution to the Riccati equation (1.1), that is $R_k = 0$, if and only if $Z_k = V_k Y_k$ is the solution to the Sylvester equation

$$A^* Z + Z \mathcal{T}_k + C^* C V_k = 0, \tag{5.6}$$

where $\mathcal{T}_k$ typically has dimensions much smaller than A. Note that this Sylvester equation is in terms of A (and not of $\mathcal{A}_k = A - B B^* X_k$), but also in terms of $\mathcal{T}_k$. Let

$$\psi_k(z) = \frac{\det(zI - T_k)}{\prod_{j=1}^k (z - s_j)} = \frac{\prod_{j=1}^k (z - \theta_j)}{\prod_{j=1}^k (z - s_j)}, \tag{5.7}$$

where θ_j are the eigenvalues of $T_k = V_k^* A V_k$. Then the following representation holds for the semi-residual $\widehat{R}_k$. The result was first proved for the Sylvester equation in [4] and then generalized to the multi-term linear case in [6]. We prove the result for C^* having a single column, the generalization to multiple columns can be obtained by working with each column of C, since the whole matrix C is used to build the approximation space.

THEOREM 5.4. *Assume that $p = 1$, that is $C^* = c \in \mathbb{R}^n$. Let ψ_k be the rational function defined in (5.7) and assume that $\mathcal{T}_k = V_k^* \mathcal{A}_k V_k$ is diagonalizable. The semi-residual $\widehat{R}_k$ of Proposition 5.3 satisfies*

$$\widehat{R}_k = \psi_k(A^*) c c^* V_k (\psi_k(-\mathcal{T}_k))^{-1}.$$

Proof. Let $\mathcal{T}_k = Q \Theta Q^{-1}$, with $\Theta = \operatorname{diag}(\theta_1, \ldots, \theta_k)$. then the result follows from standard arguments for shifted linear systems. Indeed, substituting this decomposition into $\widehat{R}_k$ in Proposition 5.3 it follows that $\widehat{R}_k Q = A^* V_k Y_k Q + V_k Y_k Q \Theta + c c^* V_k Q$. Let $Z := V_k Y_k Q = [z_1, \ldots, z_k]$, $c\eta_j := c c^* V_k Q e_j$ and $r_j = \widehat{R}_k Q e_j$, then we have

$$r_j = (A^* + \theta_j I) z_j + c\eta_j.$$

Due to the Galerkin condition, the residuals r_j are all proportional to $\hat{v}_{k+1}$, therefore using (5.7) they can be written as $r_j = \hat{\varphi}_k(A^*) c\eta_j / \hat{\varphi}_k(-\theta_j)$. Collecting all columns we get $\widehat{R}_k Q = \psi_k(A^*) c c^* V_k Q \psi_k(-\Theta)^{-1}$, where we recall that ψ_k is a multiple of $\hat{\varphi}_k$; multiplying from the right by Q^{-1} the result follows. ∎

We observe that the expression of the semi-residual generalizes the residual formula for the shifted system in (5.5) to the case of matrix equations. The quantity $(\psi_k(-\mathcal{T}_k^*))^{-1}$ plays the same scaling role as the scalar $1/\psi_k(s)$ in the shifted system in (5.5). This new relation thus appears to be of interest on its own. Indeed, while for

linear matrix equations a parallel with shifted systems had already been performed (see [38, section 4.3] and references therein), the residual matrix associated to the special Sylvester equation (5.6) had not been explicitly written down in terms of polynomials or rational functions.

The new expression for $\widehat{R}_k$ suggests a way to determine the next shift s_{k+1}. Indeed, we first recall that the numerator of the rational function ψ_k is the characteristic polynomial of T_k, which thus minimizes the numerator of ψ_k among all monic polynomials of degree k. This makes $\|\psi_k(A)c\|$ small among all rational functions ψ_k with fixed denominator and monic numerator. With the next shift we thus want to make the quantity $(\psi_k(-\mathcal{T}_k))^{-1}$ smaller in the expression for $\widehat{R}_k$. Therefore, we determine for which z in the spectral region of $\mathcal{T}_k$ the quantity $(\psi_k(-z))^{-1}$ is large, and add a root there for the construction of the next function φ_k. Therefore, s_{k+1} is chosen as the solution to the following problem

$$s_{k+1} = \arg\max_{s\in\partial\mathbb{S}_k} \left|\frac{1}{\psi_k(s)}\right| = \arg\max_{s\in\partial\mathbb{S}_k} \left|\frac{\prod_{j=1}^{k}(s-s_j)}{\det(sI-\mathcal{T}_k)}\right|, \tag{5.8}$$

where here $\mathbb{S}_k$ is a region enclosing the eigenvalues of $-\mathcal{T}_k$ and $\partial\mathbb{S}_k$ is its border. This approach should be compared with the original algorithm that uses T_k instead. This modified selection strategy can be implemented very easily, with a slight modification of the original algorithm in [15]: the algorithm needs to compute the eigenvalues of $\mathcal{T}_k = T_k - B_k B_k^* Y_k$ instead of those of T_k to determine the corresponding convex hull. It is interesting to observe that for A Hermitian, working with the non-Hermitian matrix $\mathcal{T}_k$ appears to be more complex than working with the Hermitian matrix T_k. On the other hand, the matrix $\mathcal{T}_k$ has a key role in the Riccati semi-residual matrix, and it takes into account the nonlinear term in the original equation. Clearly, if the convex hulls of T_k and $\mathcal{T}_k$ are similar, and the same for those of A and of $A - BB^*X$, then no major differences will be observed between the two selection strategies. In other words, if the field of values are similar, then the projection method based only on the linear part will be able to decrease $\|\widehat{R}_k\|$ with a similar convergence rate.

We next report an example illustrating the expected behavior of the rational Krylov method with or without the inclusion of the term $-B_k B_k^* Y_k$ in the computation of the spectral region in (5.8)[4].

EXAMPLE 5.5. *We consider a small built-up example, where A is the Toeplitz matrix $A = -\texttt{toeplitz}(-1, -1.5, \underline{2.8}, 1, 1, 1)$ of size n=700 (this small size allows us to easily compute all quantities for this theoretical analysis). Moreover, $B = t\mathbf{1}$ and $C = [1, -2, 1, -2, 1, -2, \ldots]$; this example is motivated by an example with similar data in [31]. The parameter t takes the values $t_j = 5 \cdot 10^{-j}$, so that for $j = 3$, $\|B\| \approx 1$. The left plot of Figure 5.1 shows the convergence history (relative residual norm) of the rational Krylov method for each of the three different values of t, when the shifts are adaptively computed on the spectral region of $\mathcal{T}_k$, as in (5.8). The right plot of Figure 5.1 shows the modification of the convex hull of $A^* - XBB^*$ as t varies. For the larger values of t_j, the magnitude of B significantly influences the spectral convex hull; by using the modified shift computation strategy, the method is able to adapt to this change and capture the new problem features. We remark that by using spectral information of T_k instead, the method takes about 12 iterations to converge, irrespective of the value of t. We notice that for B of rank one, the matrix XBB^**

[4]The Matlab ([32]) code for the rational Krylov subspace method for the Riccati equation is available at the author's webpage `http://www.dm.unibo.it/~simoncin/software.html`.

is also rank one, with a real positive eigenvalue whose magnitude depends on B and thus on t. For $\|B\|$ large, Figure 5.1 shows that for this example only one eigenvalue of A^* is significantly perturbed in $A^* - XBB^*$, causing the extension of the original spectrum to the left, by an amount depending on t.

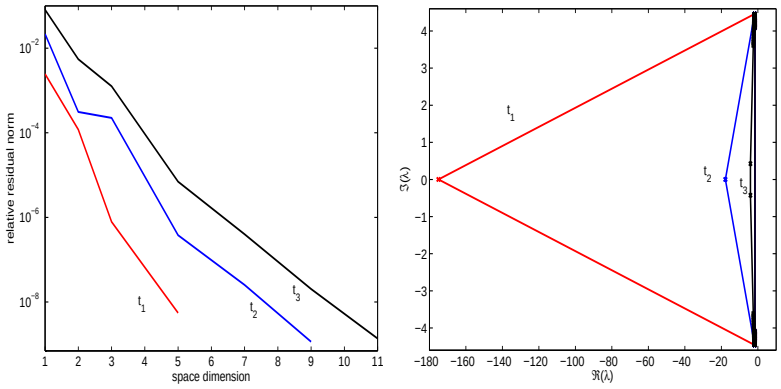

FIG. 5.1. *Example 5.5. Left: Convergence history of rational Krylov method with modified shift selection as t varies. Right: convex hull of $A^* - XBB^*$ as t varies.*

Example 5.5 shows that for these data, the magnitude of B influences the residual convergence of the modified method in a counterintuitive way: the larger its norm, the faster the method convergence. By using the modified shift selection, the isolated eigenvalue of $A^* - XBB^*$ (see Figure 5.1) is readily located, and the residual is forced to be small in that region as well.

In the next example we explore the influence of the nonsymmetry of $\mathcal{T}_k$ in the shift computation, when A is symmetric.

EXAMPLE 5.6. *We consider the same setting as for Example 5.5, except that now $A = A_0 \otimes I_{n_0} + I_{n_0} \otimes A_0$, with $A_0 = \texttt{toeplitz}(1, \underline{-2}, 1) \in \mathbb{R}^{n_0 \times n_0}$, with $n_0 = 30$ and $\otimes$ the Kronecker product, giving rise to a 900×900 symmetric negative definite matrix. These data represent the scaled finite difference discretization of the Laplacian on the unit square with homogeneous boundary conditions. As t varies, we compare the performance of the method when $\mathbb{S} \subset \mathbb{R}$ is associated with the symmetric matrix T_k, with the case when $\mathbb{S} \subset \mathbb{C}$ due to the use of $\mathcal{T}_k$; to emphasize this dependence will shall use $\mathbb{S}(\mathrm{T}_k)$ and $\mathbb{S}(\mathcal{T}_k)$, respectively. Table 5.1 shows the space dimension required by the two approaches to reach an absolute residual norm of 10^{-9}. Shown are also the absolute residual and error norms at convergence, and the norm of the exact solution. We report that all computed shifts were real also for $\mathcal{T}_k$. The table shows that the number of iterations for the residual to converge is always smaller when $\mathbb{S}(\mathcal{T}_k)$ is used, and it decreases with the magnitude growth of the B term, as in the previous example. We also notice that when using T_k, the final error is significantly smaller than in the modified version of the method; apparently, the residual lags behind in convergence, when $\mathbb{S}(T_k)$ is used.*

Figure 5.2 displays the residual convergence history for the two approaches, as t varies. The initial steep phase of the residual in the modified approach is granted by the fact that the approximation space immediately locates the isolated eigenvalue, and that the residual appears to have a large component in the corresponding eigendirection. After that, the convergence behavior depends on the rest of the spectrum. The original solver maintains the same convergence rate for all values of t.

t	Spectral Region	Space dim.	$\|R_k\|_F$	$\|X - X_k\|_F$	$\|X\|_F$
10^3	$\mathbb{S}(\mathrm{T}_k)$	21	1.8500e-10	1.6646e-13	4.9999e-03
	$\mathbb{S}(\mathcal{T}_k)$	3	8.5599e-10	1.4389e-10	
10^2	$\mathbb{S}(\mathrm{T}_k)$	23	3.1915e-10	3.0155e-13	4.9994e-02
	$\mathbb{S}(\mathcal{T}_k)$	7	4.9612e-10	1.0148e-10	
10	$\mathbb{S}(\mathrm{T}_k)$	25	9.6706e-10	2.5302e-13	4.9938e-01
	$\mathbb{S}(\mathcal{T}_k)$	9	9.0853e-10	2.2998e-10	

TABLE 5.1

Example 5.6. Comparison of performance for A symmetric. Number of iterations for the two variants for the relative residual norm and final accuracies to go below 10^{-9}.

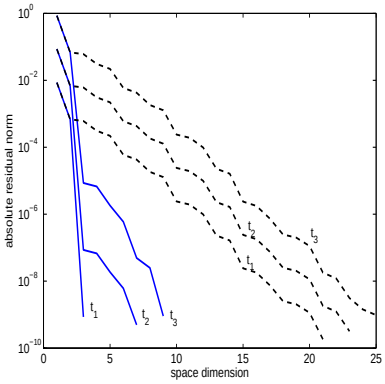

FIG. 5.2. *Example 5.6. Convergence history of rational Krylov method with and without modified shift selection as t varies. Solid curves: use of* $\mathcal{T}_k$. *Dashed curves: use of* T_k.

By generalizing field of values results in [13],[4] it may be possible to exploit the semi-residual form to analyze the convergence of the method, and its dependence on $\mathcal{T}_k$. A shortcoming in the analysis is that the field of values of the non-Hermitian matrix $\mathcal{T}_k$ depends on k, and that its relation with the field of values of $A^* - XBB^*$ is not easy to formalize, especially at an early stage of the convergence history. Resorting to the residual expression in (5.4), it is possible to exploit some of the results available in the literature for the Lyapunov equation. For instance, if the field of values of $A^* - XBB^*$ and of $A^* - X_kBB^*$ is contained in a disk of center $c > 0$ and radius equal to one for all k, then using [13, Theorem 4.11] we can state that the error satisfies

$$\overline{\lim}_{k\to\infty} \|X - X_k\|^{\frac{1}{k}} \le \frac{2c^2 + c - 1 - (2c+1)\sqrt{c^2-1}}{c + 1 + \sqrt{c^2-1}} =: \gamma.$$

The following example shows that this asymptotic bound can be descriptive of the actual behavior.

EXAMPLE 5.7. *We consider* $A = -1/(3.2)A_0 - I$ *where* A_0 *is the Grcar matrix,* $A_0 = \texttt{toeplitz}(-1, \underline{1}, 1, 1, 1) \in \mathbb{R}^{n\times n}$, $n = 1600$, $C = \mathbf{1}/\|\mathbf{1}\|$ *and* $B \in \mathbb{R}^{n\times p}$, $p = 20$ *with normally distributed random numbers, normalized so that its norm is about* $5 \cdot 10^{-2}$. *The left plot of Figure 5.3 shows the computed spectrum of A ('×' symbol), that of* $A^* - XBB^*$ *('∘' symbol), the border of the field of values of both A and* $A^* - XBB^*$ *(thin line), and the circle of center* $c = 1.25$ *and radius one, enclosing the field of values. The right plot of Figure 5.3 displays the error norm history of the modified method*

(dashed line), and $10^{-2}\gamma^k$*, The convergence rate is well captured by the theoretical estimate* γ *at the early stage of the iterations.*

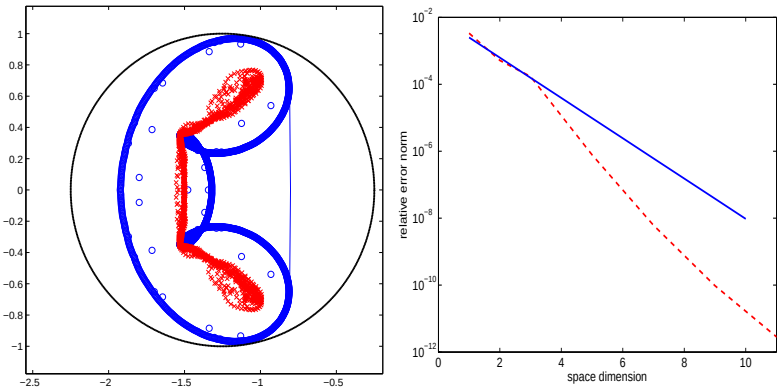

FIG. 5.3. *Example 5.7. Left: Field of values and eigenvalue location. Right: Error norm convergence history and estimate* γ^k*.*

6. Approximation of an invariant subspace. In this section we discuss the natural, albeit gone almost unnoticed, role of the approximation matrix X_k in the eigenvalue context. The problem of solving the large scale algebraic Riccati equation for $X \geq 0$ can be transformed into the problem of computing an approximate basis for the stable invariant subspace of the following Hamiltonian matrix (see, e.g., [29])

$$\mathcal{H} = \begin{bmatrix} A & -BB^* \\ -C^*C & -A^* \end{bmatrix}. \tag{6.1}$$

Several different approaches have been devised to this end, see, e.g., [1],[7],[31] and references therein. Here we show that the projection process described in the previous sections can be equivalently applied to this context, providing further motivation for the method.

Let X_k be the approximate solution to (1.1) obtained by the rational Krylov subspace method. For some $L \in \mathbb{R}^{n\times n}$ consider the eigenvalue residual

$$\mathcal{S}_k = \begin{bmatrix} A & -BB^* \\ -C^*C & -A^* \end{bmatrix}\begin{bmatrix} I \\ X_k \end{bmatrix} - \begin{bmatrix} I \\ X_k \end{bmatrix} L.$$

For $L = A - B^*BX_k$, the invariant space residual $\mathcal{S}_k$ and the matrix equation residual R_k can be easily related, since

$$\mathcal{S}_k = \begin{bmatrix} A & -BB^* \\ -C^*C & -A^* \end{bmatrix}\begin{bmatrix} I \\ X_k \end{bmatrix} - \begin{bmatrix} I \\ X_k \end{bmatrix}(A - B^*BX_k) = \begin{bmatrix} 0 \\ R_k \end{bmatrix},$$

so that $\|\mathcal{S}_k\| = \|R_k\|$. As a consequence of Proposition 5.1 the following result holds.

PROPOSITION 6.1. *The columns of the matrix* $[I; X_k]$ *span an invariant subspace of the matrix*

$$\mathcal{H}_k = \begin{bmatrix} A - f_k\hat{v}_{k+1}^* & -BB^* \\ -C^*C & -(A - f_k\hat{v}_{k+1}^*)^* \end{bmatrix},$$

and the spectrum of $T_k^* - Y_kB_kB_k^*$ *is a subset of the spectrum of* $A^* - X_kBB^* - \hat{v}_{k+1}f_k^*$*.*

Proof. Writing the eigenresidual

$$\mathcal{S}_k = \begin{bmatrix} A - f_k\hat{v}_{k+1}^* & -BB^* \\ -C^*C & -(A - f_k\hat{v}_{k+1}^*)^* \end{bmatrix}\begin{bmatrix} I \\ X_k \end{bmatrix} - \begin{bmatrix} I \\ X_k \end{bmatrix}(A - f_k\hat{v}_{k+1}^* - B^*BX_k)$$

and using Proposition 5.1 we readily see that $\mathcal{S}_k = 0$.

To prove the second assertion, we use the Arnoldi relation in (5.1). Let (θ, z) be an eigenpair of $T^* - Y_kB_kB_k^*$. Then

$$\begin{aligned}(A^* - \hat{v}_{k+1}f_k^* - X_kBB^*)V_kz &= (A^*V_k - \hat{v}_{k+1}f_k^*V_k - X_kBB^*V_k)z \\ &= (V_kT_k^* + \hat{v}_{k+1}g_k^* - \hat{v}_{k+1}f_k^*V_k - X_kBB^*V_k)z \\ &= (V_kT_k^* - X_kBB^*V_k)z = V_k(T_k^* - Y_kB_kB_k^*)z = V_kz\theta,\end{aligned}$$

and the result follows. □

The result above states that the approximate Riccati solution is associated with an invariant subspace of a modification of the original matrix in (6.1), and that the spectrum of $T_k^* - Y_kB_kB_k^*$ is a portion of the spectrum of this modified problem. These properties are a consequence of the Arnoldi relation (5.1), which indeed states that V_k is an invariant subspace basis of a modification of A^*, namely of $A^* - \hat{v}_{k+1}f_k^*$. What is noticeable in our context is that we can relate the spectral region over which we seek the next shift in (5.8) with the spectral region of a relevant matrix back in $\mathbb{R}^n$.

The approximation process leading to the computation of Y_k can be interpreted as a Galerkin method for the eigenvalue problem associated with $\mathcal{H}$. Consider the space

$$\mathbb{V}_k = \operatorname{range}\left(\begin{bmatrix} V_k & 0 \\ 0 & V_k \end{bmatrix}\right) =: \operatorname{range}(\mathcal{V}_k).$$

Then by projecting $\mathcal{H}$ onto the space we obtain,

$$\mathcal{V}_k^*\mathcal{H}\mathcal{V}_k = \begin{bmatrix} V_k^*AV_k & -V_k^*BB^*V_k \\ -V^*C^*CV_k & -V_k^*A^*V_k \end{bmatrix} = \begin{bmatrix} T_k & -B_kB_k^* \\ -C_k^*C_k & -T_k^* \end{bmatrix}.$$

The block matrix on the right-hand side is the Hamiltonian matrix associated with the reduced system. Using the reduced Riccati equation, it holds that

$$\begin{bmatrix} T_k & -B_kB_k^* \\ -C_k^*C_k & -T_k^* \end{bmatrix}\begin{bmatrix} I \\ Y_k \end{bmatrix} = \begin{bmatrix} I \\ Y_k \end{bmatrix}(T_k - B_kB_k^*Y_k),$$

with Y_k stabilizing. In terms of original space dimensions, let $\mathcal{V}_k[I; Y_k] = [V_k; V_kY_k]$ be the computed approximate eigenbasis. Then the residual is given by

$$\mathcal{S}_k = \begin{bmatrix} A & -BB^* \\ -C^*C & -A^* \end{bmatrix}\begin{bmatrix} V_k \\ V_kY_k \end{bmatrix} - \begin{bmatrix} V_k \\ V_kY_k \end{bmatrix}(T_k - B_kB_k^*Y_k).$$

It readily follows that the eigenresidual is orthogonal to the generated space, that is it holds that $(\mathcal{V}_k)^*\mathcal{S}_k = 0$, therefore it satisfies a standard Galerkin condition. As a consequence, for $T_k - B_kB_k^*Y_k$ stable, $\mathcal{V}_k[I; Y_k]$ approximates a basis of a stable invariant subspace of the matrix $\mathcal{H}$ in the sense of Galerkin projection methods.

7. Conclusions. By looking at the problem from different but highly related perspectives, we have shown that projection methods are a natural device for solving the algebraic Riccati equation. In particular, the reduced equation solves a reduced linear-quadratic optimization problem, as is typical of model order reduction techniques. By using classical arguments, we have related the residual with the error of the current approximation. Moreover, we have derived a new expression for the residual in terms of rational functions; this expression allows us to justify recent algorithmic strategies for the choice of the shift parameters used in the construction of the approximation space. In addition, this expression highlights the role of the quadratic term, and explains why it often happens that good convergence occurs even without taking the quadratic term into account during the construction of the approximation space. The new relations for the residual in terms of rational functions can be the starting point for a convergence analysis of the method. We notice that while we have focussed on generic rational Krylov subspaces in section 5, many of the stated results hold for other choices of approximation spaces, and in particular for polynomial and extended Krylov subspaces.

Finally, we have shown that the computed quantities correspond to a Galerkin approximation of the eigenvalue problem associated with the Hamiltonian matrix of the dynamical system.

Acknowledgements. We would like to thank Dario Bini and Daniel Szyld for insightful comments. This research is supported in part by the FARB12SIMO grant of the Università di Bologna, and by INdAM-GNCS under the 2016 Project *Equazioni e funzioni di matrici con struttura: analisi e algoritmi*.

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