INEXACT KLEINMAN–NEWTON METHOD FOR RICCATI EQUATIONS*

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Abstract. In this paper we consider the numerical solution of the algebraic Riccati equation using Newton's method. We propose an inexact variant which allows one control the number of the inner iterates used in an iterative solver for each Newton step. Conditions are given under which the monotonicity and global convergence result of Kleinman also hold for the inexact Newton iterates. Numerical results illustrate the efficiency of this method.

1. Introduction. The numerical solution of Riccati equations for large scale feedback control systems is still a formidable task. In order to reduce computing time in the context of Kleinman–Newton methods, it is mandatory that one uses iterative solvers for the solution of the linear systems occurring at each iteration.

In such an approach, it is important to control the accuracy of the solution of the linear systems at each Newton step in order to gain efficiency, but not to lose the overall fast convergence properties of Newton's method. This can be achieved in the framework of inexact Newton's methods.

In his classical paper, Kleinman [13] applied Newton's method to the algebraic Riccati equation, a quadratic equation for matrices of the type:

$$A^T X + X A - X B B^T X + C^T C = 0,$$

where $A \in \mathbb{R}^{n \times n}, B \in \mathbb{R}^{n \times m}, C \in \mathbb{R}^{l \times n}$.

At each Newton step, a Lyapunov equation

$$X_{k+1} \left(A - B B^T X_k \right) + \left(A - B B^T X_k \right)^T X_{k+1} = -X_k B B^T X_k - C^T C$$

needs to be solved to obtain the next iterate X_{k+1}.

In the literature, several variants of this method have been proposed. The approach taken by Banks and Ito [1] suggests to apply Chandrasekhar's method for the initial iterates and then use the computed iterate as a starting matrix for the Kleinman–Newton method. Rosen and Wang [25] apply a multilevel approach to the solution of large scale Riccati equations. Navasca and Morris [19], [20] use the Kleinman–Newton method with a modified ADI method for the Lyapunov solvers to find the feedback gain matrix directly for a discretized version of a parabolic optimal

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control problem. They also consider a version where the gain matrix is computed directly.

Benner and his co-authors use variants of the Kleinman–Newton algorithm to solve Riccati equations in their papers [2], [4], [5]. They utilize ADI methods for solving the Lyapunov equations at each step and address issues like parameter selection for ADI and parallelization among others. Incorporating line searches in a Newton procedure can often lead to a reduction in the number of iterations. This has been the focus of the research in Benner and Byers [3] and Guo and Laub [11]. The case, when the Jacobian of the nonlinear map describing the Riccati equation is singular at the solution, has been considered by Guo and Lancaster in [10].

In a recent paper Burns, Sachs, and Zietsman [6] give conditions under which the Kleinman–Newton method is mesh independent, i.e., the number of iterates remains virtually constant when the discretization of the underlying optimal control problem is refined.

Large scale Lyapunov equations usually require the use of iterative solvers like Smith's method or versions of the ADI method; for systems like this, the inexact Newton's method gives a rigorous guideline for the termination of the inner iteration for the Lyapunov equation while retaining the fast local rate of convergence. Another major effect in saving computing time is the possibility to terminate the inner iteration early when the iterates X_k are still far away from the solution of the Riccati equation. For a discussion on these methods see, for example, Kelley [12].

Whereas these aspects are typical for inexact Newton methods, the application to a Riccati equation bears some special features. Kleinman observed that the convergence is more global than usual; i.e., the starting matrix X_0 does not need to lie in a neighborhood of the solution X_∞. The proof is based on monotonicity properties of the iterates X_k as pointed out below. Obviously, this monotonicity is lost, when the iterates X_k are computed inexactly and, as a consequence, the global convergence feature of Kleinman–Newton does no longer hold. In this paper we also address the question, under which conditions the monotone convergence behavior and, hence, the larger convergence radius is maintained for the inexact Kleinman–Newton method.

The paper is organized as follows: In the next section we state the well-known convergence results for the exact Kleinman–Newton method in the case of Riccati equations and for the inexact Newton method in the general case. In the following section we formulate the inexact Newton method applied to the Riccati equation and give the convergence statement. Section 4 contains convergence results of the inexact Kleinman–Newton method including monotonicity statements for the iterates. This is achieved under certain assumptions on the residuals of the inexact Lyapunov solver. A condition on the size of the residual guarantees that the inexact Newton iterates are well defined. A stronger condition on the residuals yields the quadratic rate of convergence. The assumption on the starting data is the same as for the exact Kleinman–Newton method.

In section 5 we consider several iterative solvers for the Lyapunov equations like Smith's method and variants of the ADI method. We show how the previous conditions for the monotone convergence relate to the iterative solvers. This is followed by a section on numerical results for a discretized two-dimensional parabolic control problem. The convergence is illustrated and the savings in computing time is documented. The last section deals with another variant of the Kleinman–Newton method. We show that the inexact version of this method is unstable. The residuals accumulate as the iteration progresses, and, hence, this version should not be used in an inexact framework.

2. Inexact Newton method. The algebraic Riccati equation presented in the introduction can be written as a nonlinear system of equations.

The goal is to find a symmetric matrix $X \in \mathbb{R}^{n \times n}$ with $\mathcal{F}(X) = 0$, where the map $\mathcal{F} : \mathbb{R}^{n \times n} \to \mathbb{R}^{n \times n}$ is defined by

$$(2.1) \qquad \mathcal{F}(X) = A^T X + X A - X B B^T X + C^T C.$$

If one applies Newton's method to this system, one has to compute the derivative at X, symmetric, given by

$$\mathcal{F}'(X)(Y) = A^T Y + Y A - Y B B^T X - X B B^T Y$$
$$(2.2) \qquad = \left(A - B B^T X\right)^T Y + Y \left(A - B B^T X\right) \qquad \forall \ Y \in \mathbb{R}^{n \times n}.$$

In Newton's method, the next iterate is obtained by solving the Newton system

$$(2.3) \quad \mathcal{F}'(X_k)(X_{k+1} - X_k) = -\mathcal{F}(X_k) \quad \text{or} \quad \mathcal{F}'(X_k)X_{k+1} = \mathcal{F}'(X_k)X_k - \mathcal{F}(X_k).$$

For the Riccati equation the computation of a Newton step requires the solution of a Lyapunov equation. Corresponding to the second part of (2.3) we obtain

$$(2.4) \qquad X_{k+1} \left(A - B B^T X_k\right) + \left(A - B B^T X_k\right)^T X_{k+1} = -X_k B B^T X_k - C^T C,$$

which is a Lyapunov equation for X_{k+1}. This method is well understood and analyzed. It does not only exhibit locally a quadratic rate of convergence, but has also a monotone convergence property which is not so common for Newton's method and which is due to the quadratic form of $\mathcal{F}$ and the monotonicity of $\mathcal{F}'$. For this to hold, we introduce and impose the following definition and assumption:

DEFINITION 2.1. *Let* $A \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times m}$, *and* $C \in \mathbb{R}^{l \times n}$. *A pair* (A, BB^T) *is called stabilizable if there is a feedback matrix* $K \in \mathbb{R}^{n \times n}$ *such that* $A - BB^T K$ *is stable, which means that* $A - BB^T K$ *has only eigenvalues in the open left halfplane.* $(C^T C, A)$ *is called detectable if and only if* $(A^T, C^T C)$ *is stabilizable.*

In the following sections we make the assumption:

Assumption 2.2. (A, BB^T) *is stabilizable and* $(C^T C, A)$ *is detectable.*

Note that by [14, Lemma 4.5.4] the first assumption implies the existence of a matrix X_0 such that $A - BB^T X_0$ is stable.

As a common abbreviation we set

$$A_k := \left(A - B B^T X_k\right), \quad k \in \mathbb{N}_0$$

and $A \leq B$ means that the matrix $A - B$ is negative semidefinite. Then the next theorem is well known; see, e.g., Kleinman [13], Mehrmann [18], or Lancaster and Rodman [14].

THEOREM 2.3. *Let* $X_0 \in \mathbb{R}^{n \times n}$ *be symmetric and positive semidefinite such that* $A - BB^T X_0$ *is stable and let Assumption* 2.2 *hold. Then the Newton iterates* X_k *defined by*

$$X_{k+1} A_k + A_k^T X_{k+1} = -X_k B B^T X_k - C^T C$$

converge to some X_∞ *such that* $A - BB^T X_\infty$ *is stable, and it solves the Riccati equation* $\mathcal{F}(X_\infty) = 0$. *Furthermore, the iterates have a monotone convergence behavior*

$$0 \leq X_\infty \leq \cdots \leq X_{k+1} \leq X_k \leq \cdots \leq X_1$$

and quadratic convergence.

In the past decade, a variant of Newton's method has become quite popular in several areas of applications, the so-called inexact Newton's method. In this variant, it is no longer necessary to solve the Newton equation exactly for the Newton step, but it is possible to allow for errors in the residual. In particular, this is useful if iterative solvers are used for the solution of the linear Newton equation. We cite a theorem in Kelley [12, p. 99].

THEOREM 2.4. *Let $F : \mathbb{R}^N \to \mathbb{R}^N$ have a Lipschitz-continuous derivative in a neighborhood of some $x_\infty \in \mathbb{R}^N$ with $F(x_\infty) = 0$ and $F'(x_\infty)$ invertible. Then there exist $\delta > 0$ and $\bar{\eta}$ such that for all $x_0 \in \mathcal{B}(x_\infty, \delta)$ the inexact Newton iterates*

$$x_{k+1} = x_k + s_k,$$

where s_k satisfies

$$\|F'(x_k)s_k + F(x_k)\| \leq \eta_k \|F(x_k)\|, \qquad \eta_k \in [0, \bar{\eta}]$$

converge to x_∞. Furthermore, we have the following rate estimates:

The rate of convergence is at least linear. If, in addition, $\eta_k \to 0$, then we obtain a superlinear rate and if $\eta_k \leq K_\eta \|F(x_k)\|$ for some $K_\eta > 0$, then we have a quadratic rate of convergence.

Our goal in this paper is to analyze how we can apply the last theorem to the Riccati equation and extend the convergence Theorem 2.3 to the inexact Kleinman–Newton method. This seems to be promising, especially for this application, since the resulting linear Newton equations are Lyapunov equations which are usually solved iteratively by Smith's method or versions of the ADI method.

3. Inexact Kleinman–Newton method. Here we introduce for Riccati equations the inexact Kleinman–Newton method in the context presented in the previous chapter. Formally, the new iterate is determined by solving

$$(3.1) \qquad \mathcal{F}'(X_k)(X_{k+1} - X_k) + \mathcal{F}(X_k) = R_k$$

for X_{k+1}. This can be written more explicitly as a solution of X_{k+1}

$$(3.2) \qquad X_{k+1}A_k + A_k^T X_{k+1} = -X_k BB^T X_k - C^T C + R_k.$$

Before we come to the convergence properties, we recall an existence and uniqueness theorem for Lyapunov equations, which need to be solved at each step of the algorithm.

THEOREM 3.1. *If $A \in \mathbb{R}^{n \times n}$ is stable, then for each $Z \in \mathbb{R}^{n \times n}$ the Lyapunov equation*

$$A^T Y + YA - Z = 0$$

is uniquely solvable and its solution is given by

$$Y = -\int_0^\infty e^{A^T t} Z e^{At} dt.$$

For a proof see [14, Theorem 8.5.1].

Before we state the convergence theorem, we summarize the algorithm proposed.

Inexact Kleinman–Newton algorithm.

Step 0:   Choose X_0 and set $k = 0$.

Step 1:   Determine a solution X_{k+1},

which solves the Lyapunov equation up to a residual R_k

$$X_{k+1}A_k + A_k^T X_{k+1} = -X_k BB^T X_k - C^T C + R_k.$$

Step 2:   Set $k = k + 1$ and return to Step 1.

We can formulate the local convergence properties of this method by applying the standard theorem from the previous section.

THEOREM 3.2.   *Let $X_\infty \in \mathbb{R}^{n \times n}$ be a symmetric solution of (2.1) such that $A - BB^T X_\infty$ is stable. Then there exist $\delta > 0$ and $\bar\eta > 0$ such that for all starting values $X_0 \in \mathbb{R}^{n \times n}$ with $\|X_0 - X_\infty\| \leq \delta$ the iterates X_k of the inexact Kleinman– Newton algorithm converge to X_∞, if the residuals R_k satisfy*

$$(3.3) \qquad \|R_k\| \leq \eta_k \|\mathcal{F}(X_k)\| = \eta_k \left\|A^T X_k + X_k A - X_k BB^T X_k + C^T C\right\|.$$

The rate of convergence is linear if $\eta_k \in (0, \bar\eta]$, it is superlinear if $\eta_k \to 0$, and quadratic if $\eta_k \leq K_\eta \|\mathcal{F}(X_k)\|$ for some $K_\eta > 0$.

Proof. We apply Theorem 2.4 to the equation $\mathcal{F}(X) = A^T X + XA - XBB^T X + C^T C = 0$. This map is differentiable and has a Lipschitz continuous derivative. Since $A - BB^T X_\infty$ is assumed to be stable, $\mathcal{F}'(X_\infty)Y = 0$ implies $Y = 0$ by Theorem 3.1, and, hence, $\mathcal{F}'(X_\infty)$ is an invertible linear map. Since all assumptions in Theorem 2.4 hold, the conclusions can be applied and yield the statements in the theorem. □

4. Monotone convergence properties. An interesting fact about the Kleinman–Newton method is that the iterates exhibit monotonicity and a global convergence property, once the initial iterate X_0 is symmetric, positive semidefinite, and A_0 is stable. These properties are not common for Newton methods and depend on applications of the concavity and monotonicity results; see also Damm and Hinrichsen [7] or Ortega and Rheinboldt [21]. For the inexact version, these identities are perturbed and those results are much harder to obtain. In order to retain these properties, we have to impose certain conditions on the residuals.

Let us summarize at first a few monotonicity properties for the Lyapunov operators.

THEOREM 4.1.   *The map $\mathcal{F}$ is concave in the following sense:*

$$(4.1) \qquad \mathcal{F}'(X)(Y - X) \geq \mathcal{F}(Y) - \mathcal{F}(X) \quad \text{for all symmetric} \quad X, Y \in \mathbb{R}^{n \times n}.$$

Proof. The proof follows easily from an identity due to the quadratic nature of the Riccati equation:

$$(4.2) \qquad \mathcal{F}(Y) = \mathcal{F}(X) + \mathcal{F}'(X)(Y - X) + \frac{1}{2}\mathcal{F}''(X)(Y - X, Y - X),$$

where the quadratic term

$$(4.3) \qquad \frac{1}{2}\mathcal{F}''(Z)(W, W) = -WBB^T W$$

is independent of Z. □

THEOREM 4.2.   *Let $A - BB^T X$ be stable. Then*

$$(4.4) \qquad Z = \mathcal{F}'(X)(Y) \Longleftrightarrow Y = -\int_0^\infty e^{(A - BB^T X)^T t} Z e^{(A - BB^T X)t} dt$$

and, hence, $\mathcal{F}'(X)(Y) \geq 0$ implies $Y \leq 0$.

Proof. We have

$$Z = \mathcal{F}'(X)(Y) = \left(A - BB^T X\right)^T Y + Y \left(A - BB^T X\right).$$

Since $(A - BB^T X)$ is stable, Theorem 3.1 yields the result. $\qquad\square$

The next theorem shows that we can weaken the condition on the starting point and that the inexact Kleinman–Newton iteration is still well defined.

THEOREM 4.3. *Let X_k be symmetric and positive semidefinite such that $A - BB^T X_k$ is stable and*

$$(4.5) \qquad\qquad R_k \le C^T C$$

holds. Then

(i) *the iterate X_{k+1} of the inexact Kleinman–Newton method is well defined, symmetric and positive semidefinite,*

(ii) *and the matrix $A - BB^T X_{k+1}$ is stable.*

Proof. The inexact Newton step (3.1) is given by the solution of a Lyapunov equation

$$X_{k+1} A_k + A_k^T X_{k+1} = -X_k BB^T X_k - C^T C + R_k.$$

Since A_k is stable, the unique solution X_{k+1} exists and is symmetric by Theorem 3.1. Furthermore, requirement (4.5) leads to

$$X_{k+1} A_k + A_k^T X_{k+1} \le 0$$

and Theorem 4.2 implies $X_{k+1} \ge 0$. Equation (3.2) is equivalent to

$$(4.6) \qquad \begin{aligned} X_{k+1} A_{k+1} + A_{k+1}^T X_{k+1} = &- C^T C - X_{k+1} BB^T X_{k+1} \\ &- (X_{k+1} - X_k) BB^T (X_{k+1} - X_k) + R_k =: W. \end{aligned}$$

We define W as the right side of (4.6).

Let us assume $A_{k+1} x = \lambda x$ for λ with $Re(\lambda) \ge 0$ and $x \ne 0$. Then (4.6) implies

$$(\bar{\lambda} + \lambda) \bar{x}^T X_{k+1} x = \bar{x}^T A_{k+1}^T X_{k+1} x + \bar{x}^T X_{k+1} A_{k+1} x = \bar{x}^T W x.$$

On the one hand, the definition of W combined with requirement (4.5) leads to $W \le 0$. On the other hand, $X_{k+1} \ge 0$ implies $\bar{x}^T W x = 0$. Using the definition of W and a similar argument as before again, we obtain

$$(4.7) \qquad\qquad \bar{x}^T (X_{k+1} - X_k) BB^T (X_{k+1} - X_k) x = 0.$$

Since $BB^T \ge 0$ we have $B^T (X_{k+1} - X_k) x = 0$, and, hence, $BB^T X_{k+1} x = BB^T X_k x$, so that by definition of A_k, A_{k+1}

$$A_{k+1} x = A_k x = \lambda x,$$

contradicting the stability of A_k. Hence, A_{k+1} is also stable. $\qquad\square$

The requirements on the residuals can be weakened, e.g.,

$$(4.8) \qquad\qquad R_k \le C^T C + X_j BB^T X_j \qquad j = k, k+1$$

will also provide the previous proof.

In the following theorem we show under which requirements the monotonicity of the iterates X_k can be preserved also for the inexact Kleinman–Newton method.

THEOREM 4.4. *Let Assumption* 2.2 *be satisfied and let* X_0, *symmetric and positive semidefinite, be such that* A_0 *is stable. Assume that* (4.5) *and*

$$(4.9) \qquad 0 \leq R_k \leq (X_{k+1} - X_k)BB^T(X_{k+1} - X_k)$$

hold for all $k \in \mathbb{N}$. *Then the iterates* (3.2) *satisfy*

(i) $\lim_{k \to \infty} X_k = X_\infty$ *and* $0 \leq X_\infty \leq \cdots \leq X_{k+1} \leq X_k \leq \cdots \leq X_1$,

(ii) $(A - BB^T X_\infty)$ *is stable and* X_∞ *is the maximal solution of* $\mathcal{F}(X_\infty) = 0$,

(iii) $\|X_{k+1} - X_\infty\| \leq c\|X_k - X_\infty\|^2, k \in \mathbb{N}$.

Proof. i) Using the definition of an inexact Newton step and (4.2)

$$R_k = \mathcal{F}'(X_k)(X_{k+1} - X_k) + \mathcal{F}(X_k)$$
$$= \mathcal{F}(X_{k+1}) + (X_{k+1} - X_k)BB^T(X_{k+1} - X_k).$$

This can be inserted into the next Newton step

$$\mathcal{F}'(X_{k+1})(X_{k+2} - X_{k+1}) = -\mathcal{F}(X_{k+1}) + R_{k+1}$$
$$= R_{k+1} - R_k + (X_{k+1} - X_k)BB^T(X_{k+1} - X_k) \geq R_{k+1} \geq 0$$

by assumption (4.9). Then from Theorem 4.2 we can infer

$$X_{k+2} - X_{k+1} \leq 0, \quad k = 0, 1, 2, \dots$$

Therefore, $(X_k)_{k \in \mathbb{N}}$ is a monotone sequence of symmetric and positive semidefinite matrices and $X_k \geq 0$ due to Theorem 4.3. Hence, it is convergent to some symmetric and positive semidefinite limit matrix

$$\lim_{k \to \infty} X_k = X_\infty.$$

ii) Passing to the limit in (3.1) and (4.9) we deduce that X_∞ satisfies the Riccati equation, $X_\infty \leq X_k$ and $\mathcal{F}(X_\infty) = 0$.

We show that X_∞ is the maximal symmetric solution of the Riccati equation (2.1), which means $X_\infty \geq X$ for every symmetric solution X of (2.1). For this to hold we assume that X is a symmetric solution of the Riccati equation. Then Theorem 4.1 and (4.2) imply

$$\mathcal{F}'(X_k)(X - X_k) \geq -\mathcal{F}(X_k) = -\mathcal{F}(X_{k-1}) - \mathcal{F}'(X_{k-1})(X_k - X_{k-1})$$
$$- \frac{1}{2}\mathcal{F}''(X_{k-1})(X_k - X_{k-1}, X_k - X_{k-1}) \geq -R_{k-1}.$$

Therefore, there exists $Q_k \geq 0$ with

$$\mathcal{F}'(X_k)(X - X_k) = Q_k - R_{k-1},$$

and since A_k is stable Theorem 3.1 implies

$$(4.10) \qquad X - X_k = -\int_0^\infty e^{A_k^T t}(Q_k - R_{k-1})e^{A_k t}dt \leq \int_0^\infty e^{A_k^T t}R_{k-1}e^{A_k t}dt.$$

Passing to the limits leads to the desired result

$$X - X_\infty \leq 0$$

and X_∞ is the maximal solution. We can deduce from [14, Theorem 9.1.2] that the matrix $A - BB^T X_\infty$ is stable.

iii) To prove the quadratic rate of convergence we use the inexact Newton step

$$\mathcal{F}'(X_k)(X_{k+1} - X_k) + \mathcal{F}(X_k) - R_k = 0$$

and rewrite it using (4.2)

$$\begin{aligned}
\mathcal{F}'(X_\infty)(X_{k+1} - X_\infty) &= \mathcal{F}'(X_\infty)(X_{k+1} - X_\infty) - \mathcal{F}(X_{k+1}) + \mathcal{F}(X_\infty) \\
&\quad - \big(\, \mathcal{F}'(X_k)(X_{k+1} - X_k) - \mathcal{F}(X_{k+1}) + \mathcal{F}(X_k)\big) + R_k \\
&= (X_{k+1} - X_\infty)BB^T(X_{k+1} - X_\infty) \\
&\quad - (X_{k+1} - X_k)BB^T(X_{k+1} - X_k) + R_k.
\end{aligned}$$

Since $A_\infty := (A - BB^T X_\infty)$ is stable, Theorem 4.2 shows

$$\begin{aligned}
(4.11) \qquad 0 \leq X_{k+1} - X_\infty &= \int_0^\infty e^{A_\infty^T t}\big\{ -(X_{k+1} - X_\infty)BB^T(X_{k+1} - X_\infty) \\
&\qquad\quad + (X_{k+1} - X_k)BB^T(X_{k+1} - X_k) - R_k\big\} e^{A_\infty t} \, dt \\
&\leq \int_0^\infty e^{A_\infty^T t}((X_{k+1} - X_k)BB^T(X_{k+1} - X_k)) e^{A_\infty t} \, dt.
\end{aligned}$$

Note, that for all symmetric $A, B \in \mathbb{R}^{n \times n}$, $A \leq B$ implies $\|A\|_2 \leq \|B\|_2$, due to

$$\lambda_{\max}(A) = \max_{\|x\|_2 = 1} \frac{\bar{x}^T A x}{\bar{x}^T x} = \frac{\bar{x}_*^T A x_*}{\bar{x}_*^T x_*} \leq \frac{\bar{x}_*^T B x_*}{\bar{x}_*^T x_*} \leq \max_{\|x\|_2 = 1} \frac{\bar{x}^T B x}{\bar{x}^T x} = \lambda_{\max}(B).$$

Taking norms in (4.11) we obtain due to the stability of A_∞

$$\begin{aligned}
(4.12) \qquad 4\|X_{k+1} - X_\infty\|_2 &\leq \|X_{k+1} - X_k\|_2^2 \|BB^T\|_2 \int_0^\infty \left\|e^{A_\infty t}\right\|_2 \left\|e^{A_\infty^T t}\right\|_2 \, dt \\
&\leq c\|X_{k+1} - X_k\|_2^2,
\end{aligned}$$

and using the monotonicity of the iterates

$$(4.13) \qquad 0 \leq X_k - X_{k+1} \leq X_k - X_\infty \quad \Rightarrow \quad \|X_k - X_{k+1}\|_2 \leq \|X_k - X_\infty\|_2,$$

and, therefore,

$$\|X_{k+1} - X_\infty\|_2 \leq c\|X_k - X_\infty\|_2^2,$$

which implies quadratic convergence in any matrix norm. $\square$

We impose several requirements on the residuals in Theorem 4.3 and Theorem 4.4. Some of them restrict the size of R_k in dependence on the step, see (4.9) and (4.5); others assume the positive definiteness. The first assumption on the size of the residuals depends on the quantity X_{k+1}, which has to be computed by the iterative procedure. However, the inequalities involved can be tested as the iteration for X_{k+1} progresses. The latter assumption is a condition, which the iterative Lyapunov solver has to satisfy.

5. Methods for solving the Lyapunov equation. There is a sizeable amount of literature on how to solve Lyapunov equations with direct solvers and iterative methods. In the inexact context we do not address direct Lyapunov solvers as presented in Laub [15], Roberts [24], or Grasedyck [8], but only iterative solvers, like Smith's [27], cyclic Smith(l) [23], or ADI methods [17]. In particular, we analyze these solvers with respect to the additonal requirements for maintaining the monotonicity as stated in the previous section.

Smith's and the ADI method are iterative solvers, which can be used to solve the Lyapunov equation at each Newton step. The inexact Newton method developed previously allows for early termination of these iterations, because the convergence criterion is not so stringent far away from the solution.

We review some basic properties of these methods.

Recall that at Newton iteration step k the following Lyapunov equation needs to be solved:

$$\mathcal{F}'(X_k)(X_{k+1} - X_k) + \mathcal{F}(X_k) = 0,$$

or as in (3.2) we solve for $X = X_{k+1}$

$$(5.1) \qquad\qquad XA_k + A_k^T X + S_k = 0$$

with a stable matrix A_k

$$A_k = A - BB^T X_k \quad \text{and} \quad S_k = X_k BB^T X_k + C^T C.$$

This equation is equivalent to a Stein's equation.

LEMMA 5.1. *Given any $\mu \in \mathbb{R}^-$, then a solution X of the Lyapunov equation* (5.1) *is also a solution of Stein's equation and vice versa. Stein's equation is*

$$(5.2) \qquad\qquad X = A_{k,\mu}^T X A_{k,\mu} + S_{k,\mu}$$

with

$$A_{k,\mu} = (A_k - \mu I)(A_k + \mu I)^{-1}, \quad S_{k,\mu} = -2\mu(A_k + \mu I)^{-T} S_k (A_k + \mu I)^{-1}.$$

Note that (5.1) is equivalent to

$$(A_k + \mu I)^T X(A_k + \mu I) - (A_k - \mu I)^T X(A_k - \mu I) = -2\mu S_k,$$

and from this (5.2) follows, since $A_k + \mu I$ is invertible for $\mu < 0$ due to the stability of A_k.

Smith's method—here we consider a simple version with one shift—is a fixed point iteration for (5.2) for given starting value $Z_k^{(0)}$

$$Z_k^{(l+1)} = A_{k,\mu}^T Z_k^{(l)} A_{k,\mu} + S_{k,\mu}, \quad l = 0, 1, \ldots \quad \text{and } \mu < 0 \text{ fixed.}$$

ADI method is a fixed point iteration for (5.2) for given starting value $Z_k^{(0)}$

$$(5.3) \qquad Z_k^{(l+1)} = A_{k,\mu_l}^T Z_k^{(l)} A_{k,\mu_l} + S_{k,\mu_l}, \quad l = 0, 1, \ldots \quad \text{and } \mu_l < 0 \text{ varies.}$$

In practice, cyclic versions of both methods, where a given set of shift parameter $\mu_0, \ldots, \mu_s$ is used in a cyclic manner, became quite popular; see, e.g., [23] and [9].

Since Smith's method and the cyclic versions are special cases of the ADI method, we consider the ADI method in the following statements.

LEMMA 5.2. *Let Z_k be the solution of the Lyapunov equation* (5.1) *and let $Z_k^{(l)}$ be an iterate of the ADI method. Then*

$$(5.4) \qquad Z_k^{(l+1)} - Z_k = A_{k,\mu_l}^T \ldots A_{k,\mu_0}^T \left(Z_k^{(0)} - Z_k \right) A_{k,\mu_0} \ldots A_{k,\mu_l}.$$

Proof. Recall that by Lemma 5.1 Z_k satisfies a Stein's equation for any $\mu \in \mathbb{R}^-$; hence, for all μ_l in the ADI method

$$Z_k = A_{k,\mu_l}^T Z_k A_{k,\mu_l} + S_{k,\mu_l} \quad l = 0, 1, \ldots$$

Therefore, we have for any l

$$Z_k^{(l+1)} - Z_k = A_{k,\mu_l}^T Z_k^{(l)} A_{k,\mu_l} + S_{k,\mu_l} - \left(A_{k,\mu_l}^T Z_k A_{k,\mu_l} + S_{k,\mu_l} \right) = A_{k,\mu_l}^T \left(Z_k^{(l)} - Z_k \right) A_{k,\mu_l}.$$

If we apply this identity to $Z_k^{(l)} - Z_k$ consecutively, then we obtain the statement of the lemma. $\square$

To estimate the residual of the Lyapunov equation using some iterate from the ADI method, we prove the following lemma.

LEMMA 5.3. *Let $Z_k^{(l)}$ be an iterate of the ADI method, and then for the residuals of the Lyapunov equation we obtain*

$$\begin{aligned} R_k^{(l)} &:= Z_k^{(l)} A_k + A_k^T Z_k^{(l)} + S_k \\ (5.5) \qquad &= A_{k,\mu_{l-1}}^T \ldots A_{k,\mu_0}^T \left(Z_k^{(0)} A_k + A_k^T Z_k^{(0)} + S_k \right) A_{k,\mu_0} \ldots A_{k,\mu_{l-1}}. \end{aligned}$$

If, in particular, the initial residual $R_k^{(0)}$ is positive semidefinite, then all residuals $R_k^{(l)}$ are also positive semidefinite.

Proof. Note that

$$\begin{aligned} Z_k^{(l)} A_k + A_k^T Z_k^{(l)} + S_k &= Z_k^{(l)} A_k + A_k^T Z_k^{(l)} - Z_k A_k - A_k^T Z_k \\ &= \left(Z_k^{(l)} - Z_k \right) A_k + A_k^T \left(Z_k^{(l)} - Z_k \right). \end{aligned}$$

Next we insert (5.4) to obtain

$$\begin{aligned} (5.6) \quad Z_k^{(l)} A_k + A_k^T Z_k^{(l)} + S_k = {}& A_{k,\mu_{l-1}}^T \ldots A_{k,\mu_0}^T \left(Z_k^{(0)} - Z_k \right) A_{k,\mu_0} \ldots A_{k,\mu_{l-1}} A_k \\ &+ A_k^T A_{k,\mu_{l-1}}^T \ldots A_{k,\mu_0}^T \left(Z_k^{(0)} - Z_k \right) A_{k,\mu_0} \ldots A_{k,\mu_{l-1}}. \end{aligned}$$

Since A_k and $A_{k,\mu}$ commute for any μ, we have

$$\begin{aligned} &Z_k^{(l)} A_k + A_k^T Z_k^{(l)} + S_k \\ &\quad = A_{k,\mu_{l-1}}^T \ldots A_{k,\mu_0}^T \left(\left(Z_k^{(0)} - Z_k \right) A_k + A_k^T \left(Z_k^{(0)} - Z_k \right) \right) A_{k,\mu_0} \ldots A_{k,\mu_{l-1}} \end{aligned}$$

from which (5.5) follows. From this equation we obtain the result that if the initial residual is positive semidefinite, then this also holds for all residuals in the Lyapunov equation using any ADI iterate. $\square$

In particular, with the zero starting matrix we get the following.

LEMMA 5.4. *Let* $Z_k^{(0)} = 0$. *Then the residuals of* (5.1) *for the ADI iterates satisfy*

$$R_k^{(l)} \geq 0.$$

Proof. The residuals of (5.1) for the iterates $Z_k^{(l)}$ of the ADI method are given by Lemma 5.3:

$$R_k^{(l)} = Z_k^{(l)} A_k + A_k^T Z_k^{(l)} + S_k = A_{k,\mu_{l-1}}^T \dots A_{k,\mu_0}^T S_k A_{k,\mu_0} \dots A_{k,\mu_{l-1}} \geq 0$$

since $S_k = X_k B B^T X_k + C^T C \geq 0$. $\square$

LEMMA 5.5. *Let us consider a cyclic ADI method with a finite set of shift parameter* $\mu_0, \dots, \mu_s \in \mathbb{R}^-$. *If* $C^T C$ *is positive definite and* $Z_k^{(0)} = 0$, *there is* l_k *such that for all* $l \geq l_k$

$$0 \leq R_k^{(l)} \leq C^T C$$

holds.

Proof. $R_k^{(l)} \geq 0$ is proved in the previous Lemma. Furthermore, if $C^T C > 0$, there exists $\zeta > 0$ such that for all $x \in \mathbb{C}^n$

$$\bar{x}^T C^T C x \geq \zeta \|x\|_2^2.$$

We have $\rho(A_{k,\mu}) = \max_{\lambda \in \sigma(A_k)} |\frac{\lambda-\mu}{\lambda+\mu}| < 1$ for every $\mu \in \mathbb{R}^-$. Due to the special structure of the matrices $A_{k,\mu}, \mu \in \mathbb{R}^-$, it follows that

$$\rho(A_{k,\mu_0} \dots A_{k,\mu_s}) = \max_{\lambda \in \sigma(A_k)} \left| \prod_{i=1}^s \frac{\lambda-\mu_i}{\lambda+\mu_i} \right| \leq \prod_{i=1}^s \max_{\lambda \in \sigma(A_k)} \left| \frac{\lambda-\mu_i}{\lambda+\mu_i} \right| < 1.$$

Therefore, a consistent matrix norm $\|\cdot\|_*$ exists with $\|A_{k,\mu_0} \dots A_{k,\mu_s}\|_* < 1$.

For l large enough (depending on k) we obtain with $m := l \mod (s+1)$

$$\left\| R_k^{(l)} \right\|_2 = \left\| A_{k,\mu_m}^T \dots A_{k,\mu_0}^T \underbrace{A_{k,\mu_s}^T \dots A_{k,\mu_0}^T \dots A_{k,\mu_s}^T \dots A_{k,\mu_0}^T}_{\lfloor \frac{l}{s+1} \rfloor \text{ times}} S_k \right.$$

$$\left. \underbrace{A_{k,\mu_0} \dots A_{k,\mu_s} \dots A_{k,\mu_0} \dots A_{k,\mu_s}}_{\lfloor \frac{l}{s+1} \rfloor \text{ times}} A_{k,\mu_0} \dots A_{k,\mu_m} \right\|_2$$

$$\leq c \|A_{k,\mu_0} \dots A_{k,\mu_s}\|_2^{2\lfloor \frac{l}{s+1} \rfloor} \|S_k\|_2$$

$$\leq c_* \|A_{k,\mu_0} \dots A_{k,\mu_s}\|_*^{2\lfloor \frac{l}{s+1} \rfloor} \leq \zeta.$$

Hence, for all $x \in \mathbb{C}^n$

$$\bar{x}^T R_k^{(l)} x \leq \|x\|_2^2 \left\| R_k^{(l)} \right\|_2 \leq \zeta \|x\|_2^2 \leq \bar{x}^T C^T C x,$$

which is to be shown. $\square$

According to (4.8) it might be possible to introduce a weaker requirement compared to the positive definiteness of the matrix $C^T C$ to achieve the same results.

6. Numerical results. In this section we analyze the efficiency of the inexact Kleinman–Newton versions, developed in Theorem 3.2, compared to the standard Kleinman–Newton method. Note that we concentrate on the local convergence properties and not on the monotonicity of the iterates. The efficiency of the inexact versions cannot be tested without special consideration of the applied Lyapunov solver.

Many iterative solvers for Lyapunov equations are presented in the literature, e.g., Smith's method [27], ADI method [17], and low-rank ADI methods [22], [16]. Other iterative methods can be found in [9], [26], or [23].

In order to indicate the benefits of the inexact Kleinman–Newton method, we implement Smith's method, the ADI method, and a low-rank ADI version to solve the Newton steps.

We consider an example arising from optimal control problems. The example has been considered by Morris and Navasca [19] and is described as a two-dimensional optimal control problem with parabolic partial differential equations including convection:

$$\min_u J(u) = \frac{1}{2} \int_0^\infty \left(\| Cz(t) \|_2^2 + \| u(t) \|_2^2 \right) dt$$

s. t.

$$\frac{\partial z}{\partial t} = \frac{\partial z}{\partial x^2} + \frac{\partial z}{\partial y^2} + 20\frac{\partial z}{\partial y} + 100z = f(x,y)u(t) \qquad (x,y) \in \Omega$$

$$z(x,y,t) = 0 \qquad\qquad (x,y) \in \partial\Omega \qquad \forall t$$

with $\Omega = (0,1) \times (0,1)$ and

$$f(x,y) := \begin{cases} 100 & 0.1 < x < 0.3 \quad \& \quad 0.4 < y < 0.6, \\ 0 & \text{else.} \end{cases}$$

The discretization is carried out on a 23×23 grid and central differences are used for the approximation. We choose $C = (0.1, \ldots, 0.1)$, $X_0 = 0$. The optimal matrix X_∞ has been computed beforehand with a higher accuracy. We compare the number of the Newton steps (outer), the number of inner iterations (inner) which are needed to solve each Newton step, and the cumulative number of inner iterations (cumul). According to Theorem 3.2 we test an inexact Kleinman–Newton version with a superlinear rate of convergence. In Tables 6.1 and 6.2 we use Smith's method

TABLE 6.1
Smith's method: Exact Kleinman–Newton method.

outer	inner	cumul	$\| \mathcal{F}(X_k) \|$	$\| X_k - X_\infty \|$	$\frac{\|X_k - X_\infty\|}{\|X_{k-1} - X_\infty\|}$	$\frac{\|X_k - X_\infty\|}{\|X_{k-1} - X_\infty\|^2}$
1	97	97	$7.639e + 005$	$3.495e + 001$	$1.056e + 003$	$3.484e + 004$
2	211	308	$1.911e + 005$	$2.333e + 001$	$6.677e - 001$	$1.911e - 002$
3	144	452	$4.794e + 004$	$1.755e + 001$	$7.521e - 001$	$3.224e - 002$
4	83	535	$1.213e + 004$	$1.453e + 001$	$8.279e - 001$	$4.719e - 002$
5	66	601	$3.172e + 003$	$1.245e + 001$	$8.571e - 001$	$5.901e - 002$
6	49	650	$8.973e + 002$	$9.594e + 000$	$7.704e - 001$	$6.187e - 002$
7	66	716	$2.357e + 002$	$4.481e + 000$	$4.671e - 001$	$4.869e - 002$
8	58	774	$1.801e + 001$	$5.031e - 001$	$1.123e - 001$	$2.505e - 002$
9	43	817	$8.544e - 002$	$4.162e - 003$	$8.272e - 003$	$1.645e - 002$
10	33	850	$8.230e - 004$	$1.263e - 005$	$3.036e - 003$	$7.457e - 001$
11	21	871	$3.281e - 008$	$6.488e - 010$	$5.135e - 005$	$4.149e + 000$

TABLE 6.2
Smith's method: Inexact K-N method with superlinear convergence $\eta_k = 1/(k^3 + 1)$.

outer	inner	cumul	$\| \mathcal{F}(X_k) \|$	$\| X_k - X_\infty \|$	$\frac{\|X_k - X_\infty\|}{\|X_{k-1} - X_\infty\|}$	$\frac{\|X_k - X_\infty\|}{\|X_{k-1} - X_\infty\|^2}$
1	32	32	$7.628e + 005$	$3.490e + 001$	$1.054e + 003$	$3.479e + 004$
2	15	47	$2.294e + 005$	$2.442e + 001$	$6.997e - 001$	$2.006e - 002$
3	15	62	$6.088e + 004$	$1.827e + 001$	$7.481e - 001$	$3.065e - 002$
4	14	76	$1.581e + 004$	$1.496e + 001$	$8.191e - 001$	$4.486e - 002$
5	13	89	$4.141e + 003$	$1.284e + 001$	$8.582e - 001$	$5.738e - 002$
6	7	96	$1.162e + 003$	$1.053e + 001$	$8.203e - 001$	$6.389e - 002$
7	12	108	$3.171e + 002$	$5.560e + 000$	$5.279e - 001$	$5.012e - 002$
8	19	127	$3.797e + 001$	$9.554e - 001$	$1.718e - 001$	$3.091e - 002$
9	17	144	$2.741e - 001$	$1.483e - 002$	$1.552e - 002$	$1.625e - 002$
10	18	162	$3.396e - 003$	$5.113e - 005$	$3.448e - 003$	$2.343e - 001$
11	15	177	$1.400e - 006$	$2.267e - 008$	$4.433e - 004$	$8.886e + 000$
12	14	191	$3.477e - 010$	$3.333e - 012$	$1.471e - 004$	$6.539e + 003$

TABLE 6.3
ADI method: Exact Kleinman–Newton method.

outer	inner	cumul	$\| \mathcal{F}(X_k) \|$	$\| X_k - X_\infty \|$	$\frac{\|X_k - X_\infty\|}{\|X_{k-1} - X_\infty\|}$	$\frac{\|X_k - X_\infty\|}{\|X_{k-1} - X_\infty\|^2}$
1	24	24	$7.639e + 005$	$3.495e + 001$	$1.056e + 003$	$3.484e + 004$
2	20	44	$1.911e + 005$	$2.333e + 001$	$6.677e - 001$	$1.911e - 002$
3	22	66	$4.794e + 004$	$1.755e + 001$	$7.521e - 001$	$3.224e - 002$
4	22	88	$1.213e + 004$	$1.453e + 001$	$8.279e - 001$	$4.719e - 002$
5	21	109	$3.172e + 003$	$1.245e + 001$	$8.571e - 001$	$5.901e - 002$
6	20	129	$8.973e + 002$	$9.594e + 000$	$7.704e - 001$	$6.187e - 002$
7	22	151	$2.357e + 002$	$4.481e + 000$	$4.671e - 001$	$4.869e - 002$
8	27	178	$1.801e + 001$	$5.031e - 001$	$1.123e - 001$	$2.505e - 002$
9	34	212	$8.544e - 002$	$4.162e - 003$	$8.272e - 003$	$1.645e - 002$
10	32	244	$8.230e - 004$	$1.263e - 005$	$3.036e - 003$	$7.457e - 001$
11	24	268	$3.273e - 008$	$6.273e - 010$	$4.965e - 005$	$4.012e + 000$

TABLE 6.4
ADI method: Inexact K-N method with superlinear convergence $\eta_k = 1/(k^3 + 1)$.

outer	inner	cumul	$\| \mathcal{F}(X_k) \|$	$\| X_k - X_\infty \|$	$\frac{\|X_k - X_\infty\|}{\|X_{k-1} - X_\infty\|}$	$\frac{\|X_k - X_\infty\|}{\|X_{k-1} - X_\infty\|^2}$
1	13	13	$7.639e + 005$	$3.495e + 001$	$1.056e + 003$	$3.484e + 004$
2	4	17	$1.911e + 005$	$2.334e + 001$	$6.677e - 001$	$1.911e - 002$
3	5	22	$4.794e + 004$	$1.755e + 001$	$7.520e - 001$	$3.224e - 002$
4	5	27	$1.213e + 004$	$1.453e + 001$	$8.279e - 001$	$4.719e - 002$
5	6	33	$3.175e + 003$	$1.249e + 001$	$8.597e - 001$	$5.918e - 002$
6	3	36	$9.542e + 002$	$1.109e + 001$	$8.882e - 001$	$7.112e - 002$
7	8	44	$2.073e + 002$	$3.978e + 000$	$3.586e - 001$	$3.232e - 002$
8	5	49	$1.829e + 001$	$5.119e - 001$	$1.287e - 001$	$3.235e - 002$
9	11	60	$1.037e - 001$	$5.069e - 003$	$9.903e - 003$	$1.935e - 002$
10	16	76	$9.042e - 004$	$1.502e - 005$	$2.962e - 003$	$5.966e - 001$
11	16	92	$4.119e - 007$	$3.114e - 009$	$2.073e - 004$	$1.416e + 001$
12	15	107	$1.905e - 010$	$1.087e - 012$	$3.491e - 004$	$1.165e + 005$

for the Lyapunov solver, whereas in Tables 6.3 and 6.4 we apply the ADI method and
in Tables 6.5 and 6.6 its low-rank version. The shift parameters are determined with
a heuristic introduced by Penzl [23]. All computations were done within MATLAB.

In Table 6.7 we present a comparison of CPU times in order to test the efficiency
of the inexact versions. We include alternative stopping criteria for the inner iteration
which result according to Theorem 3.2 in a linear and a superlinear rate of convergence.
We observed for our examples a rather small linear convergence rate factor and a

TABLE 6.5
Low-rank ADI method: Exact Kleinman–Newton method.

outer	inner	cumul	$\parallel \mathcal{F}(X_k) \parallel$	$\parallel X_k - X_\infty \parallel$	$\frac{\parallel X_k - X_\infty \parallel}{\parallel X_{k-1} - X_\infty \parallel}$	$\frac{\parallel X_k - X_\infty \parallel}{\parallel X_{k-1} - X_\infty \parallel^2}$
1	24	24	$7.639e+005$	$3.495e+001$	$1.056e+003$	$3.484e+004$
2	41	65	$1.911e+005$	$2.333e+001$	$6.677e-001$	$1.911e-002$
3	25	90	$4.794e+004$	$1.755e+001$	$7.521e-001$	$3.224e-002$
4	23	113	$1.213e+004$	$1.453e+001$	$8.279e-001$	$4.719e-002$
5	24	137	$3.172e+003$	$1.245e+001$	$8.571e-001$	$5.901e-002$
6	24	161	$8.973e+002$	$9.594e+000$	$7.704e-001$	$6.187e-002$
7	25	186	$2.357e+002$	$4.481e+000$	$4.671e-001$	$4.869e-002$
8	26	212	$1.801e+001$	$5.031e-001$	$1.123e-001$	$2.505e-002$
9	33	245	$8.544e-002$	$4.162e-003$	$8.272e-003$	$1.645e-002$
10	41	286	$8.230e-004$	$1.263e-005$	$3.036e-003$	$7.457e-001$
11	42	328	$3.209e-008$	$5.735e-010$	$4.539e-005$	$3.667e+000$

TABLE 6.6
Low-rank ADI method: Inexact K-N method with superlinear convergence $\eta_k = 1/(k^3 + 1)$.

outer	inner	cumul	$\parallel \mathcal{F}(X_k) \parallel$	$\parallel X_k - X_\infty \parallel$	$\frac{\parallel X_k - X_\infty \parallel}{\parallel X_{k-1} - X_\infty \parallel}$	$\frac{\parallel X_k - X_\infty \parallel}{\parallel X_{k-1} - X_\infty \parallel^2}$
1	13	13	$7.639e+005$	$3.495e+001$	$1.056e+003$	$3.484e+004$
2	4	17	$1.908e+005$	$1.853e+001$	$5.302e-001$	$1.518e-002$
3	3	20	$4.760e+004$	$6.054e+000$	$3.267e-001$	$1.763e-002$
4	6	26	$1.208e+004$	$1.374e+001$	$2.270e+000$	$3.750e-001$
5	8	34	$3.185e+003$	$1.254e+001$	$9.122e-001$	$6.638e-002$
6	7	41	$8.998e+002$	$9.653e+000$	$7.700e-001$	$6.143e-002$
7	7	48	$2.363e+002$	$4.494e+000$	$4.655e-001$	$4.823e-002$
8	6	54	$1.788e+001$	$4.977e-001$	$1.107e-001$	$2.464e-002$
9	9	63	$8.554e-002$	$3.983e-003$	$8.002e-003$	$1.608e-002$
10	21	84	$8.871e-004$	$1.245e-005$	$3.126e-003$	$8.029e-001$
11	31	115	$5.657e-007$	$2.088e-009$	$1.677e-004$	$1.368e+001$
12	47	162	$1.449e-010$	$9.694e-013$	$4.643e-004$	$2.740e+005$

TABLE 6.7
Comparison of computing time.

Lyapunov solver	Convergence rate					
	Exact K-N		Linear		Superlinear	
	$\parallel \mathcal{F}(X_\infty) \parallel$	Time	$\parallel \mathcal{F}(X_\infty) \parallel$	Time	$\parallel \mathcal{F}(X_\infty) \parallel$	Time
Smith	$3.281e-008$	289	$6.115e-008$	68	$3.477e-010$	76
ADI	$3.273e-008$	204	$1.588e-008$	65	$1.905e-010$	81
Low-rank ADI	$3.209e-008$	145	$1.447e-008$	81	$1.449e-010$	68

rather late onset of the superlinear convergence behavior, which results in a rather good performance of the linearly convergent version compared to the superlinearly convergent version. The time needed to compute the shift parameter is not included in Table 6.7. This is an additional advantage of the inexact versions because they need fewer inner iterations and, therefore, a smaller number of shift parameters.

7. Robustness. Let us note that there is another implementation of Newton's method for the Riccati equation presented in the literature, e.g., [1], [19]. Here the Newton step is computed by a Lyapunov equation for the increment $X_{k+1} - X_k$ in the following way:

$$(7.1) \quad \begin{aligned} (X_{k+1} - X_k)\left(A - BB^T X_k\right) + \left(A - BB^T X_k\right)^T (X_{k+1} - X_k) \\ = (X_k - X_{k-1})BB^T(X_k - X_{k-1}), \end{aligned}$$

in contrast to (2.4)

$$(7.2) \qquad X_{k+1}\left(A - BB^T X_k\right) + \left(A - BB^T X_k\right)^T X_{k+1} = -X_k BB^T X_k - C^T C.$$

Note that the inhomogeneous terms in the Lyapunov equations for both variants of Newton's method differ quite substantially. The authors of [1] pointed out that (7.1) exhibits some advantages compared to the standard implementation (2.4), e.g., if BB^T has low rank.

Equation (7.1) is the matrix notation of

$$(7.3) \qquad \mathcal{F}'(X_k)(X_{k+1} - X_k) = -\mathcal{F}(X_k)$$

with the following modification due to (4.2):

$$
\begin{aligned}
-\mathcal{F}(X_k) &= -\mathcal{F}(X_{k-1}) - \mathcal{F}'(X_{k-1})(X_k - X_{k-1}) \\
&\quad -\frac{1}{2}\mathcal{F}''(X_{k-1})(X_k - X_{k-1}, X_k - X_{k-1}) \\
&= -\frac{1}{2}\mathcal{F}''(X_{k-1})(X_k - X_{k-1}, X_k - X_{k-1}).
\end{aligned}
$$
(7.4)

Both methods are identical for the exact Newton step:

LEMMA 7.1. *If a sequence X_k satisfies* (7.2), *then it also fulfills* (7.1). *If, conversely, a sequence X_k satisfies* (7.1), *then it also fulfills* (7.2), *provided the starting points X_0, X_1 satisfy* (7.2) *for $k = 0$.*

Proof. The first conclusion was shown above. For the reverse to hold, we use (7.4) and obtain

$$
\begin{aligned}
\mathcal{F}'(X_k)(X_{k+1} - X_k) &= -\tfrac{1}{2}\mathcal{F}''(X_{k-1})(X_k - X_{k-1}, X_k - X_{k-1}) \\
&= -\mathcal{F}(X_k) + \mathcal{F}(X_{k-1}) + \mathcal{F}'(X_{k-1})(X_k - X_{k-1})
\end{aligned}
$$

and, hence,

$$\mathcal{F}(X_k) + \mathcal{F}'(X_k)(X_{k+1} - X_k) = \mathcal{F}(X_{k-1}) + \mathcal{F}'(X_{k-1})(X_k - X_{k-1})$$

for all $k \geq 0$. Since it is assumed that for the starting iterates

$$(7.5) \qquad \mathcal{F}(X_0) + \mathcal{F}'(X_0)(X_1 - X_0) = 0,$$

the X_k also satisfy (2.4). $\square$

Although both methods are identical in the exact case, an inexact version of the Kleinman–Newton method based on implementation (7.1) is unstable. A reformulation of an inexact Kleinman–Newton method using (7.1) leads to

$$
\begin{aligned}
\mathcal{F}'(X_k)(X_{k+1} - X_k) &= -\frac{1}{2}\mathcal{F}''(X_{k-1})(X_k - X_{k-1}, X_k - X_{k-1}) + \tilde{R}_k \\
&= \mathcal{F}(X_{k-1}) + \mathcal{F}'(X_{k-1})(X_k - X_{k-1}) - \mathcal{F}(X_k) + \tilde{R}_k
\end{aligned}
$$

or, equivalently,

$$\mathcal{F}'(X_k)(X_{k+1} - X_k) + \mathcal{F}(X_k) = \mathcal{F}'(X_{k-1})(X_k - X_{k-1}) + \mathcal{F}(X_{k-1}) + \tilde{R}_k.$$

Using this recursively shows that the residuals accumulate during the course of the iteration

$$\mathcal{F}'(X_k)(X_{k+1} - X_k) + \mathcal{F}(X_k) = \sum_{i=1}^{k} \tilde{R}_i.$$

This means that one has to limit $R_k = \sum_{i=1}^{k} \tilde{R}_i$ (if X_1 is computed by an exact Newton step) according to the convergence Theorem 2.4 which seems to be a rather strong assumption because the residuals are cumulative.

8. Conclusion. In this paper we propose a modification of the classical Kleinman–Newton method for the numerical solution of Riccati equations. The iterative Lyapunov equation solvers for the Newton steps are terminated early to save computing time. Based on the theory of inexact Newton methods, we give termination criteria which warrant the fast local rates. In addition, we derive conditions, which guarantee the more global convergence statement for the Kleinman–Newton method. We show how these requirements can be addressed, for example, for Smith's method or the ADI method. The numerical example for a parabolic control problem illustrates the potential for substantial savings in the number of iterations and computing time.

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