

Symplectic Möbius integrators for LQ optimal control problems

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Abstract— The paper presents symplectic Möbius integrators for Riccati equations. All proposed methods preserve symmetry, positivity and quadratic invariants for the Riccati equations, and non-stationary Lyapunov functions. In addition, an efficient and numerically stable discretization procedure based on reinitialization for the associated linear Hamiltonian system is proposed.

I. INTRODUCTION

Optimal control problems for linear differential equations with quadratic cost functions are extensively studied from both theoretical and numerical standpoints. In particular, it is well-known that under some assumptions the optimal control is represented as a solution of the Pontryagin maximum principle. On the other hand, an optimal control in the feedback form may be represented by means of the Riccati matrix which solves a non-linear matrix differential Riccati equation [9]. This latter representation plays an important role in the state estimation and H_2 -filtering problems which are dual to optimal control problems [1].

In this paper we propose a class of numerical methods for solving the differential Riccati equation. This in turn allows one to construct an accurate numerical solution of the optimal control problem in feedback form and compute an observer or state estimator for a non-stationary linear system. The literature on numerical methods for Riccati equations is very rich. Without claiming completeness we mention a class of methods based on backward differentiation formulas (BDF) for symmetric and non-symmetric non-stationary differential Riccati equations [3]. These methods require on solving an algebraic Riccati equation (ARE) at each time-step.

The latter is done either using Newton's method [2] or a Schur decomposition method [7]. Another class of methods is represented by exact discretization of stationary differential Riccati equations [6].

The class of methods proposed here is based on so-called Möbius integrators for Riccati equations [10]. The basic idea behind the Möbius transformation is to make use of the fact that the solution of the Riccati equation induces a flow on a Grassmannian manifold. This flow is called a Möbius transformation (see for instance [10]). It may be constructed by solving an associated linear Hamiltonian system which has the same form as Euler-Lagrange equations associated to the Pontryagin maximum principle. We propose to construct a numerical approximation of the Möbius transform by using symplectic Runge-Kutta methods of order p and thus avoid numerical instabilities associated with Möbius transform by means of a reinitialization. The resulting symplectic Möbius integrator is stable and preserves symmetry and positivity of the Riccati matrix. Also it preserves all quadratic invariants and a non-stationary variant of a Lyapunov quadratic form (associated with the inverse Riccati matrix). The latter plays an important role in state estimation as it defines a decay rate of the state estimation error over time. We note that the algorithm proposed in [5] appears to be quite close to the symplectic Möbius integrators proposed in this paper: namely, the authors propose a numerically stable version of the so-called Davidson-Maki algorithm which represents the solution of the symmetric Riccati equation by means of Bernoulli substitution. The numerical stability of the substitution is achieved through the reinitialization over the course of computing the approximate solution of the linear Hamiltonian system. In fact, Bernoulli substitution represents a Möbius transform. Unlike [5] where explicit RK,

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linear multistep and BDF time integrators were applied to get numerical Möbius transform we construct a symplectic RK method to approximate the latter. This allows us to preserve symmetry and positivity. We illustrate the method on a numerical example which comes from the discretization of the linear non-stationary hyperbolic equation by means of the Galerkin method. The experiment shows that our implementation with reinitialization is stable unlike a standard implicit mid-point approximation of a Möbius transform and preserves symmetry and positivity as well as a non-stationary Lyapunov quadratic form. The latter is of major importance in practice of using “on-line” estimators in the form of filters[11] as the filter does not require relaunching when the new observation $\mathbf{Y}(t)$ arrives and, thus, it can be integrated for a long time. In this case, the structure preserving discretisation becomes necessary to guarantee that the error estimates hold true for the discrete system.

This paper is organized as follows. Section II.1 reviews LQ control problems, introduces linear Hamiltonian systems and Riccati equations, and discusses the relations to the dual state estimation problem. Section III introduces symplectic Möbius integrators. Section IV contains numerical assessment of the implicit midpoint version of the Möbius integrator for non-stationary linear equations. Section V contains concluding remarks.

II. REVIEW OF LQ OPTIMAL CONTROL PROBLEMS

1) *LQ problem:* The linear quadratic (LQ) optimal control problem is stated as follows. On the time interval $t \in (t_0, t_f)$ determine $x \in L^2(t_0, t_f, \mathbf{R}^n)$ and $u \in L^2(t_0, t_f, \mathbf{R}^m)$ to minimize the cost functional

$$\begin{aligned} \mathcal{L}[x, u] = & x_0^T Q_0 x_0 + \int_{t_0}^{t_f} x^T(t) Q(t) x(t) dt \\ & + \int_{t_0}^{t_f} u^T(t) R(t) u(t) dt. \end{aligned}$$

subject to the constraint:

$$\dot{x}(t) = A(t)x(t) + B(t)u(t), x(t_f) = x_f, \quad (1)$$

where $x(0) = x_0$, $Q_0 = Q_0^T \geq 0$, $Q(t) = Q^T(t) \geq 0$ and $R(t) = R^T(t) > 0$ are matrices of appropriate dimensions.

It is well known [1] that the solution of the LQ problem is in the form: $\hat{u} = R(t)^{-1}B(t)^T\lambda$ where the Lagrange multiplier $\lambda \in L^2(t_0, t_f, \mathbf{R}^n)$ solves the following linear Hamiltonian two-point boundary value problem:

$$\begin{aligned} \dot{x} &= A(t)x + B(t)R(t)^{-1}B(t)^T\lambda, x(t_f) = x_f, \\ \dot{\lambda} &= Q(t)x - A(t)^T\lambda, \lambda(t_0) = Q_0x(t_0). \end{aligned}$$

On the other hand, the optimal control \hat{u} admits a so-called feedback representation: $\hat{u} = R(t)^{-1}B(t)^TP(t)x(t)$ where P solves Riccati equation: $P(t_0) = Q_0$ and

$$\begin{aligned} \frac{dP}{dt} = & -A(t)P - PA^T(t) + Q(t) \\ & - PB(t)R^{-1}(t)B^T(t)P. \end{aligned} \quad (2)$$

It is well-known [9, p.121, Lemma 4.1] that under our assumptions on Q, R and Q_0 there exist $U(t)$ and $V(t)$ such that $U(t_0) = I$ and $V(t_0) = Q_0$ and:

$$\begin{aligned} \frac{dU}{dt} &= A(t)U + B(t)R^{-1}(t)B^T(t)V, \\ \frac{dV}{dt} &= Q(t)U - A^T(t)V, \end{aligned} \quad (3)$$

and $P(t) = V(t)U^{-1}(t)$. In particular, $x(t) = U(t)U^{-1}(t_f)x_f$ and $\lambda(t) = V(t)x_0$ so that $\lambda(t) = P(t)x(t)$. This is remarkable because in general the coupled dynamics $(x(t), \lambda(t))$ is described by a $2n \times 2n$ matrix. Here the dimension reduction follows from the coupled boundary condition at $t = t_0$. The consequence is that our solution $(x(t), \lambda(t))$ evolves on the space of n -dimensional subspaces of \mathbf{R}^{2n} , the Grassmannian $\text{Gr}(2n, n)$, as described in Section III.

Now, substituting $\hat{u}(t)$ into the cost and using (3), the cost function can be simplified along our solution as

$$\begin{aligned} \mathcal{L}[x, \lambda] &= \frac{1}{2}x_0^T Q_0 x_0 + x_0^T \left[\int_{t_0}^{t_f} \frac{d}{dt} (U(t)^T V(t)) dt \right] x_0 \\ &= \frac{1}{2}x_0^T U(t_f)^T V(t_f) x_0 = \frac{1}{2}x_f^T P(t_f) x_f \end{aligned}$$

representing the minimal value of the cost.

2) *Dual estimation problem:* The LQ problem arises in many applications. For example, it is the key object in H_2 -filtering (Kalman filtering [1]) and minimax state estimation (see for instance [8]). Namely, the cost function \mathcal{L} represents, in particular, a worst-case estimation error σ for the following state estimation problem: given an output $y(t) \in \mathbb{R}^p$ of a linear system

$$\frac{dp}{dt} = -A^T(t)p(t) + f(t), \quad p(t_0) = f_0, \quad (4)$$

in the form $y(t) = B^T(t)p(t) + \eta(t)$ find $\hat{u} \in L^2(t_0, t_f, \mathbb{R}^p)$ such that: $\sigma(\hat{u}) \leq \sigma(u)$, $\forall u \in L^2(t_0, t_f, \mathbb{R}^p)$ where

$$\sigma(u) := \sup_{f_0, f, \eta} (\ell^T p(t_f) - \int_{t_0}^{t_f} u^T(t)y(t)dt)^2,$$

assuming that

$$f_0^T Q_0^{-1} f_0 + \int_{t_0}^{t_f} f^T(t)Q^{-1}(t)f(t)dt + \eta^T(t)R^{-1}(t)\eta(t)dt \leq 1.$$

In fact, $\mathcal{L}(u, x) = \sigma(u)$ and so, by minimizing $\mathcal{L}(u)$ one finds the estimate \hat{u} of $\ell^T p(t_f)$ with the minimal worst-case error $\sigma(\hat{u})$. It turns out that $\int_{t_0}^{t_f} u^T(t)y(t)dt = \ell^T \hat{p}(t_f)$ where \hat{p} solves the so-called filter equation:

$$\frac{d\hat{p}}{dt} = (-A^T(t) - P(t)B(t)R^{-1}(t)B^T(t))\hat{p}(t) + P(t)B(t)R^{-1}(t)y(t), \quad \hat{p}(t_0) = 0.$$

Let us now assume that the estimation error $e(t) := p(t) - \hat{p}(t)$ equals e_0 at time instant $t = t^*$ and $f(t) = 0$, $\eta(t) = 0$ for $t > t^*$. Then one may write an equation for e : $e(t^*) = e_0$ and

$$\dot{e} = (-A^T(t) - P(t)B(t)R^{-1}(t)B^T(t))e(t). \quad (5)$$

We compute:

$$\begin{aligned} & (e^T(t)P^{-1}(t)e(t))' \\ &= -e^T(P^{-1}Q(t)P^{-1} + H^T(t)R^{-1}(t)H(t))e, \end{aligned}$$

so that for $t < t_f$ we get:

$$(e^T(t_f)P^{-1}(t_f)e(t_f)) \leq (e^T(t)P^{-1}(t)e(t)) \quad (A).$$

We would like to prove that this decay—of a non-stationary variant of a Lyapunov quadratic form

along the trajectory $e(t)$ —holds for the discrete dynamics which is to be presented in the following sections.

III. MÖBIUS INTEGRATORS

Each real $n \times m$ matrix Y defines a subspace of \mathbb{R}^{m+n} as follows. Partition $z \in \mathbb{R}^{m+n}$ as $z = \begin{pmatrix} u \\ v \end{pmatrix}$, where $u \in \mathbb{R}^m$ and $v \in \mathbb{R}^n$. Then consider the set of all such z satisfying $v = Yu$. This set defines an m -dimensional subspace of \mathbb{R}^{m+n} , a basis for which can easily be constructed as the column space of the matrix $Z = \begin{bmatrix} I_m \\ Y \end{bmatrix}$, where I_m denotes the m -dimensional identity matrix. Note that Z indeed has full rank m , independent of the rank of Y . As noted in [10], not all m dimensional subspaces of \mathbb{R}^{m+n} can be constructed this way, but a dense open subset of them can. The set of all m dimensional subspaces of \mathbb{R}^{m+n} that do have this property is called the Grassmannian, denoted $\text{Gr}(m+n, m)$, which can be given topological structure and is compact in \mathbb{R}^{m+n} .

Now consider the action of the Lie group $\text{GL}(m+n)$ on $\text{Gr}(m+n, m)$. Let $A \in \text{GL}(m+n)$ be close to the identity, and partitioned as $A = I + h \begin{bmatrix} a & b \\ c & d \end{bmatrix}$, where h is a small parameter and $a \in \mathbb{R}^{m \times m}$, $d \in \mathbb{R}^{n \times n}$, etc., and consider the action of A on the basis Z . Let $Z' = AZ$,

$$Z' = \begin{bmatrix} U' \\ V' \end{bmatrix}, \quad \begin{aligned} U' &= I_m + h(a + bY) \\ V' &= Y + h(c + dY) \end{aligned}$$

Under what condition does the column space of Z' define a subspace in $\text{Gr}(m+n, m)$? In this case there exists Y' such that $V' = Y'U'$, hence

$$\begin{aligned} Y + h(c + dY) &= Y' [I + h(a + bY)] \Rightarrow \\ Y' &= [Y + h(c + dY)] [I + h(a + bY)]^{-1}. \end{aligned}$$

For h small enough, the inverse exists, and hence infinitesimal generators in $\text{GL}(m+n)$ preserve the Grassmann manifold. What is more,

$$\begin{aligned} Y' &= [Y + h(c + dY)] [I - h(a + bY) + \mathcal{O}(h^2)] \\ &= Y + h(c + dY - YbY - Ya) + \mathcal{O}(h^2), \end{aligned}$$

and in the limit $h \rightarrow 0$, we see that $GL(m+n)$ induces a flow on $Gr(m+n, m)$ corresponding to the Riccati equation for $Y = VU^{-1}$

$$\frac{dY}{dt} = c + dY - YbY - Ya. \quad (6)$$

For more general elements of $GL(n+m)$, we have: $U' = \alpha + \beta Y$, $V' = \gamma + \delta Y$, $\det \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \neq 0$, and we have $V' = Y'U'$:

$$\gamma + \delta Y = Y'(\alpha + \beta Y) \Rightarrow Y' = (\gamma + \delta Y)(\alpha + \beta Y)^{-1}, \quad (7)$$

provided the inverse exists. Such a transformation is referred to as a generalized Möbius transformation in [10].

Schiff & Shnider [10] propose constructing Möbius integrators for the Riccati equation (6) by solving the related linear equation

$$\frac{d\Gamma}{dt} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \Gamma, \quad \Gamma(0) = I \quad (8)$$

over a short time interval $(0, h)$ using a numerical method or an (approximate) matrix exponential. The exact (or approximate, for that matter) solution

$$\Gamma(h) = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} = I + h \begin{pmatrix} a & b \\ c & d \end{pmatrix} + \mathcal{O}(h^2)$$

can be used to define a Möbius transformation (7) to propagate Y over (t_n, t_{n+1}) , i.e., by taking $Y = Y^n$, $Y^{n+1} = Y'$. This approach can be easily generalized to nonautonomous Riccati equations, but requires solving (8) at each time step. An advantage of the approach is that it avoids representation singularities. The stability of Möbius integrators can be directly analyzed in the context of standard linear stability theory for numerical methods applied to the auxiliary problem (8).

The efficiency of the approach of [10] can be improved slightly by directly approximating $\frac{dZ}{dt} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} Z$, $Z(0) = Z^n = \begin{bmatrix} I_m \\ Y^n \end{bmatrix}$ whose solution is $Z^{n+1} = \begin{bmatrix} \alpha + \beta Y_n \\ \gamma + \delta Y_n \end{bmatrix}$, the numerator and denominator of the desired Möbius transformation.

A. Symplectic Möbius integrator for Riccati equations

We recall that the solution P of the Riccati equation (2) may be derived from Hamiltonian system (3). Indeed, $P = VU^{-1}$ and (3) may be written as follows:

$$\begin{pmatrix} dU/dt \\ dV/dt \end{pmatrix} = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} \begin{bmatrix} -Q & A^T \\ A & BR^{-1}B^T \end{bmatrix} \begin{pmatrix} U \\ V \end{pmatrix}.$$

Thus, numerical approximation of the Riccati equation may be conducted by constructing a numerical method for the system (3).

Current wisdom [4] suggests using symplectic integrators for Hamiltonian systems. If A , B , Q and R are sparse, then partitioned RK methods or splitting methods may be an interesting alternative, but in general we must consider the class of symplectic Runge-Kutta (RK) methods. We stress that $P(t)$ is symmetric and non-negative if the initial condition $P(0)$ is symmetric and non-negative. Thus, the corresponding numerical method should preserve these properties together with the a non-stationary variant of a Lyapunov quadratic form (“decay” property (A) mentioned above). In what follows we propose s -stage implicit RK method [4, p.29] that possesses the required properties.

Following [13] we introduce a uniform grid $t_n := nh$, $n = 1, \dots, L$, $h := \frac{t_f - t_0}{L}$ on (t_0, t_f) and let $\{a_{ij}\}_{i,j=1}^s$, $\{b_i\}_{i=1}^s$ denote the coefficients of s -stage implicit RK method of order p [4, p.29] for $s \geq 1$. Let us also set $c_i := \sum_{j=1}^s a_{ij}$. Our main result – the symplectic Möbius integrator for the auxiliary system (3) – is formulated in the following theorem.

Theorem 1: Assume that $M_{jk} := b_j b_k - b_k a_{kj} - b_j a_{jk} = 0$ for $1 \leq j, k \leq s$. Define $P_n = V_n U_n^{-1}$ for $n > 0$ and $P_0 := Q_0$ and set $P_{in} = V_{in} U_{in}^{-1}$ where U_n , V_n and U_{in} , V_{in} are defined from the following equations:

$$\begin{aligned} U_{n+1} &= U_n + h \sum_{i=1}^s b_i \delta U_{in}, \\ V_{n+1} &= V_n + h \sum_{i=1}^s b_i \delta V_{in}, \end{aligned} \quad (9)$$

where $V_{in} = V_n + h \sum_{j=1}^s a_{ij} \delta V_{jn}$, $V_n = P_n$, $U_{in} = U_n + h \sum_{j=1}^s a_{ij} \delta U_{jn}$, $U_n = I$, $\delta U_{in} = A_{in} U_{in} + B_{in} R_{in}^{-1} B_{in}^T V_{in}$, $\delta V_{in} = -A_{in}^T V_{in} + Q_{in} U_{in}$, $A_{in} := A(t_n + c_i h)$ and B_{in} , Q_{in} , R_{in} are defined analogously. Then P^n is a symmetric non-negative matrix and $\|P_n - P(t_n)\| \leq O(h^p)$ for the continuous Riccati matrix $P(t)$. Moreover, for stationary A, B, Q and R such that A, B is stabilizable and $Q_0 = 0$ the ‘‘decay’’ property (A) is preserved as well.

Proof: Let us first justify the reinitialization proposed in (9), that is $V_n = P_n$ and $U_n = I$. This may be easily explained for the case of continuous time. Namely, we note that under the change of variables $U(t) := \widehat{U}(t)X$, $V(t) := \widehat{V}(t)X$, where \widehat{U} , \widehat{V} solve (3), one would get that $\widehat{P}(t) = \widehat{V}(t)\widehat{U}^{-1}(t) = V(t)U^{-1}(t) = P(t)$. Therefore, we are free to re-initialize U_n , V_n at each t_n . That is, we can compute P_{n+1} as $P_{n+1} = V_{n+1}U_{n+1}^{-1}$, where V_{n+1} , U_{n+1} are obtained through (9) with $V_n = P_n$ and $U_n = I$.

The reinitialization has one major advantage: it keeps U_n close to the identity and well-conditioned numerically, which, in turn, allows us to use standard error estimates for RK methods of order p . These imply that $\|P(t_f) - P_{t_f}\| = O(h^p)$ for $P(t_f) = V(t_f)U^{-1}(t_f)$, $P_{t_f} = V_{t_f}U_{t_f}^{-1}$.

Let us now prove that P_n is symmetric and non-negative. To this end we apply one of the key properties of symplectic RK methods (those with $M_{ij} = 0$), namely the following discrete version of the integration by parts formula:

$$U_{t_f}^T V_{t_f} = U_0^T V_0 + h \sum_{n=1}^L \sum_{i=1}^s b_i (\delta U_{in}^T V_{in} + U_{in}^T \delta V_{in}).$$

By substituting expressions for δU_{in} and δV_{in} from (9) into the above formula and multiplying both sides of the resulting equality by $U_{t_f}^{-T} := (U_{t_f}^T)^{-1}$ from the left and $U_{t_f}^{-1}$ from the right we find: $P_{t_f} = V_{t_f}U_{t_f}^{-1} = U_{t_f}^{-T}(Q_0 + h\Gamma)U_{t_f}^{-1}$, $\Gamma := \sum_{n=1}^L \sum_{i=1}^s b_i (V_{in}^T B_{in} R_{in}^{-1} B_{in}^T V_{in} + U_{in}^T Q_{in} U_{in})$. It is clear that $\Gamma = \Gamma^T$. On the other hand, $b_i \geq 0$

for all i for the symplectic Gauss-Legendre RK methods and so Γ is a symmetric non-negative matrix. Using the above representation it is easy to derive that $P_{t_f} = P_{t_f}^T \geq 0$.

Let us finally prove the ‘‘decay’’ property (A). Since the pair A, B is stabilizable and the noises are trivial after $t > t^*$ (by assumption (A)) it follows that $\lim_{t \rightarrow \infty} \|e(t)\| = 0$. Indeed, let P^∞ denote the unique equilibrium solution of the algebraic Riccati equation corresponding to (2). Then $-A^T - P^\infty B R^{-1} B^T$ is stable and since $\lim P(t) = P^\infty$ it follows that $e(t) \rightarrow 0$ monotonically at least after some $t^{**} \geq t^*$. On the other hand $P(t)$ is a non-decreasing matrix-valued function (see for instance [12, p.218]). Finally, $e_{t_n}^T P_{t_n}^{-1} e_{t_n}$ is a non-increasing function for $t > t^{**}$ as symplectic RK methods preserve quadratic invariants [4]. ■

We leave the proof of the ‘‘decay’’ property (A) in the general case of non-stationary matrices A, B for the further research.

IV. NUMERICAL EXPERIMENTS

In this experiment we approximated Riccati equation (2) using the reinitialized implicit midpoint method representing a symplectic Möbius integrator of order 2 (i.e. the method (9) with $s=1$, $a_{11} = b_1 = 1/2$) and compared it to the standard iterated midpoint method applied to (3). The matrix $A(t)$ represents the stiffness matrix of the spectral Galerkin method applied to the following 2D linear transport problem: $\partial_t I + u \partial_x I + v \partial_y I = 0$, $I(x, y, 0) = I_0(x, y)$, $I = 0$ on $\partial\Omega$, where the flow $(u(x, y, t), v(x, y, t))'$ is given. The transport equation was projected onto a finite dimensional subspace generated by the eigenfunction of the Laplacian $-\Delta$ on $\Omega = [0, 2\pi]^2$. For the simulation we took $C(t) = \text{diag}(1, 0, \dots, 0)$, $Q_0 = Q(t) = \frac{1}{100}I$, $B = \text{diag}(1, 0, \dots, 0)$, $h = 0.002$, $t_0 = 0$ and advanced Riccati equation (2) to the time-instant $t_f = 5500h$ by using the Möbius integrator in the form of reinitialized midpoint method and the non-reinitialized midpoint method. The figures below represent the simulation results. Clearly, both methods coincide for $n < 4500$ but then (for $n >$

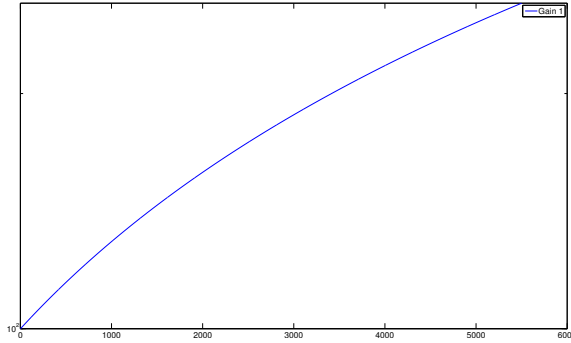


Fig. 1. The Frobenius norm of the Riccati matrix $P(t)$ computed by means of the Möbius integrator.

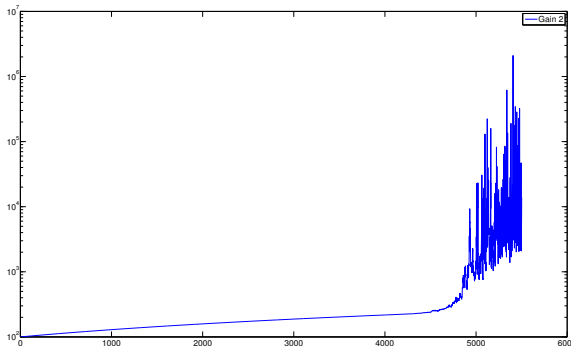


Fig. 2. The Frobenius norm of the Riccati matrix computed by means of the standard midpoint.

4500) the non-reinitialized midpoint version of the numerical Riccati matrix has growing oscillations (see Fig.1-Fig.2). This shows that the reinitialization together with symmetry and positivity preservation plays a vital role for long simulations (like filtering problems where one does not reinitialize the filter when new observations appear).

V. CONCLUSION

The paper presents a class of symplectic Möbius integrators of order p . The main advantages of the methods within this class over standard time integrators for Riccati equations are:

- Möbius integrators allow to integrate Riccati equation through “singularities” which are related only to the local coordinates and are

not present in the exact flow map over the Grassmanian manifold;

- symplectic Möbius integrators with reinitialization deliver stable numerical integration schemes of higher order;
- the proposed class of methods preserves symmetry, positivity and quadratic invariants;
- Decay of a non-stationary Lyapunov quadratic form along the trajectory of a state estimation error (see equation (A)) is preserved.

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