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DIAGONALIZATION APPROACH TO DISCRETE QUADRATIC FUNCTIONALS

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ABSTRACT. A necessary and sufficient condition for the nonnegativity of the discrete quadratic functional corresponding to a symplectic difference system is proved using the diagonalization method.

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1. INTRODUCTION

The investigation of the *nonnegativity* of discrete quadratic functionals corresponding to symplectic difference systems attracted attention in several recent papers [8, 10, 13, 14]. In this paper we continue in this research and we present an alternative approach to necessary and sufficient conditions for the nonnegativity of discrete quadratic functionals which were established in [8] by using the generalized Picone's identity and via constructing an example proving the necessity of the so-called "image condition". Here we use a different method introduced in [5] and further developed and used in [11] and [10]. This approach is based on the diagonalization of a certain "big" matrix which represents the quadratic functional under consideration. Also, the construction of an example showing the necessity of the "image condition" presented here is slightly different than the one given in [8].

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Our concern is the discrete quadratic functional

$$\begin{aligned}\mathcal{F}(x,u) &:= x_0^T\Gamma_0 x_0 + x_{N+1}^T\Gamma x_{N+1}\\ &\quad+\sum_{k=0}^{N}\{x_k^T\mathcal{C}_k^T\mathcal{A}_k x_k + 2u_k^T\mathcal{B}_k^T\mathcal{C}_k x_k + u_k^T\mathcal{B}_k^T\mathcal{D}_k u_k\}\end{aligned}$$

over the class of *admissible sequences* $\binom{x}{u}$, i.e., the sequences satisfying the *equation of motion* $x_{k+1} = \mathcal{A}_k x_k + \mathcal{B}_k u_k$, $k = 0,\dots,N$, and *endpoints constraints*

$$x_0 \in \text{Ker } \mathcal{M}_0, \quad x_{N+1} \in \text{Ker } \mathcal{M}.$$

Sometimes we speak about an admissible sequence $x = \{x_k\}_{k=0}^{N+1}$ only. By this we mean such an x for which there exist $u_0,\dots,u_N$ such that $\binom{x}{u}$ is admissible.

It is supposed that $\mathcal{A}_k, \mathcal{B}_k, \mathcal{C}_k, \mathcal{D}_k$ are $n\times n$ matrices such that the $2n\times 2n$ matrix $S_k = \begin{pmatrix}\mathcal{A}_k & \mathcal{B}_k\\ \mathcal{C}_k & \mathcal{D}_k\end{pmatrix}$ is symplectic for all k, i.e.,

$$S_k^T\mathcal{J}S_k = \mathcal{J}, \quad \text{where} \quad \mathcal{J} = \begin{pmatrix}0 & I\\ -I & 0\end{pmatrix}. \tag{1}$$

The matrices Γ_0, Γ, $\mathcal{M}_0$, $\mathcal{M}$ of the endpoints cost and boundary conditions are symmetric $n\times n$ matrices, and we assume without loss of generality that $\mathcal{M}_0$, $\mathcal{M}$ are projections and that $\Gamma_0 = (I-\mathcal{M}_0)\Gamma_0(I-\mathcal{M}_0)$, $\Gamma = (I-\mathcal{M})\Gamma(I-\mathcal{M})$. Note that these identities together with the fact that $\mathcal{M}_0$, $\mathcal{M}$ are projections imply

$$\mathcal{M}_0\Gamma_0 = 0 = \Gamma_0\mathcal{M}_0 \quad \text{and} \quad \mathcal{M}\Gamma = 0 = \Gamma\mathcal{M}.$$

The quadratic functional $\mathcal{F}$ is closely related to the symplectic difference system

$$z_{k+1} = S_k z_k \quad \text{with} \quad z_k = \begin{pmatrix}x_k\\ u_k\end{pmatrix}, \tag{2}$$

where S_k satisfies (1). This symplectic property of S translates in terms of its block entries as

$$\mathcal{A}^T\mathcal{C} = \mathcal{C}^T\mathcal{A}, \quad \mathcal{B}^T\mathcal{D} = \mathcal{D}^T\mathcal{B}, \quad \mathcal{A}^T\mathcal{D} - \mathcal{C}^T\mathcal{B} = I. \tag{3}$$

Since (1) is equivalent to $S\mathcal{J}S^T = \mathcal{J}$, identities (3) are equivalent to

$$\mathcal{A}\mathcal{B}^T = \mathcal{B}\mathcal{A}^T, \quad \mathcal{C}\mathcal{D}^T = \mathcal{D}\mathcal{C}^T, \quad \mathcal{A}\mathcal{D}^T - \mathcal{B}\mathcal{C}^T = I.$$

The fact that we consider the functional $\mathcal{F}$ over the class of sequences satisfying the separated boundary condition at $k = 0$ and $k = N+1$ actually means no loss of generality. Indeed, if we consider a more general functional

$$\tilde{\mathcal{F}}(z) := \begin{pmatrix}x_0\\ x_{N+1}\end{pmatrix}\tilde{\Gamma}\begin{pmatrix}x_0\\ x_{N+1}\end{pmatrix} + \sum_{k=0}^{N}\{x_k^T\mathcal{C}_k^T\mathcal{A}_k x_k + 2u_k^T\mathcal{B}_k^T\mathcal{C}_k x_k + u_k^T\mathcal{B}_k^T\mathcal{D}_k u_k\}$$

over the class of $z = \binom{x}{u}$ satisfying the equation of motion and the joint boundary condition $\binom{x_0}{x_{N+1}} \in \text{Ker } \tilde{\mathcal{M}}$, where $\tilde{\mathcal{M}}$ is a $2n\times 2n$ matrix, it is possible to use one of the procedures introduced in [6] and [14] to augment the problem into the "double dimension", but with separated boundary conditions at $k = 0$ and $k = N + 1$. Note also that extending the matrices in the augmented functional over the discrete interval $[-1, N + 2]$ in a suitable way, the separated boundary conditions at $k = 0$ and $k = N + 1$ can be reduced to the zero boundary conditions at $k = -1$ and $k = N+2$. However, here we will not employ this transformation, since the reformulation of the results to the extended functional brings no essential simplification of our problem.

The paper is organized as follows. In the remaining part of this section we briefly recall the history of the investigation of the positivity/nonnegativity of discrete quadratic functionals. We also compare this investigation with the same problem for (continuous–time) quadratic functionals associated with linear Hamiltonian differential systems. Then, in Section 2, we state basic results concerning symplectic difference systems and their relationship to the quadratic functionals under consideration. Section 3 is devoted to the introduction of the basic ideas of the diagonalization method. The last section contains the main result of our paper – a "diagonalization proof" of the necessary and sufficient condition for nonnegativity of the functional $\mathcal{F}$.

Consider the *linear Hamiltonian difference system*

$$\Delta x_k = A_k x_{k+1} + B_k u_k, \quad \Delta u_k = C_k x_{k+1} - A_k^T u_k, \tag{4}$$

where A, B, C are $n \times n$ matrices, B, C are symmetric and $I - A$ is invertible. Expanding the forward differences in this system, it is easy to see that (4) is a special case of (2), see [4, p. 714]. The problem of the *positivity* of the quadratic functional associated with (4)

$$\mathcal{F}_H(x, u) := \sum_{k=0}^{N} \{x_{k+1}^T C_k x_{k+1} + u_k^T B_k u_k\}$$

over the class of sequences $\binom{x}{u}$ satisfying $\Delta x_k = A_k x_{k+1} + B_k u_k$ and $x_0 = 0 = x_{N+1}$ is systematically studied in [1], where the so-called roundabout theorem is established. This theorem presents several conditions which are equivalent to the positivity of $\mathcal{F}_H$. The results of [1] were extended to "Hamiltonian" functionals $\mathcal{F}_H$ with general boundary conditions in subsequent papers [2, 3, 6, 12]. In particular, it is shown that the general joint boundary conditions can be reduced to zero separated conditions for a certain associated augmented functional. Concerning the roundabout theorem for quadratic functionals $\mathcal{F}$ corresponding to symplectic difference systems (2), the roundabout theorem (i.e., the characterization of the positivity of $\mathcal{F}$) is presented in [4]. The papers [7, 15] continue in this research and relate the oscillation properties of (2) to the number of negative eigenvalues of a certain eigenvalue problem associated with (2).

The continuous counterparts of the functional $\mathcal{F}$ and of the system (2) are the functional

$$\mathcal{F}_C(x,u) := \int_a^b [u^T(t)B(t)u(t) + x^T(t)C(t)x(t)]\,dt$$

and the linear Hamiltonian differential system

$$x' = A(t)x + B(t)u, \quad u' = C(t)x - A^T(t)u. \tag{5}$$

A comprehensive treatment of the relationship between oscillatory properties of (5) and the positivity (nonnegativity) of the functional $\mathcal{F}_C$ can be found in the books [16, 17], see also the papers [9, 18, 19, 20, 21]. Note that the problem of the positivity and the nonnegativity of $\mathcal{F}_C$ is of the same difficulty in the continuous–time case, but under a *normality condition* (or, equivalently, under a *controllability condition*), see [16, 17].

In contrast to the continuous–time case, here we suppose no normality condition. It turns out that the "gap" between the characterization of the positivity and the nonnegativity of $\mathcal{F}$ is bigger than in the continuous case, in a certain sense, as pointed out in Remark 2 of the last section.

2. AUXILIARY RESULTS

First let us recall the relationship between the symplectic system (2) and the quadratic functional $\mathcal{F}$. Functional $\mathcal{F}$ can be written in the form

$$\mathcal{F}(z) = x_0^T\Gamma_0 x_0 + x_{N+1}^T\Gamma x_{N+1} + \mathcal{F}_0(z),$$

where

$$\mathcal{F}_0(z) = \sum_{k=0}^{N} z_k^T\{S_k^T\mathcal{K}S_k - \mathcal{K}\}z_k, \quad \mathcal{K} = \begin{pmatrix} 0 & 0 \\ I & 0 \end{pmatrix},\ z = \begin{pmatrix} x \\ u \end{pmatrix}$$

and the equation of motion then reads as $\mathcal{K}z_{k+1} = \mathcal{K}S_k z_k$.

Lemma 1. *Let $z_k = \binom{x_k}{u_k}$, $\tilde z_k = \binom{\tilde x_k}{\tilde u_k}$, $k = 0,\dots,N$, satisfy the equation of motion and define the bilinear form associated with $\mathcal{F}_0$ by*

$$\mathcal{F}_0(z,\tilde z) = \sum_{k=0}^{N} z_k\{S_k^T\mathcal{K}S_k - \mathcal{K}\}\tilde z_k.$$

Then

$$\mathcal{F}_0(z,\tilde z) = \sum_{k=0}^{N}\{x_{k+1}^T(\mathcal{C}_k\tilde x_k + \mathcal{D}_k\tilde u_k - \tilde u_{k+1}) + \Delta(x_k^T\tilde u_k)\}.$$

Proof. Using the equation of motion, we have

$$\begin{aligned}\mathcal{F}_0(z,\tilde{z}) &= \sum_{k=0}^{N}\{(\mathcal{A}_k x_k + \mathcal{B}_k u_k)^T(\mathcal{C}_k\tilde{x}_k + \mathcal{D}_k\tilde{u}_k) - x_k^T\tilde{u}_k\}\\ &= \sum_{k=0}^{N}\{x_{k+1}^T(\mathcal{C}_k\tilde{x}_k + \mathcal{D}_k\tilde{u}_k - \tilde{u}_{k+1}) + x_{k+1}^T\tilde{u}_{k+1} - x_k^T\tilde{u}_k\}.\end{aligned}$$

This shows the result. □

The equivalent *time-reversed system* to (2) is the system $z_k = S_k^{-1}z_{k+1}$, which can also be studied as a discrete symplectic system [4]. In particular, this time-reversed system has the form

$$x_k = \mathcal{D}_k^T x_{k+1} - \mathcal{B}_k^T u_{k+1}, \quad u_k = -\mathcal{C}_k^T x_{k+1} + \mathcal{A}_k^T u_{k+1}. \tag{6}$$

For any two (vector or matrix) solutions $z, \tilde{z}$ of (2) we have that $z_k^T\mathcal{J}\tilde{z}_k$ is constant for $k = 0, \ldots, N+1$. This is known as the *Wronskian identity* [4, Remark 1(ii)]. In particular, if we have $Z^T\mathcal{J}Z = 0$ for a $2n\times n$ matrix solution $Z = \binom{X}{U}$ of (2), i.e., if X^TU is symmetric, then we call Z a *conjoined solution* of (2). If, in addition, $\operatorname{rank} Z = n$, then Z is called a *conjoined basis*. Two conjoined bases $Z = \binom{X}{U}$ and $\tilde{Z} = \binom{\tilde{X}}{\tilde{U}}$ are *normalized* if $Z^T\mathcal{J}\tilde{Z} = I$, i.e., if $X^T\tilde{U} - U^T\tilde{X} = I$. The *natural conjoined basis* at $k = 0$ is the solution $Z = \binom{X}{U}$ of (2) given by the initial conditions

$$X_0 = I - \mathcal{M}_0, \quad U_0 = \Gamma_0 + \mathcal{M}_0$$

and for this natural basis we have

$$X_0^T\Gamma_0 X_0 = X_0^T U_0 = \Gamma_0. \tag{7}$$

It plays the role of the principal solution of (2) at $k = 0$ used in [4] and reduces to this principal solution, when the left endpoint of $\mathcal{F}$ is zero, i.e., when $\mathcal{M}_0 = I$. In this special case one has $X_0 = 0$ and $U_0 = I$. A conjoined basis $Z = \binom{X}{U}$ is said to have *no focal points* in the interval $(k, k+1]$ if the "kernel condition"

$$\operatorname{Ker} X_{k+1} \subseteq \operatorname{Ker} X_k \tag{8}$$

and the "$\mathcal{P}$-condition"

$$\mathcal{P}_k := X_k X_{k+1}^\dagger \mathcal{B}_k \geq 0 \tag{9}$$

hold. Here Ker , † and $\geq$ stand for the kernel, the Moore–Penrose generalized inverse and the nonnegative definiteness of the matrix indicated. Note also that if (8) holds, then the matrix $\mathcal{P}$ is symmetric, see [4, p. 714 and Lemma 3]. Equivalently, Z has a focal point in $(k, k+1]$ if either $\operatorname{Ker} X_{k+1} \not\subseteq \operatorname{Ker} X_k$, or (8) holds but $\mathcal{P}_k \not\geq 0$. The nonexistence of a focal point of the principal $\binom{X}{U}$ at $k = 0$ in the discrete interval $(0, N+1]$ is a necessary and sufficient condition for *positivity* of (1) with zero boundary conditions $x_0 = 0 = x_{N+1}$, see [1, 4].

Next we define for $k = 0, \dots, N+1$ the $n \times n$ matrix

$$Q_k := U_k X_k^\dagger + (U_k X_k^\dagger \tilde{X}_k - \tilde{U}_k)(I - X_k^\dagger X_k) U_k^T, \tag{10}$$

where $Z = \binom{X}{U}$ is the natural conjoined basis at $k = 0$ and $\tilde{Z} = \binom{\tilde{X}}{\tilde{U}}$ is the conjoined basis completing Z to a pair of normalized conjoined bases of (2). The existence of $\tilde{Z}$ is proven e.g. in [10, Remark 3(ii)]. The matrix Q satisfies the identities $QX = UX^\dagger X$, $X^T Q X = U^T X$, and it solves the implicit Riccati equation $R[Q]_k X_k = 0$, where the Riccati operator $R[Q]_k$ associated with (2) is defined by

$$R[Q]_k := Q_{k+1}(\mathcal{A}_k + \mathcal{B}_k Q_k) - (\mathcal{C}_k + \mathcal{D}_k Q_k).$$

We also introduce the (symmetric) matrix

$$\tilde{\mathcal{P}}_k = \mathcal{B}_k^T \mathcal{D}_k - \mathcal{B}_k^T Q_{k+1} \mathcal{B}_k.$$

The matrices $Q, \tilde{\mathcal{P}}$ appear in the proof of the main results of our paper in the last section.

Finally, let us recall some results of the paper [15]. For a conjoined basis $Z = \binom{X}{U}$ of (2) we define the $n \times n$ matrices

$$M_k := (I - X_{k+1} X_{k+1}^\dagger)\mathcal{B}_k, \quad T_k := I - M_k^\dagger M_k, \quad P_k := T_k^T \mathcal{P}_k T_k. \tag{11}$$

Note that T_k are symmetric and the properties of the Moore–Penrose inverse imply

$$X_{k+1}^T M_k = 0, \quad M_k T_k = 0, \quad \mathcal{B}_k T_k X_{k+1} X_{k+1}^\dagger \mathcal{B}_k T_k. \tag{12}$$

Let $Z = \binom{X}{U}$ be any conjoined basis of (2). Then we have the following properties of the matrices $M, T, P, \tilde{\mathcal{P}}$. By [15, Lemma 1(ii)], the kernel condition (8) holds iff $M_k = 0$, i.e., iff $\mathcal{B}_k = X_{k+1} X_{k+1}^\dagger \mathcal{B}_k$. Further, using (6)

$$\begin{aligned}
X_k X_{k+1}^\dagger \mathcal{B}_k T_k &= (\mathcal{D}_k^T X_{k+1} - \mathcal{B}_k^T U_{k+1}) X_{k+1}^\dagger \mathcal{B}_k T_k \\
&= \mathcal{D}_k^T X_{k+1} X_{k+1}^\dagger \mathcal{B}_k T_k - \mathcal{B}_k^T U_{k+1} X_{k+1}^\dagger X_{k+1} X_{k+1}^\dagger \mathcal{B}_k T_k \\
&= \mathcal{D}_k^T \mathcal{B}_k T_k - \mathcal{B}_k^T Q_{k+1} X_{k+1} X_{k+1}^\dagger \mathcal{B}_k T_k \\
&= \mathcal{D}_k^T \mathcal{B}_k T_k - \mathcal{B}_k^T Q_{k+1} \mathcal{B}_k T_k = \tilde{\mathcal{P}}_k T_k,
\end{aligned}$$

consequently, $P_k = T_k^T \tilde{\mathcal{P}}_k T_k$ is always symmetric.

If $z = \binom{x}{u}$ satisfies the equation of motion at k, i.e., $x_{k+1} = \mathcal{A}_k x_k + \mathcal{B}_k u_k$, and if $x_k \in \operatorname{Im} X_k$, then x_{k+1} can be (uniquely) written as a sum

$$x_{k+1} = X_{k+1}\alpha_{k+1} + M_k d_k, \tag{13}$$

where, by (12), the vectors $X_{k+1}\alpha_{k+1}$ and $M_k d_k$ in the last sum are orthogonal. More precisely, suppose that $x_k = X_k \alpha_k$ and set $d_{k+1} := u_k - U_k \alpha_k$. Then

$$\begin{aligned}
x_{k+1} &= \mathcal{A}_k x_k + \mathcal{B}_k u_k = \mathcal{A}_k X_k \alpha_k + \mathcal{B}_k u_k = (X_{k+1} - \mathcal{B}_k U_k)\alpha_k + \mathcal{B}_k u_k \\
&= X_{k+1}\alpha_k + \mathcal{B}_k d_k = X_{k+1}\alpha_k + (M_k + X_{k+1} X_{k+1}^\dagger \mathcal{B}_k) d_k = X_{k+1}\alpha_{k+1} + M_k d_k,
\end{aligned}$$

where we take $\alpha_{k+1} := \alpha_k + X_{k+1}^{\dagger}\mathcal{B}_k d_k$. The previous computation means that if $x_k \in \text{Im } X_k$ (which holds e.g. if $x_0 \in \text{Im } X_0$ and if the kernel condition holds up to $k-1$), then the reachable set at $k+1$ is an orthogonal sum $\text{Im } X_{k+1} \oplus \text{Im } M_k$. Moreover, the vector x_{k+1} will stay in $\text{Im } X_{k+1}$ iff $M_k d_k = 0$.

3. ADMISSIBILITY

In this section we recall some results from [10], where the space of admissible $x = \{x_k\}_{k=0}^{N+1}$ is characterized without assuming the kernel condition.

Let us introduce (in accordance with [10], see also [5, 11]) the matrices $\Phi_{k,j} := \mathcal{A}_{k-1} \cdots \mathcal{A}_j$ for $k > j$, $\Phi_{k,k} := I$, $P_{k,j} := X_k X_{j+1}^{\dagger}\mathcal{B}_j$, $j = 0, \dots, N$, $P_{k,N+1} := X_k$, $k = 0, \dots, N$, $P_{N+1,N+1} := X_{N+1}$. Further, for $m = 0, \dots, N+1$, define

$$\mathcal{N}_m := \begin{pmatrix} P_{0,0} & P_{0,1} & \dots & P_{0,m-1} & P_{0,m} \\ -M_0 & P_{1,1} & \dots & P_{1,m-1} & P_{1,m} \\ -\Phi_{2,1}M_0 & -M_1 & \dots & P_{2,m-1} & P_{2,m} \\ \vdots & \vdots & & \vdots & \dots \\ -\Phi_{m-1,1}M_0 & -\Phi_{m-1,2}M_1 & \dots & P_{m-1,m-1} & P_{m-1,m} \\ -\Phi_{m,1}M_0 & -\Phi_{m,2}M_1 & \dots & -M_{m-1} & P_{m,m} \end{pmatrix},$$

and set $\mathcal{N} := \mathcal{N}_{N+1}$. Also, for $m = 0, \dots, N+1$ we put

$$\mathcal{K}_m := \begin{pmatrix} \mathcal{T}_0 & \mathcal{S}_0 & 0 & \dots & \dots & 0 \\ \mathcal{S}_0^T & \mathcal{T}_1 & \mathcal{S}_1 & \ddots & & \vdots \\ 0 & \mathcal{S}_1^T & \mathcal{T}_2 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & \mathcal{T}_{m-1} & \mathcal{S}_{m-1} \\ 0 & \dots & \dots & 0 & \mathcal{S}_{m-1}^T & \mathcal{T}_m \end{pmatrix},$$

where $\mathcal{T}_k := \mathcal{A}_k^T\mathcal{E}_k\mathcal{A}_k - \mathcal{A}_k^T\mathcal{C}_k - \mathcal{E}_{k-1}$, $\mathcal{S}_k := \mathcal{C}_k^T - \mathcal{A}^T\mathcal{E}_k$, $k = 0, \dots, N$, and $\mathcal{T}_{N+1} := \Gamma + \mathcal{E}_N$. The matrix $\mathcal{E}_k$ is any symmetric matrix satisfying $\mathcal{B}_k^T\mathcal{E}_k\mathcal{B}_k = \mathcal{D}_k^T\mathcal{B}_k$ (e.g. $\mathcal{E}_k = \mathcal{B}_k\mathcal{B}_k^{\dagger}\mathcal{D}_k\mathcal{B}_k^{\dagger}$), and $\mathcal{E}_{-1} := \Gamma_0$, see [10, 11]. Let

$$\Psi := \begin{pmatrix} -\Phi_{N+1,1}M_0 & -\Phi_{N+1,2}M_1 & \dots & -\Phi_{N+1,N}M_{N-1} & -M_N & X_{N+1} \end{pmatrix},$$

(i.e., Ψ is the last row in $\mathcal{N}$) and finally let

$$\mathcal{V} := \left\{ \begin{pmatrix} x_0 \\ \vdots \\ x_{N+1} \end{pmatrix}, \text{ such that } \{x_k\}_{k=0}^{N+1} \text{ is admissible} \right\}.$$

Now, by [10, Theorem 2], we have the following characterization of admissible vectors x_k, $k = 0, \dots, N+1$.

Lemma 2. [10, Theorem 2] *The vector*

$$x = \begin{pmatrix} x_0 \\ \vdots \\ x_{N+1} \end{pmatrix} \in \mathcal{V} \quad \Longleftrightarrow \quad x = \mathcal{N} d, \quad d \in \ Ker\, \mathcal{M}\Psi.$$

4. DIAGONALIZATION AND NONNEGATIVITY

The following diagonalization result extends [11, Proposition 1] to the case when the kernel condition (8) is replaced by a weaker image condition

$$x_k \in \text{ Im } X_k, \quad k = 0, \ldots, N+1, \tag{14}$$

as we will see later.

Theorem 1. *Let* $m \in \{0, \ldots, N\}$ *and* $\mathcal{U}_m = \ diag\{T_0, \ldots, T_m\}$ *with* T_k *given by* (11). *Then*

$$\mathcal{U}_{m+1}^T \mathcal{N}_{m+1}^T \mathcal{K}_{m+1} \mathcal{N}_{m+1} \mathcal{U}_{m+1} = \begin{pmatrix} \mathcal{U}_m^T \mathcal{N}_m^T \mathcal{K}_m \mathcal{N}_m \mathcal{U}_m & 0 \\ 0 & P_{m+1} \end{pmatrix}.$$

Proof. Using sightly modified computations from [5] and [11], we have

$$\mathcal{N}_{m+1}^T \mathcal{K}_{m+1} \mathcal{N}_{m+1} = \begin{pmatrix} \mathcal{N}_m^T \mathcal{K}_m \mathcal{N}_m & \Omega_m X_{m+2}^\dagger \mathcal{B}_{m+1} \\ \mathcal{B}_{m+1}^T (X_{m+2}^\dagger)^T \Omega_m^T & (X_{m+2}^\dagger \mathcal{B}_{m+1})^T \Lambda_m (X_{m+2}^\dagger \mathcal{B}_{m+1}) \end{pmatrix},$$

where

$$\begin{aligned} \Omega_m &:= \mathcal{N}_m^T \mathcal{K}_m \mathcal{Q}_m + \mathcal{N}_m^T \mathcal{R}_m X_{m+1}, \\ \Lambda_m &:= \mathcal{Q}_{m+1}^T \mathcal{K}_{m+1} \mathcal{Q}_{m+1} \\ &= \mathcal{Q}_m^T \mathcal{K}_m \mathcal{Q}_m + \mathcal{Q}_m^T \mathcal{R}_m X_{m+1} + X_{m+1}^T \mathcal{R}_m^T \mathcal{Q}_m + X_{m+1}^T \mathcal{T}_{m+1} X_{m+1}, \end{aligned}$$

with $n(m+1) \times n$ matrices

$$\mathcal{Q}_m = \begin{pmatrix} X_0 \\ \vdots \\ X_m \end{pmatrix}, \quad \mathcal{R}_m = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \mathcal{S}_m \end{pmatrix}.$$

Concerning the matrices Ω and Λ, again using computations from [5, 11]

$$\begin{aligned} \Omega_{m+1} &= \begin{pmatrix} \Omega_m \\ \mathcal{B}_{m+1}^T (X_{m+2}^\dagger)^T \{\Lambda_m + X_{m+1}^T \mathcal{S}_{m+1} X_{m+2}\} \end{pmatrix}, \\ \Lambda_m &= X_{m+1}^T [U_{m+1} + (\mathcal{A}_{m+1}^T \mathcal{E}_{m+1} \mathcal{A}_{m+1} - \mathcal{C}_{m+1}^T \mathcal{A}_{m+1}) X_{m+1}]. \end{aligned}$$

Hence, (we skip the index $m+1$ in the next computations), by using the identity

$$\mathcal{P} T = X X_{m+2}^\dagger \mathcal{B} T = \mathcal{B}^T (\mathcal{D} - Q_{m+2} \mathcal{B}) T = \tilde{\mathcal{P}} T$$

derived in Section 2, where Q is given by (10), we have

$$\begin{aligned}
&T^T\mathcal{B}^T(X^\dagger_{m+2})^T\{\Lambda_m + X^T\mathcal{S}X_{m+2}\}\\
&\quad= T^T\mathcal{B}^T(X^\dagger_{m+2})^T\{X^TU + X^T(\mathcal{A}^T\mathcal{E}\mathcal{A} - \mathcal{C}^T\mathcal{A})X + X^T\mathcal{S}X_{m+2}\}\\
&\quad= (XX^\dagger_{m+2}\mathcal{B}T)^T\{U + (\mathcal{A}^T\mathcal{E}\mathcal{A} - \mathcal{C}^T\mathcal{A})X + (\mathcal{C}^T - \mathcal{A}^T\mathcal{E})(\mathcal{A}X + \mathcal{B}U)\}\\
&\quad= T^T(\mathcal{D}^T - \mathcal{B}Q_{m+2})\{\mathcal{B}U + \mathcal{B}(\mathcal{A}^T\mathcal{E}\mathcal{A} - \mathcal{C}^T\mathcal{A})X + \mathcal{B}(\mathcal{C}^T - \mathcal{A}^T\mathcal{E})(\mathcal{A}X + \mathcal{B}U)\}\\
&\quad= T^T(\mathcal{D}^T - \mathcal{B}Q_{m+2})\{\mathcal{B}U + (\mathcal{B}\mathcal{C}^T - \mathcal{B}\mathcal{A}^T\mathcal{E})\mathcal{B}U\}\\
&\quad= T^T(\mathcal{D}^T - \mathcal{B}Q_{m+2})\{\mathcal{B}U + (\mathcal{B}\mathcal{C}^T - \mathcal{A}\mathcal{D}^T)\mathcal{B}U\}\\
&\quad= 0.
\end{aligned}$$

Consequently, since $\Omega_0 = 0$, by a similar computation as in [11, Lemma 5], we have $\Omega_m = 0$, $m = 1, \dots, N$, by the induction principle. Finally (again, no index means index $m+1$),

$$\begin{aligned}
&(X^\dagger_{m+2}\mathcal{B}T)^T\Lambda_m(X^\dagger_{m+2}\mathcal{B}T)\\
&\quad= T^T(X^\dagger_{m+2}\mathcal{B})^T\{X^TU - X^T(\mathcal{A}^T\mathcal{E}\mathcal{A} - \mathcal{C}^T\mathcal{A})X\}X^\dagger_{m+2}\mathcal{B}T\\
&\quad= (XX^\dagger_{m+2}\mathcal{B}T)^T\{U + (\mathcal{A}^T\mathcal{E}\mathcal{A} - \mathcal{C}^T\mathcal{A})X\}X^\dagger_{m+2}\mathcal{B}T\\
&\quad= T^T(\mathcal{D} - Q_{m+2}\mathcal{B})^T\{\mathcal{B}U + \mathcal{B}\mathcal{A}^T\mathcal{E}\mathcal{A} - \mathcal{B}\mathcal{C}^T\mathcal{A})X\}X^\dagger_{m+2}\mathcal{B}T\\
&\quad= T^T(\mathcal{D} - Q_{m+2}\mathcal{B})^T\{\mathcal{B}UX^\dagger_{m+2}\mathcal{B} + (\mathcal{A}\mathcal{B}^T\mathcal{E}\mathcal{A} - \mathcal{B}\mathcal{C}^T\mathcal{A})\mathcal{B}^T(\mathcal{D} - Q_{m+2}\mathcal{B})\}T\\
&\quad= T^T(\mathcal{D} - Q_{m+2}\mathcal{B})^T\{\mathcal{B}UX^\dagger_{m+2}\mathcal{B} + (\mathcal{A}\mathcal{D}^T\mathcal{B}\mathcal{A}^T - \mathcal{B}\mathcal{C}^T\mathcal{A}\mathcal{B}^T)(\mathcal{D} - Q_{m+2}\mathcal{B})\}T\\
&\quad= T^T(\mathcal{D} - Q_{m+2}\mathcal{B})^T\{\mathcal{B}UX^\dagger_{m+2}\mathcal{B} + \mathcal{A}\mathcal{B}^T(\mathcal{D} - Q_{m+2}\mathcal{B})\}T\\
&\quad= T^T(\mathcal{D} - Q_{m+2}\mathcal{B})^T\{\mathcal{B}UX_{m+2}\mathcal{B} + \mathcal{A}XX^\dagger_{m+2}\mathcal{B}\}T\\
&\quad= T^T(\mathcal{D} - Q_{m+2}\mathcal{B})^T X_{m+2}X^\dagger_{m+2}\mathcal{B}T\\
&\quad= T^T(\mathcal{D} - Q_{m+2}\mathcal{B})^T(\mathcal{B} - M)T\\
&\quad= T^T(\mathcal{B}^T\mathcal{D} - \mathcal{B}^TQ_{m+2}\mathcal{B})^TT = P.
\end{aligned}$$

The proof is complete. □

The previous statement shows what role is played by the matrices P_k in the investigation of the nonnegativity of the functional $\mathcal{F}$. They are the block diagonal entries of the "big" matrix which represents the quadratic functional $\mathcal{F}$. Another view on these matrices is presented at the end of this section.

By using the statement of Theorem 1 we can prove the following necessary and sufficient condition for the nonnegativity of $\mathcal{F}$.

Theorem 2. *Let $Z = \binom{X}{U}$ be the natural conjoined basis at $k = 0$. Then the functional $\mathcal{F}$ is nonnegative definite iff the following three statements hold true:*

(i) *The "image condition" (14) holds for every admissible $\binom{x}{u}$.*

(ii) *The "P condition" holds:*

$$P_k = T_k^T X_k X_{k+1}^\dagger \mathcal{B}_k T_k \geq 0, \quad k = 1, \dots, N. \tag{15}$$

(iii) *The "endpoint condition" holds:*

$$Q_{N+1} + \Gamma \geq 0 \quad on \quad Ker\, \mathcal{M} \cap Im\, X_{N+1}. \tag{16}$$

Proof. First we prove the sufficiency of conditions (i), (ii) and (iii) for the nonnegativity of $\mathcal{F}$. Let $\binom{x}{u}$ be any admissible pair, i.e., it satisfies the equation of motion and the boundary condition $\mathcal{M}_0 x_0 = 0 = \mathcal{M} x_{N+1}$. By Lemma 2, there exists $d = (d_0^T, \dots, d_{N+1}^T)^T \in \mathbb{R}^{n(N+2)}$, $d \in \text{Ker}\, \mathcal{M}\Psi$, such that

$$x = \begin{pmatrix} x_0 \\ \vdots \\ x_{N+1} \end{pmatrix} = \mathcal{N} d = \mathcal{N} \begin{pmatrix} d_0 \\ \vdots \\ d_{N+1} \end{pmatrix},$$

i.e.,

$$x_k = -\sum_{j=0}^{k-1} \Phi_{k,j+1} M_j + X_k \left(\sum_{j=k}^{N} X_{j+1}^\dagger \mathcal{B}_j + d_{N+1} \right).$$

For $k = 1$ (we always have $x_0 \in \text{Im}\, X_0$ even without image condition (14)),

$$x_1 = -M_0 d_0 + X_1 \alpha_1, \quad \alpha_1 := \sum_{j=1}^{N} X_{j+1}^\dagger \mathcal{B}_j d_j + d_{N+1}$$

and the condition $x_1 \in \text{Im}\, X_1$ implies $d_0 \in \text{Ker}\, M_0 = \text{Im}\, T_0$, hence $d_0 = T_0 \gamma_0$ for some $\gamma_0 \in \mathbb{R}^n$. By using the same argument, $d_k = T_k \gamma_k$, $k = 2, \dots, N$. The condition $\mathcal{M}\Psi d = 0$ then reads as $\mathcal{M} X_{N+1} d_{N+1} = 0$ and it is satisfied for $d_{N+1} \in \text{Ker}\, \mathcal{M} X_{N+1}$. Consequently, if the image condition (14) holds, then

$$\mathcal{F}(x, u) = \begin{pmatrix} \gamma_0 \\ \vdots \\ \gamma_N \\ d_{N+1} \end{pmatrix}^T \mathcal{U}_{N+1}^T \mathcal{N}_{N+1}^T \mathcal{K}_{N+1} \mathcal{N}_{N+1} \mathcal{U}_{N+1} \begin{pmatrix} \gamma_0 \\ \vdots \\ \gamma_N \\ d_{N+1} \end{pmatrix}.$$

By a similar computation as in the proof of Theorem 1,

$$\begin{aligned} \mathcal{U}_{N+1}^T \mathcal{N}_{N+1}^T \mathcal{K}_{N+1} \mathcal{N}_{N+1} \mathcal{U}_{N+1} &= \begin{pmatrix} \mathcal{U}_N^T \mathcal{N}_N^T \mathcal{K}_N \mathcal{N}_N \mathcal{U}_N & \Omega_N \\ \Omega_N^T & \mathcal{L} \end{pmatrix} \\ &= \begin{pmatrix} \text{diag}\{P_0, \dots, P_N\} & 0 \\ 0 & \mathcal{L} \end{pmatrix}, \end{aligned}$$

where

$$\mathcal{L} := \Lambda_{N-1} + X_{N+1}^T \mathcal{S}_N^T X_N + (X_N^T \mathcal{S}_N + X_{N+1}^T \mathcal{T}_{N+1}) X_{N+1}.$$

Now, substituting for Λ_{N-1}, we have (we skip the index N in the next computation)

$$\begin{aligned}
\mathcal{L} &= \Lambda_{N-1} + X^T \mathcal{S} X_{N+1} + X_{N+1}^T \mathcal{S}^T X + X_{N+1}^T \mathcal{T}_{N+1} X_{N+1} \\
&= X^T U + X^T \mathcal{A}^T \mathcal{E} \mathcal{A} X - X^T \mathcal{C}^T \mathcal{A} X + X^T (\mathcal{C} - \mathcal{A}^T \mathcal{E}) X_{N+1} \\
&\qquad + X_{N+1}^T (\mathcal{C}^T - \mathcal{E}\mathcal{A}) X + X_{N+1}^T (\Gamma + \mathcal{E}) X_{N+1} \\
&= X^T U + (-X_{N+1}^T + U^T \mathcal{B}^T) \mathcal{E} (-X_{N+1} + \mathcal{B} U) - X^T \mathcal{A}^T (\mathcal{C} X + \mathcal{E} X_{N+1}) \\
&\qquad + X^T \mathcal{C}^T X_{N+1} + X_{N+1}^T \mathcal{C} X - X_{N+1}^T \mathcal{E} \mathcal{A} X + X_{N+1}^T \Gamma X_{N+1} + X_{N+1}^T \mathcal{E} X_{N+1} \\
&= X^T U + U^T \mathcal{B}^T \mathcal{D} U - U^T (I - \mathcal{D}^T \mathcal{A}) X + X^T \mathcal{C}^T X_{N+1} + X_{N+1}^T \Gamma X_{N+1} \\
&= U^T \mathcal{D}^T (\mathcal{B} U + \mathcal{A} X) + X^T \mathcal{C}^T X_{N+1} + X_{N+1}^T \Gamma X_{N+1} \\
&= U_{N+1}^T X_{N+1} + X_{N+1}^T \Gamma X_{N+1} \\
&= X_{N+1}^T (Q_{N+1} + \Gamma) X_{N+1}.
\end{aligned}$$

Consequently,

$$\mathcal{U}_{N+1}^T \mathcal{N}_{N+1}^T \mathcal{K}_{N+1} \mathcal{N}_{N+1} \mathcal{U}_{N+1} = \operatorname{diag}\{P_0, \dots, P_N, X_{N+1}^T (Q_{N+1} + \Gamma) X_{N+1}\}.$$

This proves the sufficiency part of this theorem, since $X_{N+1}^T (Q_{N+1} + \Gamma) X_{N+1} \geq 0$ on $\operatorname{Ker} \mathcal{M} X_{N+1}$ iff $Q_{N+1} + \Gamma \geq 0$ on $\operatorname{Ker} \mathcal{M} \cap \operatorname{Im} X_{N+1}$.

Concerning the necessity part, suppose first that (i) is violated, i.e., there exists $m \in \{0, \dots, N\}$ and an admissible $z = \binom{x}{u}$ such that $x_k \in \operatorname{Im} X_k$ for $k = 0, \dots, m$, and $x_{m+1} \notin \operatorname{Im} X_{m+1}$. Then, by (13),

$$x_{m+1} = X_{m+1} \alpha_{m+1} + M_m d_m$$

for some $\alpha_{m+1}, d_m \in \mathbb{R}^n$ with $M_m d_m \neq 0$. Let S' be the $n \times n$ matrix satisfying $X_{m+1} S' = 0$, $U_{m+1} S' = M_m$, the existence of such a matrix is proven in [8]. Put $\tilde{\alpha} = t S' d_m$, define

$$\tilde{z} = \begin{pmatrix} \tilde{x} \\ \tilde{u} \end{pmatrix} := \begin{cases} \binom{X_k \tilde{\alpha}}{U_k \tilde{\alpha}}, & k = 0, \dots, m, \\ \binom{0}{0}, & k = m+1, \dots, N+1, \end{cases}$$

and let $z^* = z + \tilde{z}$. Then this z^* is admissible (since it is the sum of admissible sequences) and by a direct computation we have $\mathcal{F}(\tilde{z}) = 0$. Hence

$$\mathcal{F}(z^*) = \mathcal{F}(z) + 2\mathcal{F}(\tilde{z}, z),$$

where

$$\begin{aligned}
\mathcal{F}(\tilde{z}, z) &= \tilde{x}_0^T \Gamma_0 x_0 + \tilde{x}_{N+1}^T \Gamma x_{N+1} + \sum_{k=0}^{N} \tilde{z}_k^T \{S_k^T \mathcal{K} S_k - \mathcal{K}\} z_k \\
&= x_0^T \Gamma_0 \tilde{x}_0 + x_{N+1}^T \Gamma \tilde{x}_{N+1} + \sum_{k=0}^{N} z_k^T \{S_k^T \mathcal{K} S_k - \mathcal{K}\} \tilde{z}_k.
\end{aligned}$$

By using Lemma 1 and (7), together with $x_0 = X_0\alpha_0$ for some $\alpha_0 \in \mathbb{R}^n$, we have

$$\begin{aligned}
\mathcal{F}(\tilde{z}, z) &= x_0^T \Gamma_0 \tilde{x}_0 + x_{N+1}^T \Gamma \tilde{x}_{N+1} + \sum_{k=0}^{N} \{x_{k+1}^T(\mathcal{C}_k \tilde{x}_k + \mathcal{D}_k \tilde{u}_k - \tilde{u}_{k+1}) + \Delta(x_k^T \tilde{u}_k)\} \\
&= x_{m+1}^T(\mathcal{C}_m X_m + \mathcal{C}_m U_m)\tilde{\alpha} + \alpha_0^T(X_0^T \Gamma_0 X_0 - X_0^T U_0)\tilde{\alpha} \\
&= (X_{m+1}\alpha_{m+1} + M_m d_m)^T U_{m+1}\tilde{\alpha} \\
&= t \cdot d_m^T M_m^T U_{m+1} S' d_m \\
&= t \cdot d_m^T M_m^T M_m d_m \\
&= t\,||M_m d_m||^2 \to -\infty \qquad \text{as } t \to -\infty.
\end{aligned}$$

Consequently, $\mathcal{F}(z + \tilde{z}) = \mathcal{F}(z) + 2t(d^T M^T M d)_m < 0$ for t sufficiently negative.

Now let us suppose that (ii) does not hold, i.e., the matrix P_m fails to be nonnegative definite for some $m \in \{0, \dots, N\}$, then $\mathcal{F} \not\geq 0$ by [10, Theorem 1]. Recall that the admissible pair $z = \binom{x}{u}$ for which $\mathcal{F}(z) < 0$ is in this case e.g.

$$x_k := \begin{cases} X_k d & \text{for } k = 0, \dots, m \\ 0 & \text{for } k = m+1, \dots, N+1, \end{cases} \qquad u_k := \begin{cases} U_k d & \text{for } k = 0, \dots, m-1 \\ U_k d - T_k c & \text{for } k = m \\ 0 & \text{for } k = m+1, \dots, N+1, \end{cases}$$

where $c^T P_m c < 0$, $d := X_{m+1}^\dagger \mathcal{B}_m T_m c$ and, where $\binom{X}{U}$ is the natural conjoined basis at $k = 0$. It is shown in the proof of [10, Theorem 1] that $\mathcal{F}(z) = c^T P_m c < 0$.

Finally, suppose that (iii) does not hold, i.e. the endpoint condition (16) is not satisfied, i.e. $\tilde{d}^T(Q_{N+1} + \Gamma)\tilde{d} < 0$ for some $\tilde{d} \in$ Ker $\mathcal{M} \cap$ Im X_{N+1}, i.e., $\tilde{d} = X_{N+1}\tilde{c}$ and $\mathcal{M}\tilde{d} = 0$. Then $d = (0, \dots, 0, \tilde{c}^T)^T \in \mathbb{R}^{n(N+2)}$ satisfies $d \in$ Ker $\mathcal{M}\Psi$. Hence, $x = (x_0^T, \dots, x_{N+1}^T)^T := \mathcal{N}_{N+1} d$ is admissible and (with associated u) we have $\mathcal{F}(z) = \tilde{d}^T(Q_{N+1} + \Gamma)\tilde{d} < 0$. □

Remark 1. Observe that Theorems 1 and 2 are closely related, in a certain sense, to the generalized Picone identity [8, Proposition 2.1]. Indeed, this identity states that if $Z = \binom{X}{U}$ and $\tilde{Z} = \binom{\tilde{X}}{\tilde{U}}$ are normalized conjoined bases of (2), Q is given by (10), $z = \binom{x}{u}$ satisfies the equation of motion at k, i.e., $x_{k+1} = \mathcal{A}_k x_k + \mathcal{B}_k u_k$, and $x_k \in$ Im X_k, $x_{k+1} \in$ Im X_{k+1}, then

$$x_k^T \mathcal{C}_k^T \mathcal{A}_k x_k + 2u_k^T \mathcal{B}_k^T \mathcal{C}_k x_k + u_k^T \mathcal{B}_k^T \mathcal{D}_k u_k = s_k^T P_k s_k + \Delta(x_k^T Q_k x_k),$$

where $s_k = u_k - Q_k x_k$. Hence, if $Z = \binom{X}{U}$ is the natural conjoined basis at $k = 0$, i.e., $X_0^T \Gamma_0 X_0 = X_0^T Q_0 X_0$, then

$$\begin{aligned}
\mathcal{F}(z) &= x_{N+1}^T(\Gamma + Q_{N+1})x_{N+1} + \sum_{k=0}^{N} s_k^T P_k s_k \\
&= x_{N+1}^T(\Gamma + Q_{N+1})x_{N+1} + \begin{pmatrix} s_0 \\ \vdots \\ s_N \end{pmatrix}^T \operatorname{diag}\{P_0, \dots, P_N\} \begin{pmatrix} s_0 \\ \vdots \\ s_N \end{pmatrix} \\
&= \begin{pmatrix} s_0 \\ \vdots \\ s_N \\ x_{N+1} \end{pmatrix}^T \operatorname{diag}\{P_0, \dots, P_N, \Gamma + Q_{N+1}\} \begin{pmatrix} s_0 \\ \vdots \\ s_N \\ x_{N+1} \end{pmatrix}.
\end{aligned}$$

Remark 2. Let us compare the necessary and sufficient condition for the positivity and the nonnegativity of $\mathcal{F}$ in case of zero boundary conditions $x_0 = 0 = x_{N+1}$. The positivity of $\mathcal{F}$ is equivalently characterized by conditions (8), (9), while the nonnegativity of $\mathcal{F}$ is characterized by (14) and (15). Thus, the gap between the positivity and the nonnegativity of $\mathcal{F}$ is as big as the gap between the image condition (14) and the kernel condition (8). But since $\mathcal{F} \geq 0$ implies the image condition, the gap between $\mathcal{F} \geq 0$ and $\mathcal{F} > 0$ is in fact the kernel condition itself, see [10, Corollary 3] with $\mathcal{M} = I$. In the continuous–time case, and under the normality condition (i.e., the trivial solution $\binom{x}{u} \equiv \binom{0}{0}$ is the only solution of (5) for which $x(t) \equiv 0$ on an interval of positive length), and $B(t) \geq 0$, we have $\mathcal{F}_C(x, u) > 0$ iff the principal solution at $t = 0$ (i.e., the conjoined basis given by the initial condition $X(a) = 0, U(a) = I$) satisfies $\det X(t) \neq 0$ for $t \in (a, b]$. Moreover, under the same assumptions, $\mathcal{F}_C(x, u) \geq 0$ iff $\det X(t) \neq 0$ for $t \in (a, b)$. The last two conditions on $\det X(t)$ are much closer, in a certain sense, than conditions (8), (9) and (14), (15) in the discrete case.

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