Positive Definiteness of Discrete Quadratic Functionals

Martin Bohner, Universität Hohenheim, Institut 110,
D-70593 Stuttgart, Germany. E-Mail: bohner@uni-hohenheim.de

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Abstract

This summary of the author's talk presented in Oberwolfach motivates the importance of certain discrete quadratic functionals and characterizes so-called positive definiteness of them via a condition on the principal solution of a related linear Hamiltonian difference system.

1. Motivation: Discrete Variational Problems

Given a function $L : \mathbb{Z} \times \mathbb{R}^2 \to \mathbb{R}$, two integers $M, N \in \mathbb{Z}$ with $M \le N$, and two reals $\alpha, \beta \in \mathbb{R}$, one might be interested in minimizing the functional

$$\mathcal{L}(y) = \sum_{k=M}^{N} L\left(k, y_{k+1}, \Delta y_k\right) \quad \text{with} \quad \Delta y_k = y_{k+1} - y_k$$

subject to the boundary conditions $y_M = \alpha$ and $y_{N+1} = \beta$, i.e., in finding an "optimal sequence" $y^* = \left(y_M^*, \ldots, y_{N+1}^*\right)$ with $y_M^* = \alpha$ and $y_{N+1}^* = \beta$ such that $\mathcal{L}(y^*) \le \mathcal{L}(y)$ for all sequences $y = (y_M, \ldots, y_{N+1})$ with $y_M = \alpha$ and $y_{N+1} = \beta$ satisfying $\max_{M \le k \le N+1} |y_k - y_k^*| < \delta$ for some $\delta > 0$.

For a so-called admissible variation, i.e., a function $\eta : \mathbb{Z} \cap [M, N+1] \to \mathbb{R}$ with $\eta_M = \eta_{N+1} = 0$, and an admissible (i.e., as above) y^*, we define a function $\phi : \mathbb{R} \to \mathbb{R}$ by $\phi(\varepsilon) := \mathcal{L}(y^* + \varepsilon\eta)$. We assume that L is a C^2-function in the last two variables. Then the following necessary and sufficient conditions for a local (i.e., as above) minimum are easy to prove (see for example [5, Chapter 8]):

Theorem 1. If y^* is a local minimum, then $\dot{\phi}(0) = 0$ and $\ddot{\phi}(0) \ge 0$ (for all admissible variations).

Theorem 2. If $y_M^* = \alpha$, $y_{N+1}^* = \beta$, $\dot{\phi}(0) = 0$, and $\ddot{\phi}(0) > 0$ (for all admissible variations), then y^* is a (proper) local minimum.

At this point, of course, we are interested in how $\ddot{\phi}(0)$ looks like. An easy calculation yields

$$\ddot{\phi}(0) = \mathcal{F}(\eta) := \sum_{k=M}^{N} \left\{ L_{uu}(\cdot)\eta_{k+1}^2 + 2L_{uv}(\cdot)\eta_{k+1}\Delta\eta_k + L_{vv}(\cdot)\left(\Delta\eta_k\right)^2 \right\},$$

where $(\cdot)$ denotes $(k, y_{k+1}^*, \Delta y_k^*)$, and L_u, L_v are partial derivatives with respect to the second and third entry of L, respectively. Positive definiteness of $\mathcal{F}$ now means

$$\mathcal{F}(\eta) > 0 \quad \text{for all nontrivial admissible variations } \eta \quad .$$

It is the goal of this survey to generalize this concept and to give an easy characterization of positive definiteness. For a more general discussion of the motivation we refer to [3].

2. From Sturm-Liouville Difference Equations to Linear Hamiltonian Difference Systems

We start this section with looking at the following discrete quadratic functional:

$$\mathcal{F}(y) := \sum_{k=M}^{N} \left\{ q_k y_{k+1}^2 + p_k \left(\Delta y_k\right)^2 \right\} \quad \text{with} \quad p_k, q_k \in \mathbb{R},\ p_k \neq 0.$$

According to the introductory section, it is important to know about positive definiteness of $\mathcal{F}$, i.e., to answer the question when

$$\mathcal{F}(y) > 0 \text{ for all } y \neq 0 \text{ with } y_M = y_{N+1} = 0, \text{ we write } \mathcal{F} > 0,$$

holds. This is done by the following (at least for $p_k > 0$) well-known result.

Theorem 3. $\mathcal{F} > 0$ iff $\tilde{y}$ satisfies $\tilde{y}_k \tilde{y}_{k+1} p_k > 0$ for all $M+1 \leq k \leq N$.

Here, $\tilde{y}$ is the (unique) solution of the Sturm-Liouville difference equation

$$\Delta\left\{p_k \Delta y_k\right\} = q_k y_{k+1}$$

satisfying the initial conditions $\tilde{y}_M = 0$ and $\tilde{y}_{N+1} = \frac{1}{p_M}$. Of course, Theorem 3 provides an easy and useful characterization of positive definiteness, and it will follow from our more general result, Theorem 4 of the next section.

We now wish to generalize the present questioning in a certain sense. To do so, we introduce a state variable $x := y$ and a control variable $u := p\Delta y$. The above Sturm-Liouville difference equation now becomes a system of two difference equations

$$\Delta x_k = \frac{1}{p_k} u_k, \qquad \Delta u_k = q_k x_{k+1},$$

where the first "artificial" equation is called the equation of motion. The functional $\mathcal{F}$ now reads

$$\mathcal{F}(x,u)=\sum_{k=M}^{N}\left\{q_k x_{k+1}^2+\frac{1}{p_k}u_k^2\right\},$$

while the above $\tilde{y}$ corresponds to the solution $(\tilde{x},\tilde{u})$ of the system satisfying $\tilde{x}_M=0$ and $\tilde{u}_M=1$. Positive definiteness now means

$$\mathcal{F}(x,u)>0 \text{ for all admissible } (x,u) \text{ with } x\neq 0 \text{ and } x_M=x_{N+1}=0,$$

where an (x,u) is called admissible if it satisfies the equation of motion.

This is a perfect point to introduce general linear Hamiltonian difference systems

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

and corresponding discrete quadratic functionals

$$\mathcal{F}(x,u)=\sum_{k=M}^{N}\left\{x_{k+1}^T C_k x_{k+1}+u_k^T B_k u_k\right\}.$$

We are now dealing with real $n\times n$-matrices $A_k, B_k, C_k,\ k\in\mathbb{Z}$, satisfying our general assumptions

$$I-A_k \text{ invertible and } B_k, C_k \text{ symmetric},$$

while solutions (x,u) of the system are vectors $x_k,u_k\in\mathbb{R}^n$, $M\leq k\leq N+1$. An (x,u) satisfying the system's first equation is called admissible, and $\mathcal{F}>0$ now reads as before

$$\mathcal{F}(x,u)>0 \text{ for all admissible } (x,u) \text{ with } x\neq 0 \text{ and } x_M=x_{N+1}=0.$$

In the next section we prove a characterization of $\mathcal{F}>0$ involving the so-called principal solution $(\tilde{X},\tilde{U})$ of the Hamiltonian system, i.e., the solution of

$$\Delta X_k=A_k X_{k+1}+B_k U_k, \qquad \Delta U_k=C_k X_{k+1}-A_k^T U_k$$

satisfying the initial conditions $\tilde{X}_M=0$ (the $n\times n$-matrix with only zero entries) and $\tilde{U}_M=I$ (the $n\times n$-identity-matrix). Due to our assumptions, $(\tilde{X},\tilde{U})$ is easily calculated by the formula

$$\begin{pmatrix}\tilde{X}_k\\ \tilde{U}_k\end{pmatrix}=S_{k-1}\cdot S_{k-2}\cdot\ldots\cdot S_M\begin{pmatrix}0\\ I\end{pmatrix}, \qquad M+1\leq k\leq N+1$$

with the $2n\times 2n$-matrices (see also [1])

$$S_k=\begin{pmatrix}\tilde{A}_k & \tilde{A}_k B_k\\ C_k\tilde{A}_k & C_k\tilde{A}_k B_k+I-A_k^T\end{pmatrix}, \quad \text{where} \quad \tilde{A}_k:=(I-A_k)^{-1}.$$

Finally note that the case treated before indeed fits into this concept using $n=1$, $A_k=0$, $B_k=\frac{1}{p_k}$, and $C_k=q_k$.

3. The Main Result on Positive Definiteness

Using last section's terminology, our main result now reads as follows.

Theorem 4. $\mathcal{F} > 0$ iff $(\tilde{X}, \tilde{U})$ satisfies

$$\mathrm{Ker}\tilde{X}_{k+1} \subset \mathrm{Ker}\tilde{X}_k \text{ and } \tilde{X}_k \tilde{X}_{k+1}^\dagger \tilde{A}_k B_k \geq 0 \quad \text{for all} \quad M+1 \leq k \leq N.$$

Here, Ker and the dagger denote the nullspace and the Moore-Penrose inverse (i.e., $M^\dagger$ is the unique matrix satisfying $MM^\dagger M = M$ and $M^\dagger M M^\dagger = M^\dagger$ such that both $MM^\dagger$ and $M^\dagger M$ are symmetric), respectively, and "≥ 0" indicates positive semidefiniteness. Also, we will write Im for the image.

We devote the remainder of this paper to the proof of Theorem 5 below. This result then obviously implies our main result, Theorem 4 above.

Theorem 5. We abbreviate $\tilde{X}_k \tilde{X}_{k+1}^\dagger \tilde{A}_k B_k$ by D_k, and for admissible (x, u) we put $z_k := u_k - \tilde{U}_k \tilde{X}_k^\dagger x_k$. Let $m \in [M, N] \cap \mathbb{Z}$.

(i) Suppose $\mathrm{Ker}\tilde{X}_{m+1} \subset \mathrm{Ker}\tilde{X}_m$, and let (x, u) be admissible with $x_m \in \mathrm{Im}\tilde{X}_m$. Then D_m is symmetric, $x_{m+1} \in \mathrm{Im}\tilde{X}_{m+1}$, $x_m = \tilde{X}_m \tilde{X}_{m+1}^\dagger x_{m+1} - D_m z_m$, and

$$x_{m+1}^T C_m x_{m+1} + u_m^T B_m u_m = \Delta \left\{ x_m^T \tilde{U}_m \tilde{X}_m^\dagger x_m \right\} + z_m^T D_m z_m.$$

(ii) Suppose $\mathrm{Ker}\tilde{X}_{k+1} \subset \mathrm{Ker}\tilde{X}_k$ for all $M \leq k < m$ but $\mathrm{Ker}\tilde{X}_{m+1} \not\subset \mathrm{Ker}\tilde{X}_m$. Pick $c \in \mathrm{Ker}\tilde{X}_{m+1} \setminus \mathrm{Ker}\tilde{X}_m$. Then (x, u) defined by

$$(x_k, u_k) := \begin{cases} \left(\tilde{X}_k, \tilde{U}_k\right) c & M \leq k \leq m \\ 0 & m < k \leq N+1 \end{cases}$$

is admissible and satisfies $x \neq 0$, $x_m = x_{N+1} = 0$, and $\mathcal{F}(x, u) = 0$.

(iii) Suppose $\mathrm{Ker}\tilde{X}_{k+1} \subset \mathrm{Ker}\tilde{X}_k$ for all $M \leq k \leq N$ and $d^T D_m d < 0$ for some $d \in \mathbb{R}^n$. Put $c := -\tilde{X}_{m+1}^\dagger \tilde{A}_m B_m d$. Then (x, u) defined by

$$(x_k, u_k) := \begin{cases} \left(\tilde{X}_k, \tilde{U}_k\right) c & M \leq k < m \\ \left(\tilde{X}_m c, \left[\tilde{X}_m \tilde{X}_{m+1}^\dagger \tilde{A}_m\right]^T d\right) & k = m \\ 0 & m < k \leq N+1 \end{cases}$$

is admissible and satisfies $x \neq 0$, $x_m = x_{N+1} = 0$, and $\mathcal{F}(x, u) < 0$.

Proof. It is easy to see (e.g. as in [2, Lemma 4]) that $\mathrm{Ker}\tilde{X}_{m+1} \subset \mathrm{Ker}\tilde{X}_m$ implies

$$\tilde{X}_m \tilde{X}_{m+1}^\dagger \tilde{X}_{m+1} = \tilde{X}_m, \quad \tilde{X}_{m+1}^\dagger \tilde{X}_{m+1} \tilde{X}_m^\dagger = \tilde{X}_m^\dagger, \quad \tilde{X}_{m+1} \tilde{X}_{m+1}^\dagger \tilde{A}_m B_m = \tilde{A}_m B_m.$$

Furthermore, $\Delta\left\{\tilde X_k^T\tilde U_k-\tilde U_k^T\tilde X_k\right\}=0$ and $\tilde X_M^T\tilde U_M=0$ imply that $\tilde X_k^T\tilde U_k$ are symmetric so that

$$\begin{aligned} D_m &= \left\{(I-A_m)\tilde X_{m+1}-B_m\tilde A_m^T\left(\tilde U_{m+1}-C_m\tilde X_{m+1}\right)\right\}\tilde X_{m+1}^\dagger\tilde A_mB_m \\ &= B_m-B_m\tilde A_m^T\left(\tilde X_{m+1}^\dagger\right)^T\tilde X_{m+1}^T\left(\tilde U_{m+1}-C_m\tilde X_{m+1}\right)\tilde X_{m+1}^\dagger\tilde A_mB_m \end{aligned}$$

is symmetric. Now, $x_m=\tilde X_mc_m\in\mathrm{Im}\tilde X_m$ yields

$$\begin{aligned} x_{m+1} &= \tilde A_mx_m+\tilde A_mB_mu_m=\tilde X_{m+1}c_m+\tilde A_mB_m\left(u_m-\tilde U_mc_m\right) \\ &= \tilde X_{m+1}\left\{c_m+\tilde X_{m+1}^\dagger\tilde A_mB_m\left(u_m-\tilde U_mc_m\right)\right\}\in\mathrm{Im}\tilde X_{m+1}, \end{aligned}$$

$$\begin{aligned} \tilde X_{m+1}^\dagger\tilde A_mB_mz_m &= \tilde X_{m+1}^\dagger\left\{x_{m+1}-\tilde A_mx_m-\left(\tilde X_{m+1}-\tilde A_m\tilde X_m\right)\tilde X_m^\dagger x_m\right\} \\ &= \tilde X_{m+1}^\dagger x_{m+1}-\tilde X_m^\dagger x_m=\Delta\left(\tilde X_m^\dagger x_m\right), \end{aligned}$$

$$D_mz_m=\tilde X_m\tilde X_{m+1}^\dagger x_{m+1}-\tilde X_m\tilde X_m^\dagger x_m=\tilde X_m\tilde X_{m+1}^\dagger x_{m+1}-x_m,$$

$$\begin{aligned} \Delta\left(x_m^T\tilde U_m\right) &= (x_m+B_mu_m)^T\left(\tilde A_m^TC_m\tilde X_{m+1}+\tilde U_m\right)-x_m^T\tilde U_m \\ &= x_{m+1}^TC_m\tilde X_{m+1}+u_m^TB_m\tilde U_m \\ &= x_{m+1}^TC_m\tilde X_{m+1}+u_m^T(I-A_m)\tilde X_{m+1}-u_m^T\tilde X_m, \end{aligned}$$

and finally

$$\begin{aligned} &\left[\Delta\left(x_m^T\tilde U_m\right)\right]\tilde X_{m+1}^\dagger x_{m+1}=x_{m+1}^TC_mx_{m+1}+u_m^T(I-A_m)x_{m+1}-u_m^T\tilde X_m\tilde X_{m+1}^\dagger x_{m+1} \\ &= x_{m+1}^TC_mx_{m+1}+u_m^TB_mu_m-u_m^T\tilde X_m\left[\Delta\left(\tilde X_m^\dagger x_m\right)\right] \\ &= x_{m+1}^TC_mx_{m+1}+u_m^TB_mu_m-\left(x_m^T\tilde U_m+z_m^T\tilde X_m\right)\left[\Delta\left(\tilde X_m^\dagger x_m\right)\right] \\ &= x_{m+1}^TC_mx_{m+1}+u_m^TB_mu_m-z_m^TD_mz_m-x_m^T\tilde U_m\left[\Delta\left(\tilde X_m^\dagger x_m\right)\right]. \end{aligned}$$

This takes care of part (i). Now we look at (x,u) defined in (ii). Admissibility follows from

$$\tilde A_m\left(x_m+B_mu_m\right)=\tilde A_m\left(\tilde X_m+B_m\tilde U_m\right)c=\tilde X_{m+1}c=0=x_{m+1},$$

while an application of part (i) yields

$$\begin{aligned} \mathcal F(x,u) &= \sum_{k=M}^{m-1}\left\{x_{k+1}^TC_kx_{k+1}+u_k^TB_ku_k\right\}+x_{m+1}^TC_mx_{m+1}+u_m^TB_mu_m \\ &= x_m^T\tilde U_m\tilde X_m^\dagger x_m+\sum_{k=M}^{m-1}z_k^TD_kz_k+u_m^TB_mu_m \\ &= c^T\tilde U_m^T\tilde X_mc+c^T\tilde U_m^TB_m\tilde U_mc=c^T\tilde U_m^T(I-A_m)\tilde X_{m+1}c=0. \end{aligned}$$

Finally, we remark that (x, u) from (iii) is admissible because of

$$\tilde{A}_m (x_m + B_m u_m) = \tilde{A}_m \left(-D_m d + D_m^T d\right) = 0 = x_{m+1}.$$

Another application of part (i) yields

$$\mathcal{F}(x, u) = \sum_{k=M}^{N} z_k^T D_k z_k = z_m^T D_m z_m = d^T D_m d < 0$$

since $D_m z_m = \tilde{X}_m \tilde{X}_{m+1}^{\dagger} x_{m+1} - x_m = -x_m = -\tilde{X}_m c = D_m d$ holds. This finishes the proof of (iii) and hence yields all our desired results. ■

For a deeper discussion of this topic we refer to [4]. To finish with, we wish to remark and to emphasize that so-called Sturm-Liouville difference equations of higher order may be equivalently rewritten as certain linear Hamiltonian difference systems satisfying our general assumptions so that Theorem 4 applies to those important objects also.

References

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