ON MONOTONICITY OF SOLUTIONS OF DISCRETE-TIME NONNEGATIVE AND COMPARTMENTAL DYNAMICAL SYSTEMS

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Nonnegative and compartmental dynamical system models are widespread in biological, physiological, and pharmacological sciences. Since the state variables of these systems are typically masses or concentrations of a physical process, it is of interest to determine necessary and sufficient conditions under which the system states possess monotonic solutions. In this paper, we present necessary and sufficient conditions for identifying discrete-time nonnegative and compartmental dynamical systems that only admit monotonic solutions.

1. Introduction

Nonnegative dynamical systems are of paramount importance in analyzing dynamical systems involving dynamic states whose values are nonnegative [2, 9, 16, 17]. An important subclass of nonnegative systems is compartmental systems [1, 4, 6, 8, 11, 12, 13, 14, 15, 18]. These systems involve dynamical models derived from mass and energy balance considerations of macroscopic subsystems or compartments which exchange material via intercompartmental flow laws. The range of applications of nonnegative and compartmental systems is widespread in models of biological and physiological processes such as metabolic pathways, tracer kinetics, pharmacokinetics, pharmacodynamics, and epidemic dynamics.

Since the state variables of nonnegative and compartmental dynamical systems typically represent masses and concentrations of a physical process, it is of interest to determine necessary and sufficient conditions under which the system states possess monotonic solutions. This is especially relevant in the specific field of pharmacokinetics [7, 19] wherein drug concentrations should monotonically decline after discontinuation of drug administration. In a recent paper [5], necessary and sufficient conditions were developed for identifying continuous-time nonnegative and compartmental dynamical systems that only admit nonoscillatory and monotonic solutions. In this paper, we present analogous results for discrete-time nonnegative and compartmental systems.

The contents of the paper are as follows. In Section 2, we establish definitions and notation, and review some basic results on nonnegative dynamical systems. In Section 3, we introduce the notion of monotonicity of solutions of nonnegative dynamical systems. Furthermore, we provide necessary and sufficient conditions for monotonicity for linear nonnegative dynamical systems. In Section 4, we generalize the results of Section 3 to nonlinear nonnegative dynamical systems. In addition, we provide sufficient conditions that guarantee the absence of limit cycles in nonlinear compartmental systems. In Section 5, we use the results of Section 3 to characterize the class of all linear, three-dimensional compartmental systems that exhibit monotonic solutions. Finally, we draw conclusions in Section 6.

2. Notation and mathematical preliminaries

In this section, we introduce notation, several definitions, and some key results concerning discrete-time, linear nonnegative dynamical systems [2, 3, 10] that are necessary for developing the main results of this paper. Specifically, for $x \in \mathbb{R}^n$, we write $x \geq\geq 0$ (resp., $x \gg 0$) to indicate that every component of x is nonnegative (resp., positive). In this case, we say that x is *nonnegative* or *positive*, respectively. Likewise, $A \in \mathbb{R}^{n \times m}$ is *nonnegative* or *positive* if every entry of A is nonnegative or positive, respectively, which is written as $A \geq\geq 0$ or $A \gg 0$, respectively. (In this paper, it is important to distinguish between a square nonnegative (resp., positive) matrix and a nonnegative-definite (resp., positive-definite) matrix.) Let $\overline{\mathbb{R}}_+^n$ and $\mathbb{R}_+^n$ denote the nonnegative and positive orthants of $\mathbb{R}^n$; that is, if $x \in \mathbb{R}^n$, then $x \in \overline{\mathbb{R}}_+^n$ and $x \in \mathbb{R}_+^n$ are equivalent, respectively, to $x \geq\geq 0$ and $x \gg 0$. Finally, let $\mathbb{N}$ denote the set of nonnegative integers. The following definition introduces the notion of a nonnegative function.

Definition 2.1. A real function $u : \mathbb{N} \to \mathbb{R}^m$ is a *nonnegative* (resp., *positive*) *function* if $u(k) \geq\geq 0$ (resp., $u(k) \gg 0$), $k \in \mathbb{N}$.

In the first part of this paper, we consider discrete-time, linear nonnegative dynamical systems of the form

$$x(k+1) = Ax(k) + Bu(k), \quad x(0) = x_0, \ k \in \mathbb{N}, \tag{2.1}$$

where $x \in \mathbb{R}^n$, $u \in \mathbb{R}^m$, $A \in \mathbb{R}^{n \times n}$, and $B \in \mathbb{R}^{n \times m}$. The following definition and proposition are needed for the main results of this paper.

Definition 2.2. The linear dynamical system given by (2.1) is *nonnegative* if for every $x(0) \in \overline{\mathbb{R}}_+^n$ and $u(k) \geq\geq 0$, $k \in \mathbb{N}$, the solution $x(k)$, $k \in \mathbb{N}$, to (2.1) is nonnegative.

PROPOSITION 2.3 [10]. *The linear dynamical system given by (2.1) is nonnegative if and only if $A \in \mathbb{R}^{n \times n}$ is nonnegative and $B \in \mathbb{R}^{n \times m}$ is nonnegative.*

Next, we consider a subclass of nonnegative systems; namely, compartmental systems.

Definition 2.4. Let $A \in \mathbb{R}^{n \times n}$. A is a *compartmental matrix* if A is nonnegative and $\sum_{k=1}^n A_{(k,j)} \leq 1$, $j = 1, 2, \ldots, n$.

If A is a compartmental matrix and $u(k) \equiv 0$, then the nonnegative system (2.1) is called an *inflow-closed compartmental system* [10, 11, 12]. Recall that an inflow-closed compartmental system possesses a dissipation property and hence is Lyapunov-stable since the total mass in the system given by the sum of all components of the state $x(k)$, $k \in \mathbb{N}$, is nonincreasing along the forward trajectories of (2.1). In particular, with $V(x) = e^{\mathrm{T}}x$, where $e = [1, 1, \dots, 1]^{\mathrm{T}}$, it follows that

$$\Delta V(x(k)) = e^{\mathrm{T}}(A - I)x(k) = \sum_{j=1}^{n} \left[\sum_{i=1}^{n} A_{(i,j)} - 1 \right] x_j \leq 0, \quad x \in \overline{\mathbb{R}}_+^n. \tag{2.2}$$

Hence, all solutions of inflow-closed linear compartmental systems are bounded. Of course, if $\det A \neq 0$, where $\det A$ denotes the determinant of A, then A is asymptotically stable. For details of the above facts, see [10].

3. Monotonicity of linear nonnegative dynamical systems

In this section, we present our main results for discrete-time, linear nonnegative dynamical systems. Specifically, we consider monotonicity of solutions of dynamical systems of the form given by (2.1). First, however, the following definition is needed.

Definition 3.1. Consider the discrete-time, linear nonnegative dynamical system (2.1), where $x_0 \in \mathscr{X}_0 \subseteq \overline{\mathbb{R}}_+^n$, A is nonnegative, B is nonnegative, $u(k)$, $k \in \mathbb{N}$, is nonnegative, and $\mathscr{X}_0$ denotes a set of feasible initial conditions contained in $\overline{\mathbb{R}}_+^n$. Let $\hat{n} \leq n$, $\{k_1, k_2, \dots, k_{\hat{n}}\} \subseteq \{1, 2, \dots, n\}$, and $\hat{x}(k) \triangleq [x_{k_1}(k), \dots, x_{k_{\hat{n}}}(k)]^{\mathrm{T}}$. The discrete-time, linear nonnegative dynamical system (2.1) is *partially monotonic with respect to $\hat{x}$* if there exists a matrix $Q \in \mathbb{R}^{n \times n}$ such that $Q = \mathrm{diag}[q_1, \dots, q_n]$, $q_i = 0$, $i \notin \{k_1, \dots, k_{\hat{n}}\}$, $q_i = \pm 1$, $i \in \{k_1, \dots, k_{\hat{n}}\}$, and for every $x_0 \in \mathscr{X}_0$, $Qx(k_2) \leq\leq Qx(k_1)$, $0 \leq k_1 \leq k_2$, where $x(k)$, $k \in \mathbb{N}$, denotes the solution to (2.1). The discrete-time, linear nonnegative dynamical system (2.1) is *monotonic* if there exists a matrix $Q \in \mathbb{R}^{n \times n}$ such that $Q = \mathrm{diag}[q_1, \dots, q_n]$, $q_i = \pm 1$, $i = 1, \dots, n$, and for every $x_0 \in \mathscr{X}_0$, $Qx(k_2) \leq\leq Qx(k_1)$, $0 \leq k_1 \leq k_2$.

Next, we present a sufficient condition for monotonicity of a discrete-time, linear nonnegative dynamical system.

THEOREM 3.2. *Consider the discrete-time, linear nonnegative dynamical system given by (2.1), where $x_0 \in \overline{\mathbb{R}}_+^n$, $A \in \mathbb{R}^{n \times n}$ is nonnegative, $B \in \mathbb{R}^{n \times m}$ is nonnegative, and $u(k)$, $k \in \mathbb{N}$, is nonnegative. Let $\hat{n} \leq n$, $\{k_1, k_2, \dots, k_{\hat{n}}\} \subseteq \{1, 2, \dots, n\}$, and $\hat{x}(k) \triangleq [x_{k_1}(k), \dots, x_{k_{\hat{n}}}(k)]^{\mathrm{T}}$. Assume there exists a matrix $Q \in \mathbb{R}^{n \times n}$ such that $Q = \mathrm{diag}[q_1, \dots, q_n]$, $q_i = 0$, $i \notin \{k_1, \dots, k_{\hat{n}}\}$, $q_i = \pm 1$, $i \in \{k_1, \dots, k_{\hat{n}}\}$, $QA \leq\leq Q$, and $QB \leq\leq 0$. Then the discrete-time, linear nonnegative dynamical system (2.1) is partially monotonic with respect to $\hat{x}$.*

Proof. It follows from (2.1) that

$$Qx(k+1) = QAx(k) + QBu(k), \quad x(0) = x_0, \ k \in \mathbb{N}, \tag{3.1}$$

which implies that

$$Qx(k_2) = Qx(k_1) + \sum_{k=k_1}^{k_2-1} \left[Q(A - I)x(k) + QBu(k) \right]. \tag{3.2}$$

Next, since A and B are nonnegative and $u(k)$, $k \in \mathbb{N}$, is nonnegative, it follows from Proposition 2.3 that $x(k) \geq\geq 0$, $k \in \mathbb{N}$. Hence, since $-Q(A - I)$ and $-QB$ are nonnegative, it follows that $Q(A - I)x(k) \leq\leq 0$ and $QBu(k) \leq\leq 0$, $k \in \mathbb{N}$, which implies that for every $x_0 \in \overline{\mathbb{R}}_+^n$, $Qx(k_2) \leq\leq Qx(k_1)$, $0 \leq k_1 \leq k_2$. $\square$

COROLLARY 3.3. *Consider the discrete-time, linear nonnegative dynamical system given by (2.1), where $x_0 \in \overline{\mathbb{R}}_+^n$, $A \in \mathbb{R}^{n \times n}$ is nonnegative, $B \in \mathbb{R}^{n \times m}$ is nonnegative, and $u(k)$, $k \in \mathbb{N}$, is nonnegative. Assume there exists a matrix $Q \in \mathbb{R}^{n \times n}$ such that $Q = \text{diag}[q_1, \dots, q_n]$, $q_i = \pm 1$, $i = 1, \dots, n$, and $QA \leq\leq Q$ and $QB \leq\leq 0$ are nonnegative. Then the discrete-time, linear nonnegative dynamical system given by (2.1) is monotonic.*

Proof. The proof is a direct consequence of Theorem 3.2 with $\hat{n} = n$ and $\{k_1, \dots, k_{\hat{n}}\} = \{1, \dots, n\}$. $\square$

Next, we present partial converses of Theorem 3.2 and Corollary 3.3 in the case where $u(k) \equiv 0$.

THEOREM 3.4. *Consider the discrete-time, linear nonnegative dynamical system given by (2.1), where $x_0 \in \overline{\mathbb{R}}_+^n$, $A \in \mathbb{R}^{n \times n}$ is nonnegative, and $u(k) \equiv 0$. Let $\hat{n} \leq n$, $\{k_1, k_2, \dots, k_{\hat{n}}\} \subseteq \{1, 2, \dots, n\}$, and $\hat{x}(k) \triangleq [x_{k_1}(k), \dots, x_{k_{\hat{n}}}(k)]^{\mathrm{T}}$. The discrete-time, linear nonnegative dynamical system (2.1) is partially monotonic with respect to $\hat{x}$ if and only if there exists a matrix $Q \in \mathbb{R}^{n \times n}$ such that $Q = \text{diag}[q_1, \dots, q_n]$, $q_i = 0$, $i \notin \{k_1, \dots, k_{\hat{n}}\}$, $q_i = \pm 1$, $i \in \{k_1, \dots, k_{\hat{n}}\}$, and $QA \leq\leq Q$.*

Proof. Sufficiency follows from Theorem 3.2 with $u(k) \equiv 0$. To show necessity, assume that the discrete-time, linear dynamical system given by (2.1), with $u(k) \equiv 0$, is partially monotonic with respect to $\hat{x}$. In this case, it follows from (2.1) that

$$Qx(k + 1) = QAx(k), \quad x(0) = x_0, \ k \in \mathbb{N}, \tag{3.3}$$

which further implies that

$$Qx(k_2) = Qx(k_1) + \sum_{k=k_1}^{k_2-1} \left[Q(A - I)A^k x_0 \right]. \tag{3.4}$$

Now, suppose, *ad absurdum*, there exist $I, J \in \{1, 2, \dots, n\}$ such that $M_{(I,J)} > 0$, where $M \triangleq QA - Q$. Next, let $x_0 \in \overline{\mathbb{R}}_+^n$ be such that $x_{0J} > 0$ and $x_{0i} = 0$, $i \neq J$, and define $v(k) \triangleq A^k x_0$ so that $v(0) = x_0$, $v(k) \geq\geq 0$, $k \in \mathbb{N}$, and $v_J(0) > 0$. Thus, it follows that

$$[Qx(1)]_J = [Qx_0]_J + [Mv(0)]_J = [Qx_0]_J + M_{(I,J)}v_J(0) > [Qx_0]_J, \tag{3.5}$$

which is a contradiction. Hence, $QA \leq\leq Q$. $\square$

COROLLARY 3.5. *Consider the discrete-time, linear nonnegative dynamical system given by (2.1), where $x_0 \in \overline{\mathbb{R}}_+^n$, $A \in \mathbb{R}^{n \times n}$ is nonnegative, and $u(k) \equiv 0$. The linear nonnegative dynamical system (2.1) is monotonic if and only if there exists a matrix $Q \in \mathbb{R}^{n \times n}$ such that $Q = \mathrm{diag}[q_1, \ldots, q_n]$, $q_i = \pm 1$, $i = 1, 2, \ldots, n$, and $QA \leq\leq Q$.*

Proof. The proof is a direct consequence of Theorem 3.4 with $\hat{n} = n$ and $\{k_1, \ldots, k_{\hat{n}}\} = \{1, \ldots, n\}$. $\qquad\square$

Finally, we present a sufficient condition for *weighted monotonicity* for a discrete-time, linear nonnegative dynamical system.

PROPOSITION 3.6. *Consider the discrete-time, linear dynamical system given by (2.1), where A is nonnegative, $u(k) \equiv 0$, $x_0 \in \mathcal{X}_0 \triangleq \{x_0 \in \mathbb{R}^n : S(A - I)x_0 \leq\leq 0\}$, where $S \in \mathbb{R}^{n \times n}$ is an invertible matrix. If SAS^{-1} is nonnegative, then for every $x_0 \in \mathcal{X}_0$, $Sx(k_2) \leq\leq Sx(k_1)$, $0 \leq k_1 \leq k_2$.*

Proof. Let $y(k) \triangleq -S(A - I)x(k)$ and note that $y(0) = -S(A - I)x_0 \in \overline{\mathbb{R}}_+^n$. Hence, it follows from (2.1) that

$$y(k+1) = -S(A - I)x(k+1) = -S(A - I)Ax(k) = -SAS^{-1}S(A - I)x(k) = SAS^{-1}y(k). \tag{3.6}$$

Next, since SAS^{-1} is nonnegative, it follows that $y(k) \in \overline{\mathbb{R}}_+^n$, $k \in \mathbb{N}$. Now, the result follows immediately by noting that $y(k) = -S(A - I)x(k) \gg 0$, $k \in \mathbb{N}$, and hence $S(A - I)x(k) \leq\leq 0$, $k \in \mathbb{N}$, or, equivalently, $Sx(k+1) \leq\leq Sx(k)$, $k \in \mathbb{N}$, which implies that $Sx(k_2) \leq\leq Sx(k_1)$, $0 \leq k_1 \leq k_2$. $\qquad\square$

4. Monotonicity of nonlinear nonnegative dynamical systems

In this section, we extend the results of Section 3 to nonlinear nonnegative dynamical systems. Specifically, we consider discrete-time, nonlinear dynamical systems $\mathcal{G}$ of the form

$$x(k+1) = f(x(k)) + G(x(k))u(k), \quad x(0) = x_0, \ k \in \mathbb{N}, \tag{4.1}$$

where $x(k) \in \mathcal{D}$, $\mathcal{D}$ is an open subset of $\mathbb{R}^n$ with $0 \in \mathcal{D}$, $u(k) \in \mathbb{R}^m$, $f : \mathcal{D} \to \mathbb{R}^n$, and $G : \mathcal{D} \to \mathbb{R}^{n \times m}$. We assume that $f(\cdot)$ and $G(\cdot)$ are continuous in $\mathcal{D}$ and $f(x_e) = x_e$, $x_e \in \mathcal{D}$. For the nonlinear dynamical system $\mathcal{G}$ given by (4.1), the definitions of monotonicity and partial monotonicity hold with (2.1) replaced by (4.1). The following definition generalizes the notion of nonnegativity to vector fields.

Definition 4.1 [10]. *Let $f = [f_1, \ldots, f_n]^{\mathrm{T}} : \mathcal{D} \to \mathbb{R}^n$, where $\mathcal{D}$ is an open subset of $\mathbb{R}^n$ that contains $\mathbb{R}^n$. Then f is nonnegative if $f_i(x) \geq 0$, for all $i = 1, \ldots, n$ and $x \in \overline{\mathbb{R}}_+^n$.*

Note that if $f(x) = Ax$, where $A \in \mathbb{R}^{n \times n}$, then f is nonnegative if and only if A is nonnegative. The following proposition is required for the main theorem of this section.

PROPOSITION 4.2 [10]. *Consider the discrete-time, nonlinear dynamical system $\mathcal{G}$ given by (4.1). If $f : \mathcal{D} \to \mathbb{R}^n$ is nonnegative and $G(x) \geq\geq 0$, $x \in \overline{\mathbb{R}}_+^n$, then $\mathcal{G}$ is nonnegative.*

Next, we present a sufficient condition for monotonicity of a nonlinear nonnegative dynamical system.

THEOREM 4.3. *Consider the discrete-time, nonlinear nonnegative dynamical system $\mathcal{G}$ given by (4.1), where $x_0 \in \overline{\mathbb{R}}_+^n$, $f : \mathcal{D} \to \mathbb{R}^n$ is nonnegative, $G(x) \geq\geq 0$, $x \in \overline{\mathbb{R}}_+^n$, and $u(k)$, $k \in \mathbb{N}$, is nonnegative. Let $\hat{n} \leq n$, $\{k_1, k_2, \ldots, k_{\hat{n}}\} \subseteq \{1, 2, \ldots, n\}$, and $\hat{x}(k) \triangleq [x_{k_1}(k), \ldots, x_{k_{\hat{n}}}(k)]^{\mathrm{T}}$. Assume there exists a matrix $Q \in \mathbb{R}^{n \times n}$ such that $Q = \mathrm{diag}[q_1, \ldots, q_n]$, $q_i = 0$, $i \notin \{k_1, \ldots, k_{\hat{n}}\}$, $q_i = \pm 1$, $i \in \{k_1, \ldots, k_{\hat{n}}\}$, $Q f(x) \leq\leq Qx$, $x \in \overline{\mathbb{R}}_+^n$, and $QG(x) \leq\leq 0$, $x \in \overline{\mathbb{R}}_+^n$. Then the discrete-time, nonlinear nonnegative dynamical system $\mathcal{G}$ is partially monotonic with respect to $\hat{x}$.*

Proof. The proof is similar to the proof of Theorem 3.2 with Proposition 4.2 invoked in place of Proposition 2.3, and hence is omitted. □

COROLLARY 4.4. *Consider the discrete-time, nonlinear nonnegative dynamical system $\mathcal{G}$ given by (4.1), where $x_0 \in \overline{\mathbb{R}}_+^n$, $f : \mathcal{D} \to \mathbb{R}^n$ is nonnegative, $G(x) \geq\geq 0$, $x \in \overline{\mathbb{R}}_+^n$, and $u(k)$, $k \in \mathbb{N}$, is nonnegative. Assume there exists a matrix $Q \in \mathbb{R}^{n \times n}$ such that $Q = \mathrm{diag}[q_1, \ldots, q_n]$, $q_i = \pm 1$, $i = 1, \ldots, n$, $Q f(x) \leq\leq Qx$, $x \in \overline{\mathbb{R}}_+^n$, and $QG(x) \leq\leq 0$, $x \in \overline{\mathbb{R}}_+^n$. Then the discrete-time, nonlinear nonnegative dynamical system $\mathcal{G}$ is monotonic.*

Proof. The proof is a direct consequence of Theorem 4.3 with $\hat{n} = n$ and $\{k_1, \ldots, k_{\hat{n}}\} = \{1, \ldots, n\}$. □

Next, we present necessary and sufficient conditions for partial monotonicity and monotonicity for (4.1) in the case where $u(k) \equiv 0$.

THEOREM 4.5. *Consider the discrete-time, nonlinear nonnegative dynamical system $\mathcal{G}$ given by (4.1), where $x_0 \in \overline{\mathbb{R}}_+^n$, $f : \mathcal{D} \to \mathbb{R}^n$ is nonnegative, and $u(k) \equiv 0$. Let $\hat{n} \leq n$, $\{k_1, k_2, \ldots, k_{\hat{n}}\} \subseteq \{1, 2, \ldots, n\}$, and $\hat{x}(k) \triangleq [x_{k_1}(k), \ldots, x_{k_{\hat{n}}}(k)]^{\mathrm{T}}$. The discrete-time, nonlinear nonnegative dynamical system $\mathcal{G}$ is partially monotonic with respect to $\hat{x}$ if and only if there exists a matrix $Q \in \mathbb{R}^{n \times n}$ such that $Q = \mathrm{diag}[q_1, \ldots, q_n]$, $q_i = 0$, $i \notin \{k_1, \ldots, k_{\hat{n}}\}$, $q_i = \pm 1$, $i \in \{k_1, \ldots, k_{\hat{n}}\}$, and $Q f(x) \leq\leq Qx$, $x \in \overline{\mathbb{R}}_+^n$.*

Proof. Sufficiency follows from Theorem 4.3 with $u(k) \equiv 0$. To show necessity, assume that the nonlinear dynamical system given by (4.1), with $u(k) \equiv 0$, is partially monotonic with respect to $\hat{x}$. In this case, it follows from (4.1) that

$$Qx(k+1) = Qf(x(k)), \quad x(0) = x_0, \ k \in \mathbb{N}, \tag{4.2}$$

which implies that for every $k \in \mathbb{N}$,

$$Qx(k_2) = Qx(k_1) + \sum_{k=k_1}^{k_2-1} [Qf(x(k)) - Qx(k)]. \tag{4.3}$$

Now, suppose, *ad absurdum*, there exist $J \in \{1, 2, \ldots, n\}$ and $x_0 \in \overline{\mathbb{R}}_+^n$ such that $[Qf(x_0)]_J > [Qx_0]_J$. Hence,

$$[Qx(1)]_J = [Qx_0]_J + [Qf(x_0) - Qx_0]_J > [Qx_0]_J, \tag{4.4}$$

which is a contradiction. Hence, $Qf(x) \leq\leq Qx$, $x \in \overline{\mathbb{R}}_+^n$. □

COROLLARY 4.6. *Consider the discrete-time, nonlinear nonnegative dynamical system $\mathcal{G}$ given by (4.1), where $x_0 \in \overline{\mathbb{R}}_+^n$, $f : \mathcal{D} \to \mathbb{R}^n$ is nonnegative, and $u(k) \equiv 0$. The discrete-time, nonlinear nonnegative dynamical system $\mathcal{G}$ is monotonic if and only if there exists a matrix $Q \in \mathbb{R}^{n \times n}$ such that $Q = \operatorname{diag}[q_1, \ldots, q_n]$, $q_i = \pm 1$, $i = 1, \ldots, n$, and $Qf(x) \leq\leq Qx$, $x \in \overline{\mathbb{R}}_+^n$.*

Proof. The proof is a direct consequence of Theorem 4.5 with $\hat{n} = n$ and $\{k_1, \ldots, k_{\hat{n}}\} = \{1, \ldots, n\}$. □

Corollary 4.6 provides some interesting ramifications with regard to the absence of limit cycles of inflow-closed nonlinear compartmental systems. To see this, consider the inflow-closed ($u(k) \equiv 0$) compartmental system (4.1), where $f(x) = [f_1(x), \ldots, f_n(x)]$ is such that

$$f_i(x) = x_i - a_{ii}(x) + \sum_{j=1,\ i \neq j}^{n} [a_{ij}(x) - a_{ji}(x)] \tag{4.5}$$

and where the instantaneous rates of compartmental material losses $a_{ii}(\cdot)$, $i = 1, \ldots, n$, and intercompartmental material flows $a_{ij}(\cdot)$, $i \neq j$, $i, j = 1, \ldots, n$, are such that $a_{ij}(x) \geq 0$, $x \in \overline{\mathbb{R}}_+^n$, $i, j = 1, \ldots, n$. Since all mass flows as well as compartment sizes are nonnegative, it follows that for all $i = 1, \ldots, n$, $f_i(x) \geq 0$ for all $x \in \overline{\mathbb{R}}_+^n$. Hence, f is nonnegative. As in the linear case, inflow-closed nonlinear compartmental systems are Lyapunov-stable since the total mass in the system given by the sum of all components of the state $x(k)$, $k \in \mathbb{N}$, is nonincreasing along the forward trajectories of (4.1). In particular, taking $V(x) = e^{\mathrm{T}} x$ and assuming $a_{ij}(0) = 0$, $i, j = 1, \ldots, n$, it follows that

$$\Delta V(x) = \sum_{i=1}^{n} \Delta x_i = -\sum_{i=1}^{n} a_{ii}(x) + \sum_{i=1}^{n} \sum_{j=1,\ i \neq j}^{n} [a_{ij}(x) - a_{ji}(x)] = -\sum_{i=1}^{n} a_{ii}(x) \leq 0, \quad x \in \overline{\mathbb{R}}_+^n, \tag{4.6}$$

which shows that the zero solution $x(k) \equiv 0$ of the inflow-closed nonlinear compartmental system (4.1) is Lyapunov-stable and for every $x_0 \in \overline{\mathbb{R}}_+^n$, the solution to (4.1) is bounded.

In light of the above, it is of interest to determine sufficient conditions under which masses/concentrations for nonlinear compartmental systems are Lyapunov-stable *and* convergent, guaranteeing the absence of limit-cycling behavior. The following result is

a direct consequence of Corollary 4.6 and provides sufficient conditions for the absence of limit cycles in nonlinear compartmental systems.

THEOREM 4.7. *Consider the nonlinear nonnegative dynamical system $\mathcal{G}$ given by (4.1) with $u(k) \equiv 0$ and $f(x) = [f_1(x),\ldots,f_n(x)]$ such that (4.5) holds. If there exists a matrix $Q \in \mathbb{R}^{n \times n}$ such that $Q = \mathrm{diag}[q_1,\ldots,q_n]$, $q_i = \pm 1$, $i = 1,\ldots,n$, and $Qf(x) \leq\leq Qx$, $x \in \overline{\mathbb{R}}_+^n$, then for every $x_0 \in \overline{\mathbb{R}}_+^n$, $\lim_{k\to\infty} x(k)$ exists.*

Proof. Let $V(x) = e^{\mathrm{T}}x$, $x \in \overline{\mathbb{R}}_+^n$. Now, it follows from (4.6) that $\Delta V(x(k)) \leq 0$, $k \in \mathbb{N}$, where $x(k)$, $k \in \mathbb{N}$, denotes the solution of $\mathcal{G}$, which implies that $V(x(k)) \leq V(x_0) = e^{\mathrm{T}}x_0$, $k \in \mathbb{N}$, and hence for every $x_0 \in \overline{\mathbb{R}}_+^n$, the solution $x(k)$, $k \in \mathbb{N}$, of $\mathcal{G}$ is bounded. Hence, for every $i \in \{1,\ldots,n\}$, $x_i(k)$, $k \in \mathbb{N}$, is bounded. Furthermore, it follows from Corollary 4.6 that $x_i(k)$, $k \in \mathbb{N}$, is monotonic. Now, since $x_i(\cdot)$, $i \in \{1,\ldots,n\}$, is bounded and monotonic, it follows that $\lim_{k\to\infty} x_i(k)$, $i = 1,\ldots,n$, exists. Hence, $\lim_{k\to\infty} x(k)$ exists.   □

5. A Taxonomy of three-dimensional monotonic compartmental systems

In this section, we use the results of Section 3 to provide a taxonomy of linear three-dimensional, inflow-closed compartmental dynamical systems that exhibit monotonic solutions. A similar classification can be obtained for nonlinear and higher-order compartmental systems, but we do not do so here for simplicity of exposition. To characterize the class of all three-dimensional monotonic compartmental systems, let $\mathcal{Q} \triangleq \{Q \in \mathbb{R}^{3 \times 3} : Q = \mathrm{diag}[q_1, q_2, q_3], q_i = \pm 1, i = 1, 2, 3\}$. Furthermore, let $A \in \mathbb{R}^{3 \times 3}$ be a compartmental matrix and let $x_1(k)$, $x_2(k)$, and $x_3(k)$, $k \in \mathbb{N}$, denote compartmental masses for compartments 1, 2, and 3, respectively. Note that there are exactly eight matrices in the set $\mathcal{Q}$. Now, it follows from Corollary 3.5 that if $QA \leq\leq Q$, $Q \in \mathcal{Q}$, then the corresponding compartmental dynamical system is monotonic. Hence, for every $Q \in \mathcal{Q}$, we seek all compartmental matrices $A \in \mathbb{R}^{3 \times 3}$ such that $q_i A_{(i,i)} \leq q_i$, $i = 1, 2, 3$, and $q_i A_{(i,j)} \leq 0$, $i \neq j$, $i, j = 1, 2, 3$.

First, we consider the case where $Q = \mathrm{diag}[1, 1, 1]$. In this case, $q_i A_{(i,i)} \leq q_i$, $i = 1, 2, 3$, and $q_i A_{(i,j)} \leq 0$, $i \neq j$, $i, j = 1, 2, 3$, if and only if $A_{(1,2)} = A_{(1,3)} = A_{(2,1)} = A_{(3,1)} = A_{(3,2)} = A_{(2,3)} = 0$. This corresponds to a trivial (decoupled) case since there are no intercompartmental flows between the three compartments (see Figure 5.1(a)). Next, let $Q = \mathrm{diag}[1, -1, -1]$ and note that $q_i A_{(i,i)} \leq q_i$, $i = 1, 2, 3$, and $q_i A_{(i,j)} \leq 0$, $i \neq j$, $i, j = 1, 2, 3$, if and only if $A_{(2,2)} = A_{(3,3)} = 1$ and $A_{(1,2)} = A_{(1,3)} = A_{(2,3)} = A_{(3,2)} = 0$. Figure 5.1(b) shows the compartmental structure for this case. Finally, let $Q = \mathrm{diag}[-1, 1, 1]$. In this case, $q_i A_{(i,i)} \leq q_i$, $i = 1, 2, 3$, and $q_i A_{(i,j)} \leq 0$, $i \neq j$, $i, j = 1, 2, 3$, if and only if $A_{(1,1)} = 1$ and $A_{(2,1)} = A_{(3,1)} = A_{(3,2)} = A_{(2,3)} = 0$. Figure 5.1(c) shows the corresponding compartmental structure.

It is important to note that in the case where $Q = \mathrm{diag}[-1, -1, -1]$, there does not exist a compartmental matrix satisfying $QA \leq\leq Q$ except for the identity matrix. This case would correspond to a compartmental dynamical system where all three states are monotonically increasing. Hence, the compartmental system would be unstable, contradicting the fact that all compartmental systems are Lyapunov-stable. Finally, the remaining four cases corresponding to $Q = \mathrm{diag}[-1, 1, -1]$, $Q = \mathrm{diag}[-1, -1, 1]$, $Q = \mathrm{diag}[1, -1, 1]$, and $Q = \mathrm{diag}[1, 1, -1]$ are dual to the cases where $Q = \mathrm{diag}[1, -1, -1]$ and $Q = \mathrm{diag}[-1, 1, 1]$, and hence are not presented.
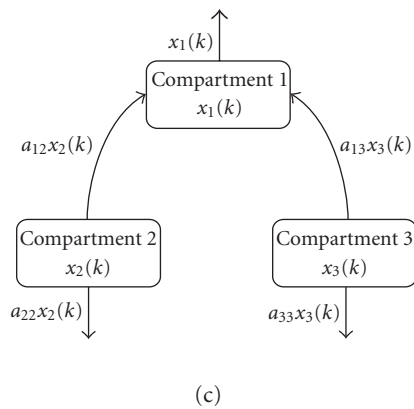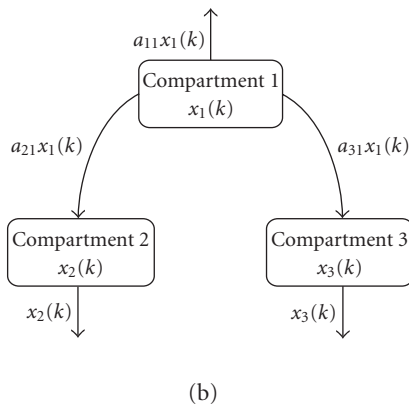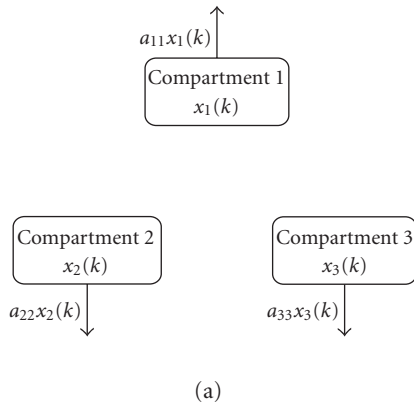
Figure 5.1. Three-dimensional monotonic compartmental systems.

6. Conclusion

Nonnegative and compartmental models are widely used to capture system dynamics involving the interchange of mass and energy between homogeneous subsystems. In this paper, necessary and sufficient conditions were given, under which linear and nonlinear discrete-time nonnegative and compartmental systems are guaranteed to possess monotonic solutions. Furthermore, sufficient conditions that guarantee the absence of limit cycles in nonlinear discrete-time compartmental systems were also provided.

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