Ladislav Adamec

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KINETICAL SYSTEMS—LOCAL ANALYSIS

Ladislav Adamec, Brno

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Abstract. The paper gives the answer to the question of the number and qualitative character of stationary points of an autonomous detailed balanced kinetical system.

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1. Introduction

Throughout this paper $\mathbb{Z}$ denotes the set of integers, $\mathbb{R}$ the set of real numbers, $\mathbb{R}^n$ the space of n-dimensional real column vectors, $\mathbb{R}^n_{\geqslant 0}$ ($\mathbb{R}^n_{>0}$) the nonnegative (positive) orthant in $\mathbb{R}^n$, $\langle u|v\rangle$ the inner product of vectors u and v and $\|u\|$ the corresponding norm $\|u\| := \langle u|u\rangle^{1/2}$. A^* denotes the conjugate transpose of the matrix A ($A^* := \overline{A}^T$). If $A \in \mathbb{R}^{r\times s}$ is an $r \times s$ matrix, then $\operatorname{col}_i(A)$ denotes the i-th column of the matrix A and $A(i_1, \ldots, i_n)$ denotes the principal submatrix of A which consists of i_1-th, …, i_n-th columns and rows of the matrix A.

In [1] an interesting class of nonlinear ordinary differential equations, widely used in chemistry, physical chemistry and biology, the so called kinetical systems, was introduced:

Definition 1.1. Consider $n \times m$ matrices $C = [c_{ij}]$, $C' = [c'_{ij}]$, where c_{ij}, $c'_{ij} \in \mathbb{Z}_{\geqslant 0}$ and $A = [a_{ij}] := C - C'$, $0 < L := \operatorname{rank}(A) < n$. Let $r_j, d_j\colon \mathbb{R} \to [0, \infty)$ be continuous functions and let $G = [G_j]$ be a m-dimensional vector such that

$$G_j(t, y) := -r_j(t) \prod_{k=1}^{n} y_k^{c_{kj}} + d_j(t) \prod_{k=1}^{n} y_k^{c'_{kj}}.$$

The system of equations

$$\dot{y} = AG(t, y), \quad (t, y) \in \mathbb{R} \times \mathbb{R}^n, \tag{1}$$

is called the *kinetical system* (KS).

Remark 1. In what follows we shall always suppose that the principal submatrix $A(1,\dots,L)$ is nonsingular.

Since $\operatorname{rank}(A) < n$ there is a real $d\times n$ matrix $U=[u_{ij}]$ of the rank $d=n-L$ such that $UA=0$. It is clear that for any vector $b\in\mathbb{R}^d$ the L–dimensional linear manifold $L(U,b) := \{y\in\mathbb{R}^n:\ Uy=b\}$ is an invariant set of (1). Other important (positively) invariant sets of (1) are the nonnegative orthant $\mathbb{R}^n_{\geqslant 0}$ and the set $H := L(U,b)\cap\mathbb{R}^n_{\geqslant 0}$. From the point of view of applications the most important case occurs if the elements u_{ij} are nonnegative integers and $\sum\limits_{i=1}^{d} u_{ij} > 0$ for $j=1,\dots,n$. Such matrix U is called the *nonnegative formula matrix* in [1]. As follows from Remark 1 there is a unique real $L\times n$ matrix $Z=[z_{ij}]$ such that

$$\operatorname{col}_j(A) = \sum_{i=1}^{L} \operatorname{col}_i(A) z_{ij} \qquad \text{for}\quad j=1,\dots,m.$$

Among all kinetical systems a very interesting subclass exists, which consists of all kinetical systems fulfilling the conditions

$$\prod_{i=1}^{L}\left[\frac{d_i(t)}{r_i(t)}\right]^{z_{ij}} = \frac{d_j(t)}{r_j(t)} \qquad \text{for}\quad j=1,\dots,m. \tag{2}$$

Such systems, denoted in [1] as *detailed balanced kinetical systems*, are in strong correspondence with critical points of (1) fulfilling the conditions $G_j(t,y)=0$ for $j=1,\dots,m$, called in [1] *balanced critical points.*

Supposing the hypotheses

- H1 *there is at least one nonnegative formula matrix U – one of them is chosen fixed.*
- H2 *there exists a vector $b\in\mathbb{R}^d_{>0}$ such that there is a nonnegative solution $y\in\mathbb{R}^d_{\geqslant 0}$ of $Uy=b$, that is the set $H := L(U,b)\cap\mathbb{R}^n_{\geqslant 0}$ is not empty. One such vector is chosen fixed.*
- H3 $r_i(t),\ d_i(t)\geqslant \xi_i > 0$ *for* $i=1,\dots,m$.
- H4 *if $y=[y_1,\dots,y_n]$ is a nonnegative solution of* (1), *then $y_i\not\equiv 0$ on the right maximal interval of existence $[t_0,\infty)$ for $i=1,\dots,n$.*

The following theorem was proved in [1] for the autonomous kinetical system

$$\dot y = AG(y). \tag{3}$$

Theorem 1.2. *Suppose that the detailed balanced system* (3) *satisfies* H1, H2, H3, H4. *If the stationary points of* (3) *are isolated, then* (3) *has exactly one stationary* *point uniformly stable with respect to the set H, other stationary points* (*if they exist*) *being unstable.*

Notice that H1 and H2 mean, that Theorem 1.2 in fact concerns the "differential-algebraic" system

$$\dot{y} = AG(y), \qquad y \in H. \tag{4}$$

In this sense Theorem 1.2 speaks about critical points, stability, closure, isolated points and so on.

This article fulfils the gap in Theorem 1.2 concerning the number and properties of stationary points of (4). The method used is the method of linearization. Perhaps the interesting point is that sometimes it is not the best way to use information about even linear first integrals of the system explored for the reduction of the system to a lower-dimensional one. At least in this case this is the path leading to the swamp of "common polynomial systems" and it is well known that for polynomial systems to answer even the simplest question is sometimes extremely difficult.

2. Asymptotic properties

Let us start with the following remark.

Remark 2. Consider a system of "differential–algebraic" equations

$$\begin{aligned} \dot{x} &= AF(x), \\ Ux &= c, \end{aligned} \tag{5}$$

where x and c are real n vectors, A is a real $n \times m$ matrix of rank L, U is a real $d \times n$ matrix of rank d, $L + d = n, Ld \neq 0$ such that $UA = 0$ and F is a real sufficiently smooth m vector. Let $\tilde{x}$ be a stationary point of (5). The transformation $y = x - \tilde{x}$ of (5) yields the system

$$\begin{aligned} \dot{y} &= Jy + f(y), \\ Uy &= 0, \end{aligned} \tag{6}$$

where $UJ = Uf(y) = 0$, $J := A\partial_x F(\tilde{x})$, $f := A\mathcal{O}(\|y\|^2)$ ($\mathcal{O}$ is the Landau order symbol). Since $UJ = 0$ and $\operatorname{rank}(U) = d$, at least d eigenvalues of J are equal to zero and there is a nonsingular real matrix T such that

$$T^{-1}JT = \begin{bmatrix} B & 0 \\ 0 & C \end{bmatrix},$$

where B is an $L \times L$ matrix and C is a $d \times d$ matrix with zero eigenvalues only. After a linear change of the variable $y = T\xi$ the system (6) becomes

$$\begin{aligned}
&\dot{\xi} = T^{-1}JT\xi + T^{-1}f(T\xi),\\
&UT\xi = 0,
\end{aligned}$$

or after denoting $\xi = [\xi_L, \xi_d]^T$, $\xi_L \in \mathbb{R}^L$, $\xi_d \in \mathbb{R}^d$, $V = [V_L, V_d] := UT$, $V_L \in \mathbb{R}^{d\times L}$, $V_d \in \mathbb{R}^{d\times d}$ and $h := T^{-1}f$, $h = [h_L, h_d]^T$, $h_L(\xi) \in \mathbb{R}^L$, $h_d(\xi) \in \mathbb{R}^d$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix}\xi_L\\ \xi_d\end{bmatrix} = \begin{bmatrix}B & 0\\ 0 & C\end{bmatrix}\begin{bmatrix}\xi_L\\ \xi_d\end{bmatrix} + \begin{bmatrix}h_L(\xi_L, \xi_d)\\ h_d(\xi_L, \xi_d)\end{bmatrix}, \tag{7}$$

$$V\xi = 0. \tag{8}$$

If the Jacobian matrix J has L nonzero eigenvalues, then B is nonsingular,

$$[\,V_L, V_d\,]\begin{bmatrix}B & 0\\ 0 & 0\end{bmatrix} = 0, \tag{9}$$

hence $V_L = 0$ and V_d is nonsingular. From (8) we have $\xi_d = 0$ and the system (7)–(8) is equivalent to the L dimensional system

$$\dot{z} = Bz + h_L(z, 0), \tag{10}$$

where $z = \xi_L$. Any assertion made about (10) yields implications for system (5) which are easily traced back using the above transformations. The asymptotic behaviour of (5) is therefore determined by the asymptotic behaviour of (10). One of simple consequences is that if for a stationary point $\tilde{x}$ the Jacobian matrix of (5) has exactly L eigenvalues with negative real parts, then $\tilde{x}$ is asymptotically stable with respect to the set $L(U, c) := \{x \in \mathbb{R}^n : Ux = c\}$.

In the proof of Theorem 2.4 we use two algebraic lemmas of independent interest.

Lemma 2.1. *Let A be a complex $n \times m$ matrix of rank r, then the Gram matrix A^*A (or AA^*) of A a) is a positive semidefinite matrix, b) is a matrix of rank r.*

Proof. Suppose $n \leqslant m$ and consider the case A^*A, the other cases being similar. a) It is clear that the matrix A^*A is a Hermitian matrix. For each m-dimensional complex vector x, $\langle x|A^*Ax\rangle = \langle Ax|Ax\rangle = \|Ax\|^2 \geqslant 0$, hence A^*A is positive semidefinite. b) Since A^*A is positive semidefinite of rank s, there is a unitary $m \times m$ matrix U such that

$$A^*A = U^* \operatorname{diag}[d_1, \dots, d_s, 0, \dots, 0]U,$$

where $d_i > 0$ for $i = 1, \ldots, s$. Then

$$\operatorname{diag}[d_1, \ldots, d_s, 0, \ldots, 0] = UA^*AU^* = (AU^*)^*(AU^*),$$

hence

$$\langle \operatorname{col}_i(AU^*) | \operatorname{col}_j(AU^*) \rangle = \begin{cases} d_i & \text{if} \quad i = j \in \{1, \ldots, s\} \\ 0 & \text{otherwise,} \end{cases}$$

in particular $\operatorname{col}_i(AU^*)$ are linearly independent for $i = 1, \ldots, s$ and $\operatorname{col}_i(AU^*) = o_n$ for $i = s+1, \ldots, m$, where o_n is the n-dimensional zero vector. Therefore

$$AU^* = [\operatorname{col}_1(AU^*), \ldots, \operatorname{col}_s(AU^*), o_n, \ldots, o_n]$$

or

$$A = [\operatorname{col}_1(AU^*), \ldots, \operatorname{col}_s(AU^*), o_n, \ldots, o_n]U,$$

and $r = \operatorname{rank}(A) = \operatorname{rank}[\operatorname{col}_1(AU^*), \ldots, \operatorname{col}_s(AU^*), o_n, \ldots, o_n] = s = \operatorname{rank}(A^*A)$.

□

Lemma 2.2. *Let $\Lambda = \operatorname{diag}[y_1, \ldots, y_n]$ be a positive definite real matrix and $V = [v_{ij}]$ a real positive definite n matrix, then all eigenvalues of the matrix*

$$A = V\Lambda \tag{11}$$

are positive.

Proof. It is well known that coefficients p_k of the characteristic polynomial of any matrix B

$$\det(B - \lambda I) = (-\lambda)^n + p_{n-1}(-\lambda)^{n-1} + \ldots + p_1(-\lambda) + p_0$$

are the sums of principal minors of order k of the matrix B, $p_k := \sum \det(B(i_1, \ldots, i_k))$ [2, p. 363].

Let $V(i_1, \ldots, i_k)$ be an arbitrary principal submatrix of V of order k, $1 \leqslant k \leqslant n$ chosen fixed and let $\xi \in \mathbb{R}$ and $u = \operatorname{col}[u_1, \ldots, u_k] \in \mathbb{R}^k$ be an eigenvalue and the corresponding eigenvector of $V(i_1, \ldots, i_k)$. Let $\tilde{u}$ be the vector created from the zero vector $o_n \in \mathbb{R}^n$ by replacing its i_1-th, …, i_k-th coordinates by numbers $u_1, \ldots, u_k$. Then

$$0 < \langle V\tilde{u} | \tilde{u} \rangle = \langle V(i_1, \ldots i_k)u | u \rangle = \langle \xi u | u \rangle = \xi \|u\|^2$$

and $\xi > 0$. Since the determinant of any matrix is equal to the product of its eigenvalues, $\det(V(i_1, \ldots, i_k)) > 0$ and similarly

$$\det(A(i_1, \ldots, i_k)) = \lambda_{i_1} \ldots \lambda_{i_k} \det(V(i_1, \ldots, i_k)) > 0.$$

Therefore all the coefficients $p_0, \dots, p_{n-1}$ of the characteristic polynomial of A are positive. The matrix $A = (\sqrt{\Lambda})^{-1}(\sqrt{\Lambda}V\sqrt{\Lambda})(\sqrt{\Lambda})$ is similar to the symmetric matrix $\sqrt{\Lambda}V\sqrt{\Lambda}$, hence its eigenvalues are real. It is clear that $\det(A - \lambda I) \geqslant p_0 > 0$ for any nonpositive λ, hence all eigenvalues of A are positive. $\square$

Corollary 2.3. If in the previous lemma we replace the positive definite matrix V by the positive semidefinite matrix V, the eigenvalues of the matrix A will be nonnegative.

Theorem 2.4. *Suppose that the detailed balanced system* (4) *satisfies* H1, H2, H3, H4. *Then any stationary point $y \in H$ of* (4) *is asymptotically stable with respect to H.*

Proof. Let the kinetical system (4) be detailed balanced and let $J(y) = [J_{is}(y)]$ denote the Jacobian matrix of (4), then on $H \cap \mathbb{R}^n_{>0}$ we have

$$J_{is}(y) = \frac{1}{y_s}\sum_{j=1}^{m}(c_{ij} - c'_{ij})\Big[-r_j c_{sj}\prod_{k=1}^{n} y_k^{c_{kj}} + d_j c'_{sj}\prod_{k=1}^{n} y_k^{c'_{kj}}\Big].$$

It follows from H4 that any stationary point $\tilde{y} \in H$ of (4) belongs to $H \cap \mathbb{R}^n_{>0}$. Since (4) is detailed balanced, $\tilde{y}$ is a balanced stationary point [1, Theorem 2.13], therefore

$$r_j \prod_{k=1}^{n} \tilde{y}_k^{c_{kj}} = d_j \prod_{k=1}^{n} \tilde{y}_k^{c'_{kj}}$$

holds and

$$\begin{aligned} J_{is}(\tilde{y}) &= -\frac{1}{\tilde{y}_s}\sum_{j=1}^{m}(c_{ij} - c'_{ij})(c_{sj} - c'_{sj})r_j\prod_{k=1}^{n}\tilde{y}_k^{c_{kj}} \\ &= -\frac{1}{\tilde{y}_s}\sum_{j=1}^{m} a_{ij}a_{sj}r_j\prod_{k=1}^{n}\tilde{y}_k^{c_{kj}} \\ &=: -\frac{1}{\tilde{y}_s}v_{is}. \end{aligned}$$

Hence at any stationary point $\tilde{y} \in H$ the Jacobian matrix J is the product

$$J = -V\Lambda,$$

where

$$V = [v_{is}] = \Big[\sum_{j=1}^{m} a_{ij}a_{sj}r_j\prod_{k=1}^{n}\tilde{y}_k^{c_{kj}}\Big]_{is}$$

and

$$\Lambda = \operatorname{diag}\left[\frac{1}{\tilde{y}_1}, \dots, \frac{1}{\tilde{y}_n}\right]$$

are real symmetric $n \times n$ matrices. As

$$V = A \operatorname{diag}\left[r_1 \prod_{k=1}^{n} \tilde{y}_k^{c_{k1}}, \dots, r_m \prod_{k=1}^{n} \tilde{y}_k^{c_{km}}\right] A^T =: ADA^T$$

and $r_i > 0 \quad i = 1, \dots, m$, the matrix V is the Gram matrix of the matrix $A\sqrt{D}$, therefore V is positive semidefinite and since $\sqrt{D}$ is regular, $\operatorname{rank}(V) = \operatorname{rank}(A) = L$.

Therefore the Jacobian matrix of the detailed balanced KS (4) at any stationary point $\tilde{y} \in H$ has exactly L negative eigenvalues and $d = n - L$ zero eigenvalues. This means that the variational equation $\dot{x} = J(\tilde{y})x$ is asymptotically stable with respect to H and (due to Remark 2) that the stationary point $\tilde{y} \in H$ of (4) is stable with respect to H. $\square$

The direct consequence of Theorem 1.2 and Theorem 2.4 is

Theorem 2.5. *Suppose that the detailed balanced system* (4) *satisfies* H1, H2, H3, H4, *then* (4) *is globally asymptotically stable with respect to the set H.*

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Author's address: *Ladislav Adamec*, Technical University of Brno, Božetěchova 2, 612 66 Brno, Czech Republic, e-mail: `adamec@dame.fee.vutbr.cz` resp. `adamec@usej.fee.vutbr.cz`.