The underlying linear dynamics of some positive polynomial systems

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Abstract

The conditions of structural dynamical similarity of two special class of positive polynomial nonlinear systems, the class of Quasi-Polynomial systems [1] and that of reaction kinetic networks with mass action kinetics [2] are investigated in this Letter. It is shown that both system classes have an underlying reduced linear dynamics. By applying the theory of X-factorable systems [3], it can be shown that the reduced linear dynamics is qualitatively similar to the original one within the positive orthant when the original nonlinear system has a unique positive equilibrium point.

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1. Introduction

The class of nonnegative dynamic systems, where the state variables remain in the nonnegative orthant while the dynamics evolves, appear naturally in many physical systems, such as thermodynamical, transportation, chemical or nuclear systems [4]. Within this class the systems that have or that are transformable to polynomial right-hand sides are of great importance: the sub-class of quasi-polynomial (QP) systems [1] and that of reaction kinetic networks with mass action kinetics [2] (reaction kinetic systems in short), the formal relationship of which is the subject of this paper.

QP systems admit an equivalence transformation, the so called quasi-monomial transformation, that splits them into equivalence classes, where a Lotka-Volterra (LV) system represents the members of the class. The dynamics of the corresponding LV system of the members of an equivalence class is the same and it is invariant under the quasi-monomial transformation. This makes the stability analysis of QP systems feasible with a Lyapunov function expressed in the variables and parameters of the LV representant member [5], [6].

Reaction kinetic systems can be seen as special QP systems, therefore they can be represented that way [7], but this results in a gross increase in the dimension of the system, while many of the important characteristic structural properties are lost. At the same time, reaction kinetic systems are

invariant at most under a variable re-scaling (and possibly variable permutation) transformation, and the analysis of their dynamical properties is quite difficult in the general case [8].

Therefore, the aim of our work was to explore the apparent similarities in the two above mentioned positive polynomial systems, the QP and reaction kinetic systems, to find formal methods to examine their dynamical similarity.

2. Basic notions

2.1. Translated X-factorable transformation and structurally similar dynamics

Assume that the following set of ordinary differential equations

$$\frac{dX}{dt} = F(X) \tag{1}$$

is defined on the positive orthant $\mathcal{P}^n$. The singular solutions of Eq. (1) are defined by $F(X) = 0$. Consider the following nonlinear translated X-factorable transformation of Eq. (1)

$$\frac{dX}{dt} = \overline{X}F(X - C) \tag{2}$$

where $\overline{X} = \mathrm{diag}(x_1, ..., x_n)$, the elements of $C = [c_1, \ldots, c_n]^T$ are positive real numbers, and $X = [x_1, ..., x_n]^T$.

Assume that $F(X)$ is composed of polynomial-type functions with a finite number of singular solutions. It can be shown [3] that the above transformation can move the singular solutions into the positive orthant, and leaves the geometry of the state (or phase) space unchanged within it (but not at or near the boundary). Therefore, the dynamics of the solutions of Eqs. (1) and (2) will be called structurally similar.

2.2. Reduced form of linear ODEs

Assume we have two full rank rectangular matrices $G \in \mathbb{R}^{m\times n}$ and $H \in \mathbb{R}^{n\times m}$ with $m \geq n$, and a set of linear ODEs

$$\frac{dZ}{dt} = G \cdot H \cdot Z \tag{3}$$

with $Z \in \mathbb{R}^m$. Using their full rank property, the matrices G, H and their product can be decomposed as

$$G = \left[\begin{array}{c} G^* \\ ---- \\ N_G G^* \end{array}\right],\ H = \left[\ H^* \mid H^* N_H\right],\ G{\cdot}H = \left[\begin{array}{cc} G^*H^* & G^*H^*N_H \\ ---- & + \quad ------ \\ N_G G^* H^* & N_G G^* H^* N_H \end{array}\right], \tag{4}$$

where G^* and H^* are nonsingular $n \times n$ matrices. Clearly, because of the rank-deficiency of the product $G \cdot H$, the solution of (3) will evolve on an n-dimesional linear manifold (translated subspace) of $\mathbb{R}^m$.

Furthermore, let us decompose the variable vector Z in (3) into two parts $Z = [\ Z_x \mid Z_+\ ]^T$ such that $\dim(Z_x) = n$. Then the decomposition of $G \cdot H$ in (4) gives rise to the following two set of linear equations

$$\frac{dZ_x}{dt} = G^*H^*Z_x + G^*H^*N_H Z_+ \tag{5}$$

$$\frac{dZ_+}{dt} = N_G G^* H^* Z_x + N_G G^* H^* N_H Z_+ = N_G \frac{dZ_x}{dt} \tag{6}$$

Eq. (6) implies $Z_+ = N_G Z_x + Z_+^0$ (with $Z_+^0 = const$) that can be substituted into (5) to obtain

$$\frac{dZ_x}{dt} = (G^*H^* + G^*H^*N_H N_G) \cdot (Z_x - Z_x^*) = M^* \cdot (Z_x - Z_x^*) \tag{7}$$

where the square $(n \times n)$ matrix $M^* = G^*H^* + G^*H^*N_H N_G$ determines the underlying *reduced minimal linear dynamics* when M^* is invertible and Z_x^* is an appropriate constant vector.

A relaxed reduction of the original dynamics (3) is still possible, when only G is of full rank, and H admits a decomposition $H = [H_x \mid H_+]$. Then the *reduced linear dynamics* is in the form

$$\frac{dZ_x}{dt} = G^* \left(H_x + H_+ N_G\right) \cdot \left(Z_x - Z_x^*\right) = M'^* \cdot \left(Z_x - Z_x^*\right) \tag{8}$$

where the square determining matrix $M'^* = G^* \left(H_x + H_+ N_G\right)$ is not necessarily of full rank.

It is important to note that both the number of equations and the number of variables are reduced during the above reduction, that can be seen as a projection of the original linear mapping charaterized by $M = G \cdot H$ to an invertible one described by M^*.

3. QP systems

QP systems form a class of nonnegative polynomial systems [1]. It can be shown that smooth nonlinear systems defined in the positive orthant and containing a wide range of non-QP functions, can be embedded into a QP system by introducing new variables [9].

The system dynamics of QP systems can be described by a set of DAEs, where the ordinary differential equations

$$\frac{dx_i}{dt} = x_i \left(\lambda_i + \sum_{j=1}^{m} \alpha_{ij} q_j\right) \ , \ i = 1, ..., n \tag{9}$$

are equiped by the so called quasi-monomial (QM) relationships

$$q_j = \prod_{i=1}^{m} x_i^{\beta_{ji}} \tag{10}$$

that are apparently nonlinear (monomial-type) algebraic equations. Two sets of variables are defined, that are (i) the differential variables $x_i, i = 1, ..., n$, and (ii) the quasi-monomials (QMs) $q_j, j = 1, ..., m$. The parameters of the above model are collected in two rectangular matrices $[A]_{ij} = \alpha_{ij}$, $[B]_{ji} = \beta_{ji}$ and a vector $[\Lambda]_i = \lambda_i$.

In order to avoid degenerate cases, we assume $m \geq n$. Furhermore, the rectangular matrices A and B are assumed to have full rank. Therefore, they admit a a decomposition in the form

$$A = [\ A^* \mid A^* N_A] \quad , \quad B = \begin{bmatrix} B^* \\ - - - - \\ N_B B^* \end{bmatrix} \tag{11}$$

by possibly permuting the columns of A and the rows of B such that both A^* and B^* is a square $(n \times n)$ invertible matrix.

3.1. The log-linear form

In order to develop the matrix-vector form of the describing equations, we define to each differential variable $x_i, i = 1, ..., n$ a log-variable $\ln x_i, i = 1, ..., n$, and form the following vectors form them:

$$X = [x_1, ..., n_n]^T \quad , \quad \underline{\ln}\ X = [\ln x_1, ..., \ln x_n]^T \tag{12}$$

Now the system dynamics is written in the following form

$$\frac{d\underline{\ln}\ X}{dt} = \Lambda + A \cdot Q \tag{13}$$

with the algebraic QM relationships

$$\underline{\ln}\ Q = B \cdot \underline{\ln}\ X \tag{14}$$

This can be used to show that there exists $m-n$ nonlinear algebraic relationships (in the $m > n$ case) between the elements of Q in (13)

$$\underline{\ln}\, Q = \begin{bmatrix} B^* \\ - - - - \\ N_B B^* \end{bmatrix} \cdot \underline{\ln}\, X = \begin{bmatrix} \underline{\ln}\, Q_X \\ - - - - \\ \underline{\ln}\, Q_+ \end{bmatrix} \tag{15}$$

with $\underline{\ln}\, Q_+ = N_B \underline{\ln}\, Q_X$. By inverting the upper block of the above equation we obtain

$$\underline{\ln}\, X = (B^*)^{-1} \cdot \underline{\ln}\, Q_X \tag{16}$$

Steady-state (SS) points. The essential (i.e. non-zero) steady-state point(s) of the dynamic equations (13) are obtained by setting the left-hand sides equal to zero, and solve the equations

$$0 = \Lambda + A \cdot Q^* \tag{17}$$

for Q^*. *Generally, this equation has a unique solution if A is quadratic and invertible. Otherwise, if $m > n$, then (15) shows that the set of equations (17) is properly determined and has generally a single solution tha is not necessarily positive. The existence of strictly positive solutions can be tested by various algorithms [10] or through simple linear programming [11].*

Transformed log-linear form. We can use any positive steady state point Q^* from (17) - if such exists - for expressing

$$\Lambda = -A \cdot Q^*$$

to the dynamic model. Thus we obtain the following form of the differential equations

$$\frac{d\underline{\ln}\ X}{dt} = A \cdot (Q - Q^*) \tag{18}$$

3.2. The log-linear LV form

The LV form can be obtained *from any QP-model* (Λ, B, A) by multiplying the matrix-vector dynamic equation (13) with B and considering the algebraic equation (14). This gives rise to

$$\frac{d\underline{\ln}\ Q}{dt} = B \cdot \lambda + M \cdot Q = \begin{bmatrix} B^*\lambda \\ ---- \\ N_B B^* \lambda \end{bmatrix} + M \cdot Q \tag{19}$$

Assume we have a unique positive steady-state point Q^*, then

$$\frac{d\underline{\ln}\ Q}{dt} = M \cdot (Q - Q^*) \quad \text{or} \quad \frac{dQ}{dt} = \overline{Q} \cdot M \cdot (Q - Q^*) \tag{20}$$

with $\Lambda = B \cdot \lambda$ and $\overline{Q} = \mathrm{diag}(q_1, ..., q_m)$.

3.3. The undelying reduced linear dynamics

The log-linear form (20) gives rise to the following underlying linear dynamics

$$\frac{dZ}{dt} = M \cdot Z \tag{21}$$

that can be transformed back to the original Q-space by translation and a nonlinear transformation using Eq. (20).

The reduced linear dynamics. This can be obtained the same way as described in subsection 2.2 using the correspondence $G \sim B$ and $H \sim A$. Then Eq. (7) implies that the square $(n \times n)$ matrix $M^* = B^*A^* + B^*A^*N_AN_B$ determines the underlying reduced linear dynamics.

4. CRNs with mass action law

Consider a set of (irreversible) chemical reactions

$$\sum_{i=1}^{K} \alpha_{\ell i} \mathcal{A}_i \xrightarrow{k_{\ell,p}} \sum_{i=1}^{K} \alpha_{pi} \mathcal{A}_i \ , \quad \ell = 1, ..., r \tag{22}$$

where the above equations define the "macro-kinetics" that obey the mass action law (MAL), and $k_{\ell,p} > 0$.

First two sets of variables are introduced, that are (i) the concentration of the components $\mathcal{A}_i$ $x_i, i = 1, ..., n$ denoted by $x_i, i = 1, ..., n$, and (ii) the reaction-monomials (RMs) $q_j, j = 1, ..., m$ and assume that $n \leq m$.

The polynomial dynamics of this systems is described by the following DAE

$$\frac{dx_i}{dt} = \sum_{j=1}^{m} \alpha_{ij} k_{ij} q_j \tag{23}$$

with the reaction monomial relationships

$$q_j = \prod_{i=1}^{m} x_i^{\alpha_{ij}} \tag{24}$$

The parameters of the dynamics are collected to the matrices

$$[Y]_{ij} = \alpha_{ij} \ , \ [A_k]_{ij} = \begin{cases} -\sum_{l=1}^{m} k_{il} & \text{if} \quad i = j \\ k_{ji} & \text{if} \quad i \neq j \end{cases} \tag{25}$$

with $A_k \in \mathbb{R}^{m \times m}$ being a Kirchhoff matrix (i.e. a square matrix with nonpositive diagonal and nonnegative off-diagonal elements and zero column sums).

4.1. The log-linear model

In order to develop the matrix-vector form of Eqs. (23) the vector variables defined in Eq. (12) can be used to obtain

$$\frac{dX}{dt} = Y \cdot A_k \cdot Q \tag{26}$$

with the reaction monomial (RM) relationships

$$\underline{\ln}\, Q = Y^T \cdot \underline{\ln}\, X \tag{27}$$

Matrix decomposition. Assume that Y is of full rank, and $m \geq n$. Then we can decompose $Y^T \in \mathbb{R}^{m\times n}$ by possibly permuting its rows to get its block-matrix form

$$Y^T = \begin{bmatrix} Y^{*T} \\ ---- \\ N_Y^T Y^{*T} \end{bmatrix} \tag{28}$$

where Y^* is a square $(n \times n)$ invertible matrix.

Similarity transformation. In order to obtain a similar form to the QP case, we first apply an X-factorable transformation of Eq. (26) according to (1) and (2) with $F(X)$ being $YA_kQ(x)$, and then multiply the result with Y^T. Making use of Eq. (27) we obtain

$$\frac{d\underline{\ln}\, Q}{dt} = Y^T \cdot Y \cdot A_k \cdot Q = M \cdot Q \tag{29}$$

Therefore, the generating matrix of the underlying linear dynamics is $M = Y^T \cdot Y \cdot A_k$.

4.2. Conservation equations in the monomial space

Because of the Kirchoff conservation matrix property of A_k, it is rank-deficient, i.e. $\text{rank}(A_k) \leq m-1$, and the sum of all but the last rows of matrix A_k equals to the last row. This enables us to write A_k in the following form

$$\tilde{A}_k = \mathcal{I}_m \cdot A_k = \begin{bmatrix} A'_k & | & A'_k N_{A_k} \\ --- & + & --- \\ 0...0 & | & 0 \end{bmatrix} \tag{30}$$

where

$$\mathcal{I}_m = \begin{bmatrix} I & | & \underline{0} \\ -- & + & -- \\ \underline{1} & | & 1 \end{bmatrix}, \ \mathcal{I}_m^{-1} = \begin{bmatrix} I & | & \underline{0} \\ -- & + & -- \\ -\underline{1} & | & 1 \end{bmatrix} \tag{31}$$

is an invertible square matrix with $\underline{0}_{m-1} = [0, ..., 0]^T$ and $\underline{1}_{m-1} = [1, ..., 1]$. Note that the variable transformation $Z = \mathcal{I}Q$ implements the replacement of the last coordinate by the sum of all coordinates.

The dynamics driven by A_k. In order to analyze this dynamics, we multiply the dynamic equation $\frac{dU}{dt} = A_k U$ by $\mathcal{I}_m$ in (31) and denote the resulting transformed vector $\mathcal{I}_m U$ by ζ to obtain

$$\frac{d\zeta}{dt} = \begin{bmatrix} A'_k & | & A'_k N_{A_k} \\ - - - - & + & - - - - \\ \underline{0}_{m-1} & | & 0 \end{bmatrix} \cdot \mathcal{I}^{-1} \cdot \zeta = \begin{bmatrix} A^*_k & | & A'_k N_{A_k} \\ - - - - & + & - - - - \\ \underline{0}_{m-1} & | & 0 \end{bmatrix} \cdot \zeta \tag{32}$$

with

$$A^*_k = A'_k - A'_k N_{A_k} \cdot \underline{1}_{m-1} \tag{33}$$

The last block in Eq. (32) implies $\zeta_m = const$, therefore the rest of Eq. (32) determines a linear dynamics with the generating matrix A^*_k of (33) in the form

$$\frac{d\tilde{\zeta}}{dt} = A^*_k \tilde{\zeta} + A'_k N_{A_k} \zeta_m = A^*_k (\tilde{\zeta} - \tilde{\zeta}^*) \tag{34}$$

with $\tilde{\zeta} = [\zeta_1, ..., \zeta_{m-1}]^T = [u_1, ..., u_{m-1}]^T$ This reduced linear dynamic system has a unique equilibrium point $\tilde{\zeta}^* = -A^{*-1}_k A'_k N_{A_k} \zeta_m$ in $\mathbb{R}^{m-1}$ if A^*_k is invertible. In this case this reduced linear dynamics is minimal.

Steady states in the monomial space. We use the column conservation property of matrix A_k in (30) to find the steady state points of (29), i.e. to find the solution of the equation $Y^T Y A_k Q = 0$. Clearly, the solution of $A_k Q = 0$ will be a solution, so we can try to solve $\mathcal{I}_m A_k Q = \tilde{A}_k Q = 0$. Let us decompose the variable vector Q into two parts as $Q = [\tilde{Q}|q_m]^T$ and use the algebraic form of $\tilde{A}_k$ in (30) to obtain

$$A'_k \left(\tilde{Q} + N_{A_k} q^*_m \right) = A'_k \left(\tilde{Q} + \tilde{Q}^* \right) = 0$$

This shows that by suitably fixing q^*_m we can have a positive steady state point $\tilde{Q}^* = N_{A_k} q^*_m \in \mathbb{R}^{(m-1)}$.

4.3. Conservation equations in the variable space

As it will be shown below, the conservation in the monomial space together with a physically plausible set of chemical reactions that obey the mass conservation law implies a conservation in the variable space, as well.

Mass conservative chemical reactions. Let us assume that the given set of chemical reactions (22) is chemically plausible, i.e. each reaction obeys the mass conservation. This means, that for each reaction, the following equality holds

$$\sum_{i=1}^{K} \alpha_{\ell i} \mathcal{M}_i \;=\; \sum_{i=1}^{K} \alpha_{pi} \mathcal{M}_i \;=\; c_s, \quad \ell = 1, ..., r \tag{35}$$

where $\mathcal{M}_i$ is the molecular weight of the component $\mathcal{A}_i$. A set of reactions with the above property will be called *mass conservative reaction set.*

Conservation in the variable space. The column conservation property of A_k can be expressed algebraically as $\underline{1}_m \cdot A_k = \underline{0}_m$. In addition, equation (35)

states that the weighted column-sum of any column in Y is the same (c_s), where the weights are the molecular weights $\mathcal{M}_i$. Therefore, we can form a weighted colunm-summation vector s such that

$$s \cdot Y = \underline{1}_m \quad \Rightarrow \quad s \cdot Y \cdot A_k = \underline{0}_m \tag{36}$$

with $s = [\frac{\mathcal{M}_1}{c_s}, ..., \frac{\mathcal{M}_1}{c_s}]^T$. that is the weighted mass conservation property in the variable space.

The dynamics driven by YA_k. In order to derive the rank of the generating matrix YA_k, we multiply the dynamic equation $\frac{dU}{dt} = YA_kU$ by $\mathcal{J}$, where

$$\mathcal{J} = \begin{bmatrix} I & | & \underline{0} \\ --- & + & -- \\ s_1, ..., s_{n-1} & | & s_n \end{bmatrix}, \; \mathcal{J}^{-1} = \begin{bmatrix} I & | & \underline{0} \\ --- & + & -- \\ -\frac{s_1}{s_n}, ..., -\frac{s_{n-1}}{s_n} & | & \frac{1}{s_n} \end{bmatrix} \tag{37}$$

By using the conservation properties of the matrices Y in Eq. (36) and A_k in Eq. (30) we obtain

$$\mathcal{J}YA_k = \begin{bmatrix} (YA_k)' \\ ---- \\ \underline{0}_m \end{bmatrix} \tag{38}$$

The above transformation shows that the linear mapping YA_k is not of full rank, but rank$(YA_k) \leq n - 1$.

4.4. The underlying reduced linear dynamics

The reduction of the underlying linear dynamics of Eq. (29) will be performed in two consecutive steps. First the linear transformation $Y^T \cdot (YA_k)$ is reduced, that is followed by further reducing it using the results from subsection 4.3 to construct the reduced minimal model.

Reduction of the mapping $Y^T(YA_k)$. Here we proceed the same way as described in subsection 2.2 using the correspondence $G \sim Y^T$ and $H \sim (YA_k)$, and observe that now YA_k is not of full rank. Let us decompose the rectangular matrix into two blocks as $YA_k = [\ W_x \mid W_+]$. Then Eq. (8) implies that the square $(n \times n)$ matrix

$$M_Y^* = Y^{*T}\left(W_x + W_+ N_Y^T\right) \tag{39}$$

determines the reduced linear mapping. However, this matrix is not of full rank, because its second factor, $(W_x + W_+ N_Y^T)$ is rank-deficient.

Similarly to the reduction of the dynamics driven by A_k, we can further reduce the dynamics driven by $(W_x + W_+ N_Y^T)$ by multiplying the dynamic equation $\frac{dU}{dt} = (W_x + W_+ N_Y^T) \cdot U$ by $\mathcal{J}$ and introduce the transformed variable $\nu = \mathcal{J}U$ to obtain

$$\frac{d\nu}{dt} = \mathcal{J}(W_x + W_+ N_Y^T)\mathcal{J}^{-1}\nu = \left[\begin{array}{ccc} \tilde{W} - \tilde{W}_+\tilde{s} & | & \frac{1}{s_n}\tilde{W}_+ \\ --- & + & -- \\ \underline{0}_{n-1} & | & 0 \end{array}\right] \cdot \left[\begin{array}{c} \tilde{\nu} \\ -- \\ \tilde{\nu}_n \end{array}\right] \tag{40}$$

with $\tilde{s} = [\frac{s_1}{s_n}, ..., \frac{s_{n-1}}{s_n}]$ The above equation shows that $\frac{d\nu_n}{dt} = 0$ and thus $\nu_n = \nu_n^* = const.$ This allows to write (40) in a reduced form as

$$\frac{d\tilde{\nu}}{dt} = (\tilde{W} - \tilde{W}_+\tilde{s})\tilde{\nu} + \frac{\nu_n^*}{s_n}\tilde{W}_+ = \tilde{W}^*(\tilde{\nu} - \tilde{\nu}^*) \tag{41}$$

with the generating square matrix $\tilde{W}^* = (\tilde{W} - \tilde{W}_+\tilde{s}) \in \mathbb{R}^{n-1 \times n-1}$ and the equilibrium point $\tilde{\nu}^* = (\tilde{W}^*)^{-1}\frac{\nu_n^*}{s_n}\tilde{W}_+$ if $\tilde{W}^*$ is invertible. In this case the reduced $(n-1)$-dimensional linear dynamics is minimal.

The reduced minimal model. The final step in the reduction is to apply the above to the dynamics $\frac{dZ}{dt} = Y^{*T}\left(W_x + W_+ N_Y^T\right) Z$, i.e. to the reduced linear

rank-deficient dynamics. Here we can use the fact that the matrix Y^{*T} is invertible, and multipy the dynamic equation by $(Y^{*T})^{-1}$. By introducing the transformed variable $\chi = (Y^{*T})^{-1}Z$ the following transformed dynamics is obtained

$$\frac{d\chi}{dt} = \left(W_x + W_+ N_Y^T\right) Y^{*T}\chi \tag{42}$$

Similarly to the previous dynamics we can again introduce a further transformed variable $\mu = \mathcal{J}\chi = \mathcal{J}(Y^{*T})^{-1}Z$ and proceed as for Eq. (41) using the derivation in Eq. (40) analogously.

5. Dynamic similarity of reaction kinetic and QP systems

5.1. Dynamic similarity criteria

A QP system is fully described by its structural paramaters n and m and by its parameters (Λ, B, A). We recall ([1], [9]) that any positive polynomial system, including reaction kinetic ones, can be written in a QP form.

Two QP systems will be called *strictly dynamically similar*, if both their structural parameters and their reduced linear dynamics is the same.

Because of the rank-deficient nature of the reduced linear dynamics of a reaction kinetic system (Y, A_k) in (39), it can only be strictly dinamically similar to a non-minimal QP system is such a way that their structural parameters (n and m) are the same, and the parameters of the QP system are $\lambda = \underline{0}_n^T$, $B = Y^T$ and $A = YA_k$.

Finally we note that the *simplest QP system with a given a reduced minimal dynamics* (M^*, Q^*) is a Lotka-Volterra system with $m = n$ and parameters (M^*, Q^*).

5.2. Illustrative example

Consider a set of chemical reactions

$$\mathcal{A}_2 + \mathcal{A}_3 \underset{k_{2,1}}{\overset{k_{1,2}}{\rightleftharpoons}} 2\mathcal{A}_1 \ , \ \mathcal{A}_1 + \mathcal{A}_3 \underset{k_{3,1}}{\overset{k_{1,3}}{\rightleftharpoons}} 2\mathcal{A}_2 \ , \ 2\mathcal{A}_1 \underset{k_{3,2}}{\overset{k_{2,3}}{\rightleftharpoons}} 2\mathcal{A}_3 \quad (43)$$

Reaction kinetic model. For the sake of simplicity, let us assume that all reaction rate constants are equal and $k_{i,j} = 1$. Then the dynamic equations are as follows.

$$\begin{aligned} \frac{dx_1}{dt} &= -4x_1^2 + x_2^2 + 2x_3^2 - x_1x_3 + 2x_2x_3 \\ \frac{dx_2}{dt} &= x_1^2 - 2x_2^2 + 2x_1x_3 - x_2x_3 \\ \frac{dx_3}{dt} &= 3x_1^2 + x_2^2 - 2x_3^2 - x_1x_3 - x_2x_3 \end{aligned}$$

The following matrices correspond to the reaction kinetic description

$$Y = \begin{bmatrix} 2 & 0 & 0 & 1 & 0 \\ 0 & 2 & 0 & 0 & 1 \\ 0 & 0 & 2 & 1 & 1 \end{bmatrix} \ , \ A_k = \begin{bmatrix} -2 & 0 & 1 & 0 & 1 \\ 0 & -1 & 0 & 1 & 0 \\ 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & -1 \end{bmatrix} \quad (44)$$

with the reaction monomial vector $Q_R = [x_1^2, x_2^2, x_3^2, x_1x_3, x_2x_3]^T$, i.e. $m_R = 5, n_R = 3$.

The time evolution of the variables of the reaction kinetic model starting from different initial conditions and with a given total mass are shown in the left sub-figure of Fig. 1. It is visible, that the trajectories move on a 2-dimensional linear manifold of the state space.

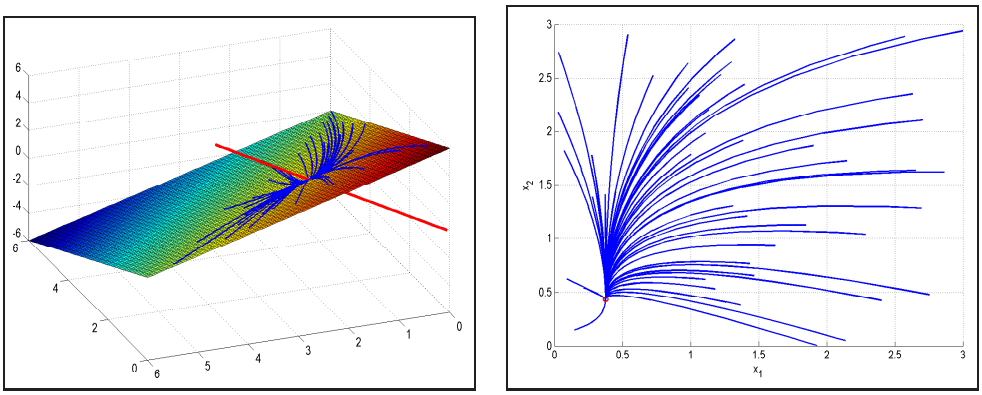

Figure 1: The phase plane of the two models with similar dynamics: CRN model (left) and reduced minimal model (right)

Strictly dynamically similar QP systems. The structural parameters of the two systems are the same, i.e. $m_{QP} = m_R = 5, n_{QP} = n_R = 3$, and the parameters of the QP systems are

$$A = YA_k = \begin{bmatrix} -4 & 1 & 2 & -1 & 2 \\ 1 & -2 & 0 & 2 & -1 \\ 3 & 1 & -2 & -1 & -1 \end{bmatrix}, \; B = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix}, \; \Lambda = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{45}$$

Reduced linear dynamics. The parameter matrices of the reaction kinetic system in (44) can be used to determine the generating matrix (39) of the reduced linear dynamics

$$M_R^* = Y^{*T}\left(W_x + W_+ N_Y^T\right) = 2 \cdot \begin{bmatrix} -5 & 3 & 3 \\ 3 & -3 & 1 \\ 2 & 0 & -4 \end{bmatrix} \tag{46}$$

The above matrix is a Kirchoff conservation matrix, therefore we have obtained that the simplest reaction kinetic system that is dynamically similar to the one in Eq. (43) has the following parameters: $m = n = n_R = 3$, $Y = I$, $A_k = M_R^*$, and it consists of linear reaction rates only.

Reduced minimal dynamics. Repeating the derivations in sub-section 4.4 in Eq. (34) the following 2-dimensional reduced minimal linear dynamics is obtained:

$$\frac{d\tilde{\zeta}}{dt} = \begin{bmatrix} -8 & 0 \\ 2 & -4 \end{bmatrix} \cdot \left(\tilde{\zeta} - \begin{bmatrix} 0.3750 \\ 0.4375 \end{bmatrix} \right) \tag{47}$$

with $\zeta_3 = 1$.

The trajectories of the reduced minimal model obtained from the reaction kinetic one are shown in the right sub-figure of Fig. 1. Now the state spce is only two-dimensional, but the phase portrait is clearly similar with the one of the original model on its 2-dimensional linear sub-space.

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