ON SOME PROPERTIES OF QUASI-POLYNOMIAL ORDINARY DIFFERENTIAL EQUATIONS (QP-ODE) AND DIFFERENTIAL ALGEBRAIC (QP-DAE) EQUATIONS

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Chapter 1

Introduction

This report summarizes our results on the properties of quasi-polynomial ordinary differential equation (QP-ODE) and differential-algebraic equation (QP-DAE) models. Lumped dynamic process models can always be transformed into either QP-ODE or QP-DAE form which serve as unifying description form of these nonlinear models.

This report is used as a basic reference for further research in two directions:

- stability analysis
- analysis of computational properties

of lumped dynamic process models.

Stability analysis The global stability analysis of general nonlinear systems needs special skills because the construction of a suitable Lyapunov function is far from being trivial. Therefore special canonical forms enabling to construct a Lyapunov function are of great theoretical and practical importance.

In this report Lotka-Volterra (LV) form is proposed for representing a wide class of lumped process systems in DAE form. Having determined the canonical Lotka-Volterra representation of a nonlinear lumped process system, local stability analysis can be performed using the invariants of the representation. A Lyapunov function for the global stability analysis can also be determined from the LV form.

The Hamiltonian description of QP-ODE systems enables us to construct a rigorous nonlinear representation of such system class and to analyze global stability and diagonal stabilizability by using linear matrix inequalities.

Computational properties Most of lumped dynamic process models are in DAE form that is the subject of the analysis of computational properties. The QP-form of DAE models is a new area with special importance here: this is, why the last chapter of this report is devoted to it.

Chapter 2

Basic notions

In this chapter, the basic notions related to quasi-polynomial and Lotka-Volterra systems are introduced, and the relationship between these two types of representation is explained.

We start with summarizing known results on quasi-polynomial ordinary differential equation (QP-ODEs) which are also called generalized Lotka-Volterra (generalized LV) models.

2.1 General form of QP-ODEs

The canonical form of a unifying representation has been introduced by Brenig and Goriely [1], and called *generalized Lotka-Volterra (GLV) form, or quasi-polynomial (QP-ODE) form*:

$$\dot{x}_i = x_i \lambda_i + x_i \sum_{j=1}^{m} A_{ij} \prod_{k=1}^{n} x_k^{B_{jk}}, \tag{2.1}$$
$$i = 1, \ldots, n, \qquad m \geq n$$

where the parameters of the model A and B are $n \times m$, $m \times n$ real matrices and $\lambda \in R^n$ is a real vector. Further we assume that every variable is strictly positive, i.e.

$$x_i > 0 \ , \quad i = 1, ..., n$$

2.1.1 The logarithmic form

Further, we make use of the logarithmic form of QP-ODEs. First we introduce the notation:

$$x_i^* = \ln x_i$$

for any scalar variable x_i.

Further we identify the so called **quasi-monomials**

$$q_j = \prod_{k=1}^{n} x_k^{B_{jk}} \quad , \quad j = 1, ..., m \tag{2.2}$$

With the above notation Eq. (2.1) can be written in the following form:

$$\begin{aligned} \dot{x_i^*} &= \lambda_i + \sum_{j=1}^{m} A_{ij} q_j, \\ i = 1, \ldots, n, & \qquad m \geq n \end{aligned} \tag{2.3}$$

Next we collect the variables into vectors of the form:

$$X^* = \begin{bmatrix} x_1^* \\ ... \\ x_n^* \end{bmatrix} \quad , \quad Q = \begin{bmatrix} q_1 \\ ... \\ q_m \end{bmatrix}$$

Then the compact vector-matrix form of Eq. (2.3) reads as:

$$\dot{X}^* = \lambda + AQ \tag{2.4}$$

2.2 Quasi-monomial transformations

The set of GLV models is closed under a special nonlinear transformation, the so-called quasi-monomial transformation [1].

A **quasi-monomial transformation** (abbreviated as **QM-transformation**) is defined as

$$x_i = \prod_{k=1}^{n} \hat{x}_k^{C_{ik}}, \qquad i = 1, \ldots, n \tag{2.5}$$

where C is an arbitrary invertible matrix.

In order to see how the above transformation changes a QP-ODE model, we investigate its effect on the logarithmic variables X^* and on the quasi-monomials Q.

First we compute the logarithm of Eq. (2.5)

$$x_i^* = \sum_{k=1}^{n} \hat{x}_k^* C_{ik}, \qquad i = 1, \ldots, n$$

The compact matrix-vector form of the above equation is:

$$X^* = C\hat{X}^* \quad \text{or} \quad \hat{X}^* = C^{-1}X^* \tag{2.6}$$

Next we take the logarithm of Eq. (2.2):

$$q_j^* = \sum_{k=1}^{n} x_k^* B_{jk}, \qquad j = 1, \ldots, m$$

which takes the following matrix-vector form:

$$Q^* = BX^* \tag{2.7}$$

With the above transformation rules for the variables we can easily deduce the **transformation rules of the QP-ODE model parameters**:

1. The QP-ODE matrices change to $\hat{B} = B \cdot C$, $\hat{A} = C^{-1} \cdot A$, $\hat{\lambda} = C^{-1} \cdot \lambda$, and the transformed set of equations will also be in QP-ODE form:

$$\dot{\hat{x}}_i = \hat{x}_i\hat{\lambda}_i + \hat{x}_i \sum_{j=1}^{m} \hat{A}_{ij} \prod_{k=1}^{n} \hat{x}_k^{\hat{B}_{jk}}, \tag{2.8}$$
$$i = 1, \ldots, n, \qquad m \geq n$$

2. the quasi-monomials remain unchanged, i.e. $\hat{Q} = Q$. This means that the transformed variables $\hat{x}_k$ will form the transformed quasi-monomials $\hat{q}_j$ using the transformed exponent matrix $\hat{B}$.

3. The above family of systems is split into classes of equivalence [5] according to the values of the products $M = B \cdot A$ and $\Lambda = B \cdot \lambda$ which are invariants under QM-transformation.

2.3 Time derivative of the monomials

Let us denote the quasi-monomials of the system as

$$U_j = \prod_{k=1}^{n} x_k^{B_{jk}}, \quad j = 1, \ldots, m \tag{2.9}$$

Then the time derivative of the monomials can be computed in the following way:

$$\dot{U}_i = \frac{\partial U_i}{\partial x}\dot{x} \tag{2.10}$$

where

$$\frac{\partial U_i}{\partial x} = \left[\begin{array}{cccc} \frac{1}{x_1}B_{i1}U_i & \frac{1}{x_2}B_{i2}U_i & \dots & \frac{1}{x_n}B_{in}U_i \end{array}\right] \tag{2.11}$$

this gives

$$\dot{U}_i = B_{i1}U_il_i + B_{i1}U_i\sum_{j=1}^{m}A_{ij}U_j + \tag{2.12}$$

$$B_{i2}U_il_i + B_{i2}U_i\sum_{j=1}^{m}A_{ij}U_j + \tag{2.13}$$

$$\dots + \tag{2.14}$$

$$B_{in}U_il_i + B_{in}U_i\sum_{j=1}^{m}A_{ij}U_j = \tag{2.15}$$

$$= \sum_{k=1}^{n}\left\{B_{ik}U_il_i + B_{ik}U_i\sum_{j=1}^{m}A_{ij}U_j\right\} = \tag{2.16}$$

$$= U_i\sum_{k=1}^{n}(B_{ik}l_i) + U_i\sum_{k=1}^{n}\sum_{j=1}^{m}(B_{ik}A_{ij}U_j) = \tag{2.17}$$

$$= U_i\underbrace{\sum_{k=1}^{n}B_{ik}l_i}_{\lambda_i} + U_i\sum_{j=1}^{m}M_{ij}U_j = \tag{2.18}$$

$$\dot{U}_i = U_i\lambda_i + U_i\sum_{j=1}^{m}M_{ij}U_j \tag{2.19}$$

This means, that a quasi-polynomial system model expressed in its quasi-monomials as system variables results in a special, quadratic QP-form, in an *LV-form*, that is a subject of the next subsection.

2.4 LV-form of QP-ODEs

The concept of Lotka-Volterra (LV) form is also based on quasi-monomial transformations. Quasi-monomial transforms define equivalence classes, in which the products $M = B \cdot A$ and $\Lambda = B \cdot \lambda$ are invariants. In addition, the quasi-monomials, which are exactly the LV variables, are also invariants of the equivalence classes.

Then the classical LV form gives the representative elements of these equivalence classes. If $rank(B) = n$, then the set of ODEs in (2.1) can be embedded into the following m-dimensional set of equations:

$$\dot{z}_f = \lambda'_f z_f + z_f \sum_{g=1}^{m} A'_{fg} z_g, \quad f = 1, \ldots, m \tag{2.20}$$

where $A' = B \cdot A$, $\lambda' = B \cdot \lambda$ and each z_f stands for a quasi-monomial:

$$\prod_{k=1}^{n} x_k^{B_{fk}}, \qquad f = 1, \ldots, m \tag{2.21}$$

It is noticeable that the LV form is a special case of the GLV system form, where the exponent matrix B is equal to a unit matrix of size m, where m is the number of the different quasi-monomials of the GLV system.

2.4.1 Obtaining LV-form by QM-transformation

Recall, that a class of QP-ODEs is invariant under QM-transformation. This is used for obtaining the LV-form being a special representative element of the invariant QP-ODE class as follows.

1. $n = m$: the number of variables is equal to the number of quasi-monomials
   Here we can simply use a QM-transformation with $C = B^{-1}$ to obtain the LV-form.

2. $m > n$: the number of variables is less than the number of quasi-monomials
   In this case we create $m - n$ dummy QP differential equations for dummy new variables to obtain the $\widetilde{n} = m$ case in the following manner:

   - we add new columns to B such that the resulting $\widetilde{B}$ is nonsingular,
   - we add new rows containing zero entries to λ and A to ensure that the new variables are constants with unit initial values.

2.5 Global stability of QP systems

2.5.1 Lyapunov function candidate

Equilibrium point: $x^* = [x_1^* \;\; x_2^* \;\; \ldots \;\; x_n^*]^T$
Notation (monomials at the equilibrium): $q_i = \prod_{k=1}^{n} (x_k^*)^{B_{ik}}$

Lyapunov function candidate in the original coordinates

$$V(x) = \sum_{i=1}^{m} a_i \left(\prod_{k=1}^{n} x_k^{B_{ik}} - q_i \ln \left(\frac{\prod_{k=1}^{n} x_k^{B_{ik}}}{q_i} \right) - q_i \right) \tag{2.22}$$

Lyapunov function candidate using monomial notation

$$V(U) = \sum_{i=1}^{m} a_i \left(U_i - q_i \ln\left(\frac{U_i}{q_i}\right) - q_i \right) \tag{2.23}$$

the k-th component in the above sum depends only on U_k

$$V_k(U) = a_k \left(U_k - q_k \ln\left(\frac{U_k}{q_k}\right) - q_k \right) \tag{2.24}$$

therefore

$$\frac{\partial V_k}{\partial U_j} = \begin{cases} 0, & k \neq j \\ a_k - a_k q_k \frac{1}{U_k}, & k = j \end{cases} \tag{2.25}$$

2.5.2 The time derivative of the Lyapunov function candidate

$$\dot{V} = \frac{\partial V}{\partial U} \cdot \dot{U} = \tag{2.26}$$

$$\sum_{k=1}^{m} \left\{ \left(a_k - a_k q_k \frac{1}{U_k} \right) \cdot \left(U_k \lambda_k + U_k \sum_{j=1}^{m} M_{kj} U_j \right) \right\} = \tag{2.27}$$

$$\sum_{k=1}^{m} \left\{ a_k U_k \lambda_k + a_k U_k \sum_{j=1}^{m} M_{kj} U_j - a_k q_k \lambda_k - a_k q_k \sum_{j=1}^{m} M_{kj} U_j \right\} = \tag{2.28}$$

$$\sum_{k=1}^{m} \left\{ a_k \lambda_k \left(U_k - q_k \right) + a_k (U_k - q_k) \sum_{j=1}^{m} M_{kj} U_j \right\} = \tag{2.29}$$

$$\sum_{k=1}^{m} \left\{ a_k (U_k - q_k) \left(\lambda_k + \sum_{j=1}^{m} M_{kj} U_j \right) \right\} \tag{2.30}$$

(2.30) can be rewritten as

$$\dot{V} = \sum_{k=1}^{m} \left\{ a_k (U_k - q_k) \left(\lambda_k + \sum_{j=1}^{m} M_{kj} (U_j - q_j + q_j) \right) \right\} = \tag{2.31}$$

$$\sum_{k=1}^{m} \left\{ a_k (U_k - q_k) \left(\underbrace{\lambda_k + \sum_{j=1}^{m} (M_{kj} q_j)}_{0} + \sum_{j=1}^{m} M_{kj} (U_j - q_j) \right) \right\}, \tag{2.32}$$

which results in

$$\dot{V} = \sum_{k=1}^{m} \sum_{j=1}^{m} a_k M_{kj} \underbrace{(U_k - q_k)}_{w_k} \underbrace{(U_j - q_j)}_{w_j}. \tag{2.33}$$

2.6 Local quadratic stability

Let us perform a coordinates shift on the LV-equations, i.e. $x = z - z^*$. Then the LV-equations in the transformed coordinates have the form

$$\dot{x} = (X + Z^*) \cdot A \cdot x, \tag{2.34}$$

where

$$X = \mathrm{diag}(x_1, \ldots, x_m), \quad Z^* = \mathrm{diag}(z_1^*, \ldots, z_m^*) \tag{2.35}$$

Let the quadratic Lyapunov function candidate be given in the following form:

$$V(x) = x^T P x \tag{2.36}$$

where P is a positive definite symmetric matrix of size $m \times m$. The time derivative of V is given by

$$\dot{V} = x^T P x + \dot{x}^T P x = \tag{2.37}$$

$$x^T P (X + Z^*) A x + x^T A^T (X + Z^*) P x = \tag{2.38}$$

$$\tag{2.39}$$

$$x^T \left\{ P(X + Z^*)A + A^T (X + Z^*) P \right\} x = \tag{2.40}$$

$$x^T \left\{ PXA + PZ^*A + A^T XP + A^T Z^* P \right\} x \tag{2.41}$$

The non-increasing nature of the quadratic Lyapunov function in a neighborhood $\mathcal{N}$ of the origin is equivalent to the validity of the following LMI

$$PXA + PZ^*A + A^T XP + A^T Z^* P \leq 0 \tag{2.42}$$

where $X = \mathrm{diag}(x_1, \ldots, x_m)$ and $[x_1, \ldots, x_m]^T \in \mathcal{N}$.

Therefore the quadratic stability region can be estimated by first solving (2.42) for P with $X = 0$, and then finding a convex neighborhood of 0 where (2.42) is valid.

Chapter 3

Nonlinear process system models in QP and LV forms

Process system models can be represented in quasi-polynomial form by embedding the non-QP model elements, most often functions, by using auxiliary variables.

Lotka-Volterra representation of process systems can be deduced from the QP model, as explained previously in Chapter 2. Because of its importance, the unambiguity of the LV form process models is also investigated and refined in this Chapter.

3.1 Embedding nonlinear process systems into QP form

A set of nonlinear ODEs can be embedded to GLV form if it satisfies two important requirements [5].

1. The set of nonlinear ODEs should be in the form:

$$\dot{x_s} = \sum_{i_{s1},\ldots,i_{sn},j_s} a_{i_{s1}\ldots i_{sn}j_s} x_1^{i_{s1}} \ldots x_n^{i_{sn}} f(\overline{x})^{j_s}, \tag{3.1}$$

$$x_s(t_0) = x_s^0, \qquad s = 1,\ldots,n$$

   where

$$a_{i_{s1}\ldots i_{sn}j_s}, i_{s1},\ldots,i_{sn}, j_s \in R, \quad s = 1,\ldots,n,$$

   and $f(\overline{x})$ is some scalar valued function, which is not reducible to *quasi-monomial form* containing terms in the form of $\prod_{k=1}^{n} x_k^{\Gamma_{jk}}$, $j = 1,\ldots,m$ with Γ being a real matrix.

2. Furthermore, we require that the partial derivatives of the system (3.1) fulfil:

$$\frac{\partial f}{\partial x_s} = \sum_{e_{s1},\dots,e_{sn},e_s} b_{e_{s1}\dots e_{sn}e_s} x_1^{e_{s1}} \dots x_n^{e_{sn}} f(\overline{x})^{e_s} \tag{3.2}$$

where

$$b_{e_{s1}..e_{sn}e_s}, e_{s1}, \dots, e_{sn}, e_s \in R, \quad s = 1, \dots, n.$$

The embedding is performed by introducing a *new auxiliary variable*

$$y = f^q \prod_{s=1}^{n} x_s^{p_s}, \qquad q \neq 0. \tag{3.3}$$

Then, instead of the non-quasi-polynomial nonlinearity f we can write the original set of equations (3.1) into GLV form:

$$\dot{x_s} = \left(x_s \sum_{i_{s1},\dots,i_{sn},j_s} \left(a_{i_{s1}\dots i_{sn}j_s} y^{j_s/q} \prod_{k=1}^{n} x_k^{i_{sk}-\delta_{sk}-j_s p_k/q} \right)\right), \qquad s = 1, \dots, n \tag{3.4}$$

where $\delta_{sk} = 1$ if $s = k$ and 0 otherwise. In addition, a new quasi-polynomial ODE appears for the new variable y:

$$\begin{aligned} \dot{y} \;\; = \;\; & y \Bigg[\sum_{s=1}^{n} \Bigg(p_s x_s^{-1} \dot{x}_s + \\ & + \sum_{\substack{i_{s\alpha},j_s \\ e_{s\alpha},e_s}} a_{i_{s\alpha},j_s} b_{e_{s\alpha},e_s} q y^{(e_s+j_s-1)/q} \times \\ & \times \prod_{k=1}^{n} x_k^{i_{sk}+e_{sk}+(1-e_s-j_s)p_k/q} \Bigg) \Bigg], \qquad \alpha = 1, \dots, n. \end{aligned} \tag{3.5}$$

It is important to observe that the embedding is not unique, because we can choose the parameters p_s and q in Eq. (3.3) in many different ways: the simplest is to choose $(p_s = 0,\; s = 1, ..., n;\; q = 1)$

3.1.1 Process system models in QP form

The state equation of a lumped process system contains additive terms corresponding to the different *mechanisms* taking place: convection, transfer and sources. Based on this understanding, the state equation of lumped process systems is nonlinear in an input-affine form

$$\dot{x} = f(x) + g(x)u$$

with x being the state and u being the input variable. If the usual and natural choice of the input variables is made, that is, they are flowrates and potential (intensive) variables at the system inlets, then the function g in the above state equation is always a *linear* function of the state vector x because of the properties of the convective terms it originates from. The nonlinear state function $f(x)$ is broken down into a linear term originating from transfer and a general nonlinear term caused by the sources (other generation and consumption terms including chemical reactions, phase changes etc.) In most of the cases, the source term contains the following special nonlinearities:

- *reaction rate expressions*
  exponential type nonlinearities which account for the temperature dependence and polynomial expressions for the concentration dependence with terms in the form of
  $$e^{-\frac{c_1}{c_2 x_T}} \prod_i x_i^{\alpha_i}$$
- *global reaction rate expressions*
  rational function type nonlinear factors in terms of $f(x)$
  $$\frac{p_1(x)}{p_2(x)}$$
  where both p_1 and p_2 are polynomials of the state vector elements x_i.

Systems containing the above two kinds of nonlinearities can easily be transformed to QP form [5].

3.2 A process system example used in the report: a batch fermenter

Let us consider an isothermal batch fermenter where a single substrate reacts with a single biomass according to a nonlinear non-monotonous reaction rate function. Assume constant physico-chemical properties and constant overall mass holdup. Then the nonlinear state-space model of the reactor is in the following form:

$$\begin{aligned} \dot{X} &= \frac{\mu_{max} X S}{K_1 + S + K_2 S^2} - \frac{F}{V} X \\ \dot{S} &= -\frac{1}{Y} \frac{\mu_{max} X S}{K_1 + S + K_2 S^2} - \frac{F}{V} S + \frac{F}{V} S_F \end{aligned} \tag{3.6}$$

Variables and their units of measure:

X:	biomass concentration (state variable),	$[g/l]$
S:	substrate concentration (state variable),	$[g/l]$
	constant parameters:	
F:	inlet feed flow rate,	$[l/h]$
V:	tank volume,	$[l]$
S_F:	inlet feed substrate concentration,	$[g/l]$
μ_{max}:	kinetic constant	1
K_1:	kinetic constant	2
K_2:	kinetic constant	3
Y:	kinetic constant	4

For the sake of simplicity the the inlet feed is omitted (that is $F = 0$) so the examined model is

$$\begin{aligned} \dot{X} &= \frac{\mu_{max} X S}{K_1 + S + K_2 S^2} \\ \dot{S} &= -\frac{1}{Y} \frac{\mu_{max} X S}{K_1 + S + K_2 S^2} \end{aligned} \tag{3.7}$$

The non-quasi-polynomial function in the above model is chosen to be

$$f(x) = (K_1 + S + K_2 S^2)^{-1} \tag{3.8}$$

3.3 Unambiguity of the LV form of process models

As it was mentioned above we have a degree of freedom in choosing a new algebraic variable (3.3) of a quasi-polynomial system.

It is a fundamental question whether the different QP models obtained by different algebraic variable selections belong to the same GLV class of equivalence. It was shown in [6] that all these QP systems lead to a unique LV model. In this section it is shown that an LV model is only unique in a restricted sense: not only the permutation of the variables is enabled, but also the re-scaling of the variables is permitted.

3.3.1 Permutation of LV variables

Let z be the vector containing the LV variables:

$$z = [z_1, z_2, \cdots, z_n] \tag{3.9}$$

Then multiplying z with a permutation matrix P (that is, P can be transformed to unit matrix with row and column changes) represents variable swapping:

$$\hat{z} = P \cdot z, \tag{3.10}$$

Any permutation can be performed step-by-step i.e. only two variables are swapped at one step. Permutation matrix P permutes the i-th and the j-th variables:

$$\hat{z} = P \cdot z = \begin{pmatrix} 1 & 0 & \dots & 0 & \dots & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 & \dots & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 & \dots & 0 & \dots & 1 \end{pmatrix} \cdot \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_i \\ \vdots \\ z_j \\ \vdots \\ z_n \end{pmatrix} = \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_j \\ \vdots \\ z_i \\ \vdots \\ z_n \end{pmatrix} \tag{3.11}$$

Now the LV matrices A and λ have to follow the changes in the order of the variables, namely columns and rows i and j of matrix A and elements i and j of λ must be swapped.
Multiplying matrix A with P from the left:

$$\begin{aligned} P \cdot A = & \\ = & \begin{pmatrix} 1 & \dots & 0 & \dots & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \dots & 1 & \dots & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & 1 & \dots & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \dots & 0 & \dots & 1 \end{pmatrix} \cdot \begin{pmatrix} a_{1,1} & \dots & a_{1,i} & \dots & a_{1,j} & \dots & a_{1,n} \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{i,1} & \dots & a_{i,i} & \dots & a_{i,j} & \dots & a_{i,n} \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{j,1} & \dots & a_{j,i} & \dots & a_{j,j} & \dots & a_{j,n} \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{n,1} & \dots & a_{n,i} & \dots & a_{n,j} & \dots & a_{n,n} \end{pmatrix} \\ = & \begin{pmatrix} a_{1,1} & \dots & a_{1,i} & \dots & a_{1,j} & \dots & a_{1,n} \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{j,1} & \dots & a_{j,i} & \dots & a_{j,j} & \dots & a_{j,n} \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{i,1} & \dots & a_{i,i} & \dots & a_{i,j} & \dots & a_{i,n} \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{n,1} & \dots & a_{n,i} & \dots & a_{n,j} & \dots & a_{n,n} \end{pmatrix} \end{aligned} \tag{3.12}$$

is not enough because rows i and j are still in order so it is necessary to multiply A with P from the right, too:

$$\hat{A} = (P \cdot A) \cdot P =$$
$$\begin{pmatrix} a_{1,1} & \dots & a_{1,i} & \dots & a_{1,j} & \dots & a_{1,n} \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{j,1} & \dots & a_{j,i} & \dots & a_{j,j} & \dots & a_{j,n} \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{i,1} & \dots & a_{i,i} & \dots & a_{i,j} & \dots & a_{i,n} \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{n,1} & \dots & a_{n,i} & \dots & a_{n,j} & \dots & a_{n,n} \end{pmatrix} \cdot \begin{pmatrix} 1 & \dots & 0 & \dots & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \dots & 1 & \dots & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & 1 & \dots & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \dots & 0 & \dots & 1 \end{pmatrix}$$
$$= \begin{pmatrix} a_{1,1} & \dots & a_{1,j} & \dots & a_{1,i} & \dots & a_{1,n} \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{j,1} & \dots & a_{j,j} & \dots & a_{j,i} & \dots & a_{j,n} \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{i,1} & \dots & a_{i,j} & \dots & a_{i,i} & \dots & a_{i,n} \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{n,1} & \dots & a_{n,j} & \dots & a_{n,i} & \dots & a_{n,n} \end{pmatrix} \tag{3.13}$$

Similarly

$$\begin{aligned} \hat{\lambda} &= P \cdot \lambda = \\ &= \begin{pmatrix} 1 & \dots & 0 & \dots & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \dots & 1 & \dots & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & 1 & \dots & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \dots & 0 & \dots & 1 \end{pmatrix} \cdot \begin{pmatrix} \lambda_1 \\ \vdots \\ \lambda_i \\ \vdots \\ \lambda_j \\ \vdots \\ \lambda_n \end{pmatrix} = \begin{pmatrix} \lambda_1 \\ \vdots \\ \lambda_j \\ \vdots \\ \lambda_i \\ \vdots \\ \lambda_n \end{pmatrix}. \end{aligned} \tag{3.14}$$

3.3.2 Multiplying LV variables with constant

Let Q be a matrix in the form $Q = \text{diag}(q_1, q_2, \cdots, q_n)$ where $q_i \in R$. If we transform the original LV variables into the form

$$\hat{z} = Q \cdot z = \begin{pmatrix} q_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & q_n \end{pmatrix} \cdot \begin{pmatrix} z_1 \\ \vdots \\ z_n \end{pmatrix} = \begin{pmatrix} q_1 z_1 \\ \vdots \\ q_n z_n \end{pmatrix} \tag{3.15}$$

then the Lotka-Volterra coefficient matrix (matrix A) must be aligned to the scaling:

$$\dot{\hat{z}}_i = \hat{z}_i\Big(\lambda_i + \sum_{j=1}^{n} \frac{a_{ij}}{q_j}\hat{z}_j\Big), \quad i = 1, \dots, n \tag{3.16}$$

i.e. the i-th column of A must be re-scaled by q_i^{-1}:

$$\begin{pmatrix} \frac{a_{11}}{q_1} & \dots & \frac{a_{1n}}{q_n} \\ \vdots & \ddots & \vdots \\ \frac{a_{n1}}{q_1} & \dots & \frac{a_{nn}}{q_n} \end{pmatrix} = \begin{pmatrix} a_{11} & \dots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \dots & a_{nn} \end{pmatrix} \cdot \begin{pmatrix} \frac{1}{q_1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \frac{1}{q_n} \end{pmatrix} \tag{3.17}$$

but the parameters λ_i are unchanged, which means

$$\hat{A} = A \cdot Q^{-1}, \qquad \hat{\lambda} = \lambda \tag{3.18}$$

being the LV system matrices.

Performing both permutation and multiplication will also keep the LV form.

3.3.3 Example: Unambiguity of the LV form of a simple batch fermenter model

In this example the batch fermenter model with non-monotonous reaction rate function is transformed to four possible QP form, to show that all four quasi-polynomial model gives rise to the same LV form.

Case A

In the first case the new algebraic variable is chosen

$$y = f(x)$$

The QP system with the above choice is:

$$\begin{aligned} \dot{X} &= X\Big(\mu_{max} S y\Big) \\ \dot{S} &= S\Big(-\frac{\mu_{max}}{Y} X y\Big) \\ \dot{y} &= y\Big(\frac{\mu_{max}}{Y} X S y^2 + 2K_2 \frac{\mu_{max}}{Y} X S^2 y^2\Big) \end{aligned} \tag{3.19}$$

The quasimonomials, i.e. the LV variables are:

$$Sy \qquad Xy \qquad XSy^2 \qquad XS^2y^2$$

From the QP system equation it is easy to determine the QP invariants A, B, λ:

$$A = \begin{pmatrix} \mu_{max} & 0 & 0 & 0 \\ 0 & -\frac{\mu_{max}}{Y} & 0 & 0 \\ 0 & 0 & \frac{\mu_{max}}{Y} & 2K_2\frac{\mu_{max}}{Y} \end{pmatrix}$$

$$B = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 2 \\ 1 & 2 & 2 \end{pmatrix}, \quad \lambda = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Case B

In this case the new algebraic variable is chosen to be

$$y = X \cdot S \cdot f(x)$$

The QP system with the above choice is:

$$\begin{aligned} \dot{X} &= X\Big(\mu_{max}X^{-1}y\Big) \\ \dot{S} &= S\Big(-\frac{\mu_{max}}{Y}S^{-1}y\Big) \\ \dot{y} &= y\Big(\mu_{max}X^{-1}y - \frac{\mu_{max}}{Y}S^{-1}y + \\ &\quad +\frac{\mu_{max}}{Y}X^{-1}S^{-1}y^2 + 2K_2\frac{\mu_{max}}{Y}X^{-1}y^2\Big) \end{aligned} \tag{3.20}$$

The quasi-monomials, i.e. the LV variables are:

$$X^{-1}y \qquad S^{-1}y \qquad X^{-1}S^{-1}y^2 \qquad X^{-1}y^2$$

The QP invariants A, B, λ:

$$A = \begin{pmatrix} \mu_{max} & 0 & 0 & 0 \\ 0 & -\frac{\mu_{max}}{Y} & 0 & 0 \\ \mu_{max} & -\frac{\mu_{max}}{Y} & \frac{\mu_{max}}{Y} & 2K_2\frac{\mu_{max}}{Y} \end{pmatrix}$$

$$B = \begin{pmatrix} -1 & 0 & 1 \\ 0 & -1 & 1 \\ -1 & -1 & 2 \\ -1 & 0 & 2 \end{pmatrix}, \quad \lambda = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Case C

The new algebraic variable is chosen as

$$y = S \cdot f(x)$$

The QP system with the above choice is:

$$\begin{aligned}
\dot{X} &= X\Big(\mu_{max} y\Big) \\
\dot{S} &= S\Big(-\frac{\mu_{max}}{Y} X S^{-1} y\Big) \\
\dot{y} &= y\Big(-\frac{\mu_{max}}{Y} X S^{-1} y + \frac{\mu_{max}}{Y} X S^{-1} y^2 + \\
&\quad +2K_2 \frac{\mu_{max}}{Y} X y^2\Big)
\end{aligned} \tag{3.21}$$

The quasi-monomials are:

$$y \qquad XS^{-1}y \qquad XS^{-1}y^2 \qquad Xy^2$$

And the QP invariants A, B, λ:

$$A = \begin{pmatrix} \mu_{max} & 0 & 0 & 0 \\ 0 & -\frac{\mu_{max}}{Y} & 0 & 0 \\ 0 & -\frac{\mu_{max}}{Y} & \frac{\mu_{max}}{Y} & 2K_2 \frac{\mu_{max}}{Y} \end{pmatrix}$$

$$B = \begin{pmatrix} 0 & 0 & 1 \\ 1 & -1 & 1 \\ 1 & -1 & 2 \\ 1 & 0 & 2 \end{pmatrix}, \quad \lambda = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Case D

The new algebraic variable is now

$$y = X \cdot f(x)$$

The QP system with the above choice is:

$$
\begin{aligned}
\dot{X} &= X\Big(\mu_{max} X^{-1} S y\Big) \\
\dot{S} &= S\Big(-\frac{\mu_{max}}{Y} y\Big) \\
\dot{y} &= y\Big(\mu_{max} X^{-1} S y + \frac{\mu_{max}}{Y} X^{-1} S y^2 + \\
&\quad +2K_2 \frac{\mu_{max}}{Y} X^{-1} S^2 y^2\Big)
\end{aligned}
\tag{3.22}
$$

The LV variables are:

$$
X^{-1}Sy \qquad y \qquad X^{-1}Sy^2 \qquad X^{-1}S^2y^2
$$

The QP invariants A, B, λ are:

$$
A = \begin{pmatrix} \mu_{max} & 0 & 0 & 0 \\ 0 & -\frac{\mu_{max}}{Y} & 0 & 0 \\ \mu_{max} & 0 & \frac{\mu_{max}}{Y} & 2K_2\frac{\mu_{max}}{Y} \end{pmatrix}
$$

$$
B = \begin{pmatrix} -1 & 1 & 1 \\ 0 & 0 & 1 \\ -1 & 1 & 2 \\ -1 & 2 & 2 \end{pmatrix} , \quad \lambda = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}
$$

Equivalence of the cases A–D

It is easy to check that the QP-invariants

$$
B \cdot A \quad , \quad B \cdot \lambda
$$

are the same in all cases with $B \cdot \lambda = 0$, therefore the LV-form will be the same irrespectively of how the new auxiliary variable is chosen.

Chapter 4

Hamiltonian description

The class of quasi-polynomial (QP) systems plays an increasingly important role in the modelling of dynamical systems since the majority of smooth nonlinear systems occurring in practice can be easily transformed to QP form [8]. It is known that the monomials of a QP system form a Lotka-Volterra (LV) system in a state space which is generally of higher dimension than that of the original QP system [6], [2].

The dissipative-Hamiltonian description of ODEs is an especially useful tool in nonlinear systems theory since it allows the solution of certain analysis and control design problems which are otherwise computationally hard in the general nonlinear case [13].

Based on the above, the purpose of this chapter is the investigation of the relationship between the stability and the dissipative-Hamiltonian structure of LV systems.

The chapter is organized as follows. The basic notions on linear matrix inequalities and stability analysis applied in this chapter can be found in section 4.1. The generalized dissipative-Hamiltonian structure and its properties are described in section 4.2. The main contributions of the chapter, which are the description of the dissipative-Hamiltonian structure in LV systems and its relation to global stability, can be found in sections 4.3 and 4.4 respectively. Section 4.5 contains a simple numerical example that illustrates the theory. Finally, a discussion and conclusions are drawn in section 4.6.

4.1 Basic notions

As we have already seen in Chapter 2, the time derivatives of the monomials of a nonlinear ODE model in QP-form constitute a Lotka-Volterra model i.e.

$$\dot{z}_i = z_i(\lambda_i + \sum_{j=1}^{n} a_{ij} z_j), \quad i = 1, \ldots, m \tag{4.1}$$

where $A = B_{QP} \cdot A_{QP} \in \mathbb{R}^{m \times m}$, $\lambda = B_{QP} \cdot \lambda_{QP} \in \mathbb{R}^{m \times 1}$, $a_{ij} = [A]_{ij}$, $\lambda_i = [\lambda]_i$, and $z_i > 0,\ i = 1, \ldots, m$.

Let us denote the equilibrium point of interest of (4.1) with

$$z^* = [z_1^* \quad z_2^* \quad \ldots \quad z_m^*]^T \in \mathrm{int}(\mathbb{R}_+^m)$$

4.1.1 Linear matrix inequalities

A (nonstrict) linear matrix inequality (LMI) is an inequality of the form

$$F(x) = F_0 + \sum_{i=1}^{m} x_i F_i \geq 0, \tag{4.2}$$

where $x \in \mathbb{R}^m$ is the variable and $F_i \in \mathbb{R}^{n \times n}$, $i = 0, \ldots, m$ are given symmetric matrices. The inequality symbol in (4.2) stands for the positive semidefiniteness of $F(x)$.

One of the most important properties of LMIs is the fact, that they form a convex constraint on the variables, i.e. the set $\{x \mid F(x) \geq 0\}$ is convex. LMIs have been playing an increasingly important role in the field of optimization and control theory since a wide variety of different problems (linear and convex quadratic inequalities, matrix norm inequalities, convex constraints etc.) can be written as LMIs and there are computationally stable and effective (polynomial time) algorithms for their solution [1], [11].

4.1.2 Global stability and diagonal stabilizability

The following Lyapunov function candidate is often used when investigating the global stability properties of (4.1) and the original (2.1) in Chapter 2.

$$V(z) = \sum_{i=1}^{m} c_i \left(z_i - z_i^* - z_i^* \ln \frac{z_i}{z_i^*} \right). \tag{4.3}$$

where $c_i \in \mathbb{R}$, $c_1 > 0$, for $i = 1, \ldots, m$.

It can be calculated (see e.g. [12]) that the time derivative of V satisfies

$$\dot{V}(z) = \frac{1}{2}(z - z^*)^T(A^TC + CA)(z - z^*), \tag{4.4}$$

where $C = \mathrm{diag}(c_1, \dots, c_m)$. This means that if the linear matrix inequality

$$A^TC + CA \leq 0 \tag{4.5}$$

can be solved for a positive definite diagonal matrix C, then z^* is a globally stable equilibrium point of (4.1) with Lyapunov function (4.3). In this case, we call A a *diagonally stabilizable matrix*. Furthermore, if the inequality (4.5) is strict, then the stability is asymptotic (A is *diagonally asymptotically stabilizable*).

Necessary and sufficient algebraic conditions of diagonal stabilizability are only available for 2×2 and 3×3 matrices [9], but it is true that a quadratic matrix A is diagonally stabilizable if and only if the LMI (4.5) has a positive definite diagonal solution, i.e the LMI

$$-(A^TC + CA) \geq 0, \quad C > 0 \tag{4.6}$$

is feasible [1].

The relationship between the stability of the original (2.1) and the derived LV-form (4.1) was studied in [4] and [2] and it was shown that the diagonal stabilizability of A implies the global stability of the equilibrium point of the original QP-model (2.1) corresponding to z^*.

We remark that the diagonal stabilizability of a quadratic matrix is an important problem in different fields such as linear systems theory ([10], [3]) and many other areas [9].

4.2 Hamiltonian systems with dissipation

The form of Hamiltonian systems with dissipation we will use is defined in [13]. In the autonomous case, this system class is defined by the differential equations

$$\dot{x} = (J(x) - R(x))\mathcal{H}_x^T(x), \tag{4.7}$$

where $x \in \mathbb{R}^n$, $\mathcal{H} : \mathbb{R}^n \mapsto \mathbb{R}$ is the Hamiltonian function, $J(x)$ is an $n \times n$ skew symmetric matrix (i.e. $J^T(x) = -J(x)$), the energy conserving part of the system, and $R(x) = R^T(x)$ is the so called dissipation matrix. $\mathcal{H}_x$ denotes the gradient of $\mathcal{H}$ (row vector).

The time derivative of the Hamiltonian function is

$$\dot{\mathcal{H}} = \mathcal{H}_x(x)(J(x) - R(x))\mathcal{H}_x^T(x) = \tag{4.8}$$

$$\underbrace{\mathcal{H}_x(x)J(x)\mathcal{H}_x^T(x)}_{0} - \mathcal{H}_x(x)R(x)\mathcal{H}_x^T(x). \tag{4.9}$$

It is visible from (4.9) that if $y^T R(x) y \geq 0$, $\forall y \in \mathbb{R}^n$ (i.e. R is positive semidefinite), then the Hamiltonian function is nonincreasing. Of course, this property might not be satisfied globally, but only in some neighborhood of the equilibrium point.

The Hamiltonian structure in Lotka-Volterra systems is not new, since it was studied in the excellent paper [7]. However, in our paper we focus on the dissipativeness of the system (4.1) and the relationship between the dissipative Hamiltonian description and the global stability with the logarithmic Lyapunov function (4.3).

4.3 Dissipative Hamiltonian description of LV systems

For the forthcoming calculations, it is comfortable to apply a coordinates shift to put the equilibrium of interest into the origin in the new coordinates. For this purpose, let us define the vector of new variables as

$$x = z - z^* \tag{4.10}$$

With this transformation, the model (4.1) in the new coordinates reads

$$\dot{x}_i = (x_i + z_i^*)\left(\lambda_i + \sum_{j=1}^{m} a_{ij}(x_j + z_j^*)\right) = \tag{4.11}$$

$$(x_i + z_i^*)\sum_{j=1}^{m} a_{ij}x_j \tag{4.12}$$

Consider a quadratic Hamiltonian function

$$\mathcal{H}(x) = \frac{1}{2}(h_1x_1^2 + h_2x_2^2 + \cdots + h_mx_m^2) \tag{4.13}$$

where $h_i > 0,\ i = 1, \ldots, m$. The gradient of $\mathcal{H}$ is then

$$H_x(x) = [h_1x_1 \quad h_2x_2 \quad \ldots \quad h_mx_m]. \tag{4.14}$$

Then the system model (4.12) can be written as

$$\dot{x} = \Gamma(x) A H^{-1} \mathcal{H}_x^T(x), \tag{4.15}$$

where

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1m} \\ a_{21} & a_{22} & \dots & a_{2m} \\ \vdots & & & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mm} \end{bmatrix}, \tag{4.16}$$

$$\Gamma(x) = \mathrm{diag}(x_i + z_i^*) = \begin{bmatrix} (x_1 + z_1^*) & 0 & \dots & 0 \\ 0 & (x_1 + z_2^*) & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & (x_n + z_n^*) \end{bmatrix} \tag{4.17}$$

and

$$H = \mathrm{diag}(h_1, \dots, h_n). \tag{4.18}$$

Let us use the notation $B(x) = \Gamma(x)AH^{-1}$. Now we decompose $B(x)$ in (4.15) to a skew symmetric and a symmetric part in the following way

$$B(x) = \frac{1}{2}\left(B(x) - B^T(x) + B(x) + B^T(x)\right). \tag{4.19}$$

Therefore $R(x) = -\frac{1}{2}(B(x) + B^T(x))$ in our model. This means that the dissipative Hamiltonian structure can be investigated through studying the definiteness of $B(x) + B^T(x)$.

It is useful to further decompose $\Gamma(x)$ as

$$\Gamma(x) = X + Z^*, \tag{4.20}$$

where $X = \mathrm{diag}(x_i)$, $Z^* = \mathrm{diag}(z_i^*)$, $i = 1, \dots, n$. Then we can write

$$B(x) + B^T(x) = \Gamma(x)AH^{-1} + H^{-1}A^T\Gamma^T(x) = \tag{4.21}$$

$$XAH^{-1} + H^{-1}A^TX + Z^*AH^{-1} + H^{-1}A^TZ^*. \tag{4.22}$$

Since X and Z^* are diagonal (and therefore symmetric), the positive definiteness of $B(x)$ leads to the following standard LMI problem

$$XAH^{-1} + H^{-1}A^TX \leq -(Z^*AH^{-1} + H^{-1}A^TZ^*) \tag{4.23}$$

There are in principle two sets of unknown in the above LMI: the coefficients of the Hamiltonian function in H^{-1} and the state variables in the matrix X.

Since we don't know the coefficients of the Hamiltonian function, first we have to solve (4.23) for a positive definite diagonal H^{-1} for $X = 0$. This is performed in the equilibrium point in matrix Z^* when the values of the other set of unknowns is being fixed to zero.

Having determined the Hamiltonian function (i.e. H^{-1}), the dissipativity region can be determined by searching a convex set which satisfies (4.23).

The **method of searching for a locally dissipative Hamiltonian description of (4.1)** can be summarized as follows

1. Determine the equilibrium point of interest (Z^*) and center the coordinates according to (4.12).

2. Try to solve the LMI

$$Z^* A H^{-1} + H^{-1} A^T Z^* \leq 0 \tag{4.24}$$

   for a positive definite diagonal H^{-1}. If the LMI is feasible, then

3. Define the Hamiltonian function with the reciprocials of the diagonal elements in H^{-1} as coefficients, i.e.

$$\mathcal{H}(x) = \sum_{i=1}^{n} h_i x_i^2. \tag{4.25}$$

4. Find a convex set around $x = 0$, for which (4.23) is valid.

4.4 Equivalence to global stability with the logarithmic Lyapunov function

Now we show that the diagonal stabilizability of A is equivalent to the solvability of (4.24), i.e. to the local dissipativity of $R(x)$. For this, we use the following well-known fact from matrix algebra.

Lemma 4.4.1 *An $n \times n$ symmetric matrix W is positive semidefinite if and only if $Q \cdot W \cdot Q^T$ is positive semidefinite for an arbitrary nonsingular quadratic matrix Q of dimension $n \times n$.*

Proof

1. Assume that $W \geq 0$ and Q is an arbitrary nonsingular quadratic matrix of appropriate dimension. Then for any $x \in \mathbb{R}^n$ $x^T W x \geq 0$ and therefore $x^T Q W Q^T x = y^T Q y \geq 0$ with $y = Q^T x$.

2. Let Q be an arbitrary invertible $n \times n$ matrix and $x^T QWQ^T x \geq 0$. Then $x^T Q^{-1} QWQ^T Q^{-T} x = y^T QWQ^T y \geq 0$ with $y = Q^{-T} x$.

Using the above lemma, we can state the following theorem.

Theorem 4.4.1 *For given $Z^* > 0$ and A, the LMI*

$$Z^* AH^{-1} + H^{-1} A^T Z^* \leq 0 \tag{4.26}$$

is solvable for a diagonal H^{-1} if and only if A is diagonally stabilizable i.e. there exists a diagonal $C > 0$ such that

$$A^T C + CA \leq 0. \tag{4.27}$$

Proof

1. Assume that (4.26) holds for a diagonal $H^{-1} > 0$. Then by Lemma 4.4.1

$$H(Z^* AH^{-1} + H^{-1} A^T Z^*)H = HZ^* A + A^T Z^* H \leq 0, \tag{4.28}$$

and therefore the positive definite diagonal C in (4.27) can be chosen as $C = HZ^* = Z^* H$, so A is diagonally stabilizable.

2. Assume that A is diagonally stabilizable i.e. (4.27) holds for a diagonal $C > 0$. Then we can write C as a product of Z^* and another positive definite diagonal matrix H, i.e. $C = HZ^* = Z^* H$. Now (4.27) can be written as $HZ^* A + A^T Z^* H \leq 0$, and again by Lemma 4.4.1

$$H^{-1}(HZ^* A + A^T Z^* H)H^{-1} = Z^* AH^{-1} + H^{-1} A^T Z^* \leq 0. \tag{4.29}$$

4.5 Example

Let the parameters of the LV system (4.1) be given as

$$A = \begin{bmatrix} -1 & 0.3 \\ 7 & -5 \end{bmatrix}, \ \lambda = \begin{bmatrix} 3.5 & -10 \end{bmatrix}^T. \tag{4.30}$$

From the parameters it's clear that the equilibrium point of interest is at $z^* = [5 \;\; 5]^T$. By solving the LMI (4.6) we get that A is diagonally stabilizable e.g. with the positive definite diagonal matrix

$$C = \begin{bmatrix} 10 & 0 \\ 0 & 1 \end{bmatrix}. \tag{4.31}$$

One can check that the eigenvalues of $A^T C + CA$ are $\lambda_1 = -26.1803$ and $\lambda_2 = -3.8197$. This means that the LV system with the parameters admits a local dissipative Hamiltonian description with a quadratic Hamiltonian function in a neighborhood of z^*. Based on Theorem 4.4.1, the Hamiltonian function in the centered coordinates can be computed as

$$\mathcal{H}(x) = 2x_1^2 + 0.2x_2^2. \tag{4.32}$$

A conservative estimate of the neighborhood of the equilibrium point where R is positive definite can be seen in Figure 4.1. The estimate was obtained by simply finding four corner points parallel to the axes of the coordinates system.

We note that often the best geometry of the level sets of the Hamiltonian function (which are ellipsoids) can be achieved by finding H with minimal condition number, and this problem is also easily solvable numerically [1].

4.6 Discussion and conclusions

The relation between the global stability and the dissipative Hamiltonian structure of QP and LV systems was investigated in this chapter.

We have shown that the monomials of a QP system form a locally dissipative Hamiltonian system with quadratic Hamiltonian function if and only if the QP (and LV) system is globally stable with the Lyapunov function (4.3).

Furthermore, we have presented a systematic method for finding the quadratic Hamiltonian function through the solution of linear matrix inequalities. The same LMI can be used for estimating the local dissipativity region.

The Hamiltonian description and the estimation of the dissipativity neighborhood was illustrated by a numerical example.

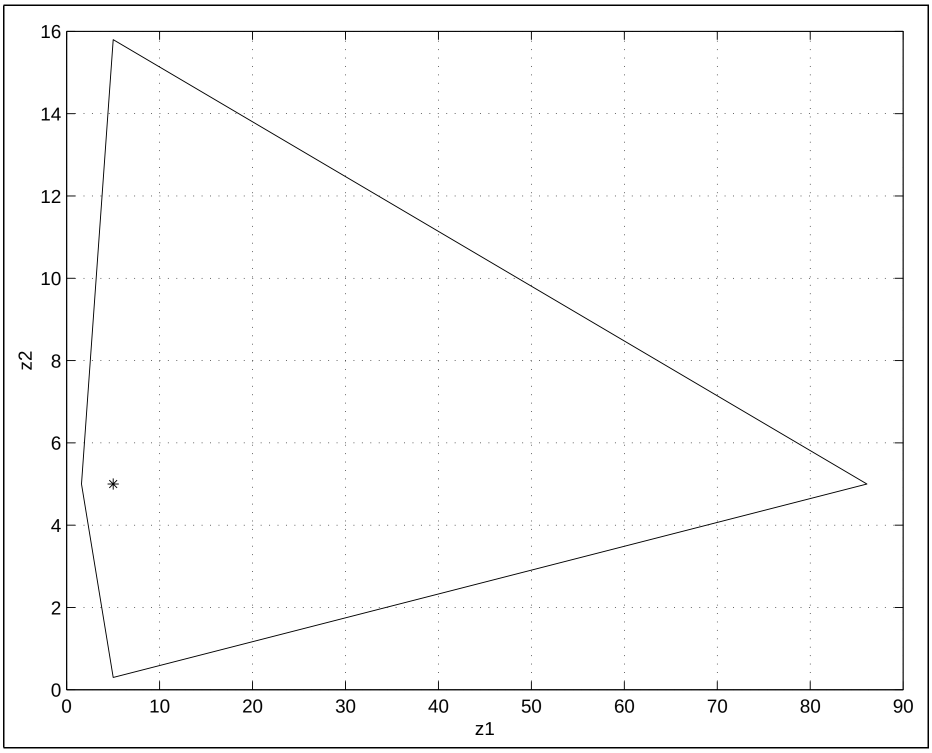

Figure 4.1: Conservative estimate of the convex quadratic dissipativity neighborhood of the equilibrium point (denoted by *).

Chapter 5

QP-DAE system models

The notion of QP type ordinary differential equation models can be easily generalized to QP differential-algebraic equation (QP-DAE) models as follows.

Consider the general form of semi-explicit DAE models:

$$\dot{x} = F(x,z) \quad , \quad x(0) = x_0 \tag{5.1}$$

$$0 = G(x,z) \tag{5.2}$$

where $F : \Re^{n\times d} \to \Re^n$ and $G : \Re^{n\times d} \to \Re^d$ with n being the dimension of the differential variable vector x and d being the dimension of the algebraic variable vector z. The above DAE model is a QP-DAE model if both F and G are in quasi-polynomial form.

5.1 The general form of QP-DAE models

The general form is obtained by extending the general form of QP-ODE models in Eq. (2.1) with suitable algebraic variables and algebraic equations as follows.

$$\dot{x_i} = x_i\lambda_i + x_i \sum_{j=1}^{m} A_{ij} \prod_{k=1}^{n} x_k^{B_{jk}} \cdot \prod_{k=1}^{d} z_k^{B_{j(n+k)}}, \qquad i = 1,\ldots,n, \tag{5.3}$$

$$0 = z_i\lambda_{n+i} + z_i \sum_{j=1}^{m} A_{(n+i)j} \prod_{k=1}^{n} x_k^{B_{jk}} \cdot \prod_{k=1}^{d} z_k^{B_{j(n+k)}}, \qquad i = 1,\ldots,d, \qquad m \geq (n+d) \tag{5.4}$$

where the parameters A and B of the model are $(n+d)\times m$, $m\times(n+d)$ real matrices and $\lambda \in R^{(n+d)}$ is a real vector. Again, we assume that every variable is strictly positive, i.e.

$$x_i > 0 \ , \quad i = 1, ..., n \quad , \quad z_i > 0 \ , \quad i = 1, ..., d$$

It is important to notice that the **quasi-monomials** of a QP-DAE model are extended versions of the original ones in the form:

$$q_j = \prod_{k=1}^{n} x_k^{B_{jk}} \cdot \prod_{k=1}^{d} z_k^{B_{j(n+k)}} \quad , \quad j = 1, ..., m \tag{5.5}$$

5.1.1 An equivalent non-minimal ODE form of QP-DAE models

QP-DAE models can be represented as *hidden DAE sytems* if the algebraic variable vector can be expressed explicitly as function of the differential variable. A necessary condition is on the invertibility of the Jacobian matrix of the algebraic equation ($G(x,z)$ in Eq. (5.4)) by the algebraic variables:

$$\exists J^{-1}, \quad \text{where} \quad J = \left[\frac{\partial G}{\partial z}\right] \tag{5.6}$$

Note that this condition is only a necessary, but not sufficient condition for the expressibility of z in terms of x, but quite enough to represent $\dot{z}$ in terms of $\dot{x}$ on a connected subset $S \subset R^{n+d}$ where Eq. (5.6) is fulfilled for every $[x, \ z]^T \in S$. It gives

$$\dot{z} = -\left[\frac{\partial G}{\partial z}\right]^{-1}\left[\frac{\partial G}{\partial x}\right]\dot{x} = \widehat{G}(x,z)\dot{x} \tag{5.7}$$

by means of the Implicit Function Theorem. Note that $\widehat{G}(x,z)$ is a matrix valued function, and the elements of $\dot{z}$ can be written in the following form:

$$\begin{aligned} \dot{z}_i &= z_i\left(\frac{1}{z_i}\sum_{l=1}^{n}\widehat{G}_{il}(x,z)\dot{x}_l\right) = \\ &= z_i\left(\sum_{l=1}^{n}\frac{\widehat{G}_{il}(x,z)}{z_i}x_l\lambda_l + \sum_{l=1}^{n}\sum_{j=1}^{m}\frac{\widehat{G}(x,z)_{il}}{z_i}x_l A_{lj} q_j\right) \\ & \quad i = 1, \ldots, d \end{aligned} \tag{5.8}$$

where $\widehat{G}_{ik}(x,z)$ denotes the appropriate element of the matrix-valued function $\widehat{G}$. The elements of $\widehat{G}$ are polynomials since the set of polynomials is closed for differentiation, and also for addition, multiplication (and therefore division) occurring in matrix inversion and multiplication. It guarantees that the new differential equations in Eq. (5.8) are indeed in QP-form.

Finally we can conclude in a nonminimal ODE representation described by Eqs. (5.3,5.8) but the set of quasi-monomials has to be extended with new participants, which come from the following terms:

$$\frac{\widehat{G}_{il}(x,z)}{z_i}x_l\lambda_l,\ \frac{\widehat{G}_{il}(x,z)}{z_i}x_lA_{lj}q_j,\quad i=1\dots d,\ j=1\dots m,\ l=1\dots n \tag{5.9}$$

With this extended set of quasi-monomials, this representation will be in the form of Eq. (2.1).

5.1.2 The logarithmic form

In order to obtain an easy-to-handle compact logarithmic form of the QP-DAE equations above, we extend the variable vectors as follows:

$$X^* = \begin{bmatrix} x^* \\ -- \\ z^* \end{bmatrix} \quad , \quad \widetilde{X}^* = \begin{bmatrix} x^* \\ -- \\ 0 \end{bmatrix}$$

Then the compact vector-matrix form of the logarithm of Eqs. (5.3)-(5.4) is as follows:

$$\dot{\widetilde{X}}^* = \lambda + AQ \tag{5.10}$$

with

$$Q^* = BX^* \tag{5.11}$$

It will be useful later, if we partition the system parameter matrices and vectors according to the variable vector partition to get:

$$A = \begin{bmatrix} A_d \\ -- \\ A_a \end{bmatrix} \quad , \quad \lambda = \begin{bmatrix} \lambda_d \\ -- \\ \lambda_a \end{bmatrix} \quad , \quad B = \begin{bmatrix} B_d & | & B_a \end{bmatrix} \tag{5.12}$$

Finally we can construct a compact linear-analogue logarithmic form of QP-DAE equations by uniting the parameters A and λ in a structure matrix $\widetilde{A} \in \Re^{(n+d)\times(m+1)}$ as follows:

$$\widetilde{A} = \begin{bmatrix} \lambda & | & A \end{bmatrix} \tag{5.13}$$

and extend the matrix B with a 0 row to have

$$\widetilde{B} = \begin{bmatrix} 0 \\ -- \\ B \end{bmatrix} \quad , \quad \widetilde{Q} = \begin{bmatrix} 1 \\ q_1 \\ \dots \\ q_m \end{bmatrix} \tag{5.14}$$

Then the compact *linear-analogue logarithmic form of QP-DAE equations* is as follows:

$$\dot{\widetilde{X}}^* = \widetilde{A}\widetilde{Q} \tag{5.15}$$

with

$$\widetilde{Q}^* = \widetilde{B}X^* \tag{5.16}$$

5.2 Form invariance of linear DAE models

Before we start investigating the form-invariance of QP-DAE models with respect to QM-transformations, let us have a look on a simple analogous case - to the case of form invariance of linear DAE models with respect to linear transformations.

Consider the following general description of linear DAE systems (with no control inputs):

$$\begin{bmatrix} \dot{x} \\ 0 \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} x \\ z \end{bmatrix} \tag{5.17}$$

where $x \in \Re^n$ is the vector of differential, $z \in \Re^d$ is

Near the assumption that the model in Eq. (5.17) has differential index equal to one (in linear case it is equivalent with the assumption that A_{22} is invertible), the algebraic variables can be expressed in terms of the differential ones:

$$z = -A_{22}^{-1} A_{21} x \tag{5.18}$$

The time-derivative of this equation gives

$$\dot{z} = -A_{22}^{-1} A_{21} \dot{x} = -A_{22}^{-1} A_{21} (A_{11} x + A_{12} z) \tag{5.19}$$

which leads to the following linear ODE:

$$\begin{bmatrix} \dot{x} \\ \dot{z} \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ -A_{22}^{-1} A_{21} A_{11} & -A_{22}^{-1} A_{21} A_{12} \end{bmatrix} \begin{bmatrix} x \\ z \end{bmatrix} \tag{5.20}$$

which is a hidden DAE system with state matrix $\widetilde{A}_{(n+d)\times(n+d)}$. This linear ODE is *nonminimal*, which means that the dynamics of the system can be described by a system with a smaller set of differential equations. If A_{11} is invertible, then the order of the system equals to $rank(A_{11}) = n$.

If the initial conditions $[x(t_0)\ z(t_0)]^T$ are *consistent* (i.e. they fulfill the algebraic equation $0 = A_{21}x(t_0) + A_{22}z(t_0)$), this model is equivalent with the DAE model in Eq. (5.17).

The application of the general invertible linear transformation

$$T = \begin{bmatrix} T_{11_{n\times n}} & T_{12_{n\times d}} \\ T_{21_{d\times n}} & T_{22_{d\times d}} \end{bmatrix} \tag{5.21}$$

to the model in Eq. (5.20) linearly combines the variables, but it won't change the rank of the transformed state matrix:

$$T \begin{bmatrix} \dot{x} \\ \dot{z} \end{bmatrix} = T \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} T^{-1} \cdot T \begin{bmatrix} x \\ z \end{bmatrix} \tag{5.22}$$

which leads to

$$\begin{bmatrix} T_{11}\dot{x} + T_{12}\dot{z} \\ T_{21}\dot{x} + T_{22}\dot{z} \end{bmatrix} = \widetilde{A} \begin{bmatrix} T_{11}x + T_{12}z \\ T_{21}x + T_{22}z \end{bmatrix} \tag{5.23}$$

where $\widetilde{A} = TAT^{-1}$.

As we can see, a general linear invertible transformation carries a nonminimal ODE to a nonminimal ODE, or in other words *a hidden DAE system to an equivalent hidden DAE system.*

5.2.1 Retrieving the algebraic equations from the transformed linear DAE

Near the index-one assumption, we can retrieve the original DAE structure from a hidden DAE system by finding an appropriate transformation. For this purpose we can use the fact that the coefficient matrix $\widetilde{A}$ is not of full rank because of construction but it is of rank n Assume that $A_1 1$ is invertible in Eq. (5.20). Then the remaining d rows (or columns) can then be expressed as a linear combination of the n rows (or columns) participating in the spanning set of the n-dimensional sub-space.

Formally speaking, consider a linear ODE model in the form of

$$\dot{\widetilde{x}} = \frac{d\widetilde{x}}{dt} = \widetilde{A}\widetilde{x} \tag{5.24}$$

such that $\widetilde{A} \in \Re^{\widetilde{n}\times\widetilde{n}}$ but rank $\widetilde{A} = n < \widetilde{n}$. The first n rows of $\widetilde{A}$ are linearly independent vectors, and the remaining rows $\widetilde{a}_j,\ j = n+1,..,\widetilde{n}$ can be expressed as linear combinations of the first n rows, i.e.

$$\widetilde{a}_j = \sum_{k=1}^{n} \alpha_{jk}\widetilde{a}_k \quad , \quad j = n+1,..,\widetilde{n} \tag{5.25}$$

The coefficient row vector α_j corresponding to x_j , $j = n+1, .., \widetilde{n}$ can be computed by solving a linear set of equations. Since $rank(\widetilde{A}) = n$, it has n independent columns. Partition $\widetilde{A}$ in such a way that its first n columns are linearly independent:

$$\widetilde{A}_{part} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \tag{5.26}$$

where the first block-column contains the linearly independent columns, the first block-row contains the linearly independent rows. The coefficient row vector α_j can be computed by solving the following linear set of equations:

$$\alpha_j M_{11} = M_{21,(j-n)} \quad , \quad j = n+1, .., \widetilde{n} \tag{5.27}$$

where $M_{21,(i)}$ denotes the i^{th} row of M_{21}. Since M_{11} is invertible, the coefficients can be computed easily. Moreover, if we collect the row vectors α_j into a combination matrix L:

$$L = \begin{bmatrix} \alpha_{n+1} \\ \vdots \\ \alpha_{n+d} \end{bmatrix} \tag{5.28}$$

we can get the combination matrix computed in a more compact form:

$$L = M_{21} M_{11}^{-1} \tag{5.29}$$

After determining the coefficients, from Eq. (5.25) we can derive a linear set of equations relating the time derivative of the corresponding state variables in $\widetilde{x}$ which reads

$$\dot{\widetilde{x}}_j = \sum_{k=1}^{n} \alpha_{jk} \dot{\widetilde{x}}_k \quad , \quad j = n+1, .., \widetilde{n}$$

Finally we can conclude in a linear dependence of the corresponding state variables integrating the equations above:

$$\widetilde{x}_j = \lambda_j + \sum_{k=1}^{n} \alpha_{jk} \widetilde{x}_k \quad , \quad j = n+1, .., \widetilde{n} \tag{5.30}$$

Since our DAE system is *linear*, $\lambda_j = 0$, $j = 1, \ldots, \widetilde{n}$. Observe that the above equations are *algebraic equations in the transformed variables.*

Finally we can construct the DAE form of the transformed ODE model in Eq. (5.24) by leaving the first n ODE unchanged but replacing the remaining ODEs by the algebraic equations in Eq. (5.30). *This way we can obtain the DAE form of any transformed ODE originating from a DAE model.*

5.2.2 From hidden linear DAE systems to minimal ODE models

Nonminimal linear ODE systems can be transformed into DAE form as it is described in the previous section. The resulted algebraic equations are explicit in their variables, so they can be substituted into the differential equations leading to a *minimal* ODE model of the system. This substitution can be performed in one step by means of a linear transformation. According to Eq. (5.28), the linear model in Eq. (5.24) can be written in the following form:

$$\frac{d}{dt}\begin{bmatrix} \widetilde{x}_{P1} \\ \widetilde{x}_{P2} \end{bmatrix} = \begin{bmatrix} \widetilde{A}_1 & \widetilde{A}_2 \\ L\widetilde{A}_1 & L\widetilde{A}_2 \end{bmatrix} \begin{bmatrix} \widetilde{x}_{P1} \\ \widetilde{x}_{P2} \end{bmatrix} \tag{5.31}$$

where

$$\widetilde{x}_{P1} = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \quad , \quad \widetilde{x}_{P2} = \begin{bmatrix} x_{n+1} \\ \vdots \\ x_{n+d} \end{bmatrix}$$

are partitions of vector $\widetilde{x}$.

Let us apply the following transformation to Eq. (5.31):

$$T_{min} = \begin{bmatrix} I_{n\times n} & 0_{n\times d} \\ -L_{d\times n} & I_{d\times d} \end{bmatrix} \tag{5.32}$$

It transforms our system to

$$\begin{bmatrix} \dot{\widetilde{x}}_{P1} \\ 0 \end{bmatrix} = \begin{bmatrix} \widetilde{A}_1 + \widetilde{A}_2 L & \widetilde{A}_2 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \widetilde{x}_{P1} \\ \lambda_{P2} \end{bmatrix} \tag{5.33}$$

where the vector λ_2 is build of λ_j -s in Eq. (5.30):

$$\lambda_{P2} = \begin{bmatrix} \lambda_{n+1} \\ \vdots \\ \lambda_{n+d} \end{bmatrix}$$

Since the second row equals to zero, only the first row has to be considered, therefore the system can be written in the following form:

$$\dot{\widetilde{x}}_{P1} = \widetilde{A}_2\lambda_{P2} + (\widetilde{A}_1 + \widetilde{A}_2 L)\widetilde{x}_{P1} \tag{5.34}$$

Note that λ_{P2} is unambiguous for given initial conditions:

$$\lambda_{P2} = \widetilde{x}_{P1}(t_0) - L\widetilde{x}_{P2}(t_0) \tag{5.35}$$

This way we get to the minimal realization of the model in Eq. (5.24) which is equivalent with the transformation which expresses the dependent (algebraic) variables in terms of the independent (differential) variables and then substitutes them into the differential equations. Moreover, this minimal model is unambiguous for given initial conditions.

5.3 Form Invariance of QP-DAE models

5.3.1 Extended QM-transformation

In this section, we show the form invariance of QP-DAE models. Due to our purpose, we transform our QP-DAE model in Eq. (5.3-5.4)into QP-ODE form. We will use the compact logarithmic form of QP-ODE models in Eq. (2.4) In order to get the characterization of a QP-DAE equivalence class, we first extend the concept of QM-transformations as follows:

$$X_{i} = \prod_{k=1}^{(n+d)} \hat{X}_{k}^{C_{ik}}, \qquad i = 1, \ldots, n+d \tag{5.36}$$

where C is an arbitrary $(n+d) \times (n+d)$ invertible matrix. Observe that now we use the extended variable vector X which contains both the differential and algebraic variables.

5.3.2 Retrieving the algebraic equations

Next, we apply this QM transformations in its logarithmic form to the QP-ODE model in its linear-analogue logarithmic form (see Eq. (2.4) to get the LV-ODE representation. The parameter matrix $\widetilde{A}_{LV_h}$ will now be rank-deficient.

This allows us to retrieve algebraic equations between the variables generated by the linearly-dependent rows

$$\widehat{\widetilde{a}}_j \quad , \quad j = n+1, ..., n+d$$

of the coefficient matrix the same way as it is in the case of transformed linear DAEs in section 5.2.

Using the same derivation as in section 5.2 we can retrieve the QP-DAE algebraic equations in the following form:

$$\widetilde{x}_j^* = \lambda_j + \sum_{k=1}^{n} \alpha_{jk} \widetilde{x}_k^* \quad , \quad j = n+1, .., n+d \tag{5.37}$$

This give rise to QP-type (quasi-monomial) algebraic equations in the original variables as

$$x_j = \lambda_j \cdot \prod_{k=1}^{n} (x_k)^{\alpha_{jk}} \quad , \quad j = n+1, .., n+d \tag{5.38}$$

It is important to observe that *there may be new quasi-monomials in the retrieved QP-algebraic set of equations.*

Note that with the method above we can retrieve a part of the algebraic equations, if they are in the form of Eq. (5.38). Unfortunately, not all of the QP-type algebraic equations can be retrieved. Further methods would focus on considering the structure of the coefficient matrix pairs (A,B) of the QP-model together.

5.4 LV-form of QP-DAE models

The results in the previous section show, that

1. It is possible to transform a QP-DAE model into LV form similarly to the case of QP-ODEs (using $C = B^{-1}$), but the resulted transformed model will be a LV-ODE, i.e. the algebraic equations formally disappear and the resulted coefficient matrix $\widetilde{A}'$ will be rank deficient.

2. We can retrieve the algebraic equation from the LV-ODE form of a QP-DAE, but then the algebraic equations will not necessarily be in a LV form (i.e. with at most 2nd order terms).

5.5 Towards the structural analysis of nonlinearity in QP-DAE systems

From all of the above and from the results of structural analysis of computational properties I have understand the following lessons concerning the structural analysis of nonlinearity in QP-DAE systems.

1. We don't need to bother ourselves with the ODE part of the model, the algebraic part of it is the one which matters anyway. *I think it is easy to show that an* ***algebraic QP set of equations is form invariant in itself and thus can be transformed into an algebraic LV-form****.*

2. The structural invariant $A' = BA$ in any "homogeneous" QP set of equations (both for QP-ODE or QP-algebraic equations) characterizes

both the convexity and nonlinearity of the set. I think I have an explanation how the Jordan forms comes into the picture but we can simply use any other characterization of the eigenvalues instead.

3. The it makes sense to use the following structure indices to characterize the structure of a QP-DAE (or any other nonlinear DAE which we can imbed into this form)

    - the number of quasi-monomials in the overall QP-DAE form,
    - the size of L-components in the structural analysis,
    - the number of quasi-monomials in every L-component (as a set of QP-algebraic equations),
    - the characterization of structural invariants $A' = BA$ in every L-components (as a set of QP-algebraic equations)

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