THE STRUCTURE AND ANALYSIS OF QP-DAE SYSTEM MODELS

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Abstract

QP-DAE system models will potentially play an important role in process systems engineering because the majority of lumped process models can be embedded into this class without approximation.

In this report two canonical forms, a hidden non-minimal Lotka-Volterra (LV) ODE form and a minimal QP-DAE form, are proposed for representing a wide class of lumped process systems in index-1 DAE form. The form invariance properties of QP-DAE models, their steady-states and local stability properties at steady-state points are discussed.

Algorithms for transforming a QP-DAE in its hidden non-minimal QP-ODE form into its minimal QP-DAE form (i.e. the retrieval of the algebraic equations) are also described.

The notions and tools are illustrated on simple examples.

Contents

Chapter 1

Introduction

Lumped dynamic process models, which have no spatial distribution of their variables, comprise sets of differential-algebraic equations (DAEs). Many lumped dynamic models of process systems can be written without approximation in quasi-polynomial differential-algebraic equation (QP-DAE) form.

The QP formalism has a great advantage: it can capture many kinds of nonlinearity without approximation in a strongly structured universal form ([5]). QP systems have both graph and matrix representations; techniques from both these disciplines can be applied.

In this report, we extend the earlier structural analysis work ([8]) to assess the static and dynamic properties of DAE process models in QP form. The QP approach allows the use not only of structural information for model analysis, but also the model's constituent mathematical functions and parameter values.

Similarly to the case of other special system classes (such as LTI, input-affine nonlinear, etc.) the various algebraically equivalent forms of QP-DAE models serve to investigate different properties such as local stability or computational decompositions.

Chapter 2

The structure of QP-DAE system models

Consider the general form of semi-explicit DAE models [1]:

$$\dot{x} = F(x, z) \quad , \quad x(0) = x_0 \tag{2.1}$$
$$0 = G(x, z) \tag{2.2}$$

where $F : \mathbb{R}^{n \times d} \rightarrow \mathbb{R}^n$ and $G : \mathbb{R}^{n \times d} \rightarrow \mathbb{R}^d$ 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.

The aim of this section is to investigate how and under which conditions can one apply the description and analysis tools developed for QP-ODE models also in the case of QP-DAE models.

2.1 The general form of QP-DAE models

The general form is obtained by extending the general form of QP-ODE models [5] with suitable algebraic variables and algebraic equations as follows.

$$\dot{x}_i = x_i \left(\lambda_i + \sum_{j=1}^{m} A_{ij} \prod_{k=1}^{n} x_k^{B_{jk}} \cdot \prod_{k=1}^{d} z_k^{B_{j(n+k)}} \right), \tag{2.3}$$
$$i = 1, \dots, n,$$
$$0 = z_i \left(\lambda_{n+i} + \sum_{j=1}^{m} A_{(n+i)j} \prod_{k=1}^{n} x_k^{B_{jk}} \cdot \prod_{k=1}^{d} z_k^{B_{j(n+k)}} \right), \tag{2.4}$$
$$i = 1, \dots, d, \qquad m \geq (n + d)$$

where the parameters A and B of the model are $(n + d) \times m$, $m \times (n + d)$ real matrices and $\lambda \in \mathbb{R}^{(n+d)}$ is a real vector.

It is important that we assume that every variable is strictly positive, i.e.

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

Inputs are regarded as parameters, thus this autonomous form can be regarded as a system model with x_i being the state variables.

It is important to notice that the **monomials**, also called **quasi-monomials**, of a QP-DAE model are present in both the differential and algebraic equations in the form:

$$q_j = \prod_{k=1}^{n} x_k^{B_{jk}} \cdot \prod_{k=1}^{d} z_k^{B_{j(n+k)}} \quad , \quad j = 1, ..., m \tag{2.5}$$

It is important to observe, that the algebraic equations (2.4) of the above QP-DAE form are ambiguous, as we can multiply any of them with a quasi-polynomial expression and they still remain QP-algebraic. Such a multiplication, however, will change the apparent quasi-monomials (2.5).

Example 1 A simple example of a QP-DAE model will be used to illustrate the concepts throughout this report. The DAE model is:

$$\dot{x}_1 = x_1(5 + 3x_1^3 x_3 + 4x_2^2) \tag{2.6}$$
$$\dot{x}_2 = x_2(2 + 7x_1 x_3^5) \tag{2.7}$$
$$x_3 = 3x_1^4 x_2^5 + 4x_2^2 \tag{2.8}$$

The above DAE can be easily transformed to the general form in Eqs. (2.3)-(2.4) to get

$$\dot{x}_1 = x_1(5 + 3x_1^3 x_3 + 4x_2^2) \tag{2.9}$$
$$\dot{x}_2 = x_2(2 + 7x_1 x_3^5) \tag{2.10}$$
$$0 = x_3(-x_3 + 3x_1^4 x_2^5 + 4x_2^2) \tag{2.11}$$

with the quasi-monomials

$$Q = \left\{x_1^3 x_3,\ x_2^2,\ x_1 x_3^5,\ x_1^4 x_2^5,\ x_3\right\} \tag{2.12}$$

The differential and algebraic variable sets are $x = [x_1 \quad x_2]^T$, $z = x_3$, so we have $n = 2$ and $d = 1$. The parameters of the model are

$$\lambda = \begin{pmatrix} 5 \\ 2 \\ 0 \end{pmatrix} \quad , \quad A = \begin{pmatrix} 3 & 4 & 0 & 0 & 0 \\ 0 & 0 & 7 & 0 & 0 \\ 0 & 4 & 0 & 3 & -1 \end{pmatrix} \quad , \quad B = \begin{pmatrix} 3 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 5 \\ 4 & 5 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{2.13}$$

Example 2: A continuous fermentation process A fermentation process with no control input (constant F and S_F) and quadratic type reaction kinetics will also be considered. Its DAE model is:

$$\dot{X} = X(-\frac{F}{V} + \mu) \tag{2.14}$$
$$\dot{S} = S(-\frac{F}{V} + \frac{S_F F}{V} S^{-1} - \frac{1}{Y} X S^{-1} \mu) \tag{2.15}$$
$$\mu = S^2 \tag{2.16}$$

The above equation can also be transformed to the general QP-DAE form:

$$\dot{X} = X(-\frac{F}{V} + \mu) \tag{2.17}$$
$$\dot{S} = S(-\frac{F}{V} + \frac{S_F F}{V} S^{-1} - \frac{1}{Y} X S^{-1} \mu) \tag{2.18}$$
$$0 = \mu(S^2 - \mu) \tag{2.19}$$

Here again we have a single algebraic variable $z = \mu$ and the set of quasi-monomials is

$$Q = \left\{\mu,\ S^{-1},\ XS^{-1}\mu,\ S^2\right\} \tag{2.20}$$

The parameters of the QP-DAE model are:

$$\lambda = \begin{pmatrix} -\frac{F}{V} \\ -\frac{F}{V} \\ 0 \end{pmatrix} \quad , \quad A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{S_F F}{V} & -\frac{1}{Y} & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix} \quad , \quad B = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & -1 & 1 \\ 0 & 2 & 0 \end{pmatrix} \tag{2.21}$$

2.2 The monomial-explicit form of QP-DAE models

In this section we will show that under mild conditions it is possible to express the *monomials of the algebraic variables* of the implicit QP-DAE model in Eqs. (2.3-2.4) explicitly (in terms of the differential ones). This monomial-explicit description is not in QP form in general, but we will show that it becomes a QP model by introducing only one new algebraic variable.

The special monomial-explicit QP-DAEs are special cases of the general QP-DAE model class where one can easily develop their QP-ODE form by direct substitution and variable embedding. This enables to apply the tools and techniques developed for QP-ODE models for this QP-DAE subclass in an easy and straightforward way.

Let us consider the algebraic equations (2.4). Construct the set of algebraic quasi-monomials Q^z by considering the differential variables as constant coefficients. Assume now that the number of these quasi-monomials is equal to the number of algebraic equations and that of the algebraic variables (d), i.e.

$$Q^z = \{q_1^z, \ldots, q_d^z\} \tag{2.22}$$

where

$$q_i^z = \prod_{j=1}^{d} z_j^{B_{ij}^z} \quad , \quad B^z \in \mathbb{R}^{d\times d} \tag{2.23}$$

This means that the logarithm of these QMs are linear combinations of the logarithm of the algebraic variables:

$$ln q_i^z = \sum B_{ij}^z ln z_j$$

which can be written in compact form:

$$q^{z*} = B^z z^* \tag{2.24}$$

where the superscript * on a vector indicates taking the logarithm element-by-element. If this assumption is fulfilled, then these quasi-monomials can be expressed explicitly from the algebraic equations with the following method. Write Eq. (2.4) in the following matrix-vector form:

$$\mu(\lambda, x) = A(x) q^z \tag{2.25}$$

where μ is a vector containing the terms which are independent of the algebraic variables, A is a matrix-valued function of the differential variables, while q^z denotes the vector made of $q_1^z, \ldots, q_d^z$. This is a linear set of equations with respect to q^z. If $\mu(\lambda, x) \neq 0$ and $det(A(x)) \neq 0$ then this set of equations can be solved for q^z by using Cramer's Rule:

$$q_i^z = \frac{det(S_i)}{det(A)} \quad \text{where} \quad \mathrm{S_i(\lambda, x) = (A_1 \ \ldots \ A_{i-1} \ \ \mu \ \ A_{i+1} \ \ldots \ A_d) \quad , \quad i = 1, \ldots, d} \tag{2.26}$$

and $A_i,\ i = 1, \ldots, d$ denotes the i-th column of A. This form of the algebraic equations is non-QP in general because $det(A)$ is generally a quasi-polynomial not a monomial, but if we introduce an additional algebraic variable

$$z_{d+1} = \frac{1}{det(A(x))} \tag{2.27}$$

then the monomial-explicit form of algebraic equations becomes a QP description:

$$q_i^z = z_{d+1} det(S_i(x)) \ , \quad i = 1, \ldots, d \tag{2.28}$$

$$z_{d+1}^{-1} = det(A(x)) \tag{2.29}$$

since $det(A(x))$ and $det(S_i(x))$, $i = 1, \ldots, d$ are polynomials of x. Thus, the monomial-explicit form of QP-DAE models given by Eqs. (2.3,2.28-2.29) consists of $m+1$ equations.

From Eq. (2.24) it follows that if B^z is of full rank, the algebraic variables can be expressed from the explicitly given algebraic monomials:

$$z^* = (B^z)^{-1} q^{z*} \tag{2.30}$$

and can be substituted into the differential equations of the model. This model is *minimal* (containing n differential equations) *but* it is *non-QP in general.* Non-QP terms in this model can be handled by variable embedding, resulting in a non-minimal, but QP differential model. For example, the embedding of z_{d+1} is performed by taking its time-derivative:

$$\frac{d}{dt} z_{d+1} = -\frac{1}{det(A(x))^2} \frac{d}{dt} det(A(x)) = -z_{d+1}^2 \frac{d}{dt} det(A(x)) \tag{2.31}$$

which results in a QP-ODE equation, since $det(A(x))$ and therefore its time-derivative are quasipolynomials.

2.2.1 A simple example

Consider the following QP-DAE model with implicit algebraic equations:

$$\dot{x} = x\big(x^2 z_1 + z_2^3\big) \tag{2.32}$$

$$0 = x^2 z_1^2 z_2 + x z_1^2 z_2 + 9x^3 + 5x + 8 + 2x z_2^{\frac{3}{2}} \tag{2.33}$$

$$0 = 3x^2 z_1^3 z_2 + 4x z_1 + z_1 z_2^{\frac{3}{2}} \tag{2.34}$$

The number of monomials of the algebraic equations is 8, and the number of algebraic monomials (q^z's) is five. It does not match with the number of the algebraic equations (which is 2). Thus, this model cannot be transformed into monomial-explicit form. But, if one divides the second algebraic equation by z_1:

$$\dot{x} = x\big(x^2 z_1 + z_2^3\big) \tag{2.35}$$

$$0 = x^2 z_1^2 z_2 + x z_1^2 z_2 + 9x^3 + 5x + 8 + 2x z_2^{\frac{3}{2}} \tag{2.36}$$

$$0 = 3x^2 z_1^2 z_2 + 4x + z_2^{\frac{3}{2}} \tag{2.37}$$

the number of algebraic monomials reduces to 2, and therefore the condition on the number of algebraic monomials is fulfilled. Write the algebraic equations in the form $\mu(\lambda, x) = A(x)q^z$:

$$\begin{bmatrix} -9x^3 - 5x - 8 \\ -4x \end{bmatrix} = \begin{bmatrix} x^2 + x & 2x \\ 3x^2 & 1 \end{bmatrix} \begin{bmatrix} z_1^2 z_2 \\ z_2^{\frac{3}{2}} \end{bmatrix} \tag{2.38}$$

By solving this set of equations with the condition that $det(A(x)) \neq 0$ and introducing

$$z_3 = \frac{1}{det(A(x))} = \frac{1}{-6x^3 + x^2 + x} \tag{2.39}$$

we get the following monomial-explicit DAE model:

$$\begin{aligned}
\dot{x} &= x\big(x^2 z_1 + z_2^3\big) && (2.40)\\
q_1^z = z_1^2 z_2 &= z_3(-9x^3 + 8x^2 - 5x - 8) && (2.41)\\
q_2^z = z_2^{\frac{3}{2}} &= z_3(27x^5 + 11x^3 + 20x^2) && (2.42)\\
z_3^{-1} &= -6x^3 + x^2 + x && (2.43)
\end{aligned}$$

As a result, we get a monomial-explicit QP-DAE description at the price of introducing a new algebraic variable. Since the exponent matrix B^z is of full rank, and its inverse,

$$(B^z)^{-1} = \begin{bmatrix} 2 & 1 \\ 0 & \frac{3}{2} \end{bmatrix}^{-1} = \begin{bmatrix} \frac{1}{2} & -\frac{1}{3} \\ 0 & \frac{2}{3} \end{bmatrix} \tag{2.44}$$

is also of full rank, the algebraic variables z_1 and z_2 can be given explicitly:

$$\begin{aligned}
z_1 &= (q_1^z)^{\frac{1}{2}}(q_2^z)^{-\frac{1}{3}} = \big(z_3(-9x^3 + 8x^2 - 5x - 8)\big)^{\frac{1}{2}}\big(z_3(27x^5 + 11^3 + 20x^2)\big)^{-\frac{1}{3}} && (2.45)\\
z_2 &= (q_2^z)^{\frac{2}{3}} = \big(z_3(27x^5 + 11^3 + 20x^2)\big)^{\frac{2}{3}} && (2.46)
\end{aligned}$$

The algebraic part can be substituted into the differential equation resulting in a minimal one-dimensional ODE that is, unfortunately, not in QP form:

$$\dot{x} = x\left(x^2\Big(\frac{-9x^3 + 8x^2 - 5x - 8}{-6x^3 + x^2 + x}\Big)^{\frac{1}{2}}\Big(\frac{27x^5 + 11^3 + 20x^2}{-6x^3 + x^2 + x}\Big)^{-\frac{1}{3}} + \Big(\frac{27x^5 + 11^3 + 20x^2}{-6x^3 + x^2 + x}\Big)^2\right)$$

To get a (non-minimal) QP-ODE representation, a possible way is embedding z_3 and then taking the time-derivative of q_1^z and q_2^z:

$$\begin{aligned}
\dot{x} &= x\big(x^2 z_1 + z_2^3\big) = x\big(x^2 (q_1^z)^{\frac{1}{2}}(q_2^z)^{-\frac{1}{3}} + (q_2^z)^2\big) && (2.47)\\
\dot{z}_3 &= -z_3^2(18x^2 + 2x + 1)\dot{x} && (2.48)\\
\dot{q}_1^z &= (-9x^3 + 8x^2 - 5x - 8)\dot{z}_3 + z_3(-27x^2 + 16x - 5)\dot{x} && (2.49)\\
\dot{q}_2^z &= (27x^5 + 11^3 + 20x^2)\dot{z}_3 + z_3(135x^4 + 33x^2 + 40x)\dot{x} && (2.50)
\end{aligned}$$

This yields a set of QP-ODEs, with variables x, q_1^z, q_2^z and z_3:

$$\begin{aligned}
\dot{x} &= x\Big[x^2 (q_1^z)^{\frac{1}{2}}(q_2^z)^{-\frac{1}{3}} + (q_2^z)^2\Big] && (2.51)\\
\dot{q}_1^z &= q_1^z\Big[(q_1^z)^{-1}\Big(z_3\big(-27x^2 + 16x - 5\big)x\big(x^2(q_1^z)^{\frac{1}{2}}(q_2^z)^{-\frac{1}{3}} + (q_2^z)^2\big) - \\
&- \big(-9x^3 + 8x^2 - 5x - 8\big)z_3^2\big(18x^2 + 2x + 1\big)x\big(x^2(q_1^z)^{\frac{1}{2}}(q_2^z)^{-\frac{1}{3}} + (q_2^z)^2\big)\Big)\Big] && (2.52)\\
\dot{q}_2^z &= q_2^z\Big[(q_2^z)^{-1}\Big(z_3\big(135x^4 + 33x^2 + 40x\big)x\big(x^2(q_1^z)^{\frac{1}{2}}(q_2^z)^{-\frac{1}{3}} + (q_2^z)^2\big) - \\
&- \big(27x^5 + 11^3 + 20x^2\big)z_3^2\big(18x^2 + 2x + 1\big)x\big(x^2(q_1^z)^{\frac{1}{2}}(q_2^z)^{-\frac{1}{3}} + (q_2^z)^2\big)\Big)\Big] && (2.53)\\
\dot{z}_3 &= z_3\Big[-z_3\big(18x^2 + 2x + 1\big)x\big(x^2(q_1^z)^{\frac{1}{2}}(q_2^z)^{-\frac{1}{3}} + (q_2^z)^2\big)\Big] && (2.54)
\end{aligned}$$

In the previous example, the four-dimensional monomial-explicit QP-DAE description could be transformed into a QP-ODE without decreasing the state-space dimension (a four-dimensional QP-DAE yields a four-dimensional QP-ODE while the minimal representation is a one-dimensional non-QP ODE).

This was the "worst case" from the viewpoint of minimality, yielding an $n + d + 1$ dimensional QP-ODE model, by embedding the reciprocal of a determinant and taking the time-derivative of the expressed algebraic monomials.

In contrast, the "best case" for transformation into QP-ODE form is when the substitution of the algebraic monomials yields a QP-ODE representation. In this case, the dimension of the state space is increased by only one - and is therefore equal to $n + 1$ - because of embedding the reciprocal of the determinant $z_{d+1} = \frac{1}{det(A(x))}$. Moreover if this determinant is a monomial only, then embedding is unnecessary, and the resulting QP model is minimal - the dimension of the resulting QP-ODE model is equal to n. Therefore the following bounds hold:

$$n \leq dim(\text{resulting QP-ODE}) \leq n + d + 1 \tag{2.55}$$

which means that the transformation of a monomial-explicit QP-DAE into QP-ODE form does not increase the state-space dimension.

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

In the previous section, the transformation of index-1 monomial-explicit QP-DAEs to QP-ODE form has been presented. In the following, the QP-ODE form of *arbitrary* index-1 QP-DAE models will be considered following the general derivation presented in [1].

Let us assume that the differential index of our DAE model is 1 on a connected subset $S \subset R^{n+d}$, which means that the first time-derivative of the algebraic variable vector can be expressed as an explicit function of the differential and the algebraic variables. A necessary condition is the invertibility of the Jacobian matrix of the algebraic equations ($G(x, z)$ in Eq. (2.4)) with respect to the algebraic variables:

$$\exists J^{-1}(x, z), \quad \text{where} \quad J = \left[\frac{\partial G}{\partial z}\right] \;, \quad \forall \; [x, \; z]^T \in S \tag{2.56}$$

Note that this condition is equivalent to $det(J) \neq 0$, $\forall \; [x, \; z]^T \in S$.

Also note that this condition is only a necessary, but not sufficient, condition for the expressibility of z in terms of x, but is quite enough to represent $\dot{z}$ in terms of $\dot{x}$ on S.

If Eq. (2.56) is fulfilled, one can differentiate the algebraic equations in the DAE model

$$\dot{z} = -\left[\frac{\partial G}{\partial z}\right]^{-1} \left[\frac{\partial G}{\partial x}\right] \dot{x} = \widehat{G}(x, z)\dot{x} \tag{2.57}$$

on S, by means of the Implicit Function Theorem. Note that $\widehat{G}(x, z)$ is a matrix valued function.

If we now consider the QP-form of the differential equations in the DAE model, then the elements of $\dot{z}$ can be written in the following form:

$$\begin{aligned} \dot{z}_i &= z_i \left(\frac{1}{z_i} \sum_{l=1}^{n} \widehat{G}_{il}(x,z)\dot{x}_l \right) = \\ &= z_i \left(\sum_{l=1}^{n} \frac{\widehat{G}_{il}(x,z)}{z_i} x_l \lambda_l + \sum_{l=1}^{n}\sum_{j=1}^{m} \frac{\widehat{G}(x,z)_{il}}{z_i} x_l A_{lj} q_j \right) \qquad (2.58) \\ & i = 1, \ldots, d \end{aligned}$$

where $\widehat{G}_{ik}(x,z)$ denotes the appropriate element of the matrix-valued function $\widehat{G}$.

Note that the elements of $\widehat{G}$ are not necessarily in a quasi-monomial form, because we need to invert the matrix $\frac{\partial G}{\partial z}$. But, if $det(\frac{\partial G}{\partial z})$ is in the form of a *quasi-monomial*, then this property is fulfilled, since the set of quasi-polynomials is closed under differentiation, and also under addition and multiplication occurring in taking the adjoint of a matrix and in matrix multiplication.

Also note that if $det(\frac{\partial G}{\partial z})$ is a quasi-polynomial, then its reciprocal can be embedded by introducing it as a new algebraic variable and taking its first time-derivative. From these it is easy to see that the resulting QP-ODE model will have the following dimension:

$$n + d \leq dim(\text{resulting QP-ODE}) \leq n + d + 1 \qquad (2.59)$$

As we can see, the "best case" dimension is much worse than that of QP-ODE models originating from monomial-explicit QP-DAEs. At the same time, the latter method is available for arbitrary index-1 models.

Non-minimal QP-ODE form One can consider the resulting set of ODEs in Eqs. (2.3) and (2.58) as a non-minimal ODE representation of the original system that is in QP form with the set of quasi-monomials extended with new members, which come from the following terms:

$$\frac{\widehat{G}_{il}(x,z)}{z_i} x_l \lambda_l, \ \frac{\widehat{G}_{il}(x,z)}{z_i} x_l A_{lj} q_j, \quad i = 1 \ldots d, \ j = 1 \ldots m, \ l = 1 \ldots n \qquad (2.60)$$

It is important to notice that *the right-hand sides of the equations (2.3) and (2.58) are related by an algebraic equation* as seen in Eq. (2.57). This fact implies the non-minimality of the pure ODE form of an index-one QP-DAE model.

Later we shall see that algebraic methods can be developed by using the equality (2.57) for retrieving the algebraic equations from a non-minimal QP-ODE form.

Example 1 (continued) First we take the time-derivative of x_3:

$$\dot{x}_3 = 4 \cdot 3x_1^4 x_2^5 (5 + 3x_1^3 x_3 + 4x_2^2) + 5 \cdot 3x_1^4 x_2^5 (2 + 7x_1 x_3^5) + 2 \cdot 4x_2^2 (2 + 7x_1 x_3^5) \qquad (2.61)$$

Arranging this equation in QP-form, we get the following QP-ODE representation:

$$\begin{aligned} \dot{x}_1 &= x_1(5 + 3x_1^3 x_3 + 4x_2^2) && (2.62) \\ \dot{x}_2 &= x_2(2 + 7x_1 x_3^5) && (2.63) \\ \dot{x}_3 &= x_3(90x_1^4 x_2^5 x_3^{-1} + 36x_1^7 x_2^5 + 48x_1^4 x_2^7 x_3^{-1} + 105x_1^5 x_2^5 x_3^4 + 16x_2^2 x_3^{-1} + 56x_1 x_2^2 x_3^4) && (2.64) \end{aligned}$$

This is a non-minimal QP model, where the third differential equation is responsible for non-minimality.

Observe that the number of quasi-monomials has increased drastically compared to the QP-DAE form in Eq. (2.12):

$$Q = \left\{ x_1^3 x_3, \ x_2^2, \ x_1 x_3^5, \ x_1^4 x_2^5 x_3^{-1}, \ x_1^7 x_2^5, \ x_1^4 x_2^7 x_3^{-1}, \ x_1^5 x_2^5 x_3^4, \ x_2^2 x_3^{-1}, \ x_1 x_2^2 x_3^4 \right\} \qquad (2.65)$$

Example 2 (continued) By taking the time-derivative of μ and arranging this equation in QP form we get the following QP-ODE representation:

$$\dot{X} = X(-\frac{F}{V} + \mu) \tag{2.66}$$

$$\dot{S} = S(-\frac{F}{V} + \frac{S_F F}{V}S^{-1} - \frac{1}{Y}XS^{-1}\mu) \tag{2.67}$$

$$\dot{\mu} = \mu(-\frac{2F}{V}S^2\mu^{-1} - \frac{2}{Y}XS + \frac{2S_F F}{V}S\mu^{-1}) \tag{2.68}$$

This is a non-minimal QP model, where the third differential equation is responsible for non-minimality.

2.4 The logarithmic form

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

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

where the natural logarithm of a scalar variable φ is denoted by φ^*, i.e.

$$\varphi^* = \ln \varphi$$

and the logarithm is taken element-wise when constructing x^* from a vector x.

It is important to note that X^* and $\widetilde{X}^*$ are equivalent under the condition when $z = 1$ with 1 being the vector of all 1 entries. This means that the time-derivatives of the algebraic variables are equal to zero, which is the case in the limit if we consider the pseudo-ODE form of a QP-DAE model.

The compact vector-matrix form of Eqs. (2.3)-(2.4) is as follows:

$$\frac{d}{dt}\widetilde{X}^* = \lambda + AQ \tag{2.69}$$

with

$$Q^* = BX^* \tag{2.70}$$

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

$$A = \begin{bmatrix} A_d \\ -- \\ A_a \end{bmatrix} \quad , \quad \lambda = \begin{bmatrix} \lambda_d \\ -- \\ \lambda_a \end{bmatrix} \quad , \quad B = \begin{bmatrix} B_d & | & B_a \end{bmatrix} \tag{2.71}$$

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 $\widetilde{A} \in \mathbb{R}^{(n+d)\times(m+1)}$ as follows:

$$\widetilde{A} = \begin{bmatrix} \lambda & | & A \end{bmatrix} \tag{2.72}$$

and extend the matrix B with a 0 row to have

$$\widetilde{B} = \begin{bmatrix} 0 \\ -- \\ B \end{bmatrix} \quad , \quad \widetilde{Q} = \begin{bmatrix} 1 \\ q_1 \\ \cdots \\ q_m \end{bmatrix} \tag{2.73}$$

The compact *linear-analogue logarithmic form of QP-DAE equations* is then as follows:

$$\frac{d}{dt}\widetilde{X}^* = \widetilde{A}\widetilde{Q} \tag{2.74}$$

with

$$\widetilde{Q}^* = \widetilde{B}X^* \tag{2.75}$$

2.5 QP algebraic equations

QP-DAE models contain both a QP-ODE part with the algebraic variables regarded as constants and a QP algebraic part. This section deals with the QP algebraic part only. It is important for calculating the steady-states of QP-DAE and QP-ODE systems.

2.5.1 The general form of QP algebraic equations

The general form of a quasi-polynomial algebraic (QP-AE) set of equations is

$$0 = z_i \left(\lambda_i + \sum_{j=1}^{m} A_{ij} \prod_{k=1}^{d} z_k^{B_{jk}} \right), \tag{2.76}$$
$$i = 1, \ldots, d, \quad m \geq d$$

where the parameters A and B of the model are $d \times m$ and $m \times d$ real matrices and $\lambda \in \mathbb{R}^d$ is a real vector.

Note that *a QP-AE can be obtained from a QP-DAE by considering its algebraic part only and regarding the differential variables as parameters.* If we characterize the nonlinearity of such a part then the solvability properties of the algebraic equations for the algebraic variables will be taken into account. This is relevant for some solution techniques for DAE models. Likewise, any subset (component) of a set of QP-algebraic equations with the number of equations equal to the number of unknown variables (e.g. an L-component) can be regarded as a QP-AE in the above form if one considers the external (known) variables as parameters.

2.5.2 QM-transformation of QP-AEs

The logarithmic form of QP-AEs is obtained if one divides each equation by $z_i > 0$:

$$0 = \lambda + AQ \quad , \quad Q^* = Bz^* \tag{2.77}$$

Note that the first equation above does not contain any logarithmic variables but puts a linear algebraic constraint of the set of quasi-monomials. The logarithmic variables appear only in the second equation.

The QM-transformation of a QP-AE model is generated by an invertible matrix $C \in \mathbb{R}^{d\times d}$ to get

$$z^* = C\widehat{z}^* \quad , \quad \widehat{z}^* = C^{-1}z^*$$

Then the transformed equations in the new variables are

$$\begin{aligned} 0 &= C^{-1}\lambda + C^{-1}AQ = \widehat{\lambda} + \widehat{A}\widehat{Q} \\ Q^* &= Bz^* = BCC^{-1}z^* = BC\widehat{z}^* = \widehat{Q}^* \\ \widehat{B} = B\cdot C \quad &, \quad \widehat{A} = C^{-1}\cdot A \quad , \quad \widehat{\lambda} = C^{-1}\cdot\lambda \end{aligned} \tag{2.78}$$

with the same invariants as for QP-ODE models, i.e. $M = A_{LV} = BA$, $\Lambda = B\lambda$ and Q.

2.5.3 Lotka-Volterra form

The Lotka-Volterra form of a QP-AE can now be obtained by extending the variable vector to form a square $m = d$ case and then following the method described for the QP-ODE models.

In the general $m \geq d$ case we extend the variable vector z with $(m-d)$ constant 1-s (and call it χ) and use the partitioned and extended compact linear-analogue logarithmic form of the model

$$\begin{bmatrix} 0 \\ Q_p^* \\ Q_s^* \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ \hline B_p & 0 \\ B_s & I \end{bmatrix} \begin{bmatrix} z^* \\ 0 \end{bmatrix} \quad , \quad 0 = \left[\begin{array}{c|cc} \lambda & A_p & A_s \\ 0 & 0 & 0 \end{array} \right] \begin{bmatrix} 1 \\ Q_p \\ Q_s \end{bmatrix} \tag{2.79}$$

Here again, there is a nonlinear QM-type algebraic relationship between the d independent primary quasi-monomials in Q_p and the rest of them in Q_s in the form of

$$Q_s^* = B_s B_p^{-1} Q_p^* \tag{2.80}$$

The Lotka-Volterra form of the original QP-AE can now be obtained by QM-transforming the above equation with

$$C = \begin{bmatrix} B_p & 0 \\ B_s & I \end{bmatrix}^{-1}$$

It is important to note that *the Lotka-Volterra form of a QP-AE model is a LV-AE* model, i.e. a set of second-order algebraic equations. This set of equations, however, is not algebraically independent, because there are $(m-d)$ QM-type algebraic dependencies between its variables in the form of Eq. (2.80).

A simple example Consider the algebraic equations of an open vessel with a one-component liquid phase:

$$0 = c_p m T - U \tag{2.81}$$

$$0 = k_0 + k_1 T + k_2 T^2 + k_3 T^3 - c_p \tag{2.82}$$

where the algebraic variables are the specific heat $z_1 = c_p$ and the temperature $z_2 = T$ while the differential variables - which are considered now as constants - are the mass m and the internal energy U. This set of algebraic equations forms a QP-AE with the following parameter matrices and the extended algebraic variable vector χ:

$$\lambda = \begin{bmatrix} -U \\ k_0 \end{bmatrix} \; , \; A = \begin{bmatrix} m & 0 & 0 & 0 & 0 \\ 0 & k_1 & k_2 & k_3 & -1 \end{bmatrix} \; , \; B = \begin{bmatrix} 1 & 1 \\ 0 & 1 \\ 0 & 2 \\ 0 & 3 \\ 1 & 0 \end{bmatrix} \; , \; \chi = \begin{bmatrix} c_p \\ T \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} z_1 \\ z_2 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

The partitioned and extended linear-analogue logarithmic form of the model is:

$$\begin{bmatrix} 0 \\ Q_p^* \\ Q_s^* \end{bmatrix} = \left[\begin{array}{cc|ccc} 0 & 0 & 0 & 0 & 0 \\ \hline 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ \hline 0 & 2 & 1 & 0 & 0 \\ 0 & 3 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \end{array}\right] \left[\begin{array}{c} z_1^* \\ z_2^* \\ \hline 0 \\ 0 \\ 0 \end{array}\right] \quad , \quad 0 = \left[\begin{array}{c|cc|ccc} -U & m & 0 & 0 & 0 & 0 \\ k_0 & 0 & k_1 & k_2 & k_3 & -1 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right] \begin{bmatrix} 1 \\ Q_p \\ Q_s \end{bmatrix}$$

where Eq. (2.80) defines the relationship between the primary and secondary monomials:

$$Q_s^* = \begin{bmatrix} 2z_2^* \\ 3z_2^* \\ z_1^* \end{bmatrix} \begin{bmatrix} 0 & 2 \\ 0 & 3 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}^{-1} \begin{bmatrix} z_1^* + z_2^* \\ z_2^* \end{bmatrix} = \begin{bmatrix} 0 & 2 \\ 0 & 3 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} z_1^* + z_2^* \\ z_2^* \end{bmatrix} \tag{2.83}$$

The Lotka-Volterra form can be achieved by a QM transformation with the following transformation matrix:

$$C = \left[\begin{array}{cc|ccc} 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ \hline 0 & 2 & 1 & 0 & 0 \\ 0 & 3 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \end{array}\right]^{-1} \tag{2.84}$$

The resulting LV model can be written in the following compact form:

$$0 = \left[\begin{array}{c|cccccc} -U + k_0 & m & k_1 & k_2 & k_3 & -1 \\ k_0 & 0 & k_1 & k_2 & k_3 & -1 \\ 2k_0 & 0 & 2k_1 & 2k_2 & 2k_3 & -2 \\ 3k_0 & 0 & 3k_1 & 3k_2 & 3k_3 & -3 \\ -U & m & 0 & 0 & 0 & 0 \end{array}\right] \begin{bmatrix} 1 \\ \widehat{\chi} \end{bmatrix} \tag{2.85}$$

where

$$\widehat{\chi}^* = C^{-1}\chi^* \tag{2.86}$$

2.6 QM-transformation

As we have seen earlier in section 2.5 the quasi-monomial transformation (QM-transformation) is generated by an invertible transformation matrix C such that

$$\hat{X}_i = \prod_{k=1}^{n} x_k^{C_{ik}} \cdot \prod_{k=1}^{d} z_k^{C_{i(n+k)}}, \quad i = 1, \ldots, n+d \tag{2.87}$$

where X is the united vector of both the differential x and algebraic z variables.

The effect of QM-transformation on the logarithmic variables can easily be computed

$$X^* = C^{-1}\hat{X}^* \quad , \quad X_i^* = lnX_i$$

with the quasi-monomials being $Q^* = BX^*$.

Similarly to the case of QM-transforming a QP-AE (see Eq. (2.78)), the effect of the QM-transformation on a QP-ODE model can be seen on its logarithmic form:

$$\dot{\hat{X}}^* = C^{-1}\lambda + C^{-1}AQ \tag{2.88}$$

$$Q^* = BX^* = BCC^{-1}X^* = BC\hat{X}^* = \hat{Q}^* \tag{2.89}$$

$$\hat{B} = B \cdot C \quad , \quad \hat{A} = C^{-1} \cdot A \quad , \quad \hat{\lambda} = C^{-1} \cdot \lambda \tag{2.90}$$

where the **invariants** of the transformation are $M = B \cdot A$, $\Lambda = B \cdot \lambda$ and Q.

2.6.1 QM-transformation of QP-DAE models

It can easily be seen that the logarithmic form (2.74) of a QP-DAE is **not invariant** with respect to QM-transformation because the differential part (a QP-ODE) and the algebraic part (a QP-AE) will be "mixed" by a general transformation matrix $C \in \mathbb{R}^{(n+d)\times(n+d)}$. However, both "pure" QP-AEs and QP-ODEs are invariant. Therefore, we have two options if we want to have a QP-DAE form that is invariant with respect to QM-transformation.

1. Construct the equivalent non-minimal QP-ODE form of the QP-DAE (see section 2.3) and perform the transformation afterwards.

2. Use a *restricted* version of QM-transformation with a block diagonal transformation matrix C such that

$$C = \begin{bmatrix} C_{n\times n} & 0 \\ 0 & C_{d\times d} \end{bmatrix}$$

Chapter 3

Form invariance

It has been shown in the previous sections that the DAE form of a QP-DAE will not generally be invariant with respect to QM-transformation but it can be embedded by introducing new variables into QP-ODEs in the index 1 case. The embedding can be seen as a transformation from the DAE form to the QP-ODE one that is not unique. The inverse of this embedding, that is the transformation that retrieves the hidden algebraic equations from a non-minimal QP-ODE, is the subject of this chapter.

The significance of the retrieval of the hidden algebraic equations from a non-minimal QP-ODE model is best explained from a control theoretical point of view. It is well known from linear and nonlinear system theory that the *minimality* of a state-space model [6] (i.e. a QP-ODE in our problem statement) is a necessary condition for designing any state feedback type controller (and most of the linearizing and stabilizing ones, as well) [4]. There exist general procedures to reduce non/minimal state-space models to find their minimal representation but these require to solve partial differential equations symbolically. Therefore, it is of great practical and theoretical importance from the viewpoint of dynamic analysis to find a feasible alternative for them.

3.1 Form invariance of linear DAE models

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

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

$$\begin{bmatrix} \dot{x} \\ 0 \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} x \\ z \end{bmatrix} \tag{3.1}$$

where $x \in \mathbb{R}^n$ is the vector of differential variables and $z \in \mathbb{R}^d$ is the vector of algebraic variables.

Let us assume that *the model in Eq. (3.1) has a differential index of one (in the linear case this is equivalent to the assumption that A_{22} is invertible)*, then the algebraic variables can be expressed in terms of the differential ones:

$$z = -A_{22}^{-1} A_{21} x \tag{3.2}$$

The DAE canonical form We can substitute the algebraic relationship (3.2) into the differential equation part of the original DAE model to obtain:

$$\dot{x} = (A_{11} - A_{12}A_{22}^{-1}A_{21})x \tag{3.3}$$

The above purely differential description contains the minimum number of differential equations describing the time-varying behaviour of the differential variables. Together with Eq. (3.2) it is equivalent to the original model in Eq. (3.1).

Observe that Eq. (3.3) is an autonomous model in itself, with the advantages of being both purely differential and minimal. Note that state-space models originating from *nonlinear* index-1 DAEs rarely have these properties.

Non-minimal ODE form The time-derivative of equation (3.2) gives

$$\dot{z} = -A_{22}^{-1}A_{21}\dot{x} = -A_{22}^{-1}A_{21}(A_{11}x + A_{12}z) \tag{3.4}$$

We can now leave out the algebraic equations and substitute them with the above algebraically equivalent set of differential equations which leads to the following linear ODE:

$$\begin{bmatrix} \dot{x} \\ \dot{z} \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ -A_{22}^{-1}A_{21}A_{11} & -A_{22}^{-1}A_{21}A_{12} \end{bmatrix} \begin{bmatrix} x \\ z \end{bmatrix} =: \begin{bmatrix} \widehat{A}_{11} & \widehat{A}_{12} \\ \widehat{A}_{21} & \widehat{A}_{22} \end{bmatrix} \begin{bmatrix} x \\ z \end{bmatrix} \tag{3.5}$$

which is a *hidden DAE system with the state matrix* $\widehat{A}$ *of dimension* $(n+d) \times (n+d)$.

This linear ODE is *non-minimal*, 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* $rank(A_{11}) = n$, *i.e.* $\widehat{A}$ *is rank-deficient.*

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 to the DAE model in Eq. (3.1).

The application of a general invertible linear transformation

$$T = \begin{bmatrix} T_{11_{n\times n}} & T_{12_{n\times d}} \\ T_{21_{d\times n}} & T_{22_{d\times d}} \end{bmatrix} \tag{3.6}$$

to the model in Eq. (3.5) linearly combines the variables, but it does not change the rank of the transformed state matrix:

$$T \begin{bmatrix} \dot{x} \\ \dot{z} \end{bmatrix} = T \begin{bmatrix} \widehat{A}_{11} & \widehat{A}_{12} \\ \widehat{A}_{21} & \widehat{A}_{22} \end{bmatrix} T^{-1} \cdot T \begin{bmatrix} x \\ z \end{bmatrix} \tag{3.7}$$

which leads to

$$\begin{bmatrix} T_{11}\dot{x} + T_{12}\dot{z} \\ T_{21}\dot{x} + T_{22}\dot{z} \end{bmatrix} = \widetilde{A} \begin{bmatrix} T_{11}x + T_{12}z \\ T_{21}x + T_{22}z \end{bmatrix} \tag{3.8}$$

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

As we can see, a general linear invertible transformation transforms a non-minimal ODE to a non-minimal ODE, or in other words *a hidden DAE system to an equivalent hidden DAE system.*

3.1.1 Retrieving the algebraic equations from the transformed linear DAE

Under the index-one assumption, we can retrieve the original DAE structure from a hidden linear DAE system in its non-minimal ODE form by finding an appropriate transformation based on the observations of the previous section.

Detection of non-minimality For this purpose we can use the fact that the coefficient matrix $\widehat{A}$ of a hidden DAE system is not of full rank because of construction, but is of rank $n < n + d$. Assume that A_{11} is invertible in Eq. (3.5) and thus the first n columns or rows are linearly independent of each other. Then the remaining d rows (or columns) can be expressed as a linear combination of the n rows (or columns) participating in the spanning set of the n-dimensional sub-space.

The retrieval algorithm Consider a linear ODE model in the form of

$$\dot{\widetilde{x}} = \frac{d\widetilde{x}}{dt} = \widehat{A}\widetilde{x} \tag{3.9}$$

such that $\widehat{A} \in \mathbb{R}^{\widetilde{n}\times\widetilde{n}}$ but rank $\widehat{A} = n < \widetilde{n}$. If we rearrange the order of variables such that he first n rows of $\widehat{A}$ are linearly independent vectors, then the remaining rows $\widehat{a}_j,\ j = n+1,..,\widetilde{n}$ can be expressed as linear combinations of the first n rows, i.e.

$$\widehat{a}_j = \sum_{k=1}^{n} \alpha_{jk}\widehat{a}_k \quad , \quad j = n+1,..,\widetilde{n} \tag{3.10}$$

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 $rank(\widehat{A}) = n$, it has n independent columns. Partition $\widehat{A}$ in such a way that its first n columns are linearly independent:

$$\widehat{A}_{part} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \tag{3.11}$$

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:

$$\alpha_j M_{11} = M_{21,(j-n)} \quad , \quad j = n+1,..,\widetilde{n} \tag{3.12}$$

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 coefficient matrix L:

$$L = \begin{bmatrix} \alpha_{n+1} \\ \vdots \\ \alpha_{\widetilde{n}} \end{bmatrix} \tag{3.13}$$

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

$$L = M_{21}M_{11}^{-1} \tag{3.14}$$

Having determined the coefficients from Eq. (3.10), we can derive a linear set of equations relating the time derivative of the corresponding state variables in $\widetilde{x}$:

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

Finally we can conclude that there is a linear dependence of the corresponding state variables by integrating the equations above:

$$\widetilde{x}_j = \varphi_j + \sum_{k=1}^{n} \alpha_{jk} \widetilde{x}_k \quad , \quad j = n+1, .., \widetilde{n} \tag{3.15}$$

Since our DAE system is *linear* (and homogeneous), $\varphi_j = 0$, $j = n+1, \ldots, \widetilde{n}$. 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. (3.9) by leaving the first n ODEs unchanged but replacing the remaining ODEs by the algebraic equations in Eq. (3.15). *This way we can obtain the DAE form of any transformed ODE originating from a DAE model.* ***This form can be regarded as a DAE canonical form*** *of a non-minimal linear ODE model.*

The *DAE canonical form of a hidden DAE system is* ***unique*** if one chooses and fixes the n independent rows of the coefficient matrix $\widehat{A}$.

3.1.2 From hidden linear DAE systems to DAE canonical form models

Non-minimal linear ODE models can be transformed into DAE canonical form as described in the previous section. The resulting algebraic equations are explicit in their variables, so they can be substituted into the differential equations leading to a ***minimal ODE form*** *of a linear non-minimal ODE model.*

Transformation to DAE canonical form This substitution can be performed in one step by using a linear transformation as follows. With the help of Eqs (3.10) and (3.13), the linear model in Eq. (3.9) can be written in the following form:

$$\frac{d}{dt} \begin{bmatrix} \widetilde{x}_{P1} \\ \widetilde{x}_{P2} \end{bmatrix} = \begin{bmatrix} \widehat{A}_1 & \widehat{A}_2 \\ L\widehat{A}_1 & L\widehat{A}_2 \end{bmatrix} \begin{bmatrix} \widetilde{x}_{P1} \\ \widetilde{x}_{P2} \end{bmatrix} \tag{3.16}$$

where

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

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

Let us apply the following transformation matrix to Eq. (3.16):

$$T_{min} = \begin{bmatrix} I_{n\times n} & 0_{n\times d} \\ -L_{d\times n} & I_{d\times d} \end{bmatrix} \tag{3.17}$$

It transforms our system to

$$\begin{bmatrix} \dot{\widetilde{x}}_{P1} \\ 0 \end{bmatrix} = \begin{bmatrix} \widehat{A}_1 + \widehat{A}_2 L & \widehat{A}_2 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \widetilde{x}_{P1} \\ \varphi_{P2} \end{bmatrix} \tag{3.18}$$

where the vector φ_{P2} is built of φ_j-s in Eq. (3.15):

$$\varphi_{P2} = \begin{bmatrix} \varphi_{n+1} \\ \vdots \\ \varphi_{\tilde{n}} \end{bmatrix}$$

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

$$\dot{\widetilde{x}}_{P1} = \widehat{A}_2\varphi_{P2} + (\widehat{A}_1 + \widehat{A}_2 L)\widetilde{x}_{P1} \tag{3.19}$$

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

$$\varphi_{P2} = \widetilde{x}_{P1}(t_0) - L\widetilde{x}_{P2}(t_0) \tag{3.20}$$

and it equals zero if our model is linear (because of homogeneity).

This way we get to the minimal realization of the model in Eq. (3.9) which is equivalent to the original one and has been generated by 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.

3.2 Form Invariance of QP-DAE models

The method of retrieving algebraic equations from a non-minimal QP-ODE model is far from being trivial. Symbolic algebraic methods are applied in [2] to construct nonlinear invariant manifolds (that correspond to the algebraic relationships between the system variables) for the 3-5 dimensional cases. Necessary conditions for the existence of quasi-polynomial invariants are presented in [3] that can be constructed recursively from the low dimensional cases.

The form invariance and the retrieval of the algebraic equations of QP-DAE models is investigated in this section by using the QP-ODE form of QP-DAE models and the known form invariance results derived therefor.

3.2.1 The Lotka-Volterra ODE form

Similarly to the case of QP-ODEs, the Lotka-Volterra form of a QP-DAE can be regarded as a canonical form representing the whole class of QM-transformation invariant models. For this we recall that the QP models that have the same invariants M, Λ and Q form an equivalence class that may contain both QP-ODE and QP-DAE models.

The Lotka-Volterra form of a QP model equivalence class can be derived in two alternative ways. We may extend the variable vector with constant elements or we may use the quasi-monomials as new variables.

Extension to the $m = n$ (square) case Note that in the general case $m \geq n$, i.e. the number of quasi-monomials is greater or equal to the number of variables. This implies that there are quasi-monomial type relationships between some $(m-n)$ quasi-monomials (see [5]). To show this, we partition the vector of quasi-monomials as follows:

$$Q = \begin{bmatrix} Q_p \\ --- \\ Q_s \end{bmatrix}$$

with $dim(Q_p) = n$ such that the $n \times n$ block B_p in the partitioned B matrix is of full rank. From

$$\begin{bmatrix} Q_p^* \\ --- \\ Q_s^* \end{bmatrix} = \begin{bmatrix} B_p \\ --- \\ B_s \end{bmatrix} X^*$$

we get

$$Q_p^* = B_p X^* \tag{3.21}$$
$$Q_s^* = B_s X^* \tag{3.22}$$

which gives the connection between the two sets of monomials:

$$Q_s^* = B_s B_p^{-1} Q_p^* \tag{3.23}$$

Moreover, we can formally extend the variable vector X of dimension n with $m-n$ constant 1-s, to get

$$\chi = \begin{bmatrix} X \\ --- \\ 1 \\ \dots \\ 1 \end{bmatrix}$$

to form a square version of the original compact logarithmic form of the QP-ODE model as

$$\begin{bmatrix} 0 \\ Q_p^* \\ Q_s^* \end{bmatrix} = B^{SQ} \cdot \begin{bmatrix} X^* \\ 0 \end{bmatrix} = \left[\begin{array}{cc} 0 & 0 \\ \hline B_p & 0 \\ B_s & I \end{array}\right] \begin{bmatrix} X^* \\ 0 \end{bmatrix} \tag{3.24}$$

$$\dot{\chi}^* = A^{SQ} \cdot \begin{bmatrix} 1 \\ Q_p \\ Q_s \end{bmatrix} = \left[\begin{array}{c|cc} \lambda & A_p & A_s \\ 0 & 0 & 0 \end{array}\right] \begin{bmatrix} 1 \\ Q_p \\ Q_s \end{bmatrix} \tag{3.25}$$

The Lotka-Volterra form of the original QP-ODE can now be obtained by QM-transforming the m-dimensional extended variable vector χ with the square invertible matrix

$$C = \begin{bmatrix} B_p & 0 \\ B_s & I \end{bmatrix}^{-1}$$

The quasi-monomials as new variables The Lotka-Volterra form of a QP-ODE or QP-DAE model is formed by choosing the quasi-monomials to be the system variables, i.e.

$$\dot{U}_i = U_i(\Lambda_i + \sum_{j=1}^{m} M_{ij} U_j), \quad i = 1, \dots, m \tag{3.26}$$

with $U_i = Q_i$. The parameters of the Lotka-Volterra form are exactly the invariants of the QP model class, being Λ and M.

It is important to note that the Lotka-Volterra form is a special QP-ODE in itself with $A = M$ and $B = I$ and thus it is a set of quadratic ODEs.

Algebraic dependencies between the quasi-monomials Recall the number of the quasi-monomials m, that is, the number of the differential variables in the Lotka-Volterra form, is greater than or equal to the number of the original differential variables n. This implies that the Lotka-Volterra form is a hidden QP-DAE, which is indicated by the fact that M is generally not of full rank. *Equation (3.23) gives the QM-type algebraic relationships between the first n and the remaining $(m-n)$ quasi-monomials.*

3.2.2 Retrieving the QM-type algebraic equations from the Lotka-Volterra ODE form model

It is important to recall that a Lotka-Volterra ODE form can be regarded as a special *non-minimal hidden QP-DAE* in the general $m > n$ case where $B_{LV} = I$ and $A_{LV} = M$. Thus the LV parameter matrix M will now be rank-deficient such that *rank* $M \leq n$.

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

$$M_j \quad , \quad j = n+1, ..., n+d$$

of the coefficient matrix in the same way as in the case of the transformed linear DAEs in section 3.1.

Using the same derivation as in section 3.1 we can retrieve the QP-DAE algebraic equations in the following form:

$$\widetilde{x}_j^* = \varphi_j + \sum_{k=1}^{n} \alpha_{jk} \widetilde{x}_k^* \quad , \quad j = n+1, .., n+d \tag{3.27}$$

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

$$x_j = \varphi_j \cdot \prod_{k=1}^{n} (x_k)^{\alpha_{jk}} \quad , \quad j = n+1, .., n+d \tag{3.28}$$

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

Note that with the method above we can retrieve a part of the hidden algebraic equations, if they are in the form of Eq. (3.28). Such equations are used when creating the Lotka-Volterra form of a QP-DAE or QP-ODE model.

Example 1 (continued) Let us consider the LV-ODE form of *Example 1*, with its matrix invariant M:

$$\dot{x} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 15 & 9 & 12 & 0 & 90 & 36 & 48 & 105 & 16 & 56 \\ 4 & 0 & 0 & 14 & 0 & 0 & 0 & 0 & 0 & 0 \\ 5 & 3 & 4 & 0 & 450 & 180 & 240 & 525 & 80 & 280 \\ 30 & 12 & 16 & 35 & -90 & -36 & -48 & -105 & -16 & -56 \\ 45 & 21 & 28 & 35 & 0 & 0 & 0 & 0 & 0 & 0 \\ 34 & 12 & 16 & 49 & -90 & -36 & -48 & -105 & -16 & -56 \\ 35 & 15 & 20 & 35 & 360 & 144 & 192 & 420 & 64 & 224 \\ 4 & 0 & 0 & 14 & -90 & -36 & -48 & -105 & -16 & -56 \\ 9 & 3 & 4 & 14 & 360 & 144 & 192 & 420 & 64 & 224 \end{pmatrix} x \tag{3.29}$$

Denote the j^{th} row of M by M_j. If one follows the retrieval algorithm above, then one can observe that the rows $\{M_2, M_3, M_4\}$ are linearly independent, giving a basis to reproduce the rows $\{M_5, \ldots, M_{10}\}$ as their linear combination (M_1 is assigned to the known monomial '1', which there is no need to retrieve). The linearly combining matrix L can be computed easily:

$$L = \begin{bmatrix} 1.5 & 2.5 & -0.5 \\ 2.5 & 2.5 & -0.5 \\ 1.5 & 3.5 & -0.5 \\ 1.5 & 2.5 & 0.5 \\ 0.0714 & 1 & -0.2143 \\ 0.0714 & 1 & 0.7857 \end{bmatrix} \tag{3.30}$$

and the algebraic relationships can be given therefrom:

$$\widetilde{x}_j^* = \varphi_j + \sum_{k=2}^{4} \alpha_{jk} \widetilde{x}_k^* \quad , \quad j = 5, \ldots, 10 \tag{3.31}$$

where α_{jk} can be given from the elements of L:

$$\alpha_{jk} = L_{(j-4,k-1)} \quad , \quad j = 5, \ldots, 10, \; k = 2, \ldots, 4$$

From this, we finally get the monomial relationships:

$$x_j = \varphi_j \cdot \prod_{k=2}^{4} (x_k)^{\alpha_{jk}} \quad , \quad j = 5, \ldots, 10 \tag{3.32}$$

where φ_j, $j = 5, \ldots, 10$ can be computed from initial conditions.

Thus, the resulting DAE model has LV differential equations complemented with QM-type algebraic relationships:

$$x_1 = 1 \tag{3.33}$$

$$\frac{dx_2}{dt} = x_2\big(15x_1 + 9x_2 + 12x_3 + 90x_5 + 36x_6 + 48x_7 + 105x_8 + 16x_9 + 56x_{10}\big) \tag{3.34}$$

$$\frac{dx_3}{dt} = x_3\big(4x_1 + 14x_4\big) \tag{3.35}$$

$$\frac{dx_4}{dt} = x_4\big(5x_1 + 3x_2 + 4x_3 + 450x_5 + 180x_6 + 240x_7 + 525x_8 + 80x_9 + 280x_{10}\big) \tag{3.36}$$

$$x_5 = \varphi_5 \cdot x_2^{1.5} \cdot x_3^{2.5} \cdot x_4^{-0.5} \tag{3.37}$$

$$x_6 = \varphi_6 \cdot x_2^{2.5} \cdot x_3^{2.5} \cdot x_4^{-0.5} \tag{3.38}$$

$$x_7 = \varphi_7 \cdot x_2^{1.5} \cdot x_3^{3.5} \cdot x_4^{-0.5} \tag{3.39}$$

$$x_8 = \varphi_8 \cdot x_2^{1.5} \cdot x_3^{2.5} \cdot x_4^{0.5} \tag{3.40}$$

$$x_9 = \varphi_9 \cdot x_2^{0.0714} \cdot x_3^{1} \cdot x_4^{-0.2143} \tag{3.41}$$

$$x_{10} = \varphi_{10} \cdot x_2^{0.0714} \cdot x_3^{1} \cdot x_4^{0.7857} \tag{3.42}$$

where the constants $\varphi_5, \ldots, \varphi_{10}$ are determined by the initial conditions of the model.

3.3 Retrieving the QP-type algebraic equations

In this section we show two algorithms for the retrieval of QP-type algebraic equations. The first is based on considering the parameter matrices A and B of the QP model *together*. The second tries to find *first integrals* of the system. Both algorithms contain heuristic steps.

3.3.1 Generalized QM retrieval algorithm

Unfortunately, only the QM-type algebraic equations can be retrieved by the approach presented in the previous section. Therefore, we have made an investigation on how one could generalize it to retrieve a broader class, namely when a variable is a quasipolynomial of the other variables.

For this purpose, we present an algorithm with heuristic elements giving back these relationships.

1. Construct the A and B matrices of the QP model sequentially, i.e. by starting with the first quasimonomial (QM) in the first differential equation, and finishing with the last QM in the last differential equation. Include the QM $'1'$ (instead of using the vector λ). Observe that A is a lower block-triangular matrix because of the way it has been built.

2. If A is not of full rank, then apply the previously presented algorithm, substitute the algebraic relationships you got, and then re-start this algorithm.

3. If A is not block-diagonal then duplicate those QMs with coefficients in the non-diagonal parts. If this step is done, the modified (expanded) A matrix is block-diagonal. Denote the diagonal elements of A (which are row vectors) with a_{row_i} , $i = 1, \ldots, m$, and their corresponding B matrix partitions by B_i , $i = 1, \ldots, m$.

4. Reproduce - if it is possible - a_{row_j} in the form:
$$\begin{aligned} a_{row_j} &= [M_1 \mid M_2 \mid \ldots \mid M_\ell] = \\ &= \left[\sum_{i=1, i\neq j}^{m} c_i^1 a_{row_i}^1 \;\middle|\; \sum_{i=1, i\neq j}^{m} c_i^2 a_{row_i}^2 \;\middle|\; \ldots \;\middle|\; \sum_{i=1, i\neq j}^{m} c_i^\ell a_{row_i}^\ell \right] \end{aligned} \tag{3.43}$$
where $c_i^1, \ldots, c_i^\ell$, $i = 1, \ldots, m$ are constants, while $a_{row_i}^k$, $i = 1, \ldots, m,\ k = 1, \ldots \ell$ denote rows made from a_{row_i} , $i = 1, \ldots m$ by permutating its elements, and by possible insertion of additional zero entries.

   Denote their accordingly arranged B_i matrices by $B_i^k,\ i = 1, \ldots m,\ k = 1, \ldots \ell$ (zero rows are inserted in the appropriate places).

5. Now construct the matrix
$$B_j^* = B_j - \begin{pmatrix} \sum_{i=1, i\neq j}^{m} B_i^1 \\ \sum_{i=1, i\neq j}^{m} B_i^2 \\ \vdots \\ \sum_{i=1, i\neq j}^{m} B_i^\ell \end{pmatrix} = \begin{pmatrix} N^1 \\ N^2 \\ \vdots \\ N^\ell \end{pmatrix} \tag{3.44}$$
If all $N^k,\ k = 1, \ldots \ell$ have identical rows in the form of $\alpha^k = [\alpha_1^k, \alpha_2^k, \ldots, -1, \ldots, \alpha_m^k]$ with their j-th columns containing -1 elements, then the algebraic relationship is of quasi-polynomial type and can be given explicitly:
$$x_j = c_0 + \sum_{k=1}^{\ell} c_k \cdot \prod_{i=1,\ i\neq j}^{m} x_i^{\alpha_i^k} \tag{3.45}$$
with the coefficients $c_k = \frac{c_k^{n_k}}{\alpha_k^{n_k}},\ k = 1, \ldots, \ell$ and $n_k \in \{1, 2, j-1, j+1, m\}$ are integers such that $\alpha_k^{n_k} \neq 0$, $k = 1, \ldots, \ell$. The coefficient c_0 can be computed from initial conditions.

3.3.2 The method of first integrals

In the previous section, an algorithm has been presented to retrieve *explicit* QP-type algebraic equations. Now we present another method, which is moreover capable to find *monomial explicit* algebraic relationships.

Take a look at the following QP-DAE model with n differential equations and a single explicit algebraic relationship:

$$\begin{aligned} \dot{x} &= f(x)\ , \quad x \in \mathbb{R}^n && (3.46) \\ z &= p(x)\ , \quad z \in \mathbb{R} && (3.47) \end{aligned}$$

where $p(x)$ is a (quasi)polynomial of x. This model can be written in an $n+1$ dimensional QP-ODE form, by simply taking the time-derivative of z:

$$\begin{aligned} \dot{x} &= f(x) && (3.48) \\ \dot{z} &= \frac{\partial p}{\partial x} f(x) = \sum_{i=1}^{n} \frac{\partial p}{\partial x_i} f_i(x) && (3.49) \end{aligned}$$

Now we will show that there exists a first integral of this system which is a function of x and z. Search for this first integral in the form $\lambda(x,z) = c$, and take its time-derivative:

$$\frac{d\lambda}{dt} = \frac{\partial \lambda}{\partial x}\dot{x} + \frac{\partial \lambda}{\partial z}\dot{z} = \frac{\partial \lambda}{\partial x} f(x) + \frac{\partial \lambda}{\partial z}\frac{\partial p}{\partial x} f(x) = 0\ , \quad \frac{\partial \lambda}{\partial x} = grad\lambda \in \mathbb{R}^{1\times n} \qquad (3.50)$$

This can be simplified to

$$\frac{\partial \lambda}{\partial x} + \frac{\partial \lambda}{\partial z}\frac{\partial p}{\partial x} = \begin{bmatrix} 0 & \dots & 0 \end{bmatrix} \in \mathbb{R}^{1\times n} \qquad (3.51)$$

which is a set of n equations. It is easy to show that

$$\lambda(x,z) = z - p(x) \in \mathbb{R}^n \qquad (3.52)$$

is a solution of this PDE, since

$$\frac{\partial \lambda(x,z)}{\partial x} + \frac{\partial \lambda(x,z)}{\partial z}\frac{\partial p}{\partial x} = -\frac{\partial p}{\partial x} + 1\frac{\partial p}{\partial x} = 0 \qquad (3.53)$$

therefore $\lambda(x,z)$ is a first integral of the system. It means that

$$z = p(x) + c \qquad (3.54)$$

therefore we retrieved our original algebraic equation, where $c = 0$ according to the initial conditions $[x(t_0),\ z(t_0)]^T$.

Experience has shown us that finding the solution is not so simple in most cases, since $\frac{\partial p}{\partial x}$ is a row vector and $p(x)$ is made of an arbitrary number of monomials, therefore the time-derivative of z can maximally contain $\ell \times m_x$ monomials, where ℓ denotes the number of monomials in $p(x)$, while m_x is the number of the monomials in the differential equations for x. However, if p is an arbitrary polynomial of one variable: $p(x) = p(x_k)$ for some k then the solution is immediately given:

$$p(x_k) = \int \frac{\dot{z}}{\dot{x}_k} dx_k \qquad (3.55)$$

If p depends on more than one variable, then a good way is to search for those parts on the RHS of $\dot{z}$ which, if they are divided by the RHS of some $\dot{x}_k$, give *monomials* without remainder:

$$\frac{part_i}{\dot{x}_k} = monomial(x) \tag{3.56}$$

These monomials (more exactly, their integrals with respect to x_k) will constitute the solution $p(x)$, if $\dot{z} = \sum_i part_i$ is fulfilled.

Example 2 (continued) Consider the QP-ODE model in Eqs. (2.66-2.68). This is the case when $z = p(x)$ depends on only one variable x_k, and therefore there is a relationship $\dot{z} = poly(x)\dot{x}_k$ where $poly(x)$ is a polynomial. It is easy to see that

$$\dot{\mu} = 2S\dot{S} \tag{3.57}$$

From this, the original algebraic equation can be easily retrieved:

$$\mu = \int \frac{\dot{\mu}}{\dot{S}}\, dS = \int 2S\, dS = S^2 + c \tag{3.58}$$

where $c = 0$ comes from the initial conditions of the model.

Example 1 (continued) Recall the QP-ODE model of this system in Eqs. (2.62-2.64):

$$\dot{x}_1 = x_1(5 + 3x_1^3x_3 + 4x_2^2) \tag{3.59}$$
$$\dot{x}_2 = x_2(2 + 7x_1x_3^5) \tag{3.60}$$
$$\dot{x}_3 = x_3(90x_1^4x_2^5x_3^{-1} + 36x_1^7x_2^5 + 48x_1^4x_2^7x_3^{-1} + 105x_1^5x_2^5x_3^4 + 16x_2^2x_3^{-1} + 56x_1x_2^2x_3^4) \tag{3.61}$$

Consider the last equation of the model - it contains the largest number of monomials, therefore this would be the differential equation coming from the time-differentiation of a polynomial in the form $x_3 = p(x_1, x_2)$. Now try to find parts of the RHS of $\dot{x}_3$ which can be divided by some $\dot{x}_k$ without remainder. Observe that

$$\frac{x_3(90x_1^4x_2^5x_3^{-1} + 36x_1^7x_2^5 + 48x_1^4x_2^7x_3^{-1})}{x_1(5 + 3x_1^3x_3 + 4x_2^2)} \tag{3.62}$$

has a remainder, but

$$\frac{x_3(60x_1^4x_2^5x_3^{-1} + 36x_1^7x_2^5 + 48x_1^4x_2^7x_3^{-1})}{x_1(5 + 3x_1^3x_3 + 4x_2^2)} = 12x_1^3x_2^5 = \frac{part_1}{\dot{x}_1} \tag{3.63}$$

gives a monomial without remainder, therefore $30x_1^4x_2^5$ should be used elsewhere. Indeed,

$$\frac{x_3(30x_1^4x_2^5x_3^{-1} + 105x_1^5x_2^5x_3^4)}{x_2(2 + 7x_1x_3^5)} = 15x_1^4x_2^4 = \frac{part_2}{\dot{x}_2} \tag{3.64}$$

For the remaining monomials,

$$\frac{x_3(16x_2^2x_3^{-1} + 56x_1x_2^2x_3^4)}{x_2(2 + 7x_1x_3^5)} = 8x_2 = \frac{part_3}{\dot{x}_2} \tag{3.65}$$

is true. Since $\dot{x}_3 = part_1 + part_2 + part_3$ we have found the partial derivatives of the monomials of $p(x_1, x_2)$. Take the integrals of these three monomials with respect to the appropriate variables:

$$\int 12x_1^3 x_2^5 dx_1 = \int 15x_1^4 x_2^4 dx_2 = 3x_1^4 x_2^5 + c_1 \tag{3.66}$$

$$\int 8x_2 dx_2 = 4x_2^2 + c_2 \tag{3.67}$$

Thus, the polynomial we searched for can be written in the form

$$x_3 = p(x_1, x_2) = 3x_1^4 x_2^5 + 4x_2^2 + c \tag{3.68}$$

which is exactly the algebraic equation of the original QP-DAE model in Eq. (2.8) with appropriate initial conditions.

3.3.3 Retrieving monomial-explicit algebraic equations

In this section we focus on the retrieval of algebraic equations in the form

$$z = p^{\alpha}(x)\ , \quad z \in \mathbb{R} \tag{3.69}$$

These equations are QP-algebraic equations, since they can be written *in monomial-explicit form*:

$$z^{\frac{1}{\alpha}} = p(x) \tag{3.70}$$

and - if their substitution spoils the QP format - they are treated by embedding. Consider the DAE model described by Eqs. (3.46,3.69). Equation (3.69) is embedded in order to have a QP-ODE representation:

$$\dot{z} = \alpha p^{\alpha-1}(x) \frac{\partial p}{\partial x} \dot{x} = \alpha z^{\frac{\alpha-1}{\alpha}} \frac{\partial p}{\partial x} f(x) \tag{3.71}$$

As we will see, the variables x, z of this QP-ODE model in Eqs. (3.46,3.71) form a first integral $\lambda(x, z) = c$. Take the time derivative of λ:

$$\frac{d\lambda}{dt} = \frac{\partial \lambda}{\partial x}\dot{x} + \frac{\partial \lambda}{\partial z}\dot{z} = \frac{\partial \lambda}{\partial x} f(x) + \frac{\partial \lambda}{\partial z} \alpha z^{\frac{\alpha-1}{\alpha}} \frac{\partial p}{\partial x} f(x) = 0 \tag{3.72}$$

This PDE can be written as

$$\frac{\partial \lambda}{\partial x} + \frac{\partial \lambda}{\partial z} \alpha \left(z^{\frac{1}{\alpha}}\right)^{\alpha-1} \frac{\partial p}{\partial x} = 0 \tag{3.73}$$

One can easily check that

$$\lambda(x, z) = z^{\frac{1}{\alpha}} - p(x) = c \tag{3.74}$$

is a solution of this PDE from which the original algebraic equation is retrieved in its monomial-explicit form in Eq. (3.70) with appropriate initial conditions.

The retrieval of embedded variables play an important role *in process systems analysis*, since a special case, when $\alpha = -1$ *is used* in describing global reaction rates in the system, *because the reaction rate equations are rational functions with quasipolynomials in the denominator.* In this case, the embedded variable is

$$z = p^{-1}(x) \tag{3.75}$$

and the differential equation for z is in the following form:

$$\dot{z} = -z^2 \sum_{i=1}^{n} \frac{\partial p}{\partial x_i} \dot{x}_i = z\Big(-z \sum_{i=1}^{n} \frac{\partial p}{\partial x_i} \dot{x}_i \Big) \tag{3.76}$$

In general, it is much easier to explore an algebraic relationship of this kind, because of the multiplier $-z$ in the monomials of $\dot{z}$. Since the elements of the gradient $\frac{\partial p}{\partial x}$ are independent of z, the powers of z in the monomials of $\dot{z}$ will be increased by one compared to the corresponding monomials in $\dot{x}_i$. Moreover, there is another connection between the coefficients of these monomials: they have opposite sign (but have the same absolute value). It can also be indicated if the monomials of some $\dot{x}_k$ do not turn up in $\dot{z}$. This is because $\frac{\partial p}{\partial x_k} = 0$ and means that $p(x)$ does not depend on x_k. This makes the retrieval easier.

To retrieve an algebraic equation of this type, one just simply applies the method of first integrals, with one modification: all integrals have to be multiplied by $-z^{-2}$, i.e. if

$$\frac{\partial part_i}{\partial x_{k_i}} = monomial_i(x, z)$$

and

$$\dot{z} = \sum_i part_i$$

then

$$p(x) = \sum_i \int -z^{-2} monomial_i(x, z) dx_{k_i}$$

Example: A continuous fermentation process with fractional reaction kinetics
Consider now the QP-DAE model of a continuous fermentation process with non-monotonous reaction kinetics:

$$\begin{aligned} \dot{X} &= X(-\frac{F}{V} + S\mu) && (3.77)\\ \dot{S} &= S(-\frac{F}{V} + \frac{S_F F}{V} S^{-1} - \frac{1}{Y} X\mu) && (3.78)\\ \mu^{-1} &= k_1 + S + k_2 S^2 && (3.79) \end{aligned}$$

This model is in *monomial-explicit* form, from which one can obtain a QP-ODE model by expressing μ and taking its time-derivative:

$$\dot{\mu} = \frac{d}{dt}(\frac{1}{k_1 + S + k_2 S^2}) = -(\frac{1}{k_1 + S + k_2 S^2})^2 (1 + 2k_2)\dot{S} = -\mu^2 (1 + 2k_2 S)\dot{S} \tag{3.80}$$

The resulting model is a QP-ODE:

$$\begin{aligned} \dot{X} &= X(-\frac{F}{V} + S\mu) && (3.81)\\ \dot{S} &= S(-\frac{F}{V} + \frac{S_F F}{V} S^{-1} - \frac{1}{Y} X\mu) && (3.82)\\ \dot{\mu} &= \mu(\frac{F}{V} S\mu + 2k_2 \frac{F}{V} S^2 \mu - \frac{S_F F}{V}\mu - 2k_2 \frac{S_F F}{V} S\mu + \frac{1}{Y} XS\mu^2 + \frac{2k_2}{Y} XS^2\mu^2) && (3.83) \end{aligned}$$

Now let's try to retrieve the algebraic equation! The coefficients of monomials in the third differential equation turn out in the second differential equation, but with an opposite sign

- it is correct. The connection between the monomials is also fulfilled, the monomials in the third equation have powers of z increased by one compared to the corresponding monomials in the second equation. Therefore our algebraic relationship would be in the form:

$$\mu = \frac{1}{p(S)} \tag{3.84}$$

Since p depends on a single variable, it can be retrieved directly:

$$p(S) = \int \frac{\dot{\mu}}{\dot{S}} \cdot (-\mu^{-2}) = \; dS = \int 2k_2 S + 1 \; dS = k_2 S^2 + S + c \tag{3.85}$$

where $c = k_1$ comes from appropriate initial conditions.

3.4 Canonical forms of QP-DAE models

Here we summarize the two previously introduced canonical forms for QP-DAE models that will be used for further analysis.

DAE canonical form of QP-DAEs The usual form of QP-DAE models

$$\dot{x}_i = x_i\big(\lambda_i + \sum_{j=1}^{m} A_{ij} \prod_{k=1}^{n} x_k^{B_{jk}} \cdot \prod_{k=1}^{d} z_k^{B_{j(n+k)}}\big), \qquad i = 1, \ldots, n, \tag{3.86}$$

$$0 = z_k\big(\lambda_{n+k} + \sum_{j=1}^{m} A_{(n+k)j} \prod_{\ell=1}^{n} x_\ell^{B_{j\ell}} \cdot \prod_{\ell=1}^{k-1} z_\ell^{B_{j(n+\ell)}}\big), \qquad k = 1, \ldots, d, \qquad m \geq (n+d) \tag{3.87}$$

where the parameters A and B of the model are $(n+d) \times m$ and $m \times (n+d)$ real matrices and $\lambda \in \mathbb{R}^{(n+d)}$ is a real vector, is called a DAE canonical form if both the blocks A_x for the rows corresponding to the differential variables and A_z for the algebraic variables are of full rank.

Example 1 (continued) Let us consider the QP-DAE of *Example 1.* It is easy to check that its DAE form in Eqs. (2.9) - (2.11) is in the canonical QP-DAE form. Defining the set of differential ($x = [x_1, \; x_2]^T$) and algebraic ($z = x_3$) variables, and using that z is positive, we get the following QP-DAE model:

$$\dot{x}_1 = x_1(5 + 3x_1^3 z + 4x_2^2) \tag{3.88}$$

$$\dot{x}_2 = x_2(2 + 7x_1 z^5) \tag{3.89}$$

$$0 = z(3x_1^4 x_2^5 + 4x_2^2 - z) \tag{3.90}$$

which is indeed in the form of Eqs. (3.86-3.87).

LV-ODE form of QP-DAE models The previously introduced (see Eq. (3.26)) form of QP-DAE models

$$\dot{U}_i = U_i(\Lambda_i + \sum_{j=1}^{m} M_{ij} U_j), \quad i = 1, \ldots, m$$

is a LV-ODE form with the following properties. It is

- a **quadratic** nonlinear model,
- **rank-deficient** M for the general $m > n$ case
- a special QP model with $A = M$ and $B = I$.

The results in the earlier sections together with the LV-form of a QP-DAE model 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 resulting transformed model will be a LV-ODE, i.e. the algebraic equations formally disappear and the resulting coefficient matrix $M = \widetilde{A}_{LV}$ will be rank deficient.
2. We can retrieve the algebraic equations 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).

Chapter 4

The steady-states of QP models

The number and properties of steady-states of QP models (QP-ODE or QP-DAE) characterize their type of nonlinearity. Generally speaking, one may call a model with single isolated steady-states more nonlinear if it has more steady-states with different local stability properties. As we shall see in this section the maximal possible number of single isolated steady-sates of a QP model is equal to the difference between the number of quasi-monomials and that of the variables.

The determination of steady-state points of a QP model is performed in two logical steps.

1. Construction of a QP algebraic (QP-AE) model by equating the time derivatives of the differential variables to zero.

2. Solution of the resulting QP-AE.

4.1 Full rank $m = (n + d)$ case

If the number of quasi-monomials is equal to the number of variables, then both A and B are square. The QP-AE to be solved for the steady-states in its logarithmic form is as follows:

$$0 = \lambda + AQ_{ss} \tag{4.1}$$

$$Q_{ss}^* = BX_{ss}^* \tag{4.2}$$

It is important to note that a necessary condition to get any admissible solution (i.e. a solution in the positive orthant) is that Eq. (4.1) possesses an element-wise positive solution.

With **invertible** (full rank) A and B we get a **unique** solution that is not necessarily admissible:

$$\begin{aligned} Q_{ss} &= -A^{-1}\lambda \\ X_{ss}^* &= B^{-1}Q_{ss}^* \end{aligned}$$

Full rank LV-case: In the rare case when the Lotka-Volterra coefficient matrix $A_{LV} = M = BA$ is of full rank (that implies that both A and B should be of full rank) and $B_{LV} = I$ is also of a full rank, the above equations become

$$U_{ss} = Q_{ss} = -M^{-1}\Lambda \tag{4.3}$$

This also means that we have a unique solution and at most a single unique admissible steady-state.

4.2 Rank-deficient cases

In the general case, however, $m \geq (n+d)$ and $rank\ M = rank\ (BA) \leq (n+d)$. That means, that the linear equation

$$0 = \lambda + AQ_{ss}$$

will not have a unique solution. Then, the vector of quasimonomials and accordingly the parameter matrices A and B can be partitioned as:

$$A = \left[\begin{array}{c|c} A_p & A_s \end{array}\right] \begin{bmatrix} Q_{p,ss} \\ Q_{s,ss} \end{bmatrix} , \quad \begin{bmatrix} Q^*_{p,ss} \\ Q^*_{s,ss} \end{bmatrix} = \left[\begin{array}{c} B_p \\ \hline B_s \end{array}\right] X^*_{ss} \tag{4.4}$$

This gives a set of solutions forming a linear subset of $\mathbb{R}^m$ that is constrained by the $m-(n+d)$ nonlinear algebraic relationship between the quasimonomials:

$$\begin{aligned} 0 &= \lambda + A_p Q_{p,ss} + A_s Q_{s,ss} && \text{containing } (n+d) \text{ equations} && (4.5) \\ Q_{s,ss} &= B_s B_p^{-1} Q_{p,ss} && \text{containing } (m-(n+d)) \text{ equations} && (4.6) \end{aligned}$$

even if both the matrices A and B are of full rank $(n+d)$.

Example 1 (continued) The parameter matrices of the DAE model of this example can be partitioned in the following way:

$$A = \left[\begin{array}{ccc|cc} 3 & 4 & 0 & 0 & 0 \\ 0 & 0 & 7 & 0 & 0 \\ 0 & 4 & 0 & 3 & -1 \end{array}\right] , \quad B = \left[\begin{array}{ccc} 3 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 5 \\ \hline 4 & 5 & 0 \\ 0 & 0 & 1 \end{array}\right] \tag{4.7}$$

for which Eqs. (4.5-4.6) are in the following form:

$$\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 5 \\ 2 \\ 0 \end{bmatrix} + \begin{bmatrix} 3 & 4 & 0 \\ 0 & 0 & 7 \\ 0 & 4 & 0 \end{bmatrix} Q_{p,ss} + \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 3 & -1 \end{bmatrix} Q_{s,ss} \tag{4.8}$$

$$Q^*_{s,ss} = \begin{bmatrix} 4 & 5 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 3 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 5 \end{bmatrix}^{-1} = \begin{bmatrix} \frac{10}{7} & \frac{5}{2} & -\frac{2}{7} \\ -\frac{1}{14} & 0 & \frac{3}{14} \end{bmatrix} Q^*_{p,ss} \tag{4.9}$$

where

$$Q_{p,ss} = \begin{bmatrix} x^3_{1,ss} x_{3,ss} \\ x^2_{2,ss} \\ x_{1,ss} x^5_{3,ss} \end{bmatrix} , \quad Q_{s,ss} = \begin{bmatrix} x^4_{1,ss} x^5_{2,ss} \\ x_{3,ss} \end{bmatrix} \tag{4.10}$$

The linear set of equations has a solution in the form of a two-dimensional subset, which is constrained by the two nonlinear equations.

In order to see what happens to the number of possible steady-state points, let us consider the LV form of the QP-ODE or QP-DAE in question. Then the equation to be solved for finding the steady-state points is

$$0 = \Lambda + MU_{ss} \tag{4.11}$$

but now $rank\ M \leq (n+d) \leq m$. Thus the steady-state points will be on an $m-n-d$ dimensional linear subspace of $\mathbb{R}^m$ constrained by the generally nonlinear algebraic relationships between the quasi-monomials, that is the LV variables, that are coded in the linear dependence of $m-n-d$ rows of M on the linearly independent ones. In the extreme case we may then obtain $m-n-d$ different isolated solutions of Eq. (4.11) as possible steady-state points. This system has no admissible steady states.

Example 3 Let us consider a simple one-dimensional example

$$\begin{aligned} \dot{x} &= x \cdot (x^3 - 3x^2 + 2x) = x^2(x-2)(x-1) \\ q_1 &= x \ , \ q_2 = x^2 \ , \ q_2 = x^3 \end{aligned}$$

that has **3** different steady-states (**two admissible ones**): $x = 0$, $x = 1$, $x = 2$. The number of variables is $n = 1$ and the number of quasi-monomials is $m = 3$.

The LV-form of the model is

$$\begin{aligned} \dot{q}_1 &= q_1 \cdot (q_3 - 3q_2 + 2q_1) \\ \dot{q}_2 &= 2q_2 \cdot (q_3 - 3q_2 + 2q_1) \\ \dot{q}_3 &= 3q_3 \cdot (q_3 - 3q_2 + 2q_1) \end{aligned} \quad , \quad M = \begin{bmatrix} 1 & -3 & 2 \\ 2 & -6 & 4 \\ 3 & -9 & 6 \end{bmatrix}$$

If one solves the related steady-state algebraic set of equations it is easy to see, that it has **infinitely many** different steady-states on the plane

$$(q_3 - 3q_2 + 2q_1) = 0$$

that is a 2-dimensional linear subspace of the 3-dimensional space.

In order to retrieve the nonlinear algebraic relationships between the quasi-monomials, we transform the equations to their minimal form by

1. retrieving the QM-type algebraic equations, and then
2. substitution

Using the LV form of the simple one-dimensional example we perform the following steps.

- rank $M = 1$, take the first row
- 2nd row $=$ 2 $\cdot$ (first row): $\dot{q}_2^* = 2\dot{q}_1^* \implies q_2^* = 2q_1^* + C_1 \implies q_2 = C_1 q_1^2$
- 3rd row $=$ 3 $\cdot$ (first row): $\dot{q}_3^* = 3\dot{q}_1^* \implies q_3^* = 3q_1^* + C_2 \implies q_3 = C_2 q_1^3$

Thus the steady-state points can be obtained as the intersection of the equations

$$(q_3 - 3q_2 + 2q_1) = 0 \quad , \quad q_2 = C_1 q_1^2 \quad , \quad q_3 = C_2 q_1^3$$

that gives 3 points, 2 in the admissible domain.

4.3 Local stability of the steady-state points

The Jacobian matrix of a QP-ODE system at a steady-state point x_{ss} can be computed from the system matrices A, B and the equilibrium point.

$$J_{QP}(x_{ss}) = \overline{X}_{ss} \cdot A \cdot \overline{Q}_{ss} \cdot B \cdot \overline{X}_{ss}^{-1}, \tag{4.12}$$

where

$$\begin{aligned} \overline{X}_{ss} &= diag([x_{1,ss}, \ldots, x_{n,ss}]), \\ \overline{Q}_{ss} &= diag([q_{1,ss}, \ldots, q_{m,ss}]) \end{aligned}$$

where $q_{j,ss},\ j = 1, ..., m$ are the quasi-monomials of the system in the equilibrium x_{ss}.

$$J_{QP}(x_{ss}) = \begin{bmatrix} \sum_{j=1}^{m} A_{1j} B_{j1} q_{j,s} & \dots & \frac{x_{1,ss}}{x_{n,ss}} \sum_{j=1}^{m} A_{1j} B_{jn} q_{j,ss} \\ \vdots & \ddots & \vdots \\ \frac{x_{n,ss}}{x_{1,ss}} \sum_{j=1}^{m} A_{nj} B_{j1} q_{j,ss} & \dots & \sum_{j=1}^{m} A_{nj} B_{jn} q_{j,ss} \end{bmatrix} \tag{4.13}$$

It is important to observe that the Jacobian matrix above is an $n \times n$ matrix and thus can have at most n different non-zero eigenvalues in the optimal full-rank A and B case.

It is also important to know that the above QP-Jacobian matrix is not invariant with respect to QM-transformation, but its eigenvalues are. To show this, transform the system with an invertible QM transformation

$$X_i = \prod_{k=1}^{n+d} \widehat{X}_k^{C_{ik}}, \qquad i = 1, \dots, n \tag{4.14}$$

where C is an arbitrary $(n+d) \times (n+d)$ invertible matrix. The effect of this transformation on the logarithmic variables at the steady state is

$$\widehat{x}^*_{ss} = C^{-1} x^*_{ss}$$

which can be written in the form

$$\widehat{x}_{ss} = exp(C^{-1} x^*_{ss})$$

where $exp(v)$ denotes element-wise exponential of vector v. Using the well-known effect of QM transformation on the parameter matrices and monomials:

$$\widehat{Q}^* = Q^* \quad , \quad \widehat{B} = B \cdot C \quad , \quad \widehat{A} = C^{-1} \cdot A \quad ,$$

the Jacobian of the transformed QP system can be written as:

$$\begin{aligned} \widehat{J}^*_{QP}(\widehat{x}_{ss}) &= \widehat{\overline{X}}_{ss} \cdot \widehat{A} \cdot \widehat{\overline{Q}}_{ss} \cdot \widehat{B} \cdot \widehat{\overline{X}}_{ss}^{-1} = \\ &= \overline{exp(C^{-1} x^*_{ss})} \cdot C^{-1} \cdot A \cdot \overline{Q}_{ss} \cdot B \cdot C \cdot \left(\overline{exp(C^{-1} x^*_{ss})}\right)^{-1} = \\ &= \overline{exp(C^{-1} x^*_{ss})} \cdot C^{-1} \cdot \overline{X}_{ss}^{-1} \cdot \overline{X}_{ss} \cdot A \cdot \overline{Q}_{ss} \cdot B \cdot \overline{X}_{ss}^{-1} \cdot \overline{X}_{ss} \cdot C \cdot \left(\overline{exp(C^{-1} x^*_{ss})}\right)^{-1} = \\ &= \left(\overline{exp(C^{-1} x^*_{ss})} \cdot C^{-1} \cdot \overline{X}_{ss}^{-1}\right) \cdot J^*_{QP}(x_{ss}) \cdot \left(\overline{exp(C^{-1} x^*_{ss})} \cdot C^{-1} \cdot \overline{X}_{ss}^{-1}\right)^{-1} = \\ &= T \cdot J^*_{QP}(x_{ss}) \cdot T^{-1} \end{aligned} \tag{4.15}$$

where $\overline{v}$ denotes the diagonal matrix made of the components of vector v.

As we can see, we get the Jacobian of the transformed system by a similarity transformation T applied to the Jacobian of the original system, and therefore the eigenvalues are preserved.

Jacobian matrix of QP models in LV form It can be shown [7] that the Jacobian matrix of the Lotka-Volterra form model is

$$J_{LV}(U_{ss}) = M diag(U_{ss}) \tag{4.16}$$

where $M = A_{LV}$ and U_{ss} is the solution of the steady state LV-AE equation

$$0 = \Lambda + MU_{ss}$$

Since the matrix M has maximal rank $n \leq m$, the LV-Jacobian matrix above is an $m \times m$ matrix with maximal rank n, and therefore it has $(m - n)$ distinct zero eigenvalues. The other (generally nonzero) eigenvalues, however, are identical with those of the QP-Jacobian matrix.

Chapter 5

Conclusions and future work

Various algebraically equivalent forms of index 1 QP-DAE models that are of importance for lumped process models are suggested in this work. These are the DAE canonical form and the LV-ODE form with a rank-deficient coefficient matrix. Form invariance and transformations for obtaining these forms from each other are also discussed.

The retrieval of the hidden algebraic equations from a non-minimal QP-ODE form of a QP-DAE model is also considered. The suggested algorithms can only retrieve special classes of QM or QP algebraic equations.

Further work will be directed to the use of these forms and the form invariants for computational and dynamic analysis of QP-DAE systems.

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