STATE ESTIMATION AND STATE FEEDBACK CONTROL IN QUASI-POLYNOMIAL AND QUANTUM MECHANICAL SYSTEMS

Theses of Ph.D. dissertation

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1 Motivation and aim

The methods and tools of modern state space representation based system and control theory [1], [2], [3], [4] has matured nowadays mainly in the fields of robust, LPV, and LQ control with numerous applications in formally difficult areas, such as process and nuclear systems, etc. However, there is still a lack of practically feasible techniques for highly nonlinear systems with a wide operating domain, such as biochemical, biomechanical, or quantum systems. This holds true despite the fact that there is a rapid development in the area of nonlinear and stochastic system and control theory (see e.g. [1],[3]).

The present thesis treats two different system classes originating from different fields of physics. Tools of modern system and control theory are applied on them in such a way that their specialities are utilized to obtain practically feasible methods for problems that are computationally hard in the general case.

The nonlinear nature of general process systems [5] makes their global stability analysis hard. Using special nonlinear system model classes that are still general enough to describe the dynamics of them might open the way of handling them efectively . In this work the so-called quasi-polynomial (QP) system class [6] [7], will be used for this purpose. Using the fact that the structure of the Lyapunov function is known for this system class will facilitate the global stability analysis of general process systems. Using the results of stability analysis, the QP system class can be used for synthesizing controllers which ensure the global stability of the closed loop system with respect to the given Lyapunov function family [8]. A further speciality is, that the state variables of process systems are typically concentrations, temperatures, pressures, etc. which are easily measurable quantities so the feedback control of them does not require state observers or estimators. Moreover, the state variables are always positive, thus process systems together with their QP representation form a sub-class of positive systems.

So far, only a few people (e.g. [9]) has tried to handle quantum mechanical systems on the control theoretical basis. The aimed subproblem in this work is reading quantum information, which asks for the design of state observers/estimators. The measurement of a quantum system has probabilistic nature and turns the whole system to be stochastic, for which reliable state estimation methods must be developed [10]. One way is to apply the Bayesian methodology to use a full probabilistic model and give a state estimate that contains a lot of information about the state to be estimated. The other direction to quantum state estimation is to develop a simple estimator which is applicable for a wide range of quantum systems and moreover it is easy to compute.

2 Methods and Tools

In what follows, the basic notions, and most important tools used in the work are summarized.

2.1 QP and LV models

Quasi-polynomial models are systems of ODEs of the following form

$$\dot{x}_i = x_i \left(\lambda_i + \sum_{j=1}^{m} A_{i,j} \prod_{k=1}^{n} x_k^{B_{j,k}} \right), \quad i = 1, \ldots, n. \tag{1}$$

where $x \in \text{int}(\mathbb{R}_+^n)$, $A \in \mathbb{R}^{n\times m}$, $B \in \mathbb{R}^{m\times n}$, $\lambda_i \in \mathbb{R}$, $i = 1, \ldots, n$. Furthermore, $\lambda = [\lambda_1 \ \ldots \ \lambda_n]^T$. It was shown in [6], that non QP nonlinear systems having *smooth* nonlinearities can easily be embedded into QP form by introducing new state variables instead of the non QP nonlinearities.

The above family of models is split into classes of equivalence [7] according to the values of the products $M = B \cdot A$ and $N = B \cdot \lambda$. The *Lotka-Volterra form* gives the representative elements of these classes of equivalence. If $rank(B) = n$, then the set of ODEs in (1) can be embedded into the following m-dimensional set of equations, the so called Lotka-Volterra model:

$$\dot{z}_j = z_j \left(N_j + \sum_{i=1}^{m} M_{j,i} z_i \right), \qquad j = 1, \ldots, m \tag{2}$$

where

$$M = B \cdot A, \quad N = B \cdot \lambda,$$

and each z_j represents a so called *quasi-monomial*:

$$z_j = \prod_{k=1}^{n} x_k^{B_{j,k}}, \qquad j = 1, \ldots, m. \tag{3}$$

Henceforth it is assumed that x^* is a positive equilibrium point, i.e. $x^* \in \text{int}(\mathbb{R}_+^n)$ in the QP case and similarly $z^* \in \text{int}(\mathbb{R}_+^m)$ is a positive equilibrium point in the LV case. For LV systems there is a well known candidate Lyapunov function family [8],[11], which is in the form:

$$V(z) = \sum_{i=1}^{m} c_i \left(z_i - z_i^* - z_i^* \ln \frac{z_i}{z_i^*} \right), \tag{4}$$

$$c_i > 0, \quad i = 1 \ldots m,$$

where $z^* = [z_1^*, \ldots, z_m^*]^T$ is the equilibrium point corresponding to the equilibrium x^* of the original QP system (1). The time derivative of the of the Lyapunov function (4) is:

$$\dot{V}(z) = \frac{1}{2}(z - z^*)(CM + M^T C)(z - z^*) \tag{5}$$

where $C = \mathrm{diag}(c_1, \ldots, c_m)$ and M is the invariant characterizing the LV form (2).

2.2 Input-affine QP system models

The general form of the state equation of an input-affine QP system model with p-inputs is as follows:

$$\begin{aligned} \dot{x}_i &= x_i \left(\lambda_{0_i} + \sum_{j=1}^{m} A_{0_{i,j}} \prod_{k=1}^{n} x_k^{B_{j,k}} \right) + \\ &+ \sum_{l=1}^{p} x_i \left(\lambda_{l_i} + \sum_{j=1}^{m} A_{l_{i,j}} \prod_{k=1}^{n} x_k^{B_{j,k}} \right) u_l \end{aligned} \tag{6}$$

where

$$i = 1, \ldots, n, \quad A_0, A_l \in \mathbb{R}^{n \times m}, \quad B \in \mathbb{R}^{m \times n},$$
$$\lambda_0, \lambda_l \in \mathbb{R}^n, \quad l = 1, \ldots, p.$$

The corresponding input-affine Lotka-Volterra model is in the form

$$\dot{z}_j = z_j \left(N_{0_j} + \sum_{k=1}^{m} M_{0_{j,k}} z_k \right) + \sum_{l=1}^{p} z_j \left(N_{l_j} + \sum_{k=1}^{m} M_{l_{j,k}} z_k \right) u_l \tag{7}$$

where

$$j = 1, \ldots, m, \quad M_0, M_l \in \mathbb{R}^{m \times m}, \quad N_0, N_l \in \mathbb{R}^m, \quad l = 1, \ldots, p,$$

and the parameters can be obtained from the input-affine QP system's ones in the following way

$$\begin{aligned} M_0 &= B \cdot A_0 \\ N_0 &= B \cdot L_0 \\ M_l &= B \cdot A_l \\ N_l &= B \cdot \lambda_l \qquad l = 1, \ldots, p. \end{aligned} \tag{8}$$

If the inputs applied on (6) are quasi-polynomial functions of the state variables, then it is easy to see, that the closed loop system will also be in QP form.

2.3 The time-reparametrization transformation

Let $\omega = [\omega_1 \quad \dots \quad \omega_n]^T \in \mathbb{R}^n$. It is shown e.g. in [11] that the following reparametrization of time

$$dt = \prod_{k=1}^{n} x_k^{\omega_k} dt' \tag{9}$$

transforms the original QP system into the following (also QP) form

$$\frac{dx_i}{dt'} = x_i \sum_{j=1}^{m+1} \tilde{A}_{i,j} \prod_{k=1}^{n} x_k^{\tilde{B}_{j,k}}, \; i = 1, \dots, n \tag{10}$$

where $\tilde{A} \in \mathbb{R}^{n\times(m+1)}$, $\tilde{B} \in \mathbb{R}^{(m+1)\times n}$ and

$$\tilde{A}_{i,j} = A_{i,j}, \;\; i = 1, \dots, n; \; j = 1, \dots, m \tag{11}$$

$$\tilde{A}_{i,m+1} = \lambda_i, \;\; i = 1, \dots, n \tag{12}$$

and

$$\tilde{B}_{i,j} = B_{i,j} + \omega_j, \;\; i = 1, \dots, m; \; j = 1, \dots, n \tag{13}$$

$$\tilde{B}_{m+1,j} = \omega_j, \;\; j = 1, \dots, n. \tag{14}$$

It can be seen that the number of monomials is increased by one and vector $\tilde{\lambda}$ is zero in the transformed system.

2.4 Linear and bilinear matrix inequalities

A (non-strict) linear matrix inequality (LMI) is an inequality of the form

$$F(x) = F_0 + \sum_{i=1}^{m} x_i F_i \leq 0, \tag{15}$$

where $x \in \mathbb{R}^m$ is the variable and $F_i \in \mathbb{R}^{n\times n}$, $i = 0, \dots, m$ are given symmetric matrices. The inequality symbol in (15) stands for the negative semi-definiteness of $F(x)$. If the equality is not allowed, then the LMI is termed *strict*.

One of the most important properties of LMIs is the fact, that they form a convex constraint on the variables, i.e. the set $\mathscr{F} = \{x \mid F(x) \leq 0\}$ is convex and thus many different kinds of convex constraints can be expressed in this way [12], [13]. It is important to note that a particular point from the convex solution set $\mathscr{F}$ can be selected using additional criteria (e.g. different kinds of objective functions) [12]. Standard LMI optimization problems are e.g. linear function minimization, generalized eigenvalue problem, etc.

Various problems in system- and control theory can be written up as a set of linear matrix inequalities. For example, the Lyapunov equation connected to the global stability of LTI systems. But they also appear in the context of *linear parameter-varying* (LPV) systems, or within μ-analysis there are also LMIs solved [14] .

On the other hand, a bilinear matrix inequality (BMI) is a diagonal block composed of q matrix inequalities of the following form

$$G_0^i + \sum_{k=1}^{p} x_k G_k^i + \sum_{k=1}^{p} \sum_{j=1}^{p} x_k x_j K_{kj}^i \leq 0, \quad i = 1, \dots, q \tag{16}$$

where $x \in \mathbb{R}^p$ is the decision variable to be determined and G_k^i, $k = 0, \dots, p$, $i = 1, \dots, q$ and K_{kj}^i, $k, j = 1, \dots, p$, $i = 1, \dots, q$ are symmetric, quadratic matrices.

The main properties of BMIs are that they are non-convex in x (which makes their solution numerically much more complicated than that of linear matrix inequalities), and their solution is NP-hard [15], so the size of the tractable problems is limited. Similarly to the LMIs, additional criteria can be used to select a preferred solution point of a feasible BMI from its solution set.

2.5 States of N-level quantum systems

For describing the states of finite quantum systems the so-called *density matrices* are used in the sequel. Density matrices χ are statistical operators acting on the Hilbert space $\mathscr{H}$, they are positive semidefinite self-adjoint matrices having unit trace:

$$\chi \in \mathbb{C}^n, \quad \chi \geq 0, \quad \chi = \chi^*, \quad \mathrm{Tr}\chi = 1 \tag{17}$$

A density operator describes a pure state if it is a rank one projection, i.e.

$$\chi = \chi^2.$$

Two level quantum systems (i.e the dimension of the underlying Hilbert space is 2) are termed *qubit*s since they are the quantum generalization of bits. Using the Pauli matrices as basis among the 2×2 density matrices, the so-called Bloch vector notation can be used to represent states of qubits:

$$\chi = \frac{1}{2}(I + x_1\sigma_1 + x_2\sigma_2 + x_3\sigma_3) \tag{18}$$

where σ_1, σ_2 and σ_3 are the so-called *Pauli matrices* [16], $x_i \in \mathbb{R}, i = 1,2,3$. This way, the state of a qubit can be represented by a vector $x = [x_1, x_2, x_3]^T$ of $\mathbb{R}^3$ instead of the density matrix χ. The positivity property of the density matrices transforms to the constraint $||x|| \leq 1$ in the Bloch vector case.

The most general parametrization of the density matrix that suits for all quantum systems uses the matrix elements as parameters:

$$\chi = \sum_{k=1}^{N} x_{kk} E_{kk} + \sum_{i<j} \left(x_{ij}(E_{ij} + E_{ji}) + x_{ji}(iE_{ij} - iE_{ji}) \right), \tag{19}$$

where E_{ij} are the matrix units (full of zeros except for the i,j-th element which is one). This way, the state of an N-level system can be given with N^2 real parameters. It can be seen that in contrast with the Bloch-parametrization (18) this parametrization does not ensure the unit trace for the density, so a reasonable modification is:

$$\begin{aligned} \chi = \sum_{k=1}^{N-1} x_{kk} E_{kk} + \left(1 - \sum_{k=1}^{N-1} x_{kk} \right) E_{NN} + \\ + \sum_{i<j} \left(x_{ij}(E_{ij} + E_{ji}) + x_{ji}(iE_{ij} - iE_{ji}) \right). \end{aligned} \tag{20}$$

This offers the use of a generalization of the Bloch-vector space [17]. The Bloch-vector of an N-level quantum system is a vector of $\mathbb{R}^{N^2-1}$.

2.6 Observables and their measurement

The measurable physical quantities of quantum systems (the so called *observables*) are represented by self-adjoint operators of $\mathscr{H}$ (i.e. self-adjoint matrices of $\mathbb{C}^{\dim \mathscr{H} \times \dim \mathscr{H}}$) [18].

The measurement of an observable O has a probabilistic nature. The possible outcomes of the measurement are the different λ eigenvalues of O, the corresponding probability is

$$\mathrm{Prob}(\lambda_i) = \mathrm{Tr} E_i \chi E_i^*,$$

where E_i are the projections onto the subspace spanned by the eigenvector corresponding to λ_i, i.e.

$$\sum_i E_i = I, \quad E_i^2 = E_i.$$

Moreover, the state of the system **S** after measuring O, and having the outcome λ_i changes to

$$\chi' = \frac{E_i \chi E_i^*}{\mathrm{Tr} E_i \chi E_i^*}$$

that means that the measurement has lost its good property of being a passive operation known from classical physics. *The measurement changes the actual state of the quantum system.*

The above measurement is called *von Neumann measurement*, the most popular example of it in the 2 level case is the spin measurement, i.e. the measurement of the *Pauli matrices* as observables.

A more general measurement type is the so-called POVM (positive operator valued measurement), see [19].

3 New scientific results

The main scientific contributions of the dissertation are summarized in the following thesis points.

Thesis 1. *The global stability analysis of nonlinear process systems being in quasi-polynomial representation has been formulated as a linear matrix inequality. The chance to prove global stability has been extended by time-reparametrization where the scaling factors were determined and the global stability is proved by solving a bilinear matrix inequality.*
(**[O1], [O2], [O3], [O4]**)
It was shown, that the negative definiteness condition of the Lyapunov function of QP and LV systems is equivalent to a linear matrix inequality, thus the stability analysis of QP systems (and general nonlinear process systems embedded into QP form) is equivalent to the feasibility of a LMI [13]. The LMI is non-strict if the model has been obtained by embedding.

It has been shown, that time-reparametrization transformation introduces a re-scaling in the QP system's quasi-monomials, such that the global stability of transformed QP system is equivalent to that of the original one. This way the global stability analysis has been extended to a wider class of QP systems by embedding the parameters of the time-reparametrization transformation into the global stability analysis, when one has to solve a bilinear matrix inequality.

Thesis 2. *The globally stabilizing quasi-polynomial state feedback design problem for quasi-polynomial systems has been expressed as a bilinear matrix inequality. The problem has been reformulated so that it can be solved by an existing iterative LMI algorithm.*
A supplementary feedback controller that shifts some coordinates of the closed loop systems's steady state has been computed from a linear set of equations. Conditions on the number of shiftable coordinates were also given.
(**[O5], [O11]**)
A globally stabilizing state feedback design problem was formulated using the global stability analysis results of **Thesis 1**. The problem has been solved as a bilinear matrix inequality feasibility problem, having two groups of variables, one for the parameters of the Lyapunov function and another for the feedback gains. The proposed method does not utilize the objective function of the BMI optimization problem (16),

thus it is a possible point to introduce some performance or robustness specifications.
If one is to solve just the BMI feasibility without additional criteria, the problem has been reformulated so that an existent iterative LMI algorithm is suitable for its' solution.

The stabilizing state feedback may shift the closed loop system's equilibrium points into unwanted values that's why the possibilities of designing an additional feedback that (partially) sets back the original steady state were proposed. It was shown that under certain conditions on the closed loop system's Lotka-Volterra coefficient matrix it is possible to design such a controller. It's parameters were determined from a linear set of equations. In most cases, however it is only possible to redesign the steady state for only a few number of state coordinates.

Thesis 3. *A Bayesian state estimation scheme was developed for a single quantum bit using Bloch parametrization. As a measurement scheme, the von Neumann measurement of the Pauli spin operators was used. Using the independency of the applied measurements, the problem was solved componentwise.*
The estimator was improved in order to avoid estimates laying out of the state space by an additional constraint.
(**[O6], [O7]**)
A relaxed state estimation problem was solved for a quantum bit using Bayesian methodology. The estimation was based on the Bloch vector representation of quantum states and on the von Neumann measurements of the three Pauli spin operator.

Since the three measurements are incompatible, the problem was regarded to be an independent estimation of the three Bloch vector components. The total estimate was obtained by multiplying the three probability density functions. The obtained Bayesian state estimator performed weak for estimation pure states, so an additional constraint was added to the problem. This step resulted in an estimator that always gives a physically meaningful result, however it's computation is more difficult.

Using the simulator Spinsim [O8] the constrained and the unconstrained Bayesian state estimation methods was compared. Their difference was outstanding in the case of estimating a pure state, or estimating based on a small measurement data.

Thesis 4. *A novel, componentwise quantum state estimation scheme was developed for N-level quantum mechanical systems. The measurement data were obtained from the von Neumann measurement of $N^2 - 1$ independent observables. The estimator uses the measurement data of the above measurement to determine the $N^2 - 1$ parameters of the density matrix.*

An algebraic and a geometric method was proposed to force the estimator to produce physically meaningful result.

The effectiveness of the estimator was compared to other estimation schemes using the mean squared error matrix.

(**[O8], [O9], [O10]**)

The quantum state estimation problem refined for quantum systems was solved for N-level quantum systems, not only for qubits.

The collection of observables consists of 3 group of von Neumann measurements. The basis of the estimation scheme is the Bloch parametrization used for general finite quantum systems. The estimator consists of $N^2 - 1$ equations for the $N^2 - 1$ parameters of the density matrix, and gives a point estimate based on the relative frequencies of certain outcomes of the observables.

It has been proven that the estimator is unbiased but suffers from the tendency to give false estimates so a modification was necessary to respect the positivity constraint of density matrices (17) .

It was shown that for invertible states the constrained estimator converges to the unconstrained one when the size of the measurement data increases. If the real state is on the boundary of the state space, then the unconstrained estimator is useless, since it is always necessary to correct its result by one of the two constraining methods proposed.

The effectiveness of the unconstrained estimator was compared to two different estimation schemes available in the literature. The comparison was based on their mean quadratic error matrices. It has been shown that the proposed scheme is more efficient than the other two.

4 Publications related to the thesis

[O1] A. Magyar and K. M. Hangos. Lotka-Volterra representation of process systems for stability analysis. *In Proceedings of on 14th International Conference on Process Control (PC'03)*, Štrbské Pleso, Slovakia, 2003. (**Thesis 1**)

[O2] A. Magyar and K. M. Hangos. Lotka-Volterra representation of process systems for stability analysis. *In Proceedings of 4th International PhD Workshop on Systems and Control*, Libverda, Czech Republic, 2003. (**Thesis 1**)

[O3] A. Magyar, G. Szederkényi, and K. M. Hangos. Quadratic stability of process systems in generalized Lotka-Volterra form. *In Proceedings of 6th IFAC Symposium on Nonlinear Control (NOLCOS 2004)*, Stuttgart, Germany, 2004. (**Thesis 1**)

[O4] G. Szederkényi, K.M. Hangos, and A. Magyar. On the time-reparametrization of quasi-polynomial systems. *Physics Letters A*, 334:288–294, 2005. **impact factor: 1.550**. (**Thesis 1**)

[O5] A. Magyar, G. Szederkényi, and K. M. Hangos. Quasi-polynomial system representation for the analysis and control of nonlinear systems. *In Proceedings of 16th IFAC World Congress*, Prague, Czech Republic, 2005. (**Thesis 2**)

[O6] A. Magyar, K. M. Hangos, and D. Petz. Bayesian qubit tomography. *In Proceedings of 6th International PhD Workshop on Systems and Control*, Izola - Simonov zaliv, Slovenia, 2005. (**Thesis 3**)

[O7] A. Magyar, D. Petz, and K. M. Hangos. Bayesian qubit state estimation. *In Proceedings of 14th IFAC Symposium on System Identification (SYSID-2006)*, Newcastle, Australia, pages 949–954, 2006. (**Thesis 3**)

[O8] D. Petz, K. M. Hangos, A. Magyar, and L. Ruppert. State estimation of n-level quantum systems. *Research report no. SCL-007/2006, Computer and Automation Research Institute*, 2006. (**Thesis 4**)

[O9] L. Ruppert and A. Magyar. The effect of constraints on LS state estimators for a qubit. *In Proceedings of 7th International PhD Workshop*, Hruba Skala, Czech Republic, ISBN: 80-903834-1-6, 2006. (**Thesis 4**)

[O10] D. Petz, K. M. Hangos, and A. Magyar. Point estimation of states of finite quantum systems. *Journal of Physics A: Math. Theor.*, 40:7955–7969, 2007. **impact factor: 1.566**. (**Thesis 4**)

[O11] A. Magyar, G. Szederkényi and K. M. Hangos. Globally stabilizing feedback control of process systems in generalized Lotka-Volterra form. *Journal of Process Control*, 2007. in print. (**Thesis 2**)

5 Application areas, directions for future work

Quasi-polynomial system representation (1) is a good tool for describing biochemical systems given in the form of reaction kinetic networks. The state variables of such systems are typically concentrations, i.e. they are also positive systems. These reaction kinetic networks are given by their *mass action law* description. This special form enables to apply the results of classical reaction kinetics together with the results of thesis points 1 and 2.

On the other hand, mixed mechanical-thermodynamical systems (e.g. gas turbines) can also be embedded into QP representation, and with a Lyapunov function (5) their global stability can be investigated. Note, that using a *quadratic Lyapunov function*, the region of their (local) stability can be conveniently determined by solving LMIs.

By formulating robustness and/or performance specifications as an objective function it will be possible to prescribe the quality of the controller to be designed. The selection of the feedback controller structure is also an important question since a wise choice can decrease the size of the BMI to be solved. That's why controller structure selection based on graph theoretic methods is another direction of future work.

The controller design BMI with the built-in robustness specifications and the controller structure design together would extend the controller design problem to a complete methodology for the stabilizing control of nonlinear process systems given in QP representation.

The measure-and-throw philosophy applied in the problem statement of quantum state estimation is in good agreement with the measurement of the polarization of photons in a photon beam, so the quantum state estimation methods presented in thesis points 3 and 4 can be applied for photon source identification. This way, the state of the system corresponds to the photon polarization, and since the polarization of photons emitted by source is not varying, there is no need to deal with the dynamics of the system.

After developing reliable state estimation methods for the quantum state estimation problem supposing no dynamics the next step would be to modify the developed methods for quantum process tomography. Its problem statement is as follows: known quantum states are sent through a quantum channel with unknown parameters and the states leaving the channel are measured. Give an estimate of the channel's parameters.

Another possible way is to include quantum dynamics to the system whose state is to be estimated. Of course, in this case a totally different kind of measurement should be applied that influences the system not as rough as the von Neumann measurement. The drawback of such measurement scheme might be the fact that it would not provide as much information as the von Neumann, or POVM type.

After having a correct method for quantum state estimation that involves also the dynamical model of the quantum system, the way is clear towards quantum control.

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