# Optimization-based analysis and control of complex networks with nonlinear dynamics

Komplex, nemlineáris dinamikájú hálózatok analízise
és irányítása optimalizálási módszerekkel

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# 1 Introduction

Dynamical models have central role in several fields of science and technology. Besides models applied in traditional engineering fields, numerous biological processes and phenomena can also be understood and explained by constructing their dynamical models [14]. Using these, the future behavior of the system can be predicted with respect to a given initial state, thus the analysis and simulation of the system is possible. An important requirement in modeling is simplification: models should most importantly describe only those phenomena which have significant effect on the dynamics of the underlying systems.

As it is known, the computational power and data processing capabilities of computers have been increasing giving us the opportunity to analyze and control large-scale systems [1]. Network-based description is often applied to describe a large-scale, complex system having many components. By identifying the individual components of a system and the connections between them the methods known from classical network theory can be applied to formulate the system model. Nodes can be corresponded to the actors and links can be refer to the corresponding connections. Usually, to describe the structure of networks in a mathematical framework, graph theory is used where nodes and links in the network are corresponding to vertices and edges in the graph, respectively. The role of the vertices and edges in the specific graph depends on the properties of the underlying system leading to a network of agents (performing some generalized computational task) or a pipeline-like network (where nodes are only connecting elements between the edges).

Due to the rapid development of computer science and technology and the available computational and analytical methods, several new application area of optimization methods appeared in system theory. Techniques applied in optimal control were further developed to the control of networked systems, such as coordinated control, synthesis

of complex process plants with a networked structure [10], etc. As the focus of the research of networked systems shifted towards the large-scale networks constructed from real-life data, the importance of the highly effective computational methods applicable for the solution of optimization problems increased.

The work summarized in this thesis focuses on the application of centralized, but parallelizable optimization-based methods in the analysis and control of networked systems having nonlinear dynamics. Two classes of networked systems are investigated because they come from basically different approaches of networked system description, while they can be handled with similar mathematical tools. The two topics include structural and dynamical analysis of kinetic reaction networks, and optimal rescheduling control of railway networks in case of delayed operation. In case of a reaction network, the model is translated into a network by defining the nodes as the chemical complexes and directed edges as the reactions (transitions) between them. In contrast to this, in case of railway networks the nodes are a topological mapping of the junctions and/or stations connected by the tracks. Along the tracks, trains are moving driven by an actual timetable.

# 2 Tools and methods

## 2.1 Optimization problems and tools

Optimization problems play an important role in several fields of system theory [3]. In particular, any controller design problem is in fact a constrained optimization problem with the control aim as loss function and the system model as a constraint. Considering the underlying computational methods, it can be said, that most of the formulated optimization problems can be traced back to mathematical programming problems which are able to handle cost functions and constraints on the variables.

**Linear Programming** (LP) is a widely applied method with

strongly detailed theoretical background and with several solution method implemented in available softwares. A linear program is a constrained convex optimization problem, where a linear function of the real-valued optimization variables is minimized (or maximized) with respect to linear equality and inequality constraints. A standard LP problem is formulated as follows:

$$\begin{cases} \min\limits_{x} c^T x \\ Ax \leq b \\ x_i \in \mathbb{R},\ i = 1, ..., k \end{cases}$$

where $x$ is the $k$-dimensional vector of *decision variables* consisting of real valued elements. The collection of $\omega$ linear inequality constraints are defined by matrix $A \in \mathbb{R}^{\omega \times k}$ called as *constraint matrix* and vector $b \in \mathbb{R}^k$. The linear function $c^T x$ with $c \in \mathbb{R}^k$ is the *objective function* to be minimized.

The solution of linear programs is a widely investigated topic: both the theoretical and implementational part of the methods have a wide literature. It should be noted, that with the help of Interior Point Methods, LPs can be solved with polynomial time complexity.

**Mixed Integer Linear Programming** (MILP) is a special case of linear programming, where some of the decision variables are integer valued. Some optimization problems having nonlinear constraints and/or nonlinear cost functions can be transformed to MILP problems. An MILP problem can be stated as follows:

$$\begin{cases} \min\limits_{x} c^T x \\ Ax \leq b \\ x_i \in \mathbb{R},\ i = 1, ..., k \\ x_j \in \mathbb{Z},\ j = k+1, ..., l \end{cases}$$

where the applied notations are similar to the LP problem, but the $l$-dimensional vector of decision variables denoted by $x$ consists of $k$ real and $l - k$ integer elements.

It has been shown that MILP problems are NP-hard to solve, hence they are usually solved by computationally very intensive heuristics-driven techniques which are sometimes unreliable in case of a large-scale problem.

## 2.2 Kinetic Reaction Networks

Kinetic Reaction Networks (KRNs) represent deterministic positive polynomial systems with mass-action kinetics [6]. The differential equations describing the system are translated into a directed graph (called reaction graph). The nodes of the graph are the $m$ complexes combined from $n$ species as it is described by matrix $Y$. The weighted edges (described by the Kirchhoff-matrix $A_k$) represent the reactions between the complexes. Considering these, the kinetic ODEs of the system are factorized as follows: $\bar{\mathbf{x}} = M \cdot \psi(\mathbf{x}) = Y \cdot A_k \cdot \psi(\mathbf{x})$, where $M$ contains the coefficients of the monomials in the ODEs describing the time-evolution of the system and the vector mapping $\psi = [\psi_1 \ \dots \ \psi_m]^T \in \mathbb{R}^n \to \mathbb{R}^m$ is defined as: $\psi_j(\mathbf{x}) = \prod_{i=1}^{n} x_i^{Y_{i,j}}$, $j = 1, \dots, m$.

**Dynamic equivalence** It is known, that multiple reaction graphs (called realizations) can generate the same dynamical behavior. Two different KRNs are called *dynamically equivalent* if they have different Kirchhoff-matrices but they describe the same dynamics: $M = Y \cdot A_k^{(1)} = Y \cdot A_k^{(2)}$, where the complex composition matrix $Y$ is fixed. Thus, we can define dynamically equivalent but structurally different reaction graphs, e.g.: *sparse graphs* containing minimal number of edges, *dense graphs* containing maximal number of edges. It is known, that for a given dynamics multiple different sparse realization can be found, but the dense realization is a unique superstructure containing all mathematically possible reactions in the network [12].

**Linear conjugacy** It is known from the literature that the kinetic property of a system of ODEs is generally preserved up to the re-ordering and positive scaling of the state variables. Hence, the phenomena of dynamical equivalence can be further generalized by introducing the

notion of linear conjugacy. Two KRNs are called *linearly conjugate* if (in the case of appropriate initial conditions) there is a positive linear diagonal mapping between the solutions of the corresponding kinetic ODEs [8]. Let us consider the kinetic systems defined by $(Y, A_k)$ and $(Y, A'_k)$:

$$\Sigma_1 : \ \dot{x} = Y \cdot A_k \cdot \psi(x)$$
$$\Sigma_2 : \ \dot{\bar{x}} = Y \cdot A'_k \cdot \psi(\bar{x}),$$

where $x, \bar{x} \in \bar{\mathbb{R}}^n_+$, $Y \in \mathbb{R}^{n \times m}$ and $A_k, A'_k \in \mathbb{R}^{m \times m}$ are Kirchhoff matrices. If there is a vector $\mathbf{d} \in \mathbb{R}^n_+$ for which $T = \mathrm{diag}(\mathbf{d})$ and $x(0) = T\bar{x}(0)$ holds, then $\Sigma_1$ and $\Sigma_2$ systems are called linearly conjugate if $x(t) = T\bar{x}(t)\ \forall t > 0$ holds. It can be also derived, that if $M = Y \cdot A_k$ holds and the two systems described by the matrices $A_k$ and $A'_k$ are linearly conjugate, then $M = T \cdot Y \cdot A'_k$ holds.

The two phenomena meet by taking the transformation $T$ to be the identity. It is also clear that the qualitative properties of the solutions (number and stability of equilibrium points, persistence/extinction of species, dimensions of invariant spaces etc.) of two linearly conjugate KRNs are always the same.

**Weak reversibility and zero deficiency** Weak reversibility has a crucial role in the theory of KRNs, since it connects structural properties of the reaction graph to qualitative features of the dynamical behavior of the reaction network. From a graph-theoretical point of view, weak reversibility holds if and only if all components (i.e. linkage classes) of the reaction graph are strongly connected components (i.e. if there exists a directed path between nodes $C_i$ and $C_j$ then there exists a directed path from $C_j$ to $C_i$, $i, j = 1...m$). Additionally, it is known that a KRN with a Kirchhoff matrix $A_k$ is weakly reversible if and only if there exists a strictly positive vector in the kernel of $A_k$ [9].

Deficiency is a structural property of a given KRN realization defined as $\delta = m - l - s$, where $m$ is the number of complexes, $l$ is the number

of reaction graph components and $s = rank(\{\rho^{(i,j)}\})$ , where $\rho^{(i,j)} = Y(\cdot,i) - Y(\cdot,j)$ for $i,j = 1,...,m$ defining the *reaction vector* for the reaction between complexes $C_i$ and $C_j$.

As it is formulated in the *Deficiency Zero Theorem* [5] for a KRN having zero deficiency and a weakly reversible structure, there exists precisely one asymptotically stable equilibrium point in each stoichiometric compatibility class.

**Mass conservation** is an important constraint when modeling physically plausible reaction sets. In [7] (stoichiometric) *mass conservation* is formulated as follows. Let us define $g_v$ as the scaled molecular weight of the species $X_v$ with strictly positive value. If reaction $C_i \to C_j$ is present in the network, the following can be written: $\sum_{v=1}^{n} \alpha_{vi} g_v = \sum_{v=1}^{n} \alpha_{vj} g_v = c_s$, where $c_s$ is a strictly positive scalar value. Let us define vector $g \in \mathbb{R}_+^n$ as a row vector formulated from the scaled molecular weights. Now the above equation can be written as $g \cdot Y(\cdot,i) = g \cdot Y(\cdot,j) = c_s$ where $Y(\cdot,i)$ refers to the $i$th column of matrix $Y$. It can be said that a reaction is mass conservative if the following holds: $g \cdot \rho^{(i,j)} = 0$, where $\rho^{(i,j)}$ is a reaction vector and $g$ is strictly positive. Let us define the *mass conservative reaction set* which is a set of the reactions having the above property.

A given KRN is said to be mass conservative if all of its reactions are in the mass conservative reaction set and a common strictly positive $g$ can be determined for them.

## 2.3 Transportation networks

Transportation networks are interesting and widely investigated examples of networks with complex dynamics with the topological network of routes (air corridors, railway tracks, highways, streets) and the vehicles moving along them. To avoid the disadvantageous effects of the accidents/disturbances ruining the flow of the traffic, control methods are applied to reschedule or reroute vehicles in the network if it is needed.

The ever increasing load on the railway networks in recent years poses serious challenges for network managers. To ensure the smooth operation of the network especially in case of delayed operation, a lot of research effort has been put in the topic of timetable design. Proper rescheduling of the trains give us the opportunity to limit the propagation of the delay and recover the nominal operation of the network as soon as possible. Different solutions of the delay-management are known from the literature based on mixed-integer programming [11] or greedy algorithms [13].

In [2] a permutation-based methodology was proposed which uses max-plus algebra to derive a Mixed Integer Linear Programming (MILP) to find optimal rescheduling patterns in a Model Predictive Control framework. The applied feedback controller is able to predict the future behavior of the railway network with a cyclic timetable and reorder the trains using the same track in an optimal way to minimize the sum of the delays along the prediction horizon in the network. The model of the system consists of trains moving along tracks between (virtual) stations. A linear constraint set is formulated describing the dependency between the events in the railway network. The nominal departure and arrival times are defined in an original timetable which is perturbed by the current delays.

It has been shown that this method can efficiently reduce the amount of delays over the prediction horizon, but in case of large and dense networks the increase of solution speed is needed.

# 3 New scientific results

The new scientific results presented in this work are summarized in the following thesis points. For each thesis point, the corresponding publications of the author are listed, too.

## Thesis I. Numerically efficient algorithms to find sparse and dense realizations of kinetic reaction networks.

*I have proposed two algorithms both based on linear programming (LP) having polynomial time complexity to compute dynamically equivalent alternative realizations of a kinetic reaction network (KRN). I have showed that with the help of the proposed methods alternative realizations of large scale, biologically motivated KRNs can be computed, too. The algorithms are compared with the mixed-integer linear programming (MILP) based algorithm available in the literature and the correctness of the solutions is shown. I have also concluded that the introduced new methods outperform the MILP-based solution in terms of the time consumption of the solution.*

Corresponding publications: [J1, C3]

### Thesis I.a

*I have proposed an LP-based algorithm to compute dynamically equivalent realizations of a KRN containing minimal number of reactions. The so-called sparse realization of the reaction network is computed via the column-wise L1-norm minimization of the off-diagonal elements of the Kirchhoff-matrix.*

The method uses the result that the L1-minimal description of large, under-determined system of linear equations is a sparse realization [4]. The resulting LP problem can be solved efficiently with the help of publicly available solvers. I have found, that the proposed method outperforms the MILP-based methods and other, LP-based methods known from the literature.

### Thesis I.b

*I have proposed an LP-based algorithm to compute a dynamically equivalent realization of a KRN containing maximal number of reactions*

*which is proven to contain all possible realizations of the reaction graph as a subgraph. The method to compute the so-called dense realization of the reaction network is based on the relaxation of the MILP-based method known from the literature: the column-wise sum of the introduced real-valued auxiliary variables corresponding to the off-diagonal elements of the Kirchhoff-matrix has been maximized.*

The algorithm proposed for the computation of the dense realization can be considered as an improvement of the MILP-based solution known from the literature [12]. According to the completed measurements, the obtained algorithm outperforms the other known methods in terms of computation time. Besides the computations completed on randomly generated KRNs, a large-scale, biologically relevant network is investigated, too, describing the *ErbB* intracellular regulator pathway. With the help of the presented method the dense realization is computed. The resulting new realization contains 29 extra reactions originating from 15 different complexes.

## Thesis II. New methods to compute weakly reversible and mass conserving realizations of kinetic reaction networks.

*I have proposed new methods to compute dynamically equivalent and linearly conjugate alternative realizations of a kinetic reaction network while constraints in terms of the structural properties of the reaction graph and/or dynamical properties of the described system are present, too.*

Corresponding publications: [J2, C1]

### Thesis II.a.

*A new, linear programming-based method with polynomial time complexity is proposed to compute linearly conjugate, weakly reversible re-*

*alizations of a kinetic reaction network (KRN). I have compared the method to other linear programming- and mixed-integer linear programming-based algorithms from the literature and it is shown that it outperforms all the others in terms of computational time, hence the algorithm is capable to handle large scale KRNs, too.*

The proposed method is based on the one presented in [9]. I have formulated the problem in an LP framework while the method is extended to handle linearly conjugate networks, too. I have exploited the fact, that the structural equivalence of two Kirchhoff matrices (meaning that the zero and non-zero elements of the matrices are at the same positions) can be formulated as linear constraints.

I have shown the correctness of the method through several examples. The advantageous computational properties of the proposed method has been shown via comparative tests on randomly generated KRNs having different sizes.

**Thesis II.b.**

*I have proposed a mixed-integer linear programming-based algorithm to compute dynamically equivalent realizations of a kinetic reaction network with mass-conservation property. The correctness of the results was shown through examples taken from the literature.*

The proposed method incorporates the constraints for mass conservation and dynamical equivalence into a single MILP problem. The size of the emerging MILP problem is mainly determined by the number of appearing auxiliary binary variables which has the magnitude $\mathcal{O}(m^2)$ where $m$ is the number of the complexes in the network. The correctness of the presented method is shown on an example taken from the literature.

## Thesis III. New solution methods of scheduling problems in traffic networks.

*I have proposed a model formulation method for model-predictive controllers which aim to deal with the scheduling problem of railway*

*networks in case of delayed operation. The controller reorders the trains in order to minimize the total delay in the network over the prediction horizon. The model is described with the help of linear constraints. Thus, the controlling problem is formulated as a mixed-integer linear programming (MILP) problem. I have showed the effectiveness of the proposed control technique and a method is proposed for the sensitivity analysis of the model in case of single delays.*

Corresponding publications: [C2, J3]

**Thesis III.a.**

*I have proposed a reordering method of the constraint matrix that can speed up the solution of the MILP problem in the presence of the solver's preprocessor, too. The method is based on the track-based reordering of the constraint matrix. The track-based reordering means that the constraints corresponding to a given track are collected into one block resulting that the constraint matrix of the emerging MILP problem has a clear block-angular structure.*

Simulations were completed on the model of the Dutch railway network where the original timetable were perturbed with complex delay scenarios. By applying the proposed reordering of the constraint matrix an average speedup ratio 1.813 has been achieved with respect to the unordered case.

**Thesis III.b.**

*I have proposed an algorithm to reformulate the constraints in order to achieve a more simple model formulation. The resulting model shows a clear and simple correspondence between the continuous variables describing the schedule of the events in the network and the binary control variables. Considering these, further analysis of the internal relations of the network model can be done, while problem-specific solution methods can be developed instead of the application of the general-purpose MILP solvers.*

The proposed reformulation of the constraints results a constraint structure where a variable describing an event depends directly only on known constants and/or binary control variables. The obtained structure contains more constraints than the original formulation but enables us to directly investigate the effect of the individual control variables on the delay reduction.

# 4 Application of the results

In this thesis the topic of the analysis and control of complex, nonlinear dynamical systems with networked structure has been investigated through two open problems.

Firstly, a set of new or improved methods were presented to compute dynamically equivalent or linearly conjugate KRNs with additional structural or dynamical constraints. The introduced algorithms give us the opportunity to analyze large scale, biologically relevant networks, too. Furthermore, it has been shown that the search for realizations having prescribed properties can be done with the applied optimization-based framework. Some of the emerging optimization tasks can be reformulated in order to achieve problems which can be solved in polynomial time.

Secondly, new model formulations were proposed for the dynamical railway scheduling problem in case of delayed operation. With the help of a model predictive controller-based framework, new timetables are obtained from the nominal one in order to reduce total delays along the prediction horizon. The effectiveness of the proposed control technique has been shown through extensive simulations using the model of the Dutch railway network. It has been shown, that by applying the presented model formulations, in one hand, the solution speed of the emerging optimization problems can be increased. On the other hand, with proper reformulation, a very clean model structure can be obtained which can serve as a basis of the development of problem-specific solvers. The results emphasize the importance of the structured problem formulation based on problem-specific knowledge.

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# The Author's Publications

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