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An improved method for inference of piecewise linear systems by detecting jumps using derivative estimation

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ABSTRACT

Inference of dynamical systems using piecewise linear models is a promising active research area. Most of the investigations in this field have been stimulated by the research in functional genomics. In this article we study the inference problem in piecewise linear systems. We propose first identifying the state transitions by detecting the jumps of the derivative estimates, then finding the guard conditions of the state transitions (thresholds) from the values of the state variables at the state transition time and finally using the conventional gene regulatory network inference methods to infer the regulatory relations. This approach does not require a priori information or assumption on the guard conditions and provides robustness to environmental or measurement noise underlined by the used jump detection filter. We discuss the particular problems where the suggested method can improve the efficiency and demonstrate the results on a comparative basis.

1. Introduction

Inferential modeling of nonlinear dynamical systems has received growing interest. Development of instrumentation technologies providing high throughput data, increased computational power, more efficient inference algorithms, better understanding of various important but complicated dynamical systems have enabled inference of dynamical features of those systems from empirical observations. Some exemplary challenges where the inference methodology can suggest promising results can be given as:

Inference of gene expression dynamics which grabbed the attention of researchers after the development of expression microarray technology [1–3] and suggests potential use in intervention planning and drug discovery [4]. Calibration of ecosystem models for marine ecology by using satellite ocean color data [5] which can be utilized for longer term forecasts. Parameter estimation in flux balance models for batch fermentation [6] aimed at finding the optimal parameters for fermentation processes.

Some of the challenging nonlinear dynamical system inference problems, including but not limited to the gene regulatory networks exhibit a switching nature due to the threshold phenomenon. Dynamical properties of those types of networks and their simplified versions were already studied as abstract gene network models [7]. Besides, some dynamical systems which do not fit to global models expressed by elementary mathematical expressions can be approximated by fitting each portion of the model locally to a simple expression.

Without using any approximations or simplifications, a very limited range of nonlinear dynamics can be modeled due to immense complexity. Thus, a reasonable effort to reduce the complexity is to characterize nonlinearity based on the way of violation of linear intuition. Considering a characterization based on the 'type' of nonlinearity, to select simple nonlinear

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model structures has been used for model-based control [8]. With a similar motivation, in this study we concentrated on piecewise linearity for modeling switching dynamical systems. For this framework we suggest piecewise linear hybrid systems with the state space partitioned by single threshold per each variable. The first advantage of piecewise linear systems is the capability of modeling a wide range of dynamics. When an abstraction for modeling a dynamical system is necessary, qualitative behavior matching becomes a very important criterion [8]. That is the model should be capable of exhibiting the essential features of the real world system. In that context, piecewise linear systems with single threshold per variable were investigated and many features supported by them was demonstrated [9,7]. Thus, we know that they can model systems exhibiting fixed point stable, periodic, quasiperiodic, chaotic, multistationary behavior, computation etc. Secondly, piecewise linear systems were studied and in the literature there exist known methodologies for analysis and synthesis of them [10]. Therefore, piecewise linear approximations of switching networks can be used for applications like long term forecasting, intervention planning and control wherever possible.

The piecewise linear systems have already been extensively studied for modeling and analyzing gene regulatory networks [7,11]. On the other hand Random Boolean Networks and regarding NK models also suggest several advantages in modeling and analyzing similar networks [12,13]. An important advantage of Boolean approach is its use in inference and intervention planning [4]. This work concerns inference into piecewise linear models by using sampled continuous variables.

A switching dynamical system subject to threshold phenomenon can be considered as a hybrid system where continuous and discrete variables regulate each other. In the simplest scheme, we can assign only two type of phases for each variable in the system, ON and OFF, to be observed during the evolution of continuous variables in time. Denoting ON and OFF by 0 and 1 respectively, the state of hybrid system can be defined as the the vector formed by all Boolean states at a certain time.

In this study, we assumed that within a given system state, the evolution of continuous variables can be modeled with linear ordinary differential equations (ODEs). Change of system state can be observed as switching of a variable and threshold phenomenon explains this switching by another variable (the corresponding activator or repressor) attaining a certain value (the threshold). Threshold phenomenon is observed in various dynamical systems and its relation with switching systems has been studied in the literature [14–16]. The different evolution schemes in distinct states are introduced to the model by changing the parameters of the system of linear ODEs. This formulation brings the following advantages:

- The physical,chemical and biological interpretation of the states and linear ODEs are simple; the states stand for the combinations of ON-OFF conditions of continuous variables in the network and the coefficients of ODEs exhibit the relation between values of continuous variables and their time derivatives.
- The piecewise linearity enables approximation to arbitrary nonlinear system dynamics up to a certain extent.
- The analytical and computational complexity of linear ODEs are less than other equations used in modeling similar systems, like functional differential equations, integral equations, differential algebraic equations etc.

While modeling the switching systems with piecewise linear formulation, state transitions stimulate a switching in the governing differential equations which typically cause a jump in the derivatives of one or more variables. This fact provides us a way of distinguishing the state transitions by detecting those jumps. The best-fit parameters of the linear discrete system, which can be calculated by L2 error minimization on the given sample, are estimates of the parameters of the system of ODEs governing the continuous evolution in the corresponding state.

In the Section 2, the studied piecewise linear systems will be introduced and their basic properties will be discussed. Section 3 explains the problem of inference and defines the model parameters we want to infer explicitly. In Section 4, we discuss and study the gene networks as they display the appropriate dynamics to be modeled by the considered model. We also discuss similar approaches used in gene network inference and modeling. A concrete example on partial inference of cell division process for fission yeast is also covered in that part. In Section 5, we conclude with the discussion on the performance and feasibility of the inference method and possible improvement strategies for future development of the inference method.

2. Used piecewise linear system

In mathematical modeling of dynamical systems, there is always a tradeoff between complexity and model fit quality. Piecewise linear formulation can approximate complex systems with an adjustable approximation accuracy [34]. Moreover, some advantages of linear systems can be preserved with this formulation [9]. Hence, the piecewise linear systems have favorable properties in the aspect of this tradeoff. In this study, we focused on inferring regulatory relations in linear switched hybrid systems which are governed by threshold phenomenon. The specifications of these systems can be abstracted as follows:

$$\dot{y}_t = M_{S(y_t)}(y_t) + b_{S(y_t)} \tag{1}$$

where, the parameters M and b are determined by the system state at time t and y denotes the continuous variable(s). As mentioned previously, we focused on systems in which the regulatory relations are explained by a single threshold per variable. The state of the system $S(y_t)$ is a vector formed by 0 or 1 values where each 0 means that the corresponding variable is below its threshold and 1 means the corresponding variable is above its threshold at that instant. It is obvious that, there are 2^n states for a system composed of n variables. With this definition, a state transition can be interpreted as the change in a single element of the Boolean sequence that represents the state. Let $S(t)$ be the state of the system at time t and $B_i(t)$