Network Structure Preserving Model Reduction: Results of a Simulation Study

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Abstract— **Reconstructed models of biochemical networks often reflect the high level of complexity inherent in the biological system being modeled. The difficulties of predicting gene expression and analyzing the effects of individual perturbations at a system-wide resolution are exacerbated by model complexity. This paper extends a state projection method for structure preserving model reduction to a particular model class of reconstructed networks known as dynamical structure functions. In contrast to traditional approaches where a priori knowledge of partitions on unmeasured species is required, dynamical structure functions require a weaker notion of system structure, specifying only the causal relationship between measured chemical species of the system. The resulting technique, like similar approaches, does not provide theoretical performance guarantees, so an extensive computational study is conducted, and it is observed to work fairly well in practice. Moreover, sufficient conditions, characterizing edge loss resulting from the reduction process, are presented.**

I. Introduction

Simplified representations of biological systems play an important role in simulating and controlling their underlying dynamic phenomena. This can be especially true in situations where the underlying system is large and structured in a complex network of interconnections.

For such networks, the input-output dynamics alone may not be an adequate measure of the strength of a reduced order model. *System structure* may be an equally important characteristic for understanding, or controlling the system since, for example, only distributed interaction may be feasible. In this case, model reduction must not only approximate the dynamics of the system, but it also must reflect a priori knowledge of the system structure to the extent possible.

Unfortunately, traditional approaches to model reduction focus only on dynamic approximation and do not generally preserve interconnection structure. Nevertheless, recent work has considered this issue, and a number of structure-preserving methods have been presented in [5], [10], [1], [7], [8], [9]. These methods, however, all assume that the structure of the complex system is known a priori in a very strong sense. In particular, a partition of the entire state space is assumed to be known, enabling a decomposition of the system into the interconnection of a finite set of subsystems.

However, when modeling a chemical reaction network of a biological system, assuming a priori knowledge of a partition over the entire state space of the complex system could be unreasonable. For example, one may not even be aware of many of the chemical species involved in intermediate reactions, much less their reaction pathways. As a result, it could be unreasonable to expect that one would know how to meaningfully partition all of the states of the system into distinct subsystems. In these situations, a weaker notion of a priori structural information is necessary to formulate a meaningful structure-preserving model reduction problem.

A weaker notion of system structure has been developed in the context of the network reconstruction of biochemical systems [3]. This notion of structure is characterized by a factorization of a system's transfer function, called the *dynamical structure function*, and it characterizes the causal relationship between measured chemical species and inputs without imposing any particular structural form on the rest of the system. This paper formulates the structure-preserving model reduction problem assuming only weaker a priori structural information, as characterized by the dynamical structure function of the system. A state projection technique similar to that in [9] is then applied, and it is found to deliver reduced models with good dynamic fidelity. Nevertheless, unlike situations where strong a priori structural information is available, the technique is shown to not necessarily preserve structure in the weaker sense, and conditions for structure preservation are then provided.

II. Background: Characterizing Structure

This section compares and contrasts different ways of characterizing partial structure information of the system. First, note that *complete structural information* is characterized by the state-space equations describing how the system actually computes its outputs given the input and initial conditions; we call this the *complete* or *computational structure* of the system. We next discuss *strong partial structure information* vs. *weak partial structure information* of the system and show that, the type of a priori information requirements they impose are very different.

A. Strong Partial Structure Information

One way to encode partial structure information about a system is to decompose the composite system into $q + 1$ distinct subsystems. One of these subsystems, $N(s)$, is a special module that characterizes the system structure and interconnects the other q subsystems; the others, $G_i(s), i = 1, 2, ..., q$, are completely distinct and decoupled and do not interact except through $N(s)$. In this setting, replacing

any subsystem $G_i(s)$ with another system, $\hat{G}_i(s)$, preserves the composite system structure, as encoded in $N(s)$, as long as the dimensions of the inputs and outputs of $\hat{G}_i(s)$ conform to the ports made available by removing $G_i(s)$. The mathematical representation of the composite system then becomes the lower fractional transformation of the system $N(s)$ and a block diagonal system $G(s)$, $\mathcal{F}_l(N, G)$, with $G_i(s)$ on the ith block of G.

The strong sense of structural understanding required by this definition of structure is a global partition on all the states of the complex, composite system resulting in the diagonalization of G. Other names for this strong type of partial structural information include *subsystem structure* or the *solid-state structure* of the system.

B. Weak Partial Structure Information

The notion of weak partial structure does not require knowledge or existence of a global partition of all system states in order to be meaningful; rather, it characterizes the network of interactions among measured chemical species and inputs as causal relationships.

The mathematical representation of the weak partial structure of a system employs a pair of matrix functions, similar to transfer functions, called the *dynamical structure function* of the system.

To see how the dynamical structure function is derived, consider the system given by:

$$\begin{bmatrix} \dot{z}_1 \\ \dot{z}_2 \end{bmatrix} = \begin{bmatrix} \bar{A}_{11} & \bar{A}_{12} \\ \bar{A}_{21} & \bar{A}_{22} \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} + \begin{bmatrix} \bar{B}_1 \\ \bar{B}_2 \end{bmatrix} u$$
$$y = \begin{bmatrix} \bar{C}_1 & \bar{C}_2 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} + \begin{bmatrix} \bar{D} \end{bmatrix} u \tag{1}$$

where $\begin{bmatrix} z_1' & z_2' \end{bmatrix}' \in \mathbb{R}^n$, is the full state vector with $z_1 \in \mathbb{R}^p$, $y \in \mathbb{R}^p$ $(p < n)$ are the measured outputs, and $u \in \mathbb{R}^m$ is the control input. Without significant loss of generality, we assume $\begin{bmatrix} \bar{C}_1 & \bar{C}_2 \end{bmatrix}$ has full row rank and $\bar{D} = 0$ (these assumptions simplify the exposition but do not restrict the results). We first consider the change of basis on the state variables yielding:

$$\begin{bmatrix} \dot{y} \\ \dot{x} \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} + \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} u$$
$$y = \begin{bmatrix} I & 0 \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix}. \tag{2}$$

Taking Laplace Transforms of the signals in (2), we find

$$\begin{bmatrix} sY \\ sX \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} Y \\ X \end{bmatrix} + \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} U \tag{3}$$

Solving for X, gives

$$X = (sI - A_{22})^{-1} A_{21} Y + (sI - A_{22})^{-1} B_2 U$$

Substituting into the first equation of (3) then yields

$$sY = WY + VU$$

where $W = A_{11} + A_{12}(sI - A_{22})^{-1}A_{21}$ and $V = A_{12}(sI - A_{22})^{-1}B_2 + B_1$. Let D be a matrix with the

diagonal term of W, i.e. $D = \text{diag}(W_{11}, W_{22}, ..., W_{pp})$. Then,

$$(sI - D)Y = (W - D)Y + VU$$

Note that $W - D$ is a matrix with zeros on its diagonal. We then have $Y = QY + PU$ where

$$Q = (sI - D)^{-1}(W - D) \tag{4}$$

and

$$P = (sI - D)^{-1}V. \tag{5}$$

The matrix Q is a matrix of transfer functions from Y_i to Y_j, $i \neq j$, or relating each measured signal to all other measured signals (note that Q is zero on the diagonal). Likewise, P is a matrix of transfer functions from each input to each output without depending on any additional measured state Y_i. Together, the pair $(Q(s), P(s))$ is the dynamical structure function for the system (1).

Note that when discussing the structure of a system, it is often convenient to distinguish between the *dynamical structure*, given by (Q, P), and its *network structure*, characterized by the Boolean structure of (Q, P). The Boolean structure of a matrix function Q is simply a matrix $\mathcal{B}(Q)$ with elements $\mathcal{B}(Q)_{ij} = 0$ if and only if $Q_{ij} = 0$, otherwise $\mathcal{B}(Q)_{ij} = 1$. The network structure of a system is thus given by $\mathcal{B}(Q, P)$.

III. PROBLEM FORMULATION

Realization problems transition to model reduction problems when the order of the representation is reduced beyond some threshold: systems with order greater than this threshold can exactly produce the desired behavior, while those with order less than the threshold must approximate the desired behavior. The context for model reduction is thus characterized by the minimal threshold defining this transition. This motivates the following definition.

Definition 3.1: Given a structure (Q, P) of the transfer function G, with $G = (I - Q)^{-1}P$, then a realization of G with order n is *dynamically minimal* if every realization of G has order $\bar{n} \geq n$, and it is *structurally minimal* if it generates (Q, P), in the sense of satisfying (2)-(5), and if every other realization that generates (Q, P) has order $\bar{n} \geq n$. We call the order of a dynamically minimal realization the *degree* of the system, and the order of a structurally minimal realization the *structural degree* of the system.

With this notion of minimal model complexity, the problem we want to solve then becomes:

Problem: Given a system G with dynamical structure function (Q, P) and structural degree n, for a non-negative integer $\tilde{n} < n$, find an approximate system $\tilde{G}$ with dynamical structure function $(\tilde{Q}, \tilde{P})$ and structural degree $\tilde{n}$ such that
1) $\mathcal{B}(\tilde{Q}, \tilde{P}) = \mathcal{B}(Q, P)$, and
2) $\tilde{G}(s) = \arg \min \|G - \tilde{G}\|_\infty$.

This research does not solve this problem.

Nevertheless, we demonstrate that a state projection reduction method known to preserve structure in the strong sense (when it exists) can be adapted to perform reasonably well

Q Size	Connectivity	Chop	Unstable	n	p	States Chopped	Edges in Q	Edges Lost	Scaled Error
Small	Sparse	Low	4%	19.8	2.3	3.7	2.6	0	ϵ
Small	Sparse	Med	6%	22.4	2.66	10.2	3.3	0	.0609
Small	Sparse	High	0%	20.0	2.5	12.2	2.8	0	0.0119
Small	Mid	Low	0%	20.5	2.8	3.7	5.2	0	ϵ
Small	Mid	Med	0%	22.7	2.7	10.8	4.1	0	ϵ
Small	Mid	High	0%	21.6	3.1	12.9	5.9	.5	.0184
Small	Dense	Low	0%	29.1	4.2	4.9	14.6	0	ϵ
Small	Dense	Med	2%	27.1	4.1	12.6	13.6	0	ϵ
Small	Dense	High	4%	29.4	4.2	18.1	14.8	0	.0060
Med	Sparse	Low	0%	22.2	6.3	3.7	21.2	0.1	.0014
Med	Sparse	Med	0%	22.5	6.7	3.8	13.2	0	ϵ
Med	Sparse	High	0%	25.01	6.7	13.1	11.8	1.9	.0140
Med	Mid	Low	2%	25.7	3.7	4.1	11.1	.2	.0075
Med	Mid	Med	0%	22.5	6.4	9.0	23.3	0	.0106
Med	Mid	High	0%	23.3	6.6	11.6	23.4	.5	.0028
Med	Dense	Low	0%	25.9	7.8	3.6	60.2	0	.0303
Med	Dense	Med	0%	28.1	8.0	10.2	62.2	0	.0959
Med	Dense	High	0%	24.7	7.2	12.4	49.7	0	.3147
High	Sparse	Low	0%	22.1	10.0	2.9	23.8	0	ϵ
High	Sparse	Med	0%	23.5	10.0	7.3	19.5	0	.0081
High	Sparse	High	0%	18.6	2.2	11.0	2.46	0	.0863
High	Mid	Low	0%	20.2	9.0	2.6	49.6	0	ϵ
High	Mid	Med	0%	20.6	8.9	6.5	44.5	2.0	.0013
High	Mid	High	0%	23.3	6.6	11.6	23.4	.5	.0028
High	Dense	Low	0%	24.4	11.1	2.8	130.5	0	.0588
High	Dense	Med	0%	27.1	12.0	8.3	145.1	0	.0085
High	Dense	High	0%	26.8	11.3	10.2	133.2	0	.0375

TABLE I

RESULTS FROM THE COMPUTATIONAL STUDY

with only weak structural information. Moreover, although it does not necessarily preserve structure in the weak sense, conditions for when it fails to do so are provided. The next sections describe the method, empirically explore its performance, and analyze its ability to preserve structure as described by the Boolean structure of (Q, P).

IV. STRUCTURED BALANCED TRUNCATION

Standard approaches to the unstructured version of the above problem, such as Hankel norm approximation or balanced truncation, are suboptimal in the H_∞ sense. Likewise, the approach taken here is also suboptimal, and it is an extension of balanced truncation adapted to accommodate system structure.

We apply a strong structure technique from [9], writing the system (2) as the linear fractional transform of two subsystems, one subsystem representing the measured variables y and one subsystem representing the hidden variables x. The technique prescribes a block diagonal transformation to balance diagonal blocks of the controllability and observability gramians. It can be shown that such a *structured transformation* always exists and is unique, generating a local change of basis within each subsystem such that the resulting controllability gramian and observability gramian have a particular structure, with diagonal blocks that are 1) equal, 2) diagonal, 3) positive semidefinite, and 4) with entries ordered from largest to smallest within the block– while the off diagonal blocks have no particular relationship or structure.

The structure preserving model reduction method described above preserves structure in the strong sense, see

[9], [5], [11], [6], [9]. As there are few theoretical guarantees characterizing how the weak structure of a system is preserved, the next section presents the results of an extensive computational study exploring the performance of the procedure for a variety of systems.

V. RESULTS FROM A COMPUTATIONAL STUDY

Since the state projection technique for reduction suggested in the previous section does not necessarily preserve stability of a system, nor provide bounds on the dynamic fidelity of the reduced model, nor guarantee structure preservation in the weak sense, we engaged a computational study to explore the performance of the technique. The results of the study are displayed in Table 1. First, note that although instability is possible, it was rare to lose stability through truncation. Although this may have been affected by our use of diagonally dominate A matrices in the system realization when generating stable random systems, it is still encouraging to note that even without stability guarantees the procedure generally delivers stable reduced order models.

Second, we observe that although weak structure was preserved most of the time, an average as high as 15% of the edges in Q can be lost by the procedure. This motivates the characterization of edge loss discussed in the next section.

Finally, the dynamic fidelity of the procedure appears to be excellent. Although one category reports an average error as high as 30% of the norm of G, generally the error is well below $1-3\%$. Note that ϵ refers to values smaller than 10^{-3}.

VI. SUFFICIENT CONDITIONS FOR EDGE LOSS

It is easy to understand how an edge may be lost through the reduction process. If, for example, the edge connecting

two measured outputs y_1 and y_2 is realized through a hidden state x_n, so that $y_1 \longrightarrow x_n \longrightarrow y_2$, and that hidden state is eliminated in the truncation process, then we would expect the edge not to be present in the network structure of the reduced model. These observations lead us to the following characterization of edge loss.

Definition 6.1: A realization of the form (2) is *hidden balanced* if its controllability and observability gramians (with block structure conformal to the partition in (2)),

$$X_c = \left[\begin{array}{cc} X_{c11} & X_{c12} \\ X_{c21} & X_{c22} \end{array} \right], \quad Y_o = \left[\begin{array}{cc} Y_{o11} & Y_{o12} \\ Y_{o21} & Y_{o22} \end{array} \right],$$

satisfy $X_{c22} = Y_{o22} = \Sigma$, were $\Sigma > 0$ is diagonal.

Theorem 6.1: Given a system G with network structure $\mathcal{B}(Q, P)$ and a hidden balanced realization given by

$$\left[\begin{array}{c} \dot{y} \\ \dot{x}_1 \\ \dot{x}_2 \end{array} \right] = \left[\begin{array}{ccc} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{array} \right] \left[\begin{array}{c} y \\ x_1 \\ x_2 \end{array} \right] + \left[\begin{array}{c} B_1 \\ B_2 \\ B_3 \end{array} \right] u$$
$$y = \left[\begin{array}{ccc} I & 0 & 0 \end{array} \right] \left[\begin{array}{c} y \\ x_1 \\ x_2 \end{array} \right],$$

(6)

where x_1 and x_2 partition the hidden states of the system. Let $a^T = [a_2^T \ a_3^T]$ be the ith row of $[A_{12} \ A_{13}]$, $b = [b_2^T \ b_3^T]^T$ be the jth column of $[A_{21}^T \ A_{31}^T]^T$, and T_2 be the unitary transformation constructing the Schur form of A_{22}. Consider the system $\tilde{G}$ with network structure $\mathcal{B}(\tilde{Q}, \tilde{P})$ and hidden balanced realization given by

$$\left[\begin{array}{c} \dot{y} \\ \dot{x}_1 \end{array} \right] = \left[\begin{array}{cc} A_{11} & A_{12} \\ A_{21} & A_{22} \end{array} \right] \left[\begin{array}{c} y \\ x_1 \end{array} \right] + \left[\begin{array}{c} B_1 \\ B_2 \end{array} \right] u$$
$$y = \left[\begin{array}{cc} I & 0 \end{array} \right] \left[\begin{array}{c} y \\ x_1 \end{array} \right],$$

(7)

obtained by truncating x_2 from the system (6). Then an edge in the ij^{th} position is lost as a result of truncation, meaning $[\mathcal{B}(Q)]_{ij} = 1$ and $[\mathcal{B}(\tilde{Q})]_{ij} = 0$, if $[A_{11}]_{ij} = 0$, $[\mathcal{B}(Q)]_{ij} = 1$, and the matrix $T_2 a_2 b_2^T T_2^*$ is lower triangular with zero on the diagonals.

This theorem characterizes sufficient alignment conditions for an edge to be lost through the truncation process discussed in this paper. A proof of this theorem can be found in [2]. Although as a practical matter it may be easy to compute $\mathcal{B}(\tilde{Q}, \tilde{P})$ and directly compare it with $\mathcal{B}(Q, P)$ to detect edge loss, these conditions help distinguish situations where truncation is guaranteed to simplify the dynamical structure of the reduced order model.

This loss of edges can actually be valuable in situations where a structured system is identified from noisy data. In these situations, network reconstruction algorithms will find fully connected structures fit the data as well or better than sparse structures. As a result, there is a tendency to overestimate structure, and many approaches actively work to compensate for this tendency by explicitly rewarding sparsity of the estimate [4].

The alignment conditions provided in Theroem 6.1 offer the hope for a new approach to this problem by using model reduction to both simplify the dynamic expression of a model and to purposefully simplify the structure estimate, eliminating only those edges that result from noise. Future work will explore these issues.

VII. Conclusion

This paper extended a state projection technique for structure preserving model reduction to situations where only a weak notion of system structure is available. Strong partial structure information and weak partial structure information were defined and compared, An extensive computational study of the reduction process was conducted, demonstrating that it typically performs well in spite of the lack of theoretical guarantees on stability or performance bounds. Nevertheless, the technique does not always strictly preserve structure in the weak sense, and sometimes a reduced model may lose edges compared with the network structure of the original system. Sufficient conditions for edge loss were then provided, demonstrating certain alignment properties that reveal how this approach to model reduction may contribute in the future to network reconstruction from noisy data.

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