

Dynamical Structure Function Identifiability Conditions Enabling Signal Structure Reconstruction

J. Adebayo, T. Southwick, V. Chetty, E. Yeung,
Y. Yuan, J. Gonçalves, J. Grose, J. Prince, G.B. Stan, S. Warnick*

Abstract—Networks of controlled dynamical systems exhibit a variety of interconnection patterns that could be interpreted as the structure of the system. One such interpretation of system structure is a system’s signal structure, characterized as the open-loop causal dependencies among manifest variables and represented by its dynamical structure function. Although this notion of structure is among the weakest available, previous work has shown that if no a priori structural information is known about the system, not even the Boolean structure of the dynamical structure function is identifiable. Consequently, one method previously suggested for obtaining the necessary a priori structural information is to leverage knowledge about target specificity of the controlled inputs. This work extends these results to demonstrate precisely the a priori structural information that is both necessary and sufficient to reconstruct the network from input-output data. This extension is important because it significantly broadens the applicability of the identifiability conditions, enabling the design of network reconstruction experiments that were previously impossible due to practical constraints on the types of actuation mechanisms available to the engineer or scientist. The work is motivated by the proteomics problem of reconstructing the Per-Arnt-Sim Kinase pathway used in the metabolism of sugars.

I. INTRODUCTION: NETWORK RECONSTRUCTION

Two fundamental properties characterizing networks of controlled dynamical systems include their overall, dynamic behavior and their network structure. Since interconnections of systems are themselves systems, standard mathematical representations of systems can be used to describe networks of controlled dynamical systems. Nevertheless, while different representations may describe the same overall dynamic behavior of the network, they can convey very different information about the network’s underlying structure.

Consider, for example, an n^{th} order, causal linear time-invariant system with m inputs and p outputs. This system may be described both by a $p \times m$ transfer function (TF) matrix $G(s)$ and a state space realization characterized by the matrices (A, B, C, D) . If $G(s) = C(sI - A)^{-1}B + D$, then both of these representations describe the overall dynamic

behavior of the system. Nevertheless, these representations carry very different information about the system’s internal network structure.

In particular, the sparsity pattern of G reveals closed-loop dependencies of the outputs on inputs. Thus, for example, if G were diagonal, then any dependencies that output i may have on any other input, other than input i , must be exactly cancelled internally within the system. This sparsity structure of the TF is the weakest notion of system structure that we typically consider.

On the other hand, the state space realization describes detailed information about the dependencies among inputs, state variables, and outputs. This offers a much stronger understanding of system structure; it conveys everything revealed by the sparsity structure of the TF and much more about system structure. For example, knowing the state realization can determine whether a system with a diagonal TF G is truly decoupled, or whether off-diagonal dependencies between inputs and outputs are externally hidden by exact cancellations within the system.

Because different representations of the same system describe different amounts of structural information, they need different experimental conditions to be correctly identified. For example, a rich theory of system identification has detailed sufficiency of excitation and sample complexity requirements necessary to determine a system’s TF from input-output data [10]. Discovering richer structural information than the sparsity structure of the TF, however, demands additional a priori knowledge about the system. For example, if one not only met the requirements to identify a system’s TF from input-output data, but also knew that the measured outputs were, in fact, the system’s state variables, then the state space representation of the system could also be identified.

For many applications, the experimental burden necessary to identify a network’s state space realization is prohibitive, while the burden necessary to identify the associated TF may be reasonable. In these situations, and when additional structural information about the system is desired, another representation of the system may be employed that describes more structural information than the TF yet less than the state space realization (and thus incurring less of an experimental burden). The dynamical structure function (DSF) of a linear time-invariant system is just such a *partial-structure* representation.

This paper describes the experimental burden necessary and sufficient to identify a system’s DSF. This burden is

J. Adebayo is with the Systems Biology Department at Harvard Medical School, T. Southwick, V. Chetty, and S. Warnick are with the Information and Decision Algorithms Laboratories, Brigham Young University; E. Yeung is with the Control and Dynamical Systems group at the California Institute of Technology; Ye Yuan and Jorge Gonçalves are with the Control Group, Department of Engineering, University of Cambridge; J. Grose is with the Department of Microbiology and Molecular Biology at Brigham Young University; J. Prince is with the Department of Chemistry and Biochemistry at Brigham Young University, and Guy-Bart Stan is with the Department of Bioengineering and the Centre for Synthetic Biology and Innovation, Imperial College London. The BYU team gratefully acknowledges the generous support of AFRL FA8750-09-2-0219.

* Corresponding author, sean.warnick@gmail.com.

characterized in terms of parts of the DSF that must be known a priori so that knowledge of the TF, identified from input-output data, would then uniquely specify the remaining parts of the DSF. Previous work has shown that if only the input-output data necessary to identify the system's TF are known a priori, then not even the Boolean structure, which denotes the presence of a causal relationships without its effects, of the DSF can be reconstructed. On the other hand, if one additionally knows that each input, u_i , exhibits *target specificity*, in that it only affects outputs y_j through its associated output, y_i , then the DSF can be uniquely reconstructed from sufficiently informative input-output data or knowledge of the system's TF [2].

In this paper we show that, while target specificity is a sufficient condition for reconstruction of the DSF, it is not necessary. By providing a complete set of necessary and sufficient conditions for reconstruction of a system's DSF, we significantly broaden the applicability of the associated reconstruction results [1], [9], [11], [3]. The next section details mathematical preliminaries concerning DSF as a partial-structure representation of a system. The main result then follows, with necessary and sufficient identifiability conditions for reconstructing a system's DSF. The last section motivates the utility of these new results with a network reconstruction problem from proteomics where target specificity can not be guaranteed. Conclusions follow.

II. DYNAMICAL STRUCTURE FUNCTIONS

This section gives an overview of the derivation of DSF as discussed in [2]. To see how the DSF is derived, consider the system given by:

$$\begin{aligned} \begin{bmatrix} \dot{y} \\ \dot{x} \end{bmatrix} &= \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} + \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} u \\ y &= \begin{bmatrix} I & 0 \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix}. \end{aligned} \quad (1)$$

Note that $C = [I \ 0]$ allows the variables to be separated into the measured states, y , and the unmeasured states, x .

Equation (1) describes the state space realization of the system, which contains information about the dependency among input, state, and output variables and defines both the structure and dynamics of the entire network.

The next step in the derivation of the DSF is to take Laplace Transforms of the signals in (1). Assuming zero initial conditions we get:

$$\begin{bmatrix} sY \\ sX \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} Y \\ X \end{bmatrix} + \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} U \quad (2)$$

Solving for X , gives:

$$X = (sI - A_{22})^{-1} A_{21}Y + (sI - A_{22})^{-1} B_2U$$

Substituting into the first equation of (2) 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. $D = \text{diag}(W_{11}, W_{22}, \dots, W_{pp})$. Then,

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

Note that $sI - D$ is always invertible since D is always proper. We then have:

$$Y = QY + PU \quad (3)$$

where

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

and

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

Note that since $W - D$ is a hollow matrix (a matrix with zeros along the diagonal), then Q is also a hollow matrix.

The matrix Q is a matrix of strictly proper TF from Y_i to Y_j , $i \neq j$ relating each measured signal to all other measured signals. Likewise, P is a matrix of strictly proper TF from each input to each output without depending on any additional measured state Y_i .

Definition 1: Given the system (1), we define the *dynamical structure function* of the system to be (Q, P) , where Q and P are the *internal structure* and *control structure*, respectively, and are given as in (4) and (5).

A. Meaning of the Dynamical Structure Function

The DSF describes the network structure of the system (1) in the sense that the matrix Q can be interpreted as the weighted adjacency matrix of a directed graph, an example of which is shown in Figure 1, indicating the causal relationships between measured states. Also, P is the weighted adjacency matrix of a directed graph indicating the causal relationships between inputs and measured states. The weights on the edges of this graph are TFs between relevant variables. This graphical representation of the system is referred to as the *signal structure* of the system.

Note that the TF matrix of the graph in Figure 1 would be full because every input affects each output, whether it be directly or indirectly. This can be readily seen from the figure since there is a path from each input, u_i , to every measured output of the system, y_j .

The DSF, on the other hand, contains more information about the structure of the system than the TF. It describes the original TF as an interconnection of systems characterized by the elements of Q and P . In this sense, we describe the DSF as the *open-loop causal dependencies among the manifest variables*, distinguishing it from the *closed loop dependencies* characterized by the TF.

This notion of the DSF as characterizing open loop causal dependencies among manifest variables is further described by the following theorem:

Theorem 1: Let (A, B) be the matrices from the state-space representation of an LTI system, and (Q, P) its dynamical structure function.

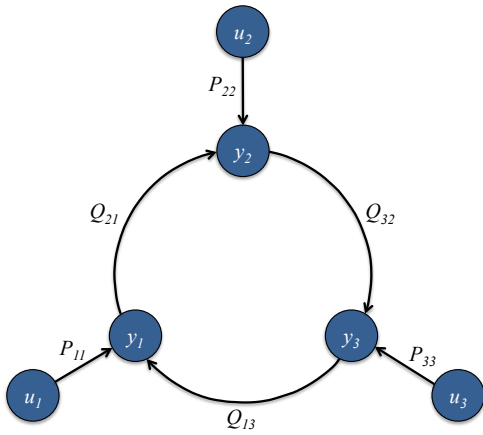


Fig. 1. Signal Structure representation of a system with three inputs and three outputs. Note that the transfer function for this system is fully connected, while the dynamical structure function, and its associated signal structure, exhibits a particular ring structure.

- 1) If Q_{ij} is nonzero, then either A_{ij} is nonzero or there exists a sequence k_1, k_2, \dots of indices corresponding to hidden states such that $A(i, k_1), A(k_1, k_2), \dots, A(k_{m-1}, k_m), A(k_m, j)$ are nonzero
- 2) If P_{ij} is nonzero, then either B_{ij} is nonzero or there exists a sequence k_1, k_2, \dots of indices corresponding to hidden states such that $A(i, k_1), A(k_1, k_2), \dots, A(k_{m-1}, k_m), A(k_m, j)$ and $B(k_m, j)$ are nonzero

Proof: We proceed with a proof by contradiction. Assume that Q_{ij} is nonzero, but that A_{ij} is zero and there does not exist a sequence k_1, k_2, \dots of indices corresponding to hidden states such that $A(i, k_1), A(k_1, k_2), \dots, A(k_{m-1}, k_m), A(k_m, j)$ are nonzero. Then, we see that:

$$W_{ij} = A_{ij} + (A_{12}(sI - A_{22})^{-1}A_{21})_{ij} = 0$$

From the definition of Q in (4), we note that the off-diagonal values of Q are nonzero (zero) when the off-diagonal values of W are nonzero (zero). Thus,

$$W_{ij} = 0 \implies Q_{ij} = 0$$

which gives us a contradiction. The proof for part (b) is similar. ■

Note that there are subtle differences between a system's DSF and its subsystem interconnection structure. In particular, while the DSF does, in fact, describe a system as an interconnection of systems, as described by the Q and P matrices, these systems are not necessarily *subsystems* of the original system. In particular, describing a system as an interconnection of subsystems requires one to *partition* the states of the system into distinct parts, where each part of the state vector corresponds to the state of an associated subsystem. The DSF, on the other hand, does not demand the existence of such a partition when describing the open-loop causal dependencies among manifest variables [10].

B. Relationship of the Dynamical Structure Function to a System's Transfer Function

Given any system (1), its DSF, like its TF, is uniquely specified. However, although the system's TF contains the dynamics of the system, it yields no information about the structure of the network. The direct relationship between a system's DSF and its TF can be defined as:

Lemma 1: [2] The transfer function, G , of the system (1), is related to its dynamical structure, (Q, P) , by

$$G = (I - Q)^{-1}P \quad (6)$$

This follows from (3) and $Y = GU$.

C. Signal Structure Reconstruction

Network reconstruction considers the problem of finding the DSF of a given system, which is consistent with its TF. This makes it similar to the realization problem, which is concerned with finding the state-space description that is consistent with a system's TF, shown in Figure 2.

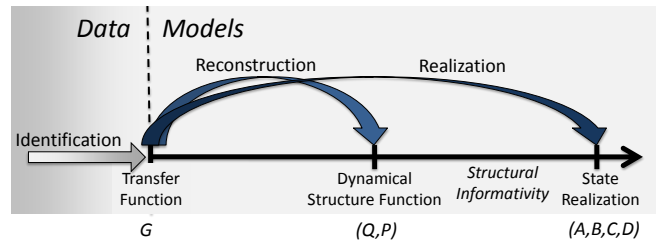


Fig. 2. Different types of models of the same system describe different amounts of structural information. The reconstruction problem, like the realization problem, requires additional information about the system above and beyond the input-output data necessary to identify the transfer function.

Like realization, the problem of reconstruction is ill-posed, however, since there are many different DSFs that are consistent with a given TF. The next lemma makes this idea precise:

Lemma 2: [3] Given a transfer function G , the set \mathcal{S}_G of all dynamical structure functions consistent with G can be parameterized by a $p \times p$ internal structure function, \tilde{Q} , and is given by

$$\mathcal{S}_G = \left\{ (Q, P) : \begin{bmatrix} Q' \\ P' \end{bmatrix} = \begin{bmatrix} 0 \\ G' \end{bmatrix} + \begin{bmatrix} I \\ -G' \end{bmatrix} \tilde{Q}, \tilde{Q} \in \mathcal{Q} \right\}, \quad (7)$$

where \mathcal{Q} is the set of internal structure functions, and where A' is the conjugate transpose of a matrix A . Moreover, the set \mathcal{S}_G has $p^2 - p$ degrees of freedom.

Thus, the reconstruction problem can be characterized as in [3] with the following theorem:

Theorem 2: Given any $p \times m$ transfer function G , with $p > 1$ and no other information about the system, dynamical and boolean reconstruction is not possible. Moreover, for any internal structure Q , there is a dynamical structure function (Q, P) that is consistent with G .

However, since the DSF (Q, P) is a partial structure representation of the network, less information is needed for

the DSF to be reconstructed than for the entire state space to be realized. The following corollary from previous work indicates what partial-structure information, which refers to a priori knowledge of some of the elements of Q or P , is sufficient for dynamical structure reconstruction.

Corollary 1: [3] If $m = p$, G is full rank, and there is no information about the internal structure, Q , then the dynamical structure can be reconstructed if each input controls a measured state independently, that is, without loss of generality, the inputs can be indexed such that P is diagonal.

This section served to describe the reconstruction methodology from [2] and the basic requirements for reconstruction of the DSF of a system such as (1). Equipped with this description, we are now prepared to extend the details discussed in this section in order to allow for systems whose measured states cannot be independently controlled. These systems have a P matrix that is not diagonal, hence previous methods have to be extended to accommodate them.

III. MAIN RESULT

Identifiability conditions fundamentally concern the definition of a map from model parameters to data and ensuring that it is injective. In this way, a particular set of parameters is uniquely specified by the data, identifying the correct model from the set of models under consideration.

Identifying a system's DSF from data involves the standard issues related to identifying a TF from data (sufficiency of excitation, etc.), along with additional issues related to the fact that many DSF generate the same TF (consider Lemma 2). In the sequel we will ignore the standard issues and focus on the additional identifiability issues unique to DSF. Consequently we will assume that the system's TF has been successfully identified from data and focus on necessary and sufficient conditions for then recovering the DSF. To accomplish this, we will construct the map from the elements of the DSF to the associated TF and establish conditions ensuring this map is injective.

To facilitate the discussion, we introduce the following notation. Let $A \in \mathbb{C}^{n \times m}$ and $B \in \mathbb{C}^{k \times l}$. Then:

- $\text{blkdiag}(A, B)$ is the block diagonal matrix given by

$$\begin{bmatrix} A & 0 \\ 0 & B \end{bmatrix},$$

- a_i is the i^{th} column of matrix A ,
- A_{-i} is the matrix A without its i^{th} column,
- a_{ij} is the $(i, j)^{\text{th}}$ entry of matrix A ,
- A' is the conjugate transpose of matrix A ,
- $\mathcal{R}(A)$ is the range of A ,
- \vec{a} is the vector stack of the columns of A , given by

$$\begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \end{bmatrix}$$

- and \overleftarrow{a} is the vector stack of the columns of A' .

The construction of a map from elements of the DSF to the associated TF begins by rearranging the relationship from Lemma 1 in Equation (6) to yield:

$$\begin{bmatrix} I & G' \end{bmatrix} \begin{bmatrix} P' \\ Q' \end{bmatrix} = G' \quad (8)$$

Noting that

$$AX = B \iff \text{blkdiag}(A, \dots, A)\vec{x} = \vec{b}$$

and defining $X = \begin{bmatrix} P' & Q' \end{bmatrix}$ then allows us to rewrite Equation (8) as

$$\begin{bmatrix} I & \text{blkdiag}(G', \dots, G') \end{bmatrix} \overleftarrow{x} = \overleftarrow{g}. \quad (9)$$

Further noting that since the diagonal elements of Q are identically zero and the dimensions of P , Q , and G are $p \times m$, $p \times p$, and $p \times m$ respectively, then exactly p elements of \overleftarrow{x} are always zero. Abusing notation, we can then redefine \overleftarrow{x} to remove these zero elements, reducing Equation (9) to the following:

$$\begin{bmatrix} I & \text{blkdiag}(G'_{-1}, G'_{-2}, \dots, G'_{-p}) \end{bmatrix} \overleftarrow{x} = \overleftarrow{g}. \quad (10)$$

Equation (10) reveals the mapping from elements of the DSF, contained in \overleftarrow{x} , to its associated TF, represented by \overleftarrow{g} . The mapping is clearly a linear transformation represented by the matrix operator $\begin{bmatrix} I & \text{blkdiag}(G'_{-1}, G'_{-2}, \dots, G'_{-p}) \end{bmatrix}$. This matrix has dimensions $(pm) \times (pm + p^2 - p)$, and thus the transformation is certainly not injective. This is why not even the Boolean structure of a system's DSF can be identified – even from perfect information about the system's TF – without additional a priori structural information.

Identifiability conditions will thus be established by determining which elements of \overleftarrow{x} must be known a priori in order to reduce the corresponding transformation to an injective map. To accomplish this, consider the $(pm + p^2 - p) \times k$ transformation T such that

$$\overleftarrow{x} = Tz \quad (11)$$

where z is an arbitrary vector of size k . The following lemma describes technical conditions on T establishing necessary and sufficient identifiability conditions for DSF reconstruction.

Lemma 3: Let

$$M = LT, \quad (12)$$

where $L = \begin{bmatrix} I & \text{blkdiag}(G'_{-1}, G'_{-2}, \dots, G'_{-p}) \end{bmatrix}$ and T is a $(pm + p^2 - p) \times k$ matrix operator as in Equation (11). Then M is injective if and only if

- 1) $k \leq pm$, and
- 2) $\text{rank}(T) = k$ (i.e. T is injective).

Proof: Since $\begin{bmatrix} I & \text{blkdiag}(G'_{-1}, G'_{-2}, \dots, G'_{-p}) \end{bmatrix}$ has $\text{rank } pm$, $\text{rank}(M) = \min(pm, \text{rank}(T))$. If $\text{rank}(T) > pm$, implying $k > pm$, then M is clearly not injective. If $\text{rank}(T) \leq pm$, then $\text{rank}(M) = \text{rank}(T)$ and M will be injective if and only if $k = \text{rank}(T)$. ■

Theorem 3: (Identifiability Conditions) Given a system characterized by the transfer function G , its DSF (Q, P) can be identified if and only if

- 1) M , defined as in Equation (12), is injective, and
- 2) $\overleftarrow{g} \in \mathcal{R}(M)$.

Proof: The proof follows immediately from the observation that M is the mapping from unidentified model parameters to the system TF. Under these conditions one can clearly solve for z given G and then construct the DSF from \overleftarrow{x} , where $\overleftarrow{x} = Tz$, and T is precisely the a priori system information that is necessary and sufficient for reconstruction. ■

We will now illustrate this reconstruction result on some simple examples.

Example 1: Consider a system with square TF given by

$$G = \begin{bmatrix} G_{11} & G_{12} & \dots & G_{1p} \\ G_{21} & G_{22} & & G_{2p} \\ \vdots & & \ddots & \vdots \\ G_{p1} & G_{p2} & \dots & G_{pp} \end{bmatrix}.$$

Previous work has shown that if G is full rank and it is known, a priori, that the control structure P is diagonal that reconstruction is possible [2]. Here we validate that claim by demonstrating that the associated T matrix becomes:

$$\begin{bmatrix} P_{11} \\ P_{12} \\ \vdots \\ P_{21} \\ P_{22} \\ \vdots \\ P_{pp} \\ Q_{12} \\ \vdots \\ Q_{p(p-1)} \end{bmatrix} = \begin{bmatrix} 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \ddots & & \ddots & \vdots \\ 0 & \dots & 1 & \dots & 0 \\ 0 & \dots & 0 & 1 & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} P_{11} \\ P_{22} \\ \vdots \\ P_{pp} \\ Q_{12} \\ \vdots \\ Q_{p(p-1)} \end{bmatrix}$$

yielding the operator $M = LT$ as:

$$M = \begin{bmatrix} e_1 & 0 & 0 & G'_{-1} & \dots & 0 \\ 0 & \ddots & 0 & 0 & \ddots & 0 \\ 0 & \dots & e_p & 0 & \dots & G'_{-p} \end{bmatrix}$$

where e_i is a zero vector with 1 in the i^{th} position. Note that M is a square matrix with dimensions $p^2 \times p^2$ and will be invertible provided G is full rank, thus enabling reconstruction.

Example 2: Given the following TF of a system:

$$G = \begin{bmatrix} \frac{s+2}{s^2+3s+1} & -\frac{s^2+3s+3}{(s+2)(s^2+3s+1)} \\ \frac{s+2}{(s+1)(s^2+3s+1)} & \frac{s^2+s-1}{(s+1)(s^2+3s+1)} \end{bmatrix}$$

We attempt to find the DSF (Q, P) of the system:

$$Q = \begin{bmatrix} 0 & Q_{12} \\ Q_{21} & 0 \end{bmatrix} \text{ and } P = \begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix}$$

yielding the vector of unknowns $\vec{x} = [P_{11} \ P_{12} \ P_{21} \ P_{22} \ Q_{12} \ Q_{21}]'$. This gives us the system of equations of the form $L\vec{x} = \vec{b}$:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & \frac{s+2}{(s+1)(s^2+3s+1)} & 0 \\ 0 & 1 & 0 & 0 & \frac{s^2+s-1}{(s+1)(s^2+3s+1)} & 0 \\ 0 & 0 & 1 & 0 & 0 & \frac{s+2}{s^2+3s+1} \\ 0 & 0 & 0 & 1 & 0 & -\frac{s^2+3s+3}{(s+2)(s^2+3s+1)} \end{bmatrix} \begin{bmatrix} P_{11} \\ P_{12} \\ P_{21} \\ P_{22} \\ Q_{12} \\ Q_{21} \end{bmatrix} = \begin{bmatrix} \frac{s+2}{s^2+3s+1} \\ -\frac{s^2+3s+3}{(s+2)(s^2+3s+1)} \\ \frac{s+2}{(s+1)(s^2+3s+1)} \\ \frac{s^2+s-1}{(s+1)(s^2+3s+1)} \end{bmatrix}$$

Without additional information a priori structural information, we can not reconstruct. Suppose, however, that we know a priori that P takes the form:

$$P = \begin{bmatrix} P_{11} & -P_{11} \\ 0 & P_{22} \end{bmatrix}$$

Note that this non-diagonal P fails to meet the previous conditions for reconstruction [2], [1]. Nevertheless, the vector of unknowns \vec{x} can then be decomposed into the form $T\vec{z}$ as follows:

$$T = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \text{ and } \vec{z} = [P_{11} \ P_{22} \ Q_{12} \ Q_{21}]'$$

Replacing \vec{x} with $T\vec{z}$ above yields the system of equations of the form $M\vec{z} = \vec{b}$, where $M = LT$:

$$\begin{bmatrix} 1 & 0 & \frac{s+2}{(s+1)(s^2+3s+1)} & 0 \\ -1 & 0 & \frac{s^2+s-1}{(s+1)(s^2+3s+1)} & 0 \\ 0 & 0 & 0 & \frac{s+2}{s^2+3s+1} \\ 0 & 1 & 0 & -\frac{s^2+3s+3}{(s+2)(s^2+3s+1)} \end{bmatrix} \begin{bmatrix} P_{11} \\ P_{22} \\ Q_{12} \\ Q_{21} \end{bmatrix} = \begin{bmatrix} \frac{s+2}{s^2+3s+1} \\ -\frac{s^2+3s+3}{(s+2)(s^2+3s+1)} \\ \frac{s+2}{(s+1)(s^2+3s+1)} \\ \frac{s^2+s-1}{(s+1)(s^2+3s+1)} \end{bmatrix}$$

In this case M is full rank, from theorem 3 we know that the system is reconstructible. By solving for $\vec{x} = (M)^{-1}\vec{b}$ we get the DSF to be:

$$Q = \begin{bmatrix} 0 & \frac{1}{s+2} \\ \frac{1}{s+1} & 0 \end{bmatrix} \text{ and } P = \begin{bmatrix} \frac{1}{s+1} & -\frac{1}{s+1} \\ 0 & \frac{1}{s+2} \end{bmatrix}$$

IV. MOTIVATING EXAMPLE: THE PAS KINASE PATHWAY

An example of such a network is the Per-Arnt-Sim (PAS) Kinase pathway. Human mutations in the PAS Kinase pathway have recently been linked to the early development of type 2 diabetes [7]. The PAS Kinase pathway is composed of proteins that interact in specific ways to direct the metabolism of sugars in eukaryotic cells. Each of these proteins have both an activated and a deactivated

form that serves a distinct function within the network. The identification of network structure in this system is an ideal application of signal structure theory.

Several PAS Kinase networks have been proposed such as in [5], so analysis of such a pathway with the DSF method would help to indicate flaws or validate proposed biological pathways. Yeast serves as a model biological organism for understanding the basic processes of life due to the ease of study and the conservation of many pathways. In fact, the best characterized PAS Kinase pathway, the Ugp1 pathway, was first identified in yeast [6].

One of the proposed networks for the PAS Kinase Ugp1 pathway is indicated in Fig. 3. In this pathway there are three proteins that are directly formed from a gene: PSK, Ugp1, and Glc7; the others are activated forms or complexes involving these three proteins. The species of interest in the pathway are Ugp1, Ugp1* and the Ugp1*Glc7. The asterisk implies an activated form of the protein, e.g Ugp1* is the activated form of Ugp1 that is produced when PAS Kinase modifies the Ugp1 protein [6]. Once Ugp1 is activated, it partitions the use of cellular glucose towards structural components at the expense of storage carbohydrates [8]. The last species, Ugp1*Glc7, is theoretical and may be formed by a direct interaction between Ugp1* and Glc7 [6]. It is hypothesized that Ugp1* is deactivated by this process, however this needs to be verified. Other key network players include the Snf1 protein, which is required for the activation of PAS Kinase in response to available nutrients [4].

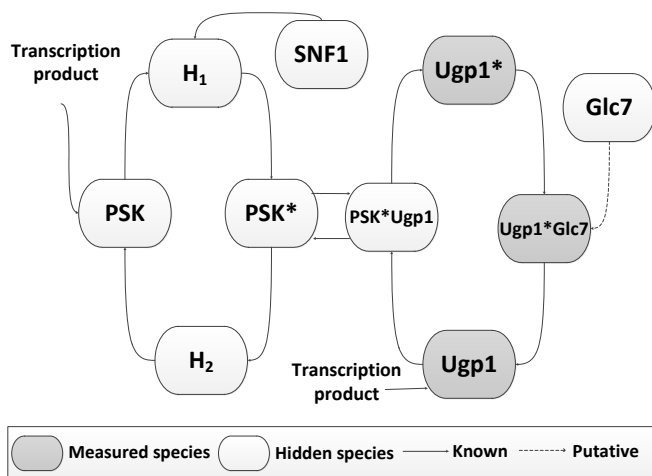


Fig. 3. PAS Kinase Pathway with H_1 and H_2 representing networks of unobserved nodes

As shown, the current theoretical network involves ten species, with the majority of the pathway verified. It is not easy to directly perturb each of the three nodes of interest since PSK affects two of the observed nodes however, it is possible to create experiments that directly affect two of the species. These experiments consist of turning on or off a specified gene by modifying the yeast cell or its environment. This is commonly done through the use of a plasmid, a small circular piece of DNA inserted into the

yeast cell that expresses the protein in response to external stimulus (such as the addition of a particular chemical to the growth media). The experiments for the PAS Kinase network include manipulation of the genes Glc7, Ugp1, and PSK. The plasmids with PSK will directly affect two observed nodes: Ugp1* and Ugp1. However, this will be done in an equal amount; it will increase the activated form of Ugp1* while decreasing the inactive form, Ugp1. The experimental setup is shown below in Fig. 4.

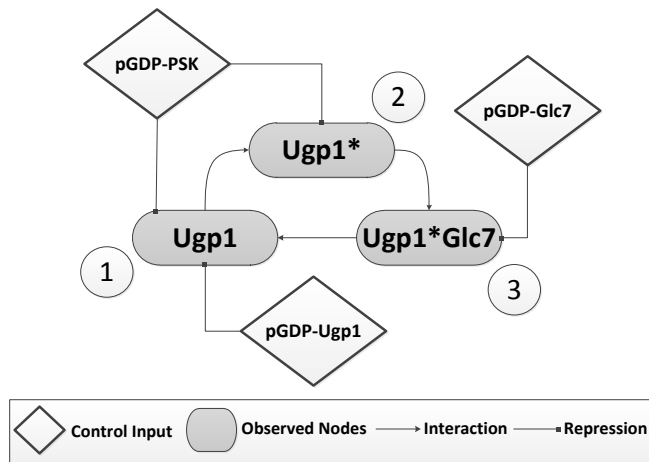


Fig. 4. Experimental setup for PAS Kinase Pathway

As expected, the exact mechanisms by which phosphorylation and dephosphorylation occur are hidden in this formulation. As indicated earlier, previous formulation required a direct perturbation for each observed node in any given network. However, methods or experimental conditions that independently perturb observed nodes in biological networks are usually not feasible. This becomes even more difficult to do when biological networks have several observed nodes; in many cases it is even impossible to independently perturb all the observed nodes. However, with the extensions indicated in Section III, reconstruction is still possible despite multiple perturbations of observed nodes in a given experiment. This is demonstrated for the Pas Kinase pathway as indicated in Fig. 4

A. Reconstruction for PAS Kinase Pathway

We can define Q , P , and G for the pathway as follows:

$$G_{PAS} = \begin{bmatrix} G_1 & G_2 & G_3 \\ G_4 & G_5 & G_6 \\ G_7 & G_8 & G_9 \end{bmatrix} \quad (13)$$

$$Q_{PAS} = \begin{bmatrix} 0 & Q_1 & Q_2 \\ Q_3 & 0 & Q_4 \\ Q_5 & Q_6 & 0 \end{bmatrix} \quad (14)$$

$$P_{PAS} = \begin{bmatrix} P_1 & P_2 & P_3 \\ P_4 & P_5 & P_6 \\ P_7 & P_8 & P_9 \end{bmatrix} \quad (15)$$

However, from the experimental design indicated in Fig. 4, we know the true representation of the control matrix P is

as follows:

$$P_{PAS} = \begin{bmatrix} -P_{PSK} & P_{Ugp1} & 0 \\ P_{PSK} & 0 & 0 \\ 0 & 0 & P_{Glc7} \end{bmatrix}$$

Where $P_{PSK} = P_1$, $P_{Ugp1} = P_2$, and $P_{Glc7} = P_9$. This true representation of P serves as the prior knowledge for this system. Given $L\vec{x} = \vec{b}$ such that:

$$\mathbf{I} \begin{bmatrix} G_4 & G_7 & 0 & 0 & 0 & 0 \\ G_5 & G_8 & 0 & 0 & 0 & 0 \\ G_6 & G_9 & 0 & 0 & 0 & 0 \\ 0 & 0 & G_1 & G_7 & 0 & 0 \\ 0 & 0 & G_2 & G_8 & 0 & 0 \\ 0 & 0 & G_3 & G_9 & 0 & 0 \\ 0 & 0 & 0 & 0 & G_1 & G_4 \\ 0 & 0 & 0 & 0 & G_2 & G_5 \\ 0 & 0 & 0 & 0 & G_3 & G_6 \end{bmatrix} \times \begin{bmatrix} P_1 \\ P_2 \\ \vdots \\ P_9 \\ Q_1 \\ \vdots \\ Q_6 \end{bmatrix} = \begin{bmatrix} G_1 \\ G_2 \\ \vdots \\ G_9 \end{bmatrix}$$

This system has 15 unknowns and 9 equations, so it is easy to see that no unique solution exists as is. However, taking into account a priori information given the true structure of P , we can decompose \vec{x} into $T\vec{z}$ as follows:

$$T = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \text{ and } \vec{z} = \begin{bmatrix} P_1 \\ P_2 \\ P_9 \\ Q_1 \\ \vdots \\ Q_6 \end{bmatrix}$$

The total number of variables in \vec{z} is 9, and T is full column rank. In this case, $k = pm$, given $M\vec{z} = \vec{b}$ ($M = LT$), and since M is square and full rank, $(M)^{-1}$ exists. Therefore, $\vec{z} = (M)^{-1}\vec{b}$, hence reconstruction is possible, and the signal structure of the system can be uniquely identified from the overall structure of Q

V. CONCLUSION

This paper extends the identifiability conditions required for the reconstruction of the signal structure of an LTI system. The notion of the DSF (Q, P), of system was introduced in [2] and the required conditions for reconstruction were also indicated. In that work, it was shown that if no additional information is known about the system besides its TF, not even Boolean network reconstruction, that is, correctly identifying the presence or absence of network edges, is possible.

This work identifies precisely the a priori information that is necessary and sufficient for network reconstruction. Previous results showed that a priori knowledge that P is diagonal is sufficient to reconstruct the DSF from a system's TF; this work extends these results to situations where P may not be known to be diagonal. This extension is significant because it identifies when systems that do not necessarily have independent perturbation of measured states are reconstructible.

Although these results identify the precise conditions for reconstruction of a system's complete dynamical structure function, future work may consider how these conditions may be relaxed to obtain weaker characterizations of a system's network structure. These weaker characterizations may include the Boolean structure of the system's DSF, or structurally-accurate reduced-order models of the system.

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