On the Necessity of Full-State Measurement for State-Space Network Reconstruction

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***Abstract*—Network reconstruction is an important research topic in many different applications, including biochemical reactions, critical infrastructures, social media, and wireless mesh networks. This paper shows that, for a certain important class of systems, all the states in a system must be measured in order to ensure correct reconstruction of the network. Furthermore, we show that this result is strongly necessary, in that if only one state is not measured, the structure of the recovered network could be arbitrarily different from the structure of the actual network. Finally, we note that our results motivate the need for dynamical structure functions, a partial structure system representation that reveals important structural information about the system but requires much less a priori information (than knowledge of full state measurements) for reconstruction from data.**

***Index Terms*—network reconstruction, full–state measurement, dynamical structure functions**

I. Introduction

The network reconstruction problem, also referred to as reverse engineering or network inference, is the attempt to discover the underlying structure of a system, typically from input-output data, [1]. Traditional system identification for linear time-invariant systems recovers a system's transfer function, $G(s)$, from rich input-output data. Many reconstruction techniques try to recover a more detailed representation of a system, namely the state-space model, [2]–[4]. The state-space model is generally represented by a system of equations of the form:

$$\begin{array}{rcl} \dot{x}(t) & = & Ax(t) + Bu(t) \\ y(t) & = & Cx(t) + Du(t), \end{array} \tag{1}$$

where $x(t) \in \mathbb{R}^n$ is a vector of the states of the system, $u(t) \in \mathbb{R}^m$ is the vector of inputs, $y(t) \in \mathbb{R}^p$ is the vector of outputs. The A matrix is called the *dynamics matrix*, the B matrix is called the *control matrix*, the C matrix is called the *sensor matrix*, and the D matrix is called the *direct term*, [5]. The one-to-many relationship between a system's transfer function and its state-space model is given by:

$$G(s) = C(sI - A)^{-1}B + D. \tag{2}$$

where s is the Laplace variable and the true state-space model (A, B, C, D) is a minimal realization of $G(s)$, meaning that it is both controllable and observable.

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In this work we take the perspective that the system's state-space model, and thus its associated transfer function, is fixed but unknown, and we are using input-output data to attempt to discover not only its correct transfer function, but also the particular state-space realization that generates it. We assume the transfer function has been obtained through standard system identification techniques, and we therefore explore the conditions when the true state realization can be identified from knowledge of its transfer function. That is to say, we present conditions under which a transfer function has a unique state realization.

The transfer function details the input-output dynamics of the network, but it reveals very little structural information about the system. The state-space realization, on the other hand, exposes very detailed interconnection information of the system. Structural information, in either case, is disclosed through the sparsity pattern of the associated system representation; Example 1 illustrates how a system with an unstructured transfer function nevertheless may be very structured, as revealed by its state realization.

Example 1. *Consider the system in Figure 1, with $B = I$, $C = I$, $D = 0$ and the associated dynamics matrix, A, and transfer function matrix, $G(s)$, given by:*

$$A = \begin{bmatrix} 0 & 0 & -1 \\ -2 & -3 & 0 \\ 0 & -2 & -3 \end{bmatrix}, \tag{3}$$

$$G(s) = \begin{bmatrix} \frac{(s+3)^2}{(s+1)^2(s+4)} & \frac{2}{(s+1)^2(s+4)} & \frac{-(s+3)}{(s+1)^2(s+4)} \\ \frac{-2(s+3)}{(s+1)^2(s+4)} & \frac{s(s+3)}{(s+1)^2(s+4)} & \frac{2}{(s+1)^2(s+4)} \\ \frac{4}{(s+1)^2(s+4)} & \frac{-2s}{(s+1)^2(s+4)} & \frac{s(s+3)}{(s+1)^2(s+4)} \end{bmatrix}. \tag{4}$$

This system exhibits a very clear ring-structure, revealed by the sparsity pattern of the dynamics matrix. Nevertheless, the sparsity pattern of the transfer function would suggest that the system is unstructured, and reveals nothing of the underlying ring structure.

From this example we note that the state-space model is a better representation of system structure than the transfer function. Nevertheless, realizing a system, even minimally, is known to be ill-posed, since any change of basis on the state variables yields another state-space model that is consistent with the same transfer function. In fact, without any other

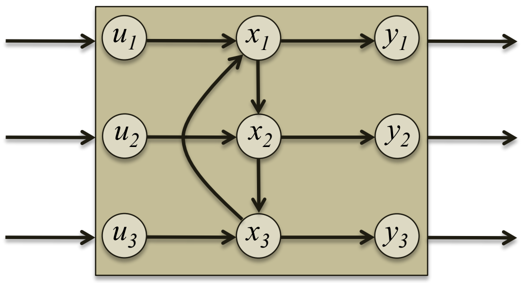

Fig. 1: System with a ring structure, given by Equations (3) and (4).

a priori system information, the most detailed representation that can be determined from input-output data is the system's transfer function [6].

The problem of structural identifiability was studied extensively in the systems theory community in the 1970's. Structural identifiability, or the ability to identify internal structure, was introduced and formulated in [7]. The authors also explained the necessary and sufficient conditions for several classes of systems; single–input single–output single–state, diagonal dynamics matrix, observable canonical form, sensor matrix equal to the identity ($C = I$), and compartmental models. In [8], the author provided conditions for identifiability using a fair amount of assumptions and invertibility of the information matrix. In [9], the authors provided conditions for identifiability using an arbitrary vector of unknown parameters of the system.

The generalization results of the structural identifiability problem were in terms of the information matrix, or an arbitrary parameterization of unknowns, and not in terms of the specific a priori information of the realization needed to recover the complete realization. In contrast, this work is leading towards quantifying the exact information needed for network reconstruction of all classes of systems. However in this paper, we focus on network reconstruction of a specific class of systems and the exact information needed to recover the structure of this class. This could be seen as an extension of [7], considering they show that the class of systems defined by $C = I$ is identifiable. Nevertheless, here we show that this condition is not only sufficient, but also necessary for the partial–state measurement class of systems, where $C = [I\ 0]$.

II. Necessity and Sufficiency of the Full–State Measurement Assumption

For this section we will focus on systems that directly measure some of their states. This type of system is common in many applications, such as biochemical reaction networks. The states of biochemical reaction networks represent different chemical species, and the system dynamics describe the reaction kinetics associated with the relevant chemistry. For in vivo experiments on these systems, it is often naive to assume that all the system states are measured, since reactions transforming one measured species to another may involve intermediate steps where a number of unmeasured species can significantly influence the overall reaction. Moreover, this situation is common in other complex systems, where our sensor technologies are designed to measure particular system states but can not possibly hope to capture all possible state measurements.

Based on this idea, we say that a system has **partial–state measurement** if it directly measures a proper subset of the set of all states. The unmeasured states are referred to as **hidden states**. These type of systems give motivation for the following class of state-space models,

$$\begin{aligned} \dot{x}(t) &= Ax(t) + Bu(t) \\ y(t) &= [\ I_p\ 0\ ]x(t), \end{aligned} \tag{5}$$

where I_p is the $p \times p$ identity matrix. A system has **full–state measurement** when $p = n$, yielding $C = I$ and $y = x$.

We will now show that full–state measurement is necessary for network reconstruction of systems of the form found in Equation (5) with no prior information about A and B.

Theorem 1. *Consider a system as given by Equation (5), for some $p \leq n$, with no prior information about A and B. The matrices (A,B) are uniquely specified by $G(s)$ if and only if $p = n$, i.e. there is full–state measurement.*

Proof. ($\Rightarrow$) We will prove necessity by contraposition.

Assume $p < n$. This implies $C = \begin{bmatrix} I_n & 0_{n-p} \end{bmatrix}$ with $n - p > 0$, thus $C \neq I$. Moreover, for any system there exists a minimal pair of matrices (A, B), not necessarily unique, that realize $G(s)$:

$$G(s) = C(sI - A)^{-1}B. \tag{6}$$

Consider the state transformation T and its inverse:

$$T = \begin{bmatrix} I_n & 0 \\ K & I_{n-p} \end{bmatrix},\ T^{-1} = \begin{bmatrix} I_n & 0 \\ -K & I_{n-p} \end{bmatrix}, \tag{7}$$

where K is an arbitrary $(n - p) \times n$ nonzero matrix.

The resulting transformed system, $A_2 = TAT^{-1}$, $B_2 = TB$, and $C_2 = CT^{-1}$, is still of the form (5), since $CT^{-1} = C$, and clearly has the same transfer function $G(s)$. Nevertheless, different values of K will clearly result in various dynamics matrices, A_2, and control matrices, B_2, thus showing that $p < n$ implies the existence of multiple minimal realizations consistent with $G(s)$.

($\Leftarrow$) Assume $n = p$, $C = I$ and that $G(s)$ is realized by (A_1, B_1, C_1) and (A_2, B_2, C_2). This implies there exists an invertible matrix T such that $A_2 = TA_1T^{-1}$, $B_2 = TB_1$, and $C_2 = C_1T^{-1}$. Since $C_1 = C_2 = I$ and $C_2 = C_1T^{-1}$ the only acceptable T matrix is clearly the identity matrix. Therefore $A_1 = A_2$ and $B_1 = B_2$ and only one set of matrices (A, B) realizes $G(s)$.

$\square$

This theorem states that network reconstruction cannot recover a network in the class of models depicted in Equation (5)

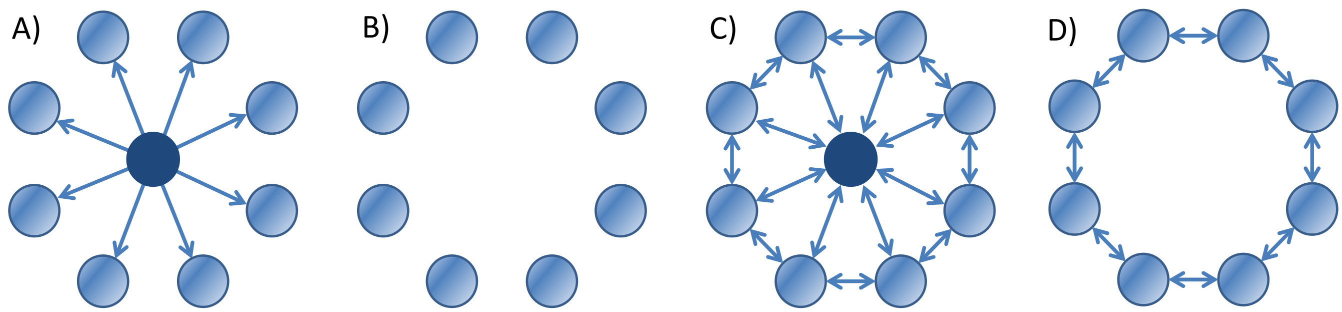

Fig. 2: In Example 2, if $n = 9$, the actual system can be a nine-node network ranging from A) to C). The hidden node is the darker node and can affect every node. Network reconstruction on A) would yield the network in B) and network reconstruction on C) would yield D).

unless you have full–state measurement. However, it does not tell us how different from the actual network the result could be if you fail to meet this full–state measurement condition. In Example 2 we show that even if only one state in a network is not measured, then the structure of the smaller system yielded from a reconstruction algorithm could be completely different from that of the original network. This is done by presenting a pair of $n \times n$ A matrices with $n-1$ measured states.

Example 2. *Consider a hub-spoke network (Figure (2A)) with $n-1$ nodes on the outside driven by the n^{th} node in the center. Systems with this structure occur commonly in transportation systems, communication networks, and social networks, just to name a few applications. The dynamics matrix for such a system is of the form*

$$A_1 = \begin{bmatrix} I_{n-1} & \Gamma \\ 0 & 1 \end{bmatrix}, \qquad (8)$$

where Γ is a column vector with no zero entries. This structure is depicted in Figure (2A). Moreover, let $B = \begin{bmatrix} 0 & \cdots & 0 & 1 \end{bmatrix}^T$, which will be controllable when Γ has no zero entries.

Note that the only observable partial–state measurement configuration for this system, with only one hidden state, is $C = [I_{n-1}\ 0]$. Nevertheless, it is easy to see that the set of minimal realizations that preserve the same partial state configuration (i.e. preserve $C = [I_{n-1}\ 0]$) span all possible Boolean structures for the dynamics matrix.

To see this, consider the state transformation $T = A_1^T$. The new, transformed dynamics matrix then becomes:

$$\begin{aligned} A_2 = TA_1T^{-1} &= \begin{bmatrix} I_{n-1} & 0 \\ \Gamma & 1 \end{bmatrix} \begin{bmatrix} I_{n-1} & \Gamma \\ 0 & 1 \end{bmatrix} \begin{bmatrix} I_{n-1} & 0 \\ -\Gamma & 1 \end{bmatrix} \\ &= \begin{bmatrix} I_{n-1} & \Gamma \\ \Gamma & * \end{bmatrix} \begin{bmatrix} I_{n-1} & 0 \\ -\Gamma & 1 \end{bmatrix} = \begin{bmatrix} \hat{\Gamma} & * \\ * & * \end{bmatrix} \end{aligned} \qquad (9)$$

where $*$ indicates a nonzero entry of the appropriate dimension. The non-diagonal entries of $\hat{\Gamma}$ are equal to $\hat{\gamma}_{ij} = -\gamma_i\gamma_j = -ij$, which is always nonzero by the construction of Γ. This results in the structure shown in Figure (2C). Notice that $C = CT^{-1}$, demonstrating that this state transformation preserves the partial state configuration of the system.

Clearly the transfer functions for both systems are equal, since they differ only by a change of state coordinates. Nevertheless, notice that the portion of the underlying realization corresponding to the measured states, i.e. the sub matrix $\hat{\Gamma}$ in the transformed system, can have any Boolean structure, from diagonal, as in Equation (8), to completely full, as in Equation (9) (or anything in between). Thus, any network reconstruction technique that attempts to recover this system–even knowing a priori that the system is both controllable and observable–can not distinguish even the Boolean structure relating the measured nodes to each other without more information than the input-output behavior of the system.

From Example 2 we can see that even if a network had 1000 states, and we only missed measuring a single hidden state, then a reconstruction method may reasonably recover a ring network (like Figure 2D), and it could actually have been completely disconnected (like Figure 2B).

Thus we have shown, for systems of the form in Equation (5), that reconstruction techniques which recover the sparsity pattern of the A matrix must rely on full–state measurement. If reconstruction algorithms do not strictly meet this assumption, e.g. measuring 999 out of 1000 states, their solutions can be arbitrarily incorrect. In [3], [4] they do not explicitly make the full–state measurement assumption however it is implied in their problem formulation. We see from Theorem 1 and Example 2 the full–state measurement assumption must be met for them to have a chance of success. Moreover, we reiterate that this full–state measurement assumption can be very difficult or expensive to achieve in practice for many complex-systems applications.

III. Dynamical Structure Functions

The necessity and sufficiency of full–state measurements to reconstruct systems of the form given in Equation (5) motivates the need for partial structure representations that require less stringent assumptions than full–state measurement, but have more structural information than a system's transfer function. One such representation is a system's dynamical structure function, [10], which may be interpreted as a particular left factorization of a system's transfer function such that

$$G(s) = (I - Q(s))^{-1} P(s)$$

where $Q(s)$ is a strictly proper transfer matrix with zeros on the diagonal, representing how measured states within the system affect each other, and $P(s)$ is a strictly proper transfer matrix, representing how external inputs affect the measured states. The dynamical structure function of a network is uniquely defined for a system's state-space model of the form given in Equation (5), and requires less a priori information to reconstruct than the state-space representation of a system; in particular, full–state measurements are not necessary. See [11] for a discussion of the dynamical structure function of more general systems.

An important aspect of dynamical structure functions that make them useful system representations for network reconstruction is that they represent the structure and dynamics of a system at a resolution consistent with the number of measured states. So, as more states are measured in the system, the dynamical structure function becomes more consistent with the state-space representation, but if less states are measured, the dynamical structure function becomes more consistent with a system's transfer function; when only a single state is measured, the dynamical structure function is the transfer function. Moreover, necessary and sufficient conditions for ensuring a one-to-one correspondence between a system's input-output map and its dynamical structure function are given in [6].

To reconstruct the dynamical structure function of a system, it is not necessary to measure every state in the network, which can be a difficult task for complex networks. Rather, the conditions needed to reconstruct are very reasonable for many applications, essentially being equivalent to requiring target specificity in the system. Target specificity means that every *measured* state in the system can be manipulated independently, no requirements are necessary for manipulating the hidden states in the system. Target specificity can be achieved, for example, when studying in vivo experiments of genomic networks where each measured gene can be switched off or on independently. Furthermore, an assumption similar to target specificity that meets the exact conditions from [6] can often be achieved for proteomic networks, where not all proteins from an in vivo experiment can be measured, but the measured proteins can be manipulated somewhat independently. Thus, although full–state measurements may be an unrealistic condition for many applications, thereby preventing full–state network reconstruction, dynamical structure functions offer a more reasonable approach to the network reconstruction problem.

IV. Conclusion

We have shown that full–state measurement is necessary and sufficient for recovering the state-space model of systems of the form presented in Equation (5) given no a priori information about A and B. Given this result, we showed that even if one state in the system was not measured, that network reconstruction algorithms could return structures that were arbitrarily wrong. This result showed that reconstruction techniques which claim to recover systems of the given form without a priori information about A and B must assume full–state measurement or they could be arbitrarily incorrect. This result also helped motivate the need of the dynamical structure function, a partial structure representation, as an alternative system representation. Dynamical structure functions provide more structural information than a system's transfer function and have less costly assumptions to ensure correct network reconstruction than the state-space model. More information on dynamical structure functions can be found in [6], [10].

References

[1] M. Hecker, S. Lambeck, S. Toepfer, E. van Someren, & R. Guthke. "Gene Regulatory Network Inference: Data Integration in Dynamic Models – A Review." Biosystems, vol. 96, pp. 86-103, 2009.

[2] E. Sontag. "Network Reconstruction Based on Steady-State Data." *Essays Biochem*, vol. 45, pp. 161-176, 2008.

[3] C. Cosentino, W. Curatola, F. Montefusco, M. Bansal, D. di Bernardo, & F. Amato. "Linear Matrix Inequalities Approach to Reconstruction of Biological Networks. Systems Biology IET, vol. 1(3), pp. 164-173, 2007.

[4] T.S. Gardner, D. di Bernardo, D. Lorenz, & J.J. Collins. "Inferring Genetic Networks and Identifying Compound Mode of Action via Expression Profiling." Science Signalling, vol. 301(5629), pp. 102, 2003.

[5] K.J. Astrom, & R.M. Murray, Feedback Systems: An Introduction for Scientists and Engineers. Princeton University Press, 2008.

[6] J. Adebayo, T. Southwick, V. Chetty, E. Yeung, Y. Yuan, J. Goncalves, J. Grose, J. Prince, G.B. Stan, & S. Warnick. "Dynamical Structure Function Identifiability Conditions Enabling Signal Structure Reconstruction." IEEE 51st Annual Conference on Decision and Control, pp. 4635-4641, 2012.

[7] R. Bellman & K. J. Astrom. "On structural identifiability." Mathematical Biosciences 7.3 (1970): 329-339.

[8] T. Rothenberg. "Identification in Parametric Models." Econometrica , Vol. 39, No. 3 (May, 1971), pp. 577-591

[9] K. Glover & J. Willems. "Parametrizations of linear dynamical systems: canonical forms and identifiability." IEEE Transactions on Automatic Control, 19.6 (1974): 640-646.

[10] J. Goncalves & S. Warnick. "Necessary and Sufficient Conditions for Dynamical Structure Reconstruction of LTI Networks." IEEE Transactions on Automatic Control, vol. 53, pp. 1670-1674, 2008.

[11] E. Yeung, J. Goncalves, H. Sandberg, & S. Warnick. "The Meaning of Structure in Interconnected Dynamic Systems." arXiv:1108.2755. 2011.